Configurational forces and variational mesh adaption in solid dynamics

Thesis by

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To my wife Alejandra

To my son Sebastian

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Abstract

This thesis is concerned with the exploration and development of a variational finite element mesh adaption framework for non-linear solid dynamics and its conceptual links with the theory of dynamic configurational forces. The distinctive attribute of this methodology is that the underlying variational principle of the problem under study is used to supply both the discretized fields and the mesh on which the discretization is supported. To this end a mixed-multifield version of Hamilton's principle of stationary action and Lagrange-d'Alembert principle is proposed, a fresh perspective on the theory of dynamic configurational forces is presented, and a unifying variational formulation that generalizes the framework to systems with general dissipative behavior is developed. A mixed finite element formulation with independent spatial interpolations for deformations and velocities and a mixed variational integrator with independent time interpolations for the resulting nodal parameters is constructed. This discretization is supported on a continuously deforming mesh that is not prescribed at the outset but computed as part of the solution. The resulting space-time discretization satisfies exact discrete configurational force balance and exhibits excellent long term global energy stability behavior. The robustness of the mesh adaption framework is assessed and demonstrated with a set of examples and convergence tests.

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Chapter 1

Introduction

This thesis is concerned with the exploration and development of a *variational finite element mesh adaption* framework for non-linear solid *dynamics* and its conceptual links with the concept of *dynamic configurational forces.* The distinctive attribute of this methodology is that the underlying variational principle of the problem under study is used to supply *both* the discretized fields *and* the mesh on which the discretization is supported. To this end a *mixed-multifield* (as opposed to the standard, single-field) version of the governing variational principles is proposed, an expanded perspective on the theory of dynamic configurational forces is presented, and a unifying variational formulation that generalizes the framework to dissipative systems with viscous, inelastic, and thermal processes is developed.

Dynamic applications often exhibit solutions with steep gradients at some regions of the domain of analysis and smooth gradients at others. These steep regions may change their locations and shapes both in space and time. It is therefore advantageous to vary the resolution of the computational grid, i.e., to *adapt the mesh,* according to the behavior of the solution, to ensure that the spatial mesh and time step are sufficiently fine in those regions and stages of steep gradients and reasonably coarse in other areas of less interest. In this way the accuracy and reliability of the numerical approximation is increased and evolving, and developing small scale features of the solution are explicitly resolved. We shall explore and develop in this work a mesh adaption framework particularly targeted for the challenging conditions just described.

In traditional finite element mesh adaption strategies mesh improvement is a post-processing operation based on *error estimation.* For static applications this approach might be summarized as follows: The user first selects an initial mesh. Then the *error* in the finite element solution corresponding to that mesh is *estimated.* Next, using this error as a measure of mesh quality, another mesh is designed by refining and coarsening the initial mesh in those areas where the estimated error is beyond a prescribed limit. This cycle is continued until a finite element solution with an error below the target tolerance is found. The same methodology can be extended to dynamic applications when only space adaption (and no time adaption) is pursued. In this case the (space) mesh adaption process is exercised at each time step of the computation using as initial mesh for the adaption loop the adapted mesh of the previous time step, see for example [55].

While considerable success has been achieved on error estimation and adaptivity for linear, static (elliptic) problems (see for example [61]), the theory concerning error estimation and the formulations and implementation of adaptive methods for dynamic (hyperbolic) applications is comparatively less developed, ([32], [55]). For this class of analysis the development of alternative mesh adaption paradigms is therefore desirable.

One possible approach in this direction that applies naturally to non-linear *variational* problems and that sidesteps the use of error estimation is the framework of *variational* mesh adaption. In this approach the mesh is not prescribed at the outset but regarded as an *unknown* of the problem to be handled jointly with the main unknowns, the evolving fields of the dynamical system under study. Then the variational principle that governs the evolution of the system is used to determine both the main unknowns *and* the mesh. For dynamics, the governing variational principle is *Hamilton's principle of stationary action* in the conservative case and *Lagrange-d'Alembert principle* in the non-conservative case.

The concept of using the underlying variational principle to optimize the mesh enjoys a long tradition in the context of linear *static* elasto and structural mechanics problems and traces back at least to [10], [11], [33]. The idea was to use the principle of minimum potential energy (the governing variational principle for static applications) as a measure of mesh quality and to regard as a better mesh the particular mesh that produces a lower potential energy. The total energy functional was thus minimized not only with respect to nodal field values but also with respect to the triangulation of the domain of analysis. Up to that moment, the computation of the analytic derivative of the discretized potential energy with respect to the discretization was regarded "a hopeless task in the case of arbitrary two and three-dimensional grids," (see [10]) and only optimization techniques based on energy *evaluation* (as opposed to energy differentiation) were thus implemented. These techniques proved to be too costly for the computational resources available at the time.

By contrast, the connection between energy minimization with respect to the triangulation and *configurational forces* was only recognized recently ([24], [35], [36], [37], [59], [60]). A closed form expression for the analytical derivative of the total potential energy with respect to nodal mesh placements was derived (see also [57]) and feasible solution strategies for the minimization process were successfully implemented [49]. Configurational forces, also known as material forces, arise in applications involving the evolution of defects or interfaces in continuum bodies. Unlike standard (Newtonian) forces that drive the spatial motion, configurational forces drive the motion of entities that migrate relative to the material. Examples include vacancies, inclusions, dislocations, cracks, inhomogeneities, or evolving interfaces. From a variational point of view, configurational forces may be described as those energetically conjugate to rearrangements of defects. When the continuum is discretized, artificial defects are induced due to the non-smooth nature of the discretized fields. The forces energetically conjugate to changes in the discretization can thus be uderstood as discrete configurational forces.

As opposed to static applications, the generalization of the concept of variational mesh adaption to *solid dynamics* is far from being fully explored. The idea, as it applies to dynamical systems, was originally conceptualized within the context of the theory of *discrete mechanics* and *variational integrators* [29], [31], [30], [63]. For finite degree-of-freedom dynamical systems the notion of applying the underlying variational principle, i.e., Hamilton's principle, to find the time mesh was originally studied in Kane, Marsden & Ortiz [20]. Then, the possibility of extending this concept to solid dynamics for both space and time adaption was theoretically conceived in [28], [29], [30], [63] and an implementation restricted to one-dimensional low dimensionality problems was attempted in [60].

Despite of the conceptual appeal of generalizing the methodology conceived for the time domain to the space-time domain, we have found, as we shall explain as we proceed in this work, that the application of this approach to non-linear multidimensional solid dynamic problems is not without difficulty. Concisely, the main idea of the theory of discrete mechanics as it applies to finite-dimensional (time-only-dependent) dynamical systems is to derive time-stepping algorithms by discretizing Hamilton's principle. The continuous trajectory of the dynamical system is first discretized. Then the discrete trajectory is obtained by invoking Hamilton's principle, i.e., by rendering the *discrete action sum*, discrete version of the *action* integral of the system, stationary with respect to the parameters that define the discrete trajectory. The main consequence of this methodology is that the resulting time-stepping algorithms, referred to as variational integrators, preserve *part* of the geometric structure of the continuous system, in particular they are simplectic methods and exactly conserve momenta associated to symmetries of the system [31], [30]. However they do not preserve *exactly* energy (see [20], [31], [30]) although they do exhibit long time energy stability. Kane, Marsden & Ortiz [20] noticed that this lack of *exact* energy balance was artificially induced by the discretization since in the continuous setting, energy balance *follows directly from Hamilton's principle as Euler-Lagrange equations* or, alternatively, as conserved momenta associated to symmetries with respect to time translations of the continuous action integral. They then proposed to *compute* the time steps in such a way that the energy of the discrete system is exactly conserved. Furthermore, they showed that this was equivalent to render the discrete action sum stationary not only with respect to the discrete trajectory but also with respect to the discrete times where that trajectory was sampled, i.e., the mesh. This resulted in *variational time adaption* in as much as the time set was not prescribed at the outset but determined as part of the solution by invoking the variational principle of the problem, namely, Hamilton's principle.

The generalization of the idea of variational integrators to space-time-dependent systems was studied in [29], [30], [31], [63], see also references therein. Within this context it was established that, in this expanded space-time framework, not only energy balance but also *configurational force balance* arise directly from Hamilton's principle and follow necessarily from momentum balance. Furthermore it was observed that this is not the case when space-time is discretized. The approximations derived by invoking Hamilton's principle are (multi)simplectic and preserve momenta associated to symmetries of the system but do not preserve exactly discrete energy and do not result in the automatic balance of discrete configurational forces. It was then suggested to generalize the variational mesh adaption notion proposed by Kane, Marsden & Ortiz [20] for the time domain to the space-time domain by computing the space-time mesh using Hamilton's principle. More precisely it was theoretically proposed to require the stationarity of the discrete action sum with respect to the space-time mesh. This would result in a new set of equations from which both space and time adaptivity eventually could be driven. The resulting discretization would exhibit the desirable feature of (multi)simplecticity and momentum conservation and at the same time the also desirable property of exact discrete energy and discrete configurational force balances, see for example [30], §7.3., [63], §6.2.3., [28], §5.6.

This space-time generalization approach was attempted in [60] by discretizing the space-time domain with isoparametric space-time finite elements. The method was implemented for one-dimensional elastodynamics and tested in a low dimensionality linear elastic problem. One essential problem of this generalization is the issue of solvability for the time step. The energy balance equation from which the time step should be solved for involves the unknown time step in a very highly non-linear way and do not always delivers physically admissible solutions as reported in [20], [29]. Since variational integrators do exhibit good average energy stability and since exact energy conservation was too costly and not always possible, it was then suggested to restrict the methodology to *space adaption only* while the global time step would be estimated rather than computed to exactly preserve energy. This was the approach of [60], where space-time isoparametric finite elements were implemented by taking the space coordinates of the space-time nodes as unknown while prescribing the time coordinate at the outset. This can be regarded as the starting point of this thesis where we have reexamined and expanded the theoretical developments to establish a powerful, efficient and robust variational space adaptivity framework.

We begin by observing that since time adaptivity is no longer pursued, there is no need to resort to the simultaneous discretization of the space-time domain, which requires the machinery of space-time finite elements and is supported on the expanded space-time theoretical framework. The approach we shall follow instead is to *uncouple the space and time discretization* by effecting a *space* semidiscretization in a first stage, keeping the time variable continuous and leading to the construction of a finite dimensional dynamical system. The latter is then discretized in time in a second stage using an appropriate time integrator. We shall therefore pursue a finite element space semidiscretization supported on a spatial mesh that, as a result of adaption, evolves continuously in time. The evolution of this continuously varying mesh shall not be prescribed but *computed* as part of the solution simultaneously with the motion of the dynamical system under study. Both the evolution of the body and the evolution of the mesh will be derived using Hamilton's principle. This will result, as we shall prove in the following, in nodal configurational force balance, which unlike the continuous setting is not automatically satisfied.

We next observe that the expanded *space-time* based configurational bundle framework that serves as a theoretical basis for the analysis of space-time variational integrators and variational space-time mesh adaption, is not advantageous when the spatial and time discretization are decoupled By contrast, much more insight might be gained by adopting a *space-space* configuration bundle approach, that notably highlights the structure of mesh adaption framework while remarkably simplifying its analysis and implementation.

We proceed to show in an illustrative example that the use of the *standard* Hamilton's principle to supply both the motion and the evolution of the spatial mesh usually results in unstable and meaningless solutions. These instabilities are attributed to inaccurate approximations for the *velocity field* resulting from the approximation for the motion of the mechanical system. To overcome this difficulty we shall make use of an *independent, assumed* velocity approximation different from that derived by time differentiation of the motion and we shall develop a *mixed, multifield version of Hamilton's principle* that allows for *independent* interpolations of velocities *and* deformations. This *mixed* variational principle, which shall be referred to as *mixed Hamilton's principle*, has been also linked to the Pontryagin's maximum principle in optimal control [54] and is thus referred to as *Hamilton's Pontryagin variational principle*, see [64] for a historical overview. Within the full space-time context and for small strains it was theoretically conceptualized by Washizu, see [62], §15.2. This mixed version of Hamilton's principle is invoked and the corresponding Euler-Lagrange equations might be collected to form an extended system of equations to determine the time evolution of nodal displacements, velocities, and the mesh.

We finally consider the problem of time discretization. After the space is discretized one is left with a finite degree-of-freedom dynamical system that evolves continuously in time. More precisely, the action integral of the system transitions from a *mixed space-time*-dependent field functional to a *mixed semidiscrete* functional whose arguments depend only on time. A complete discrete system is then obtained by recourse of time discretization. To this end we shall develop an extended family of variational time integrators, which will be referred to as *mixed variational time integrators*, that allow for the use of independent *time* interpolations for velocities and configurations.

Chapter 2 reviews the process just outlined with particular emphasis in the conceptual transition from variational adaption in *time,* to variational mesh adaption in *space-time* and finally to variational adaption in *space-space*. To simplify the exposition and to keep the technicalities to a minimum only one-dimensional solid dynamics is considered. This chapter provides a simple overview of the mixed version of Hamilton's principle both in time and space-time as well as its semidiscrete and full discrete versions.

In attempting to apply the variational adaptivity framework to problems with evolving shocks and steep gradients we are required to consider systems with viscosity. In this case the governing variational principle is the Lagrange-d'Alembert principle. One intrinsic difficulty in non-conservative systems is the formulation of a variational framework from which the equations of balance of configurational forces in the presence of viscosity can be established and can provide the basis for mesh adaption. For conservative systems it was demonstrated, as we shall review as we proceed, that *configurational force balance* follows directly from Hamilton's principle as Euler-Lagrange equations corresponding to spatial translations or reparametrizations of the base space, i.e., space-time. Motivated by the ideas developed in [44] for general dissipative behavior, we shall develop an extended version of Lagrange-d'Alembert principle in both standard-single-field and mixed-multifield versions from which both mechanical and configurational force balance equations in the presence of viscosity can be established. The mixed version of this extended version of Lagrange-d'Alembert principle will operate as the driving variational principle for mesh adaptivity in the framework of solid dynamics for elastic materials with viscosity.

Chapter 3 reviews this variational formulation of configurational forces for isothermal elastodynamics with and without viscosity. The development follows the spirit of the space-time based concept analyzed within the context of variational integrators by [29], [30], [31], [63] but using a *space-space* bundle as opposed to a *space-time* based bundle. This space-space perspective provides a more intuitive and appropriate conceptual framework for the class of approximations considered in this work, i.e., based on uncoupled space and time discretization. The derivation of the equations of balance of configurational forces from Hamilton's principle is reviewed and the extension of Lagrange-d'Alembert principle to drive configurational force balance in the presence of viscosity is presented. Particular emphasis has been placed on geometrical considerations where we have added some innovative concepts relevant to the analysis of the structure of the method.

In Chapter 4 we consider the formulation of a generalized variational framework to account for general dissipative behavior to include not only viscosity, but also thermal and inelastic processes. Thermal processes are incorporated by taking as primitive thermal variables the so-called *thermal displacements*, an idea suggested in [13] and considered within the context of the theory of configurational forces in [3], [18], [47], [48]. Thermal displacements are defined as the time integral of the temperature field or, equivalently, as the scalar field whose rate is the temperature. The main consequence of introducing thermal displacements as primitive variables is that a *correspondence* or *analogy* between mechanical variables and thermal variables can be established. For each quantity in the equation of mechanical force balance, parallel quantities can be identified in the equation of entropy balance. In order to extend the variational adaptivity framework to problems with thermal and internal variables we shall take this analogy further by assuming an additive decomposition for the heat flux into a conservative, dissipationless part and a non-conservative (or dissipative) part in complete analogy to the well-established additive decomposition of the mechanical stress into elastic (or conservative) and viscous parts. We shall furthermore pursue equivalent decompositions for the thermodynamic stresses conjugate to the internal variables and for the mechanical body forces and heat sources. Then, mirroring the formulation of the extended Lagrange-d'Alembert principle developed for isothermal elasticity with viscosity, we shall formulate an *extended thermomechanical* analog of Lagrange-d'Alembert principle from which all governing equations, i.e., mechanical force balance, entropy balance, internal force balance, and configurational force balance, can be derived and from which adaptivity eventually can be driven.

A central attribute of the variational principles we consider in this work is its *mixed or multifield* character, which allows for the combination of multiple interpolation spaces as an approach to control stability. Mixed variational principles have been widely used in the formulation of finite element procedures (see for example [1]) mainly in elliptic (static) boundary value problems. In chapter 5 we develop the mixed version of Hamilton's principle as it will be used for variational space adaptivity. These mixed principles might be regarded as the dynamic analog of well-known DeVeubeke-Hu-Washizu mixed variational principles for statics and related principles [62], [9]. In particular the two-field (deformation-velocity) mixed version of Hamilton's principle from which we shall drive adaptivity corresponds to the deformation-strain dual of the well-known Hellinger-Reissner principle. We shall also develop in this chapter a mixed version of the *extended* Lagrange-d'Alembert principle (in its mechanical and thermomechanical versions) targeted to drive adaptivity in problems with viscosity. In this mixed version of the extended Lagrange-d'Alembert principle a total assumed viscous force field is incorporated into the model as a new unknown, and independent test functions are used to enforce compatibility between the assumed viscous field and the physical viscous stresses.

Chapter 6 fully develops the finite element formulation and implementation and variational time integration within the context of elastodynamics with and without viscous processes. Since the full space-time discretization is effected in stages, the first part of the chapter focuses in the spatial discretization using the mixed Hamilton's principle and leads to a semidiscrete, finite degree-of-freedom dynamical system, while the second part focuses in the time discretization using mixed variational time integrators. Particular emphasis has been placed in geometrical aspects of the method and in highlighting differences and similitudes between the semidiscrete and continuous pictures. A comparison between the formulations based on the standard, single-field and mixed-multifield versions of Hamilton's principle is presented and the need for driving adaptivity with the latter is demonstrated with an illustrative example. Several one dimensional and three-dimensional numerical examples and tests designed to assess the performance, robustness and potential of the adaptivity framework are presented in Chapter 7. In particular we assess the convergence in a wave propagation example and explore the use of this methodology in a dynamic fracture mechanics test problem.

Chapter 2

Variational Mesh Adaption in 1D

In this chapter we present an overview of the fundamental aspects of the variational methods developed in this work. To simplify the exposition and to keep the technicalities to a minimum we shall restrict the presentation to one-dimensional hyperelastodynamics. The general formulation will be developed in the following chapters. We start by reviewing Hamilton's principle, Lagrange-d'Alembert's principle and variational integrators, highlighting the fundamental concept of horizontal variations. We next review the concept of variational adaptivity as it applies to finite dimensional Lagrangian systems. We proceed then to study a *mixed* version of Hamilton's principle in which not only configurations but also velocities are taken as independent functions. This mixed variational principle, which will be referred to as *mixed-Hamilton's principle*, is then used to formulate an extended family of time integrators that makes use of different time interpolations for velocities and trajectories. The first section of this chapter focuses on systems where the only independent variable is time t, i.e., finite-dimensional Lagrangian systems, and provides a background for the upcoming developments. In the second section we turn to systems that depend on both space X and time t (Lagrangian *field* theory). When the space variable is incorporated into the picture, we are obviously required to consider the problem of discretization in time *and* space. Within this context we review Hamilton's principle, highlighting the fundamental concept of space-time horizontal variations and horizontal Euler-Lagrange equations and we study the mixed version of Hamilton's principle for space-time-dependent systems. After reviewing the concept of variational adaptivity as it applies to static problems, we present the *space-time* generalization of this idea and its implementation in terms of space-time isoparametric elements. This methodology is then restricted to *space adaption only*, which results in a particular class of space-time finite elements where the same time step is used for all nodes in the mesh, i.e., space-time is discretized with an *homogeneous time step.* We will show that for this particular class of space-time finite elements there is no need to resort to the machinery of the space-time formalism and its implementation in terms of finite elements since, as we shall prove, this discretization is *equivalent* to effect the space-time discretization in two separated and *uncoupled* stages, the first stage (semidiscretization in space) where the space variable is discretized keeping the time continuous and *over a continuously deforming spatial mesh*, followed by a second stage in which the time is discretized using an appropriate time integrator. We finally present a mixed variational adaptive finite element formulation governed by the mixed version of Hamilton's principle and characterized by an *independent, assumed* spatial interpolation for the material velocity field and independent *time* interpolations for nodal displacement and velocity parameters. The use of an independent interpolation for the velocity field is proposed as an approach to overcome instability problems inherent to the use of finite elements supported over moving meshes.

In summary, the resulting mesh adaption framework is characterized by the following features:

1. The unknown field of the problem (deformation) and its time derivative (velocity) are interpolated in space over a continuously deforming spatial mesh.

2. The evolving mesh itself is regarded as a new unknown to be handled jointly with the original unknown field and its time rate.

3. The mixed version of Hamilton's principle is used to supply not only the main unknowns but also the deforming mesh.

4. Space interpolation and time interpolation are decoupled and effected in two separated stages. The first spatial discretization over the continuously deforming mesh leads to the construction of a finite-dimensional (time-only-dependent) Lagrangian system. The latter is then discretized in time leading to the construction of a full discrete (in space and time) system.

5. Equations for the evolution of all unknowns (original unknown, fields, their velocities and the mesh) are obtained by invoking the stationarity of the mixed action with respect to variation of all its arguments. These equations correspond to the equations of mechanical force balance (or balance of linear momentum), configurational force balance (balance of material momentum), and compatibility between assumed and consistent velocity interpolations.

6. Since the governing differential equations follow from the *mixed* Hamilton's principle, its integration can be directly accomplished by making use of a *mixed* variational integrator of the class analyzed in the first part of this chapter.

2.1 Mixed variational principles for dynamics and mixed variational integrators

2.1.1 Hamilton's principle

We consider a finite-dimensional dynamical system with configurations specified by the set of generalized coordinates $q(t)$ and with Lagrangian $L(q, \dot{q})$ typically defined as the difference between kinetic and potential energies of the system. As we mentioned in the introduction to this chapter, in this section we will consider only *time* as independent variable. The action functional is defined as

$$S[q(t)] = \int_{t_0}^{t_f} L(q, \dot{q})\, dt$$

where t_0 and t_f are the initial and final times. Given the forces that act in and on the dynamical system, we would like to find its time evolution, namely the curve $q(t)$. Hamilton's principle states that among all the possible trajectories that join a given initial configuration $q(t_0)$ with a final configuration $q(t_f)$, the actual motion of the system corresponds to the particular trajectory that renders the action functional stationary with respect to every *admissible* variation δq of the trajectory $q(t)$, i.e., variations δq that vanish in the initial and final times $\delta q(t_0) = \delta q(t_f) = 0$. This implies that the variation of the action functional vanishes, namely

$$\begin{aligned} \langle \delta S, \delta q \rangle &= \frac{d}{d\varepsilon} S[q + \varepsilon \delta q] \bigg|_{\varepsilon=0} = \\ &= \int_{t_0}^{t_f} \left(\frac{\partial L}{\partial q} \delta q + \frac{\partial L}{\partial \dot{q}} \delta \dot{q} \right) dt = 0 \end{aligned}$$

for every δq in the set of admissible variations. Integrating by parts we find

$$\langle \delta S, \delta q \rangle = \int_{t_0}^{t_f} \left\{ \left(\frac{\partial L}{\partial q} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}} \right) \right) \delta q \right\} dt + \frac{\partial L}{\partial \dot{q}} \delta q \bigg|_{t_0}^{t_f} = 0$$

Since this identity must be satisfied for every admissible variations δq, and assuming that the latter is continuous in the time interval, the previous implies the well-known *Euler-Lagrange* equations

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}} \right) - \frac{\partial L}{\partial q} = 0$$

The magnitudes

$$\begin{aligned} p &= \frac{\partial L}{\partial \dot{q}} \\ f^e &= -\frac{\partial L}{\partial q} \end{aligned}$$

are, respectively, the generalized momentum and generalized (conservative) forces, and in terms of them the Euler-Lagrange equations reduce to

$$\frac{dp}{dt} + f^e = 0$$

which correspond to the equation of mechanical force balance, or equations of momentum balance.

In particular we will consider Lagrangian systems of the form

$$L(q, \dot{q}) = \frac{1}{2} m(q) \dot{q}^2 - I(q) \tag{2.1}$$

where $m(q)$ is the mass, possibly configuration-dependent, $I(q)$ is the potential energy, and the Lagrangian is given simply by the difference between kinetic and potential energies. For this particular Lagrangian the momentum and conservative forces follow as

$$\begin{aligned} p &= m(q)\dot{q} \\ f^e &= -\frac{\partial}{\partial q}\left(\frac{1}{2} m \dot{q}^2\right) + \frac{\partial I}{\partial q} \end{aligned}$$

and the Euler-Lagrange equations reduce to

$$\frac{d}{dt}(m(q)\dot{q}) + f^e(q) = 0 \tag{2.2}$$

2.1.2 Lagrange-d'Alembert principle

We will consider also systems with viscosity. In this case the total force is given by

$$f = f^e + f^v$$

where f^v are the viscous (non-equilibrium or non-conservative) forces assumed to depend explicitly on velocity and possibly on the instantaneous configuration, i.e.,

$$f^v = f^v(q, \dot{q})$$

Furthermore we shall assume that the viscous force derives from a kinetic potential $\phi(q, \dot{q})$ in the form

$$f^v = \frac{\partial \phi}{\partial \dot{q}}$$

In this case the total force balance equation is given by

$$\frac{d}{dt}(m(q)\dot{q}) + f^e(t, q) + f^v(q, \dot{q}) = 0 \tag{2.3}$$

or in terms of the Lagrangian and kinetic potentials as

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right)-\frac{\partial L}{\partial q}+\frac{\partial \phi}{\partial \dot{q}}=0$$

Unlike the case of conservative systems, this equation does not derive from Hamilton's principle. It can be established instead from the *Lagrange d'Alembert* principle

$$\langle \delta S, \delta q\rangle-\int_{t_0}^{t_f} f^v\left(q, \dot{q}\right)\delta q dt=0$$

where S is the action defined as in the case of conservative systems as

$$S\left[q\right]=\int_{t_0}^{t_f} L\left(q, \dot{q}\right)dt$$

and where the above identity must be satisfied for every admissible variation δq. For viscous forces deriving from a kinetic potential the Lagrange-d'Alembert principle becomes

$$\langle \delta S, \delta q\rangle-\int_{t_0}^{t_f} \frac{\partial \phi}{\partial \dot{q}}\left(q, \dot{q}\right)\delta q dt=0 \qquad \forall \delta q$$

2.1.3 Horizontal variations

Of key importance to understanding the methods studied in this work is the concept of *horizontal variations* and the Euler-Lagrange equations associated to the stationarity of the action functional with respect to the latter, which will be referred to as *horizontal Euler-Lagrange equations.* Consider the *graph* of the function $q\left(t\right)$, i.e., the curve $\left(t, q\left(t\right)\right)\in\mathbb{R}\times\mathbb{Q}$, where $\mathbb{Q}$ is the configuration space, figure 2.1. The components t and q are, respectively, the *horizontal* and *vertical* coordinates of each point on this curve. Hamilton's principle involves the stationarity of the action functional with respect to vertical variations δq, which implies the Euler-Lagrange equation

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right)-\frac{\partial L}{\partial q}=0$$

the equation of momentum balance. We now focus attention on the study of variations of the action with respect to the horizontal variable δt. To this end we follow the usual procedure (c.f. references [20], [29], [31]) of introducing a *change of parametrization of the horizontal variable*

$$t=\psi\left(\tau\right)$$

where τ is a new parameter and $\psi:\mathbb{R}\rightarrow\mathbb{R}$ is an invertible function that maps the parameter domain $\left[\tau_0, \tau_f\right]$ into the time domain $\left[t_0, t_f\right]$ as depicted in figure 2.1.

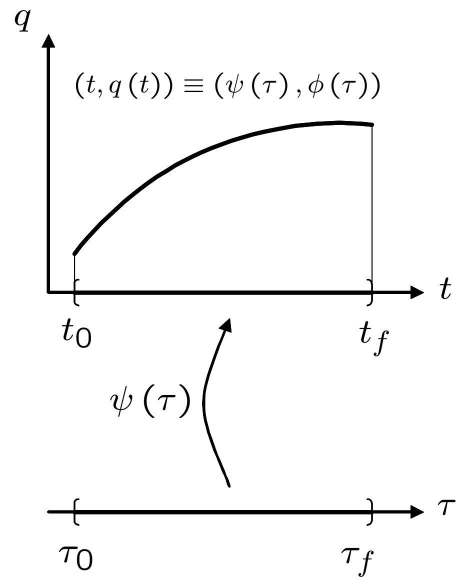

Figure 2.1: Trajectory of the dynamical system. Graph and representation of a change of parametrization of the horizontal (time) domain.

Let

$$\phi = q \circ \psi \tag{2.4}$$

or

$$\phi(\tau) = q(\psi(\tau))$$

be the composition function. It follows from these definitions that the pair $(\psi(\tau), \phi(\tau))$ represents a change of parametrization of the graph of the function $q(t)$, namely, each point of this graph might be parametrized as

$$(t, q(t)) = (\psi(\tau), \phi(\tau))$$

We next refer the action integral to the parameter domain (τ_0, τ_f) to obtain

$$\begin{aligned} S &= \int_{t_0}^{t_f} L(q, \dot{q})\, dt = \\ &= \int_{\tau_0}^{\tau_f} L(q \circ \psi, \dot{q} \circ \psi)\, \psi'(\tau)\, d\tau = \\ &= \int_{\tau_0}^{\tau_f} L\left(\phi(\tau), \frac{\phi'(\tau)}{\psi'(\tau)}\right) \psi'(\tau)\, d\tau = \\ &= S[\psi, \phi] \end{aligned}$$

where we the prime symbol $'$ denotes the derivative with respect to the parameter τ (as opposed to the dot symbol, which denotes the derivative with respect to time t) and where we have made use of the identity

$$\dot{q} \circ \psi = \frac{\phi'}{\psi'}$$

that follows by differentiation of (2.4) with respect to the parameter τ. Horizontal variations of S are defined as the variations of the latter with respect to ψ, namely,

$$\begin{aligned} \langle \delta S, \delta\psi \rangle &= \frac{d}{d\varepsilon} S\left[\psi + \varepsilon\delta\psi, \phi\right]\Big|_{\varepsilon=0} = \\ &= \int_{\tau_0}^{\tau_f} \left(L - \frac{\partial L}{\partial \dot{q}} \frac{\phi'(\tau)}{\psi'(\tau)} \right) \delta\psi'(\tau)\, d\tau \end{aligned}$$

Referring the previous back to the original time domain $[t_0, t_f]$ we find

$$\langle \delta S, \delta\psi \rangle = \int_{t_0}^{t_f} \left(L - \frac{\partial L}{\partial \dot{q}} \dot{q} \right) \frac{d}{dt} \left(\delta\psi \circ \psi^{-1} \right) d\tau$$

where we have made use of the identity

$$\begin{aligned} \frac{d}{dt}\left(\delta\psi \circ \psi^{-1} \right) &= \left(\delta\psi' \circ \psi^{-1} \right) \frac{d}{dt}\left(\psi^{-1} \right) = \\ &= \left(\frac{\delta\psi'}{\psi'} \right) \circ \psi^{-1} \end{aligned}$$

Integrating by parts yields

$$\begin{aligned} \langle \delta S, \delta\psi \rangle &= \int_{t_0}^{t_f} -\frac{d}{dt} \left(L - \frac{\partial L}{\partial \dot{q}} \dot{q} \right) \left(\delta\psi \circ \psi^{-1} \right) d\tau \\ &\quad + \left(L - \frac{\partial L}{\partial \dot{q}} \dot{q} \right) \left(\delta\psi \circ \psi^{-1} \right) \Big|_{t_0}^{t_f} \end{aligned} \tag{2.5}$$

Horizontal Euler-Lagrange equations follow then by invoking the stationarity of the action functional S with respect to all *admissible* horizontal variations $\delta\psi$, i.e., variations $\delta\psi$ continuous and vanishing at the initial and final times $\delta\psi(\tau_0) = \delta\psi(\tau_f) = 0$,

$$\langle \delta S, \delta\psi \rangle = 0 \quad \forall \delta\psi$$

On account of identity (2.5), the previous implies the following *horizontal Euler-Lagrange equation:*

$$-\frac{d}{dt}\left(L - \frac{\partial L}{\partial \dot{q}} \dot{q} \right) = 0$$

Three important observations follow:

(i) The horizontal Euler-Lagrange equation is independent of the parametrization $\psi(\tau)$. We shall therefore and occasionally write δt instead of $\delta\psi$.

(ii) For Lagrangian systems of the form

$$L = \frac{1}{2} m(q)\,\dot{q}^2 - I(q)$$

$I(q)$ is the potential energy; the horizontal Euler-Lagrange equation reduces to

$$\frac{dE}{dt} = 0$$

where

$$\begin{aligned} E &= -\left(L - \frac{\partial L}{\partial \dot{q}}\dot{q}\right) = \\ &= \frac{1}{2} m(q)\,\dot{q}^2 + I(q) \end{aligned} \tag{2.6}$$

is the total energy of the system. The horizontal balance equations for finite-dimensional (time-only-dependent) Lagrangian systems is therefore the equation of energy balance.

(iii) For conservative systems, horizontal and vertical Euler-Lagrange equations are *equivalent*, in the sense that if one equation is satisfied, the other is automatically satisfied. This can be directly verified by defining the following operators (left hand side of the vertical and horizontal Euler-Lagrange equations)

$$\begin{aligned} \mathcal{F}_q(q) &= \frac{d}{dt}\frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} \\ \mathcal{F}_t(q) &= -\frac{d}{dt}\left(L - \frac{\partial L}{\partial \dot{q}}\dot{q}\right) \end{aligned}$$

whereupon the vertical and horizontal balance equations can be rewritten as

$$\begin{aligned} \mathcal{F}_q &= 0 \\ \mathcal{F}_t &= 0 \end{aligned}$$

Then, it is straightforward to prove the identity

$$\mathcal{F}_t = -\dot{q}\mathcal{F}_q \tag{2.7}$$

which implies

$$\mathcal{F}_q = 0 \Longleftrightarrow \mathcal{F}_t = 0$$

As will be illustrated shortly, this equivalence is broken in the discrete setting, and discrete energy conservation does not follow automatically from discrete momentum conservation in general but only for particular and appropriate selection of the time discretization.

2.1.4 Variational integrators

We review in this subsection the basic formulation of variational integrators as a background for the upcoming developments. An extensive analysis of this class of integrators may be found for example in [20], [29], [30], [31] and references therein.

As opposed to standard integrators that discretize (in time) the Euler-Lagrange equations, in a variational integrator it is the *action functional* what is discretized. To this end we partition the time interval $[t_0, t_f]$ into discrete times $\left(t^0 = t_0, \cdots, t^k, \cdots, t^K = t_f\right)$, where K is the number of time subintervals and where we use a supraindex to denote time step. This partition results in a sequence of discrete configurations $\left(q^0 = q_0, \cdots, q^k, \cdots, q^K = q_f\right)$. We then interpolate the trajectories $q(t)$ in each interval $\left[t^k, t^{k+1}\right]$ with appropriate interpolating functions. Different choices of interpolation spaces will give place to different integrators. To fix ideas and by way of example assume that we choose linear interpolation, namely,

$$q(t) = q^k \frac{t^{k+1} - t}{t^{k+1} - t^k} + q^{k+1} \frac{t - t^k}{t^{k+1} - t^k}$$

Inserting this interpolation into the action integral result in the *action sum*

$$S_d\left(q^0, \cdots, q^k, \cdots, q^K\right) = \sum_{k=0}^{K-1} L_d\left(q^k, q^{k+1}, t^k, t^{k+1}\right)$$

where

$$L_d\left(q^k, q^{k+1}, t^k, t^{k+1}\right) = \int_{t^k}^{t^{k+1}} L\left(\frac{t^{k+1} - t}{t^{k+1} - t^k} q^k + \frac{t - t^k}{t^{k+1} - t^k} q^{k+1}, \frac{q^{k+1} - q^k}{t^{k+1} - t^k}\right) dt$$

is the *discrete-Lagrangian.* We next approximate the integral by recourse of an appropriate quadrature rule. Different quadrature rules will give different integrators. We take as a particular example the simple "midpoint" rule

$$L_d\left(q^k, q^{k+1}, t^k, t^{k+1}\right) = \left(t^{k+1} - t^k\right) L\left((1-\alpha) q^k + \alpha q^{k+1}, \frac{q^{k+1} - q^k}{t^{k+1} - t^k}\right)$$

where the integrand is evaluated at the intermediate time (midpoint)

$$t^{k+\alpha} = (1-\alpha) t^k + \alpha t^{k+1}$$

with $\alpha \in [0, 1]$ an integration parameter. Discrete trajectories are then obtained by invoking the stationarity of the discrete action sum S_d with respect to variations of the discrete trajectories q^k:

$$\frac{\partial S}{\partial q^k} = D_1 L_d \left(q^k, q^{k+1}, t^k, t^{k+1}\right) + D_2 L_d \left(q^{k-1}, q^k, t^{k-1}, t^k\right) = 0 \tag{2.8}$$

where we have made use of the standard notation $D_i L_d$ to indicate the derivative of L_d with respect to its i-th argument. This identity is the *discrete Euler-Lagrange equation* (DEL). It represents an equation to be solved for q^{k+1} given q^k and q^{k-1} and defines therefore a time-stepping algorithm.

Introducing the discrete momentum

$$p^k = -D_1 L_d \left(q^k, q^{k+1}, t^k, t^{k+1}\right) = D_2 L_d \left(q^{k-1}, q^k, t^{k-1}, t^k\right) \tag{2.9}$$

the algorithm may be rewritten in the so-called *position-momentum* form:

$$\begin{aligned} p^k &= -D_1 L_d \left(q^k, q^{k+1}, t^k, t^{k+1}\right) \\ p^{k+1} &= D_2 L_d \left(q^k, q^{k+1}, t^k, t^{k+1}\right) \end{aligned}$$

Given the pair $\left(p^k, q^k\right)$ the first equation provides an (implicit) equation to be solved for q^{k+1} and the second serves as an update equation for the momentum p^{k+1}. The pair provides therefore an update system for the determination of $\left(p^{k+1}, q^{k+1}\right)$ given $\left(p^k, q^k\right)$.

For the particular Lagrangian of the form (2.1) and making use of linear time interpolation and the midpoint integration rule we obtain the discrete Lagrangian

$$L_d \left(q^k, q^{k+1}, t^k, t^{k+1}\right) = \left(t^{k+1} - t^k\right) \left(\frac{1}{2} m^{k+\alpha} \left(\frac{q^{k+1} - q^k}{t^{k+1} - t^k}\right)^2 - I^{k+\alpha}\right) \tag{2.10}$$

where

$$\begin{aligned} t^{k+\alpha} &= (1-\alpha)\, t^k + \alpha t^{k+1} \\ q^{k+\alpha} &= q\left(t^{k+\alpha}\right) = \\ &= (1-\alpha)\, q^k + \alpha q^{k+1} \end{aligned}$$

are, respectively, the intermediate time and configuration, and

$$\begin{aligned} m^{k+\alpha} &= m\left(q^{k+\alpha}\right) \\ I^{k+\alpha} &= I\left(q^{k+\alpha}\right) \end{aligned}$$

are the mass and potential energy evaluated at the midpoint. The discrete momenta follow in this case as

$$\begin{aligned} p^k &= m^{k+\alpha}\left(\frac{q^{k+1}-q^k}{t^{k+1}-t^k}\right)+(1-\alpha)\left(t^{k+1}-t^k\right)f^{e-(k+\alpha)} \\ p^{k+1} &= m^{k+\alpha}\left(\frac{q^{k+1}-q^k}{t^{k+1}-t^k}\right)-(\alpha)\left(t^{k+1}-t^k\right)f^{e-(k+\alpha)} \end{aligned}$$

where

$$\begin{aligned} f^{e-(k+\alpha)} &= -\frac{\partial}{\partial q}\left(\frac{1}{2}m(q)\left(\frac{q^{k+1}-q^k}{t^{k+1}-t^k}\right)^2-I(q)\right)\Bigg|_{q^{k+\alpha}}= \\ &= -\left(\frac{1}{2}\frac{\partial m}{\partial q}^{k+\alpha}\left(\frac{q^{k+1}-q^k}{t^{k+1}-t^k}\right)^2-\frac{\partial I}{\partial q}^{k+\alpha}\right) \end{aligned}$$

is the midpoint force and the DEL reduce to

$$\begin{gathered} m^{k+\alpha}\left(\frac{q^{k+1}-q^k}{t^{k+1}-t^k}\right)-m^{k-1+\alpha}\left(\frac{q^k-q^{k-1}}{t^k-t^{k-1}}\right)+ \\ +(1-\alpha)\left(t^{k+1}-t^k\right)f^{e-(k+\alpha)}+(\alpha)\left(t^k-t^{k-1}\right)f^{e-(k-1+\alpha)}=0 \end{gathered} \tag{2.11}$$

which clearly represent a discretization of (2.2)

2.1.5 Extension for non-conservative systems

For discrete systems with non-conservative forces we may extend the previous integrator by making use of the following discretized version of Lagrange d'Alembert principle ([29], [30], [30]):

$$\frac{\partial S_d}{\partial q^k}\delta q^k-\sum_{k=0}^{K}f_d^{v-}\left(q^k,q^{k+1},t^k,t^{k+1}\right)\delta q^k+f_d^{v+}\left(q^k,q^{k+1},t^k,t^{k+1}\right)\delta q^{k+1}=0 \qquad \forall k$$

where f^{v-} and f^{v+} are the so-called "left" and "right" non-conservative forces that should approximate the non-conservative part $\int_{t_0}^{t_f} f^v \delta q dt$ of the Lagrange-d'Alembert principle, namely,

$$\sum_{k=0}^{K}f_d^{v-}\left(q^k,q^{k+1},t^k,t^{k+1}\right)\delta q^k+f_d^{v+}\left(q^k,q^{k+1},t^k,t^{k+1}\right)\delta q^{k+1}\approx\int_{t_0}^{t_f}f^v\left(q,\dot{q}\right)\delta q dt \tag{2.12}$$

Enforcing this principle for every variation in the discretized trajectory δq^k results in the identity

$$\begin{gathered} D_1L_d\left(q^k,q^{k+1},t^k,t^{k+1}\right)+D_2L_d\left(q^{k-1},q^k,t^{k-1},t^k\right)+ \\ -f_d^{v-}\left(q^k,q^{k+1},t^k,t^{k+1}\right)-f_d^{v+}\left(q^{k-1},q^k,t^{k-1},t^k\right)=0 \end{gathered} \tag{2.13}$$

which provides the time-stepping algorithm in the presence of non-conservative forces. Defining the discrete momentum now as

$$\begin{aligned} p^k &= -D_1 L_d\left(q^k, q^{k+1}, t^k, t^{k+1}\right) + f_d^{v-}\left(q^k, q^{k+1}, t^k, t^{k+1}\right) = \\ &= D_2 L_d\left(q^{k-1}, q^k, t^{k-1}, t^k\right) - f_d^{v+}\left(q^{k-1}, q^k, t^{k-1}, t^k\right) \end{aligned}$$

the "position-momentum" form of the algorithm may be rewritten as

$$\begin{aligned} p^k &= -D_1 L_d\left(q^k, q^{k+1}, t^k, t^{k+1}\right) + f_d^{v-}\left(q^k, q^{k+1}, t^k, t^{k+1}\right) \\ p^{k+1} &= D_2 L_d\left(q^k, q^{k+1}, t^k, t^{k+1}\right) - f_d^{v+}\left(q^k, q^{k+1}, t^k, t^{k+1}\right) \end{aligned}$$

As in the case of conservative systems, the previous equations define the update algorithm to compute the updated position and momentum $\left(q^{k+1}, p^{k+1}\right)$ given the current position and momentum $\left(q^k, p^k\right)$.

We consider by way of example the particular case of linear time interpolation for $q\left(t\right)$ and one single quadrature point located at $t^{k+\gamma} = \left(1-\gamma\right) t^k + \left(\gamma\right) t^{k+1}$ with $\gamma \in [0,1]$, another integration parameter (possibly coincident with α). The non-conservative part of the Lagrange-d'Alembert results are approximated then as

$$\int_{t_0}^{t_f} f^v\left(q\left(t\right), \dot{q}\left(t\right)\right) \delta q dt \approx \sum_{k=0}^{K} \left(t^{k+1} - t^k\right) f^v\left(q^{k+\gamma}, \frac{q^{k+1} - q^k}{t^{k+1} - t^k}\right) \delta q^{k+\gamma}$$

with

$$q^{k+\gamma} = \left(1-\gamma\right) q^k + \left(\gamma\right) q^{k+1}$$

and

$$\delta q^{k+\gamma} = \left(1-\gamma\right) \delta q^k + \left(\gamma\right) \delta q^{k+1}$$

Rearranging in the approximation we find

$$\int_{t_0}^{t_f} f^v\left(q\left(t\right), \dot{q}\left(t\right)\right) \delta q dt \approx \sum_{k=0}^{K} f_d^{v-} \delta q^k + f_d^{v+} \delta q^{k+1}$$

where

$$\begin{aligned} f_d^{v-} &= \left(1-\gamma\right)\left(t^{k+1} - t^k\right) f^{v-(k+\gamma)} \\ f_d^{v+} &= \left(\gamma\right)\left(t^{k+1} - t^k\right) f^{v-(k+\gamma)} \end{aligned}$$

with

$$f^{v-(k+\gamma)} = f^{v}\left(q^{k+\gamma}, \frac{q^{k+1}-q^{k}}{t^{k+1}-t^{k}}\right) = \frac{\partial \phi}{\partial \dot{q}}\left(q,\dot{q}\right)\Big|_{\left(q^{k+\gamma}, \frac{q^{k+1}-q^{k}}{t^{k+1}-t^{k}}\right)}$$

In particular, if the Lagrangian is of the form 2.1, the discrete momentum reduce to

$$\begin{aligned} p^{k} &= m^{k+\alpha}\left(\frac{q^{k+1}-q^{k}}{t^{k+1}-t^{k}}\right) + \left(t^{k+1}-t^{k}\right)\left(\left(1-\alpha\right) f^{e-(k+\alpha)} + \left(1-\gamma\right) f^{v-(k+\gamma)}\right) \\ p^{k+1} &= m^{k+\alpha}\left(\frac{q^{k+1}-q^{k}}{t^{k+1}-t^{k}}\right) - \left(t^{k+1}-t^{k}\right)\left(\left(\alpha\right) f^{e-(k+\alpha)} + \left(\gamma\right) f^{v-(k+\gamma)}\right) \end{aligned}$$

which clearly represents a discretization of equations (2.3).

2.1.6 Variational integrators and incremental potentials

We analyze whether the DEL equations (2.8) or their counterpart for dissipative systems (2.13) derive from the so-called *incremental potential*. An incremental potential is a function $\Phi\left(q^{k-1}, q^{k}, q^{k+1}\right)$ such that the update equations that map the pair $\left(q^{k-1}, q^{k}\right)$ to the updated pair $\left(q^{k}, q^{k+1}\right)$ (or a linear combination of them) can be written as

$$\frac{\partial \Phi}{\partial q^{k+1}} = 0$$

In this way the configuration at the new time step q^{k+1} can be found by minimizing the incremental potential Φ.

Consider the following hypothesis:

1. A Lagrangian of the form (2.1).
2. Constant mass matrix $m\left(q\right) = m$.
3. A variational integrator based on linear time interpolation for $q\left(t\right)$ and midpoint quadrature rule.
4. A constant time step Δt.
5. A viscous force independent of q and only dependent on $\dot{q}$.
6. Integration parameters $\alpha = \gamma$

In this case the update equations reduce to

$$m\left(\frac{q^{k+1}-q^{k}}{\Delta t} - \frac{q^{k}-q^{k-1}}{\Delta t}\right) + \Delta t\left(\left(1-\alpha\right)\left(\frac{\partial I}{\partial q} + \frac{\partial \phi}{\partial \dot{q}}\right)\Big|_{k+\alpha} + \left(\alpha\right)\left(\frac{\partial I}{\partial q} + \frac{\partial \phi}{\partial \dot{q}}\right)\Big|_{k-1+\alpha}\right) = 0$$

A straightforward differentiation shows that the previous equation may be written as

$$\frac{\partial \Phi}{\partial q^{k+1}} = 0$$

where

$$\Phi\left(q^{k-1}, q^k, q^{k+1}\right) = \frac{m}{2\Delta t}\left(q^{k+1} - q^{pre}\right)^2 + \Delta t \frac{1-\alpha}{a}\left(\left.(I + \alpha \Delta t \phi)\right|_{k+\alpha} - \left.(I + \alpha \Delta t \phi)\right|_{k-1+\alpha}\right)$$

is the incremental potential, with

$$\begin{aligned} q^{pre} &= q^k + \left(q^k - q^{k-1}\right) - \alpha \frac{\Delta t^2}{m}\left.\left(\frac{\partial I}{\partial q} + \frac{\partial \phi}{\partial \dot{q}}\right)\right|_{k-1+\alpha} = \\ &= q^k + \left(q^k - q^{k-1}\right) - \frac{\Delta t^2}{m}\frac{\partial}{\partial q^k}\left(\left|(I + \alpha \Delta t \phi)\right|_{k-1+\alpha}\right) \end{aligned}$$

and

$$\begin{aligned} I^{k+\alpha} &= I\left((1-\alpha)\, q^k + \alpha q^{k+1}\right) \\ &= I\left(q^{k+\alpha}\right) \\ \phi^{k+\alpha} &= \phi\left(\frac{q^{k+1} - q^k}{\Delta t}\right) \\ &= \phi\left(\frac{q^{k+\alpha} - q^k}{\alpha \Delta t}\right) \end{aligned}$$

2.1.7 Variational time adaption

In this section we illustrate the concept of variational adaptivity within the context of finite dimensional Lagrangian systems. As opposed to standard variational integrators, where the set of discrete times $\left(t^0 = t_0, \cdots, t^k, \cdots, t^K = t_f\right)$ is given or estimated, we shall regard the latter as *unknowns* and we shall make use of Hamilton's principle to *compute* those unknowns. As was explained in Chapter 1, this idea was originally studied in Kane, Marsden & Ortiz [20] and the class of variational integrators so obtained exactly preserve discrete energy.

We recall that in standard variational integrators (see §2.1.4), only the vertical coordinates q^k of the discretized trajectory (see figure 2.2) are computed and only one equation is derived. This equation is the discrete (vertical) Euler-Lagrange equation (equation 2.8)

$$D_1 L_d\left(q^k, q^{k+1}, t^k, t^{k+1}\right) + D_2 L_d\left(q^{k-1}, q^k, t^{k-1}, t^k\right) = 0 \tag{2.14}$$

where

$$L_d\left(q^k, q^{k+1}, t^k, t^{k+1}\right)$$

is the discrete Lagrangian.

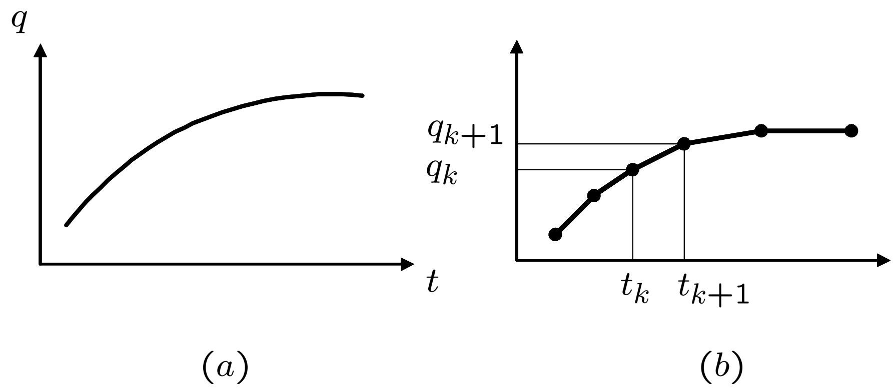

Figure 2.2: Continuous (a) and discrete (b) trajectory of the dynamical system. The complete set of parameters that define the discretization is given not only by the vertical coordinates q^k but also by the horizontal coordinates t^k (the mesh).

We regard now as unknowns not only the vertical coordinates q^k but also the horizontal coordinates t^k and we use the the *same* variational principle from which the (vertical) unknowns q^k are obtained (discrete Hamilton's principle) to derive equations for the determination of the discrete times t^k (horizontal unknowns). In other words we assume that an *optimal* set of discrete times t^k is obtained by rendering the discrete action sum S_d stationary with respect to the horizontal coordinates t^k. We recall that the discrete action sum is given by

$$S_d\left(\cdots, t^k, q^k, \cdots\right) = \sum_{k=0}^{K} L_d\left(q^k, q^{k+1}, t^k, t^{k+1}\right)$$

Invoking the latter stationary with respect to horizontal coordinates t^k we find

$$D_3 L_d\left(q^k, q^{k+1}, t^k, t^{k+1}\right) + D_4 L_d\left(q^{k-1}, q^k, t^{k-1}, t^k\right) = 0 \tag{2.15}$$

This equation coupled with the first discrete Euler-Lagrange equation (2.14) enables the simultaneous determination of both q^k (vertical coordinates) and the mesh t^k (horizontal coordinates).

Consider for example the particular case of Lagrangian systems of the form

$$L\left(q, \dot{q}\right) = \frac{1}{2} m\left(q\right) \dot{q} - I\left(q\right)$$

discretized with piecewise linear and continuous interpolation and a single quadrature point

$$L_d\left(q^k, q^{k+1}, t^k, t^{k+1}\right) = \left(t^{k+1} - t^k\right)\left(\frac{1}{2} m^{k+\alpha}\left(\frac{q^{k+1} - q^k}{t^{k+1} - t^k}\right)^2 - I^{k+\alpha}\right)$$

In this case we have

$$\begin{aligned} D_4L_d\left(q^k,q^{k+1},t^k,t^{k+1}\right) &= -E^k \\ D_3L_d\left(q^k,q^{k+1},t^k,t^{k+1}\right) &= E^k \end{aligned}$$

where

$$E^k = \frac{1}{2}m^{k+\alpha}\left(\frac{q^{k+1}-q^k}{t^{k+1}-t^k}\right)^2 + I^{k+\alpha}$$

is the discrete energy. Equation (2.15) then yields

$$E^k - E^{k-1} = 0$$

Motivated by this example we arrive to the following two important conclusions:

(i) Enforcing horizontal balance equations at the discrete level is equivalent to choosing discrete times t^k such that the *discrete energy is exactly conserved.*

(ii) As opposed to the continuum setting where energy conservation (horizontal balance) follows *automatically* from momentum conservation (vertical balance) (see §2.1.3), in the discrete setting this equivalence is broken. Arbitrary selection of discrete times t^k will not result in general in the automatic satisfaction of a discrete energy conservation law. Vertical and horizontal balance equations are equivalent in the continuum setting but are *not* equivalent in the discrete setting. Therefore, the stationarity of the discrete action with respect to the vertical coordinates q^k will not imply stationarity of the discrete action with respect to horizontal coordinates t^k.

This discrepancy between continuous and discrete settings is illustrated graphically in figure 2.3 (c.f. reference ([29]), see also Chapter 3). Every vertical variation can be interpreted as an horizontal variation in the continuous case. In the discrete case however, horizontal and vertical variations do not lead to the same variation and therefore, horizontal and vertical discrete balance equations are not equivalent.

2.1.8 Mixed Hamilton's principle

In this section we study a *mixed* variational formulation that allows for independent variations of trajectories $q(t)$ and velocities $V(t)$ and an extended class of variational integrators based on this mixed formulation. The mixed variational formulation and corresponding integrator will be referred, respectively, to as the *mixed Hamilton's principle* and *mixed variational integrators.* This mixed principle might be understood as the analogous for *dynamics* of the well-known DeBeuveke-Hu-Washizu variational principle for *statics* and has been linked to the Pontryagin maximum principle

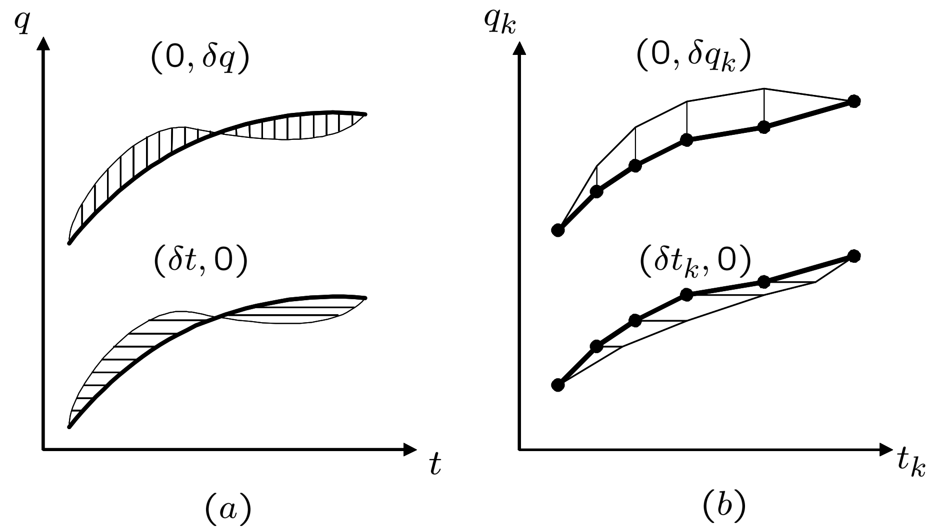

Figure 2.3: Horizontal and vertical variations in the continuous (a) and discrete (b) settings. In the continuous case every horizontal variation might be interpreted as a vertical variation and reciprocally. In the discrete setting, however, horizontal and vertical variations are not equivalent leading to independent horizontal and vertical balance equations.

in optimal control (c.f. [54]). Due to the conceptual link with Pontryagin's maximum principle the name *Hamilton-Pontryagin variational principle* has also been proposed [64]. The formulation of this mixed variational principle follows standard Lagrange multiplier arguments, where the *compatibility* condition $\dot{q} - V = 0$ is imposed by recourse of a Lagrange multiplier p that is itself taken as independent variable. The *mixed action* follows then as

$$S[q, V, p] = \int_{t_0}^{t_f} \left(L(q, V) + p(\dot{q} - V)\right) dt$$

The variations of this functional with respect to each of its arguments are

$$\begin{aligned}
\langle \delta S, \delta q \rangle &= \int_{t_0}^{t_f} \left(\frac{\partial L}{\partial q} \delta q + p \delta \dot{q} \right) dt = 0 \\
\langle \delta S, \delta V \rangle &= \int_{t_0}^{t_f} \left(\frac{\partial L}{\partial V} - p \right) \delta V dt = 0 \\
\langle \delta S, \delta p \rangle &= \int_{t_0}^{t_f} (\dot{q} - V) \delta p dt = 0
\end{aligned}$$

Integrating by parts in the first identity we obtain

$$\langle \delta S, \delta q \rangle = \int_{t_0}^{t_f} \left(\frac{\partial L}{\partial q} - \frac{dp}{dt} \right) \delta q dt + p \delta q|_{t_0}^{t_f} = 0$$

Demanding now the stationarity of the mixed action with respect to admissible variations of all of its arguments, namely, variations $(\delta q, \delta V, \delta p)$ with the first component δq vanishing on the initial and final times t_0 and t_f we find the Euler-Lagrange equations

$$\begin{aligned} \frac{dp}{dt} - \frac{\partial L}{\partial q} &= 0 \\ p &= \frac{\partial L}{\partial V} \\ \dot{q} &= V \end{aligned}$$

We obtain then a system of equations that is equivalent to the Euler-Lagrange equations corresponding to the standard (one-field-dependent) Hamilton's principle. It follows from this identities that the Lagrange multiplier p is nothing more than the momentum evaluated in V instead of $\dot{q}$.

We next eliminate the Lagrange multiplier p by making use of the Euler-Lagrange equation corresponding to variations of V. In this way we build the following (two-field-dependent) mixed action functional

$$S[q,V] = \int_{t_0}^{t_f} \left(L(q,V) + \left.\frac{\partial L}{\partial V}\right|_{(q,V)} (\dot{q} - V) \right) dt$$

The variations of the previous with respect to each of its arguments are

$$\begin{aligned} \langle \delta S, \delta q \rangle &= \int_{t_0}^{t_f} \left(\frac{\partial L}{\partial q}\delta q + \frac{\partial L}{\partial V}\delta\dot{q} + \frac{\partial^2 L}{\partial q \partial V}(\dot{q} - V)\,\delta q \right) dt = 0 \\ \langle \delta S, \delta V \rangle &= \int_{t_0}^{t_f} \frac{\partial^2 L}{\partial V^2}(\dot{q} - V)\,\delta V dt = 0 \end{aligned}$$

Integrating by parts in the first identity we obtain

$$\langle \delta S, \delta q \rangle = \int_{t_0}^{t_f} \left(\frac{\partial L}{\partial q} - \frac{d}{dt}\left(\frac{\partial L}{\partial V}\right) + \frac{\partial^2 L}{\partial q \partial V}(\dot{q} - V) \right) \delta q dt + \left.\frac{\partial L}{\partial V}\delta q\right|_{t_0}^{t_f} = 0$$

Stationarity of the mixed action with respect to independent variations of each of the two arguments $(\delta q, \delta V)$ (with δq vanishing in the initial and final times) implies the Euler-Lagrange equations

$$\begin{aligned} \frac{\partial L}{\partial q} - \frac{d}{dt}\left(\frac{\partial L}{\partial V}\right) + \frac{\partial^2 L}{\partial q \partial V}(\dot{q} - V) &= 0 \\ \frac{\partial^2 L}{\partial V^2}(\dot{q} - V) &= 0 \end{aligned}$$

It easy to see that, if $\frac{\partial^2 L}{\partial V^2}$ is not singular, the previous is equivalent to the Euler-Lagrange equations corresponding to the standard (single-field-dependent) Hamilton's principle.

To simplify the notation we will occasionally use the notation

$$L^{mix}(q,\dot{q},V) = L(q,V) + \left.\frac{\partial L}{\partial V}\right|_{(q,V)} (\dot{q} - V)$$

The new magnitude L^{mix} will be referred to as the *mixed Lagrangian.* Using this new symbol the mixed Hamilton's principle becomes

$$S\left[q,V\right]=\int_{t_0}^{t_f}L^{mix}\left(q,\dot{q},V\right)dt$$

Written in terms of L^{mix} the variations of the mixed action are

$$\begin{aligned}\langle\delta S,\delta q\rangle &= \int_{t_0}^{t_f}\left(\frac{\partial L^{mix}}{\partial q}\delta q+\frac{\partial L^{mix}}{\partial\dot{q}}\delta\dot{q}\right)dt=0\\ \langle\delta S,\delta V\rangle &= \int_{t_0}^{t_f}\frac{\partial L^{mix}}{\partial V}\delta V\,dt=0\end{aligned}$$

and the Euler-Lagrange equation take the compact form

$$\begin{aligned}\frac{d}{dt}\left(\frac{\partial L^{mix}}{\partial\dot{q}}\right)-\frac{\partial L^{mix}}{\partial q} &= 0\\ \frac{\partial L^{mix}}{\partial V} &= 0\end{aligned}$$

For the particular class of Lagrangians of the form $L\left(q,\dot{q}\right)=\frac{1}{2}m\left(q\right)\dot{q}^2-I\left(q\right)$ the mixed (two-field) action is given by

$$S\left[q,V\right]=\int_{t_0}^{t_f}\left(\frac{1}{2}m\left(q\right)V^2-I\left(q\right)+Vm\left(q\right)\left(\dot{q}-V\right)\right)dt$$

The corresponding Euler-Lagrange equations are in this case

$$\begin{aligned}\frac{d}{dt}\left(m\left(q\right)V\right)+f^e &= 0\\ m\left(q\right)\left(\dot{q}-V\right) &= 0\end{aligned}$$

where

$$\begin{aligned}f^e\left(q,\dot{q},V\right) &= -\frac{\partial}{\partial q}\left(\frac{1}{2}m\left(q\right)V^2-I\left(q\right)+Vm\left(q\right)\left(\dot{q}-V\right)\right)=\\ &= -\frac{\partial L^{mix}}{\partial q}\left(q,\dot{q},V\right)\end{aligned}$$

2.1.9 Relation with Hamilton's equations

A straightforward derivation shows that the mixed (two-field) variational formulation just outlined may be transformed into another functional that operates as a variational principle for Hamilton's equations. We recall that Hamilton's equations are

$$\begin{aligned}\dot{p} &= -\frac{\partial H}{\partial q}\\ \dot{q} &= \frac{\partial H}{\partial p}\end{aligned}$$

where $H(q,p)$ is the Hamiltonian defined as

$$H(q,p) = -L(q,V) + pV$$

with V written in terms of (p,q), using for this the inverse of the equation that defines the momentum, namely

$$p = \frac{\partial L}{\partial V}(q,V)$$

To establish this relation, we simply rearrange the mixed (two field) action in the form

$$S[q,V] = \int_{t_0}^{t_f} \left(\left(L(q,V) - V\frac{\partial L}{\partial V}\right) + \frac{\partial L}{\partial q}\dot{q}\right) dt$$

and define

$$-H(q,V) = L(q,V) - V\frac{\partial L}{\partial V}$$

Using this notation the mixed variational principle becomes

$$S[q,V] = \int_{t_0}^{t_f} \left(-H(q,V) - \frac{\partial L}{\partial q}\dot{q}\right) dt$$

Inverting now the relation

$$p = \frac{\partial L}{\partial V}(q,V)$$

to obtain V as function of (q,p) and composing the mixed functional $S(q,V)$ with the obtained function $V(q,p)$, the following new mixed functional arise

$$\begin{aligned}S'[q,p] &= S[q,V(q,p)]\\ &= \int_{t_0}^{t_f} (-H(q,p) - p\dot{q})\, dt\end{aligned}$$

where $H(q,p)$ is the Hamiltonian. Stationarity of the S' with respect to each one of its arguments implies

$$\begin{aligned} \langle \delta S', \delta q \rangle &= \int_{t_0}^{t_f} \left(-\frac{\partial H}{\partial q} \delta q - p \delta \dot{q} \right) dt = 0 \\ \langle \delta S', \delta p \rangle &= \int_{t_0}^{t_f} \left(-\frac{\partial H}{\partial p} - \dot{q} \right) \delta p dt = 0 \end{aligned}$$

with corresponding Euler-Lagrange equations

$$\begin{aligned} \dot{p} - \frac{\partial H}{\partial q} &= 0 \\ \dot{q} + \frac{\partial H}{\partial q} &= 0 \end{aligned}$$

Therefore the stationarity of the new mixed functional $S'[q,p] = S[q, V(q,p)]$ with $V(q,p)$ defined implicitly by $p = \frac{\partial L}{\partial V}(q,V)$ with respect to its arguments implies Hamilton's equations.

2.1.10 Mixed Variational Integration

We proceed now to use the mixed action $S(q,V)$ as an operative variational principle to formulate an extended class of time-stepping algorithms. To this end we partition the time interval $[t_0, t_f]$ into discrete times $\left(t^0 = t_0, \cdots, t^k, \cdots, t^K = t_f\right)$ where K is the number of time subintervals. We proceed by interpolating the trajectories $q(t)$ and velocities $V(t)$ in each interval $\left[t^k, t^{k+1}\right]$ with some interpolating functions. As is standard in mixed formulations, the question that immediately arise is how to select the interpolating spaces. We will provide an insight to the answer of this question by analyzing by way of example the following two possibilities:

1. Trajectories $q(t)$ are interpolated linearly and velocities $V(t)$ are interpolated with a constant $V^{k+\beta}$, namely,

$$\begin{aligned} q(t) &= q^k \frac{t^{k+1} - t}{t^{k+1} - t^k} + q^k \frac{t - t^k}{t^{k+1} - t^k} \\ V(t) &= V^{k+\beta} \end{aligned}$$

   for every $t \in \left[t^k, t^{k+1}\right]$.

2. Both trajectories and velocities are interpolated linearly, namely, for every $t \in \left[t^k, t^{k+1}\right]$

$$\begin{aligned} q(t) &= q^k \frac{t^{k+1} - t}{t^{k+1} - t^k} + q^k \frac{t - t^k}{t^{k+1} - t^k} \\ V(t) &= V^k \frac{t^{k+1} - t}{t^{k+1} - t^k} + V^k \frac{t - t^k}{t^{k+1} - t^k} \end{aligned}$$

Using these two examples we now proceed to build the mixed action sum, discrete-mixed Lagrangian, and discrete-mixed Euler-Lagrange equations. To simplify the derivations we assume the classical Lagrangian

$$L(q,V) = \frac{1}{2}m(q)V^2 - I(q)$$

for which the mixed Lagrangian is given by

$$\begin{aligned} L^{mix}(q,\dot{q},V) &= L(q,V) + \frac{\partial L}{\partial V}(\dot{q} - V) = \\ &= \frac{1}{2}m(q)V^2 - I(q) + Vm(q)(\dot{q} - V) \end{aligned}$$

Inserting the first of these interpolations into the mixed action functional, the following *mixed action sum* is obtained

$$S_d\left(\left(\cdots, q^k, \cdots\right), \left(\cdots, V^{k+\beta}, \cdots\right)\right) = \sum_{k=0}^{K} L_d^{mix}\left(q^k, q^{k+1}, V^{k+\beta}, t^k, t^{k+1}\right) \tag{2.16}$$

where

$$\begin{gathered} L_d^{mix}\left(q^k, q^{k+1}, V^{k+\beta}, t^k, t^{k+1}\right) = \\ = \int_{t^k}^{t^{k+1}} L^{mix}\left(q(t), \frac{q^{k+1} - q^k}{t^{k+1} - t^k}, V^{k+\beta}\right) dt = \\ \int_{t^k}^{t^{k+1}} \left(\frac{1}{2}m(q(t))\left(V^{k+\beta}\right)^2 - I(q(t)) + V^{k+\beta}m(q(t))\left(\frac{q^{k+1} - q^k}{t^{k+1} - t^k} - V^{k+\beta}\right)\right) dt \end{gathered} \tag{2.17}$$

with

$$q(t) = \frac{t^{k+1} - t}{t^{k+1} - t^k}q^k + \frac{t - t^k}{t^{k+1} - t^k}q^{k+1}$$

Inserting the second of the interpolations into the mixed action functional, the mixed action sum follow instead as

$$S_d\left(\left(\cdots, q^k, \cdots\right), \left(\cdots, V^k, \cdots\right)\right) = \sum_{k=0}^{K} L_d^{mix}\left(q^k, q^{k+1}, V^k, V^{k+1}, t^k, t^{k+1}\right)$$

with corresponding discrete-mixed Lagrangian given by

$$L_d^{mix}\left(q^k, q^{k+1}, V^k, V^{k+1}, t^k, t^{k+1}\right) =$$

$$= \int_{t^k}^{t^{k+1}} L^{mix}\left(q\left(t\right), \frac{q^{k+1}-q^k}{t^{k+1}-t^k}, V\left(t\right)\right) dt =$$

$$= \int_{t^k}^{t^{k+1}} \left(\frac{1}{2} m\left(q\left(t\right)\right)\left(V\left(t\right)\right)^2 - I\left(q\left(t\right)\right) + V\left(t\right) m\left(q\left(t\right)\right)\left(\frac{q^{k+1}-q^k}{t^{k+1}-t^k} - V\left(t\right)\right)\right) dt$$

with

$$\begin{aligned} q\left(t\right) &= \frac{t^{k+1}-t}{t^{k+1}-t^k} q^k + \frac{t-t^k}{t^{k+1}-t^k} q^{k+1} \\ V\left(t\right) &= \frac{t^{k+1}-t}{t^{k+1}-t^k} V^k + \frac{t-t^k}{t^{k+1}-t^k} V^{k+1} \end{aligned}$$

The formulation of time integrators is then completed by the appropriate selection of a quadrature rule. If for example we use a single quadrature point located at $t^{k+\alpha} = (1-\alpha)\, t^k + (\alpha)\, t^{k+1}$ the following discrete-mixed Lagrangians are obtained: for the first set of interpolating spaces (linear for q and constant for V):

$$L_d^{mix}\left(q^k, q^{k+1}, V^{k+\beta}, t^k, t^{k+1}\right) =$$

$$\left(t^{k+1}-t^k\right)\left(\frac{1}{2} m^{k+\alpha}\left(V^{k+\beta}\right)^2 - I^{k+\alpha} + V^{k+\beta} m^{k+\alpha}\left(\frac{q^{k+1}-q^k}{t^{k+1}-t^k} - V^{k+\beta}\right)\right)$$

where

$$\begin{aligned} I^{k+\alpha} &= I\left(q^{k+\alpha}\right) \\ m^{k+\alpha} &= m\left(q^{k+\alpha}\right) \\ q^{k+\alpha} &= (1-\alpha)\, q^k + (\alpha)\, q^{k+1} \end{aligned}$$

and

$$V^{k+\beta} = \text{constant}$$

per time interval. For the second set of spaces (linear for both q and V) we obtain

$$L_d^{mix}\left(q^k, q^{k+1}, V^k, V^{k+1}, t^k, t^{k+1}\right) =$$

$$\left(t^{k+1}-t^k\right)\left(\frac{1}{2} m^{k+\alpha}\left(V^{k+\alpha}\right)^2 - I^{k+\alpha} + V^{k+\alpha} m^{k+\alpha}\left(\frac{q^{k+1}-q^k}{t^{k+1}-t^k} - V^{k+\alpha}\right)\right)$$

where $m^{k+\alpha}$, $I^{k+\alpha}$ and $q^{k+\alpha}$ is given as before but where $V^{k+\alpha}$ is given now by

$$V^{k+a} = (1-\alpha)\,V^{k} + (\alpha)\,V^{k+1}$$

While these two discrete-mixed Lagrangians seem to be identical, there is a very important difference: in the first case the Lagrangian is assumed to be function of one velocity $V^{k+\beta}$ per time interval $\left[t^{k}, t^{k+1}\right]$ while in the second case the Lagrangian is assumed to depend on two velocities V^{k} and V^{k+1} per time interval. As we will illustrate shortly this derives in the existence of "modes" for the velocity.

The discrete trajectories and velocities follow now by invoking the stationarity of the discrete-mixed action sum S_d with respect to each and all of its arguments. In the first case we obtain

$$\frac{\partial S_d}{\partial q^k} = D_1 L_d^{mix}\left(q^k, q^{k+1}, V^{k+\beta}, t^k, t^{k+1}\right) + D_2 L_d^{mix}\left(q^{k-1}, q^k, V^{k-1+\beta}, t^{k-1}, t^k\right) = 0 \quad (2.18)$$

$$\frac{\partial S_d}{\partial V^{k+\beta}} = D_3 L_d^{mix}\left(q^k, q^{k+1}, V^{k+\beta}, t^k, t^{k+1}\right) = 0 \quad (2.19)$$

while in the second case we get

$$\frac{\partial S_d}{\partial q^k} = D_1 L_d^{mix}\left(q^k, q^{k+1}, V^k, V^{k+1}, t^k, t^{k+1}\right) + D_2 L_d^{mix}\left(q^{k-1}, q^k, V^{k-1}, V^k, t^{k-1}, t^k\right) = 0$$

$$\frac{\partial S_d}{\partial V^k} = D_3 L_d^{mix}\left(q^k, q^{k+1}, V^k, V^{k+1}, t^k, t^{k+1}\right) + D_4 L_d^{mix}\left(q^{k-1}, q^k, V^{k-1}, V^k, t^{k-1}, t^k\right) = 0$$

These equations are the *discrete-mixed Euler-Lagrange equations* (DMEL). For the particular discrete-mixed Lagrangians under study the DMEL reduce to

$$0 = -\left(m^{k+\alpha}V^{k+\beta} - m^{k-1+\alpha}V^{k-1+\beta}\right) + \left(t^{k+1}-t^k\right)(1-\alpha)\,f^{k+\alpha} + \left(t^k - t^{k-1}\right)(\alpha)\,f^{k-1+\alpha}$$

$$0 = m^{k+\alpha}\left(V^{k+\beta} - \frac{q^{k+1}-q^k}{t^{k+1}-t^k}\right)$$

with

$$f^{k+\alpha} = \frac{1}{2}\frac{\partial m}{\partial q}^{k+\alpha}\left(V^{k+\beta}\right)^2 - \frac{\partial I}{\partial q}^{k+\alpha} + V^{k+\beta}\frac{\partial m}{\partial q}^{k+\alpha}\left(\frac{q^{k+1}-q^k}{t^{k+1}-t^k} - V^{k+\beta}\right)$$

$$f^{k-1+\alpha} = \frac{1}{2}\frac{\partial m}{\partial q}^{k-1+\alpha}\left(V^{k-1+\beta}\right)^2 - \frac{\partial I}{\partial q}^{k-1+\alpha} + V^{k-1+\beta}\frac{\partial m}{\partial q}^{k-1+\alpha}\left(\frac{q^{k}-q^{k-1}}{t^{k}-t^{k-1}} - V^{k-1+\beta}\right)$$

in the first case and

$$0 = -\left(m^{k+\alpha}V^{k+\alpha} - m^{k-1+\alpha}V^{k-1+\alpha}\right) + \left(t^{k+1}-t^k\right)(1-\alpha)\,f^{k+\alpha} + \left(t^k - t^{k-1}\right)(\alpha)\,f^{k-1+\alpha}$$

$$0 = (1-\alpha)\,m^{k+\alpha}\left(V^{k+\alpha} - \frac{q^{k+1}-q^k}{t^{k+1}-t^k}\right) + (\alpha)\,m^{k-1+\alpha}\left(V^{k-1+\alpha} - \frac{q^{k}-q^{k-1}}{t^{k}-t^{k-1}}\right)$$

with

$$
\begin{aligned}
f^{k+\alpha} &= \frac{1}{2}\frac{\partial m}{\partial q}^{k+\alpha}\left(V^{k+\alpha}\right)^2 - \frac{\partial I}{\partial q}^{k+\alpha} + V^{k+\alpha}\frac{\partial m}{\partial q}^{k+\alpha}\left(\frac{q^{k+1}-q^k}{t^{k+1}-t^k} - V^{k+\alpha}\right) \\
f^{k-1+\alpha} &= \frac{1}{2}\frac{\partial m}{\partial q}^{k-1+\alpha}\left(V^{k-1+\alpha}\right)^2 - \frac{\partial I}{\partial q}^{k-1+\alpha} + V^{k-1+\alpha}\frac{\partial m}{\partial q}^{k-1+\alpha}\left(\frac{q^{k}-q^{k-1}}{t^{k}-t^{k-1}} - V^{k-1+\alpha}\right)
\end{aligned}
$$

in the second case.

We can see that in the first case we have a system of two equations for the unknowns $\left(q^{k+1}, V^{k+\beta}\right)$ given $\left(q^{k-1}, q^k, V^{k-1+\beta}\right)$ and discrete trajectories and velocities result univocally determined given initial conditions $\left(q^0, q^1, V^{0+\beta}\right)$. However only two of these are required since the Euler-Lagrange equation for V at the initial time is just

$$
V^{0+\beta} - \frac{q^1-q^0}{t^1-t^0} = 0
$$

Therefore, and as expected, given the initial data $\left(q^0, V^{0+\beta}\right)$ the complete discrete trajectories for q and V are well defined by this algorithm. Analyzing now the DMEL equations for the second case we observe that we obtain a system of two equations for the unknowns $\left(q^{k+1}, V^{k+\alpha}\right)$ that can only be solved if we are given $\left(q^{k-1}, q^k, V^{k-1+\alpha}\right)$. A discrete trajectory will therefore be generated if we provide as initial conditions the triple $\left(q^0, q^1, V^{0+\alpha}\right)$. However, unlike the first case, the three values $\left(q^0, q^1, V^{0+\alpha}\right)$ are required to generate a unique trajectory and the algorithm does not provide a unique way to generate the additional required value q^1. We thus conclude that the second algorithm will exhibit *arbitrary global modes in time*. This means that the resulting trajectory for $q(t)$ and $V(t)$ will be unique up to an arbitrary global mode fixed only by the arbitrary selection of the initial data q^1.

We also observe that in the first case we recover the variational integrator based on the single field Lagrangian (2.10). This can be easily verified by eliminating $V^{k+\beta}$ from the second DMEL equation and substituting the result into the first to obtain

$$
\begin{aligned}
0 = & -\left(m^{k+\alpha}\frac{q^{k+1}-q^k}{t^{k+1}-t^k} - m^{k-1+\alpha}\frac{q^{k}-q^{k-1}}{t^{k}-t^{k-1}}\right) + \\
& + \left(t^{k+1}-t^k\right)(1-\alpha)\left(\frac{1}{2}\frac{\partial m}{\partial q}^{k+\alpha}\left(\frac{q^{k+1}-q^k}{t^{k+1}-t^k}\right)^2 - \frac{\partial I}{\partial q}^{k+\alpha}\right) \\
& + \left(t^{k}-t^{k-1}\right)(\alpha)\left(\frac{1}{2}\frac{\partial m}{\partial q}^{k-1+\alpha}\left(\frac{q^{k}-q^{k-1}}{t^{k}-t^{k-1}}\right)^2 - \frac{\partial I}{\partial q}^{k-1+\alpha}\right)
\end{aligned}
$$

that correspond to the DEL equations (2.11). This will happen in general when the interpolation space for $V(t)$ coincides with the space that results from taking derivatives in time of the interpolating functions selected for $q(t)$. More precisely, let $\mathcal{Q}$ be the global interpolation space for $q(t)$

and $\mathcal{V}$ be the global interpolating space for V, i.e., the functions $q(t)$ and $V(t)$ (in the complete time interval $[t_0, t_f]$) are linear combinations of functions of $\mathcal{Q}$ and $\mathcal{V}$. Then If $\mathcal{V} = \dot{\mathcal{Q}}$, that is to say, functions of $\mathcal{V}$ are time derivatives of functions of $\mathcal{Q}$, then both methods will be equivalent. If on the other hand the space $\mathcal{V}$ is too rich compared to the space $\dot{\mathcal{Q}}$ then the method will exhibit velocity modes.

2.1.11 Mixed Variational Integration with selective quadrature rules

Consider again the case of piecewise linear (and continuous) interpolation for trajectories $q(t)$ and piecewise constant (and discontinuous) interpolation for the velocity $V(t)$, namely,

$$\begin{aligned} q(t) &= q^k \frac{t^{k+1} - t}{t^{k+1} - t^k} + q^k \frac{t - t^k}{t^{k+1} - t^k} \\ V(t) &= V^{k+\beta} \end{aligned}$$

for $t \in \left[t^k, t^{k+1}\right]$ and for every k. As was explained in the previous subsection, inserting this interpolation into the mixed action functional, the following *mixed action sum* is obtained:

$$S_d\left(\left(\cdots, q^k, \cdots\right), \left(\cdots, V^{k+\beta}, \cdots\right)\right) = \sum_{k=0}^{K} L_d^{mix}\left(q^k, q^{k+1}, V^{k+\beta}, t^k, t^{k+1}\right)$$

with a discrete-mixed Lagrangian given by

$$L_d^{mix}\left(q^k, q^{k+1}, V^{k+\beta}, t^k, t^{k+1}\right) =$$

$$= \int_{t^k}^{t^{k+1}} L^{mix}\left(q(t), \frac{q^{k+1} - q^k}{t^{k+1} - t^k}, V^{k+\beta}\right) dt =$$

$$\int_{t^k}^{t^{k+1}} \left(\frac{1}{2} m(q(t)) \left(V^{k+\beta}\right)^2 - I(q(t)) + V^{k+\beta} m(q(t)) \left(\frac{q^{k+1} - q^k}{t^{k+1} - t^k} - V^{k+\beta}\right)\right) dt$$

Different alternative time-stepping algorithms follow by an appropriate selection of quadrature rule.

A class of mixed variational integrators might be designed by making use of *selective quadrature rules*, that is to say, different quadrature rules for the different terms in the previous integral. For example, if we use one single quadrature point located at $t^{k+\beta}$ for the kinetic energy term and Lagrange multiplier terms, but a two point quadrature rule (located at $t^{k+\alpha} = (1-\alpha) t^k + (\alpha) t^{k+1}$ and $t^{k+1-\alpha} = (\alpha) t^k + (1-\alpha) t^{k+1}$) for the potential energy term, we obtain the discrete-mixed

Lagrangian

$$L_d^{mix}\left(q^k, q^{k+1}, V^{k+\beta}, t^k, t^{k+1}\right) =$$
$$\left(t^{k+1}-t^k\right)\left(\frac{1}{2}m^{k+\beta}\left(V^{k+\beta}\right)^2 - \frac{1}{2}\left(I^{k+\alpha}+I^{k+1-\alpha}\right) + V^{k+\beta}m^{k+\beta}\left(\frac{q^{k+1}-q^k}{t^{k+1}-t^k} - V^{k+\beta}\right)\right) \quad (2.20)$$

where

$$\begin{aligned} I^{k+\alpha} &= I\left(\left(1-\alpha\right)q^k + \left(\alpha\right)q^{k+1}\right) \\ I^{k+1-\alpha} &= I\left(\left(\alpha\right)q^k + \left(1-\alpha\right)q^{k+1}\right) \end{aligned}$$

In this case the discrete-mixed Euler-Lagrange equations take the form

$$\begin{aligned} 0 &= -\left(m^{k+\beta}V^{k+\beta} - m^{k-1+\beta}V^{k-1+\beta}\right) \\ &\quad + \left(t^{k+1}-t^k\right)e^{k+\beta}\left(1-\beta\right) + \\ &\quad + \left(t^k - t^{k-1}\right)e^{k-1+\beta}\left(\beta\right) + \\ &\quad + \left(t^{k+1}-t^k\right)\frac{1}{2}\left(f^{k+\alpha}\left(1-\alpha\right) + f^{k+1-\alpha}\left(\alpha\right)\right) \\ &\quad + \left(t^k - t^{k-1}\right)\frac{1}{2}\left(f^{k-1+\alpha}\left(\alpha\right) + f^{k-\alpha}\left(1-\alpha\right)\right) && (2.21) \\ 0 &= m^{k+\beta}\left(V^{k+\beta} - \frac{q^{k+1}-q^k}{t^{k+1}-t^k}\right) && (2.22) \end{aligned}$$

with

$$\begin{aligned} e^{k+\beta} &= \frac{1}{2}\frac{\partial m}{\partial q}^{k+\beta}\left(V^{k+\beta}\right)^2 + V^{k+\beta}\frac{\partial m}{\partial q}^{k+\beta}\left(\frac{q^{k+1}-q^k}{t^{k+1}-t^k} - V^{k+\beta}\right) \\ e^{k-1+\beta} &= \frac{1}{2}\frac{\partial m}{\partial q}^{k-1+\beta}\left(V^{k-1+\beta}\right)^2 + V^{k-1+\beta}\frac{\partial m}{\partial q}^{k-1+\beta}\left(\frac{q^{k}-q^{k-1}}{t^{k}-t^{k-1}} - V^{k-1+\beta}\right) \end{aligned}$$

and

$$\begin{aligned} f^{k+\alpha} &= \frac{\partial I}{\partial q}^{k+\alpha} = \left.\frac{\partial I}{\partial q}\right|_{\left(\left(1-\alpha\right)q^k + \left(\alpha\right)q^{k+1}\right)} \\ f^{k+1-\alpha} &= \frac{\partial I}{\partial q}^{k+1-\alpha} = \left.\frac{\partial I}{\partial q}\right|_{\left(\left(\alpha\right)q^k + \left(1-\alpha\right)q^{k+1}\right)} \\ f^{k-1+\alpha} &= \frac{\partial I}{\partial q}^{k-1+\alpha} = \left.\frac{\partial I}{\partial q}\right|_{\left(\left(1-\alpha\right)q^{k-1} + \left(\alpha\right)q^{k}\right)} \\ f^{k-\alpha} &= \frac{\partial I}{\partial q}^{k-\alpha} = \left.\frac{\partial I}{\partial q}\right|_{\left(\left(\alpha\right)q^{k-1} + \left(1-\alpha\right)q^{k}\right)} \end{aligned}$$

2.1.12 Mixed Variational Integration and mixed incremental potential

For non-conservative systems, we may extend the update equations for a mixed variational integrator (2.18) and (2.19) in the form

$$\begin{aligned} 0 &= D_1 L_d^{mix}\left(q^k, q^{k+1}, V^{k+\beta}, t^k, t^{k+1}\right) + D_2 L_d^{mix}\left(q^{k-1}, q^k, V^{k-1+\beta}, t^{k-1}, t^k\right) + \\ & \quad - f_d^{v-}\left(q^k, q^{k+1}, t^k, t^{k+1}\right) - f_d^{v+}\left(q^{k-1}, q^k, t^{k-1}, t^k\right) \\ 0 &= D_3 L_d^{mix}\left(q^k, q^{k+1}, V^{k+\beta}, t^k, t^{k+1}\right) \end{aligned}$$

where f_d^{v-1} and f_d^{v+} are the left and right discrete viscous forces defined such that relation (2.12) is satisfied. It becomes useful to analyze whether these equations derive from a mixed-incremental potential, i.e., a function $\Phi\left(q^{k+1}, V^{k+\beta}\right)$ such that the previous can be written as

$$\begin{aligned} \frac{\partial \Phi}{\partial q^{k+1}} &= 0 \\ \frac{\partial \Phi}{\partial V^{k+\beta}} &= 0 \end{aligned}$$

Consider the following hypothesis:

1. A Lagrangian of the form (2.1).
2. Constant mass matrix $m(q) = m$.
3. A variational integrator based on linear time interpolation for $q(t)$, piecewise constant interpolation for $V(t)$ and midpoint quadrature rule.
4. A constant time step Δt.
5. A viscous force independent of q and only dependent on $\dot{q}$.
6. Integration parameters $\alpha = \gamma$

In this case the updated equations reduce to

$$\begin{aligned} m\left(V^{k+\beta} - V^{k-1+\beta}\right) + \Delta t\left((1-\alpha)\left(\frac{\partial I}{\partial q} + \frac{\partial \phi}{\partial \dot{q}}\right)\Big|_{k+\alpha} + (\alpha)\left(\frac{\partial I}{\partial q} + \frac{\partial \phi}{\partial \dot{q}}\right)_{k-1+\alpha}\right) &= 0 \\ m\left(V^{k+\beta} - \frac{q^{k+1} - q^k}{\Delta t}\right) &= 0 \end{aligned}$$

A straightforward differentiation shows that the previous equation derive from the following incremental potential:

$$\begin{aligned}\Phi\left(q^{k-1},q^{k},V^{k-1+\beta},q^{k+1},V^{k+\beta}\right) &= \frac{m}{2}\left(V^{k+\beta}-V^{pre}\right)^{2}+\\ &+\Delta t\frac{1-\alpha}{a}\left(\left.\left|(I+\alpha\Delta t\phi)\right|_{k+\alpha}-\left|(I+\alpha\Delta t\phi)\right|_{k-1+\alpha}\right)+\\ &+\left(V^{k+\beta}-V^{pre}\right)m\left(\frac{q^{k+1}-q^{pre}}{\Delta t}-\left(V^{k+\beta}-V^{pre}\right)\right)\end{aligned}$$

with

$$\begin{aligned}q^{pre} &= q^{k}+\Delta tV^{k-1+\beta}-\alpha\frac{\Delta t^{2}}{m}\left.\left(\frac{\partial I}{\partial q}+\frac{\partial\phi}{\partial\dot q}\right)\right|_{k-1+\alpha}=\\ &= q^{k}+\Delta tV^{k-1+\beta}-\frac{\Delta t^{2}}{m}\frac{\partial}{\partial q^{k}}\left.(I+\alpha\Delta t\phi)\right|_{k-1+\alpha}\\ V^{pre} &= V^{k-1+\beta}-\alpha\frac{\Delta t^{2}}{m}\left.\left(\frac{\partial I}{\partial q}+\frac{\partial\phi}{\partial\dot q}\right)\right|_{k-1+\alpha}=\\ &= V^{k-1+\beta}-\frac{\Delta t^{2}}{m}\frac{\partial}{\partial q^{k}}\left.(I+\alpha\Delta t\phi)\right|_{k-1+\alpha}\end{aligned}$$

and

$$\begin{aligned}I^{k+\alpha} &= I\left((1-\alpha)\,q^{k}+\alpha q^{k+1}\right)\\ &= I\left(q^{k+\alpha}\right)\\ \phi^{k+\alpha} &= \phi\left(\frac{q^{k+1}-q^{k}}{\Delta t}\right)\\ &= \phi\left(\frac{q^{k+\alpha}-q^{k}}{\alpha\Delta t}\right)\end{aligned}$$

2.2 Mixed variational principles for Solid dynamics and variational mesh adaption

We proceed in this section to incorporate the space variable X into the picture and to highlight the salient features of the variational principles and the variational finite element mesh adaption framework analyzed in this thesis. To keep the presentation simple we will consider for the duration of this chapter only one-dimensional (in space) problems and the particular case of isothermal elasticity with no viscosity. The full three-dimensional formulation in the presence of viscous, thermal, and internal processes will be treated in the following chapters.

2.2.1 Lagrangian formulation for elastodynamics

We begin by reviewing Hamilton's principle in the context of one-dimensional elasticity. The extension of Hamilton's principle and its mixed version to the space-time context is accomplished by defining the Lagrangian L of the the body B in terms of a density $\mathcal{L}$

$$L = \int_B \mathcal{L} dX$$

Consider a one-dimensional body $B = [0, L]$ where L is the undeformed length L of the body. The body subsequently moves under the action of externally applied forces and we are interested in finding its motion $\varphi(X, t)$, i.e., the function that specifies the spatial position $x = \varphi(X, t)$ for each material particle $X \in B$ and each time t in the time interval $[t_0, t_f]$ of analysis. Let $B(X, t)$ be the external body forces per unit of undeformed length and assume that the material is elastic and possibly inhomogeneous, i.e., its constitutive relation is given by

$$P = \frac{\partial A}{\partial F}$$

where P is the (Piolla-Kirchhoff) stress, $F = \frac{\partial \varphi}{\partial X}$ is the deformation gradient, and $A(X, F)$ is the strain-energy density (assumed to depend explicitly on X to account for the possible inhomogeneity). To simplify the derivations we will assume zero traction and displacement boundary conditions, i.e.,

$$\begin{aligned} \varphi(0, t) &= \varphi(L, t) = 0 \\ P(0, t) &= P(L, t) = 0 \end{aligned}$$

The Lagrangian density is defined as

$$\mathcal{L}(X, t, \varphi, V, F) = \frac{1}{2} R V^2 - W(X, t, \varphi, F) \tag{2.23}$$

where $V = \dot{\varphi}$ is the material velocity, R is the mass density per unit of undeformed length, and W is the total potential energy given in this case as

$$W(X, t, \varphi, F) = A(X, F) - B(X, t)\varphi$$

The (standard, single-field) action functional $S(\varphi)$ follows by integrating in space and time the

Lagrangian density in the form

$$S[\varphi] = \int_{t_0}^{t_f} \int_0^L \mathcal{L}(X, t, \varphi, \dot{\varphi}, D\varphi)\, dX dt = $$
$$= \int_{t_0}^{t_f} \int_0^L \left(\frac{1}{2} R \dot{\varphi}^2 - W(X, t, \varphi, D\varphi) \right) dX dt \tag{2.24}$$

where we are using the notation

$$\dot{\varphi} = \frac{\partial \varphi}{\partial t}$$
$$D\varphi = \frac{\partial \varphi}{\partial X}$$

for the partial derivatives with respect to time and space. The variations of the action functional with respect to its argument are

$$\langle \delta S, \delta\varphi \rangle = \int_{t_0}^{t_f} \int_0^L \left(\frac{\partial \mathcal{L}}{\partial \varphi} \delta\varphi + \frac{\partial \mathcal{L}}{\partial V} \delta\dot{\varphi} + \frac{\partial \mathcal{L}}{\partial F} D\delta\varphi \right) dX dt$$

where we have used the usual commutative assumption

$$\delta(\dot{\varphi}) = \delta\left(\frac{\partial \varphi}{\partial t}\right) = \frac{\partial}{\partial t}(\delta\varphi) = \delta\dot{\varphi}$$
$$\delta(D\varphi) = \delta\left(\frac{\partial \varphi}{\partial X}\right) = \frac{\partial}{\partial X}(\delta\varphi) = D\delta\varphi$$

Integrating by parts in time for the second factor and in space for the third factor we obtain the variations in the form

$$\langle \delta S, \delta\varphi \rangle = \int_{t_0}^{t_f} \int_0^L \left(\frac{\partial \mathcal{L}}{\partial \varphi} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial V} - \frac{d}{dX}\frac{\partial \mathcal{L}}{\partial F} \right) \delta\varphi dX dt + $$
$$\int_{t_0}^{t_f} \frac{\partial \mathcal{L}}{\partial F} \delta\varphi \Big|_0^L dt + \int_0^L \frac{\partial \mathcal{L}}{\partial V} \delta\varphi \Big|_{t_0}^{t_f} dX$$

Hamilton's principle states the actual motion $\varphi(X,t)$ that joins prescribed initial and final configurations $\varphi_0(X)$ and $\varphi_f(X)$ will be the particular motion that renders the action functional stationary with respect to all admissible variations, i.e., variations that vanish in the initial and final times and in the Dirichlet part of the boundary. This implies the Euler-Lagrange equations

$$\frac{\partial \mathcal{L}}{\partial \varphi} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial V} - \frac{d}{dX}\frac{\partial \mathcal{L}}{\partial F} = 0 \tag{2.25}$$

For a Lagrangian density of the form $\mathcal{L} = \frac{1}{2} R V^2 - W(X, t, \varphi, F)$ the previous yields

$$-B - \frac{dP}{dX} + \frac{d}{dt}(RV) = 0 \tag{2.26}$$

that corresponds to the equations of balance of mechanical forces or balance of linear momentum.

2.2.2 Horizontal variations and Euler-Lagrange equations

As in the case of finite-dimensional Lagrangian systems, the concept of horizontal variations and horizontal Euler-Lagrange equations will play a fundamental role in the analysis of the methods presented in this thesis. This variational formulation was developed within the context of the theory of multisimplectic continuum mechanics in [29], [30] and the procedure we will present in what follows is its particularization to one-dimensional elasticity rewritten in a less abstract notation.

The motion of the body is defined as the function

$$x = \varphi\left(X, t\right)$$

Consider the graph of this function, i.e., the surface

$$\left(X, t, \varphi\left(X, t\right)\right)$$

which belongs to the combined space-time-space bundle with coordinates (X, t, x) and its one of its sections. Figure 2.4 depicts this surface. With this picture in mind, we shall refer to (X, t) as the *horizontal* variables and to $x = \varphi\left(X, t\right)$ as the *vertical* variable.

In the previous subsection we invoked the stationarity of the action functional $S\left[\varphi\right]$ with respect to variations of the vertical variable φ, or vertical variations. The corresponding Euler-Lagrange equation (equation 2.25) evaluated to

$$\frac{\partial \mathcal{L}}{\partial \varphi} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial V} - \frac{d}{dX}\frac{\partial \mathcal{L}}{\partial F} = 0$$

We focus the attention now in variations with respect to the horizontal variables and the Euler-Lagrange equations corresponding to the stationarity of the action functional with respect to horizontal variations, which shall be referred to as *horizontal Euler-Lagrange equations.* We recall from §2.1.3 that for finite-dimensional Lagrangian systems, the Euler-Lagrange equation corresponding to horizontal variations was nothing more than the energy balance equation. When the base space is *space-time*, we are allowed to take horizontal variations both in the direction of space and the direction of time. We shall find as we proceed, that the horizontal Euler-Lagrange equation in the direction of time corresponds to the equation of *energy balance* while the horizontal Euler-Lagrange equation associated to the space direction yields the *equation of balance of dynamic configurational forces.*

To this end, and as it was done for the finite-dimensional case (see §2.1.3), we introduce a change

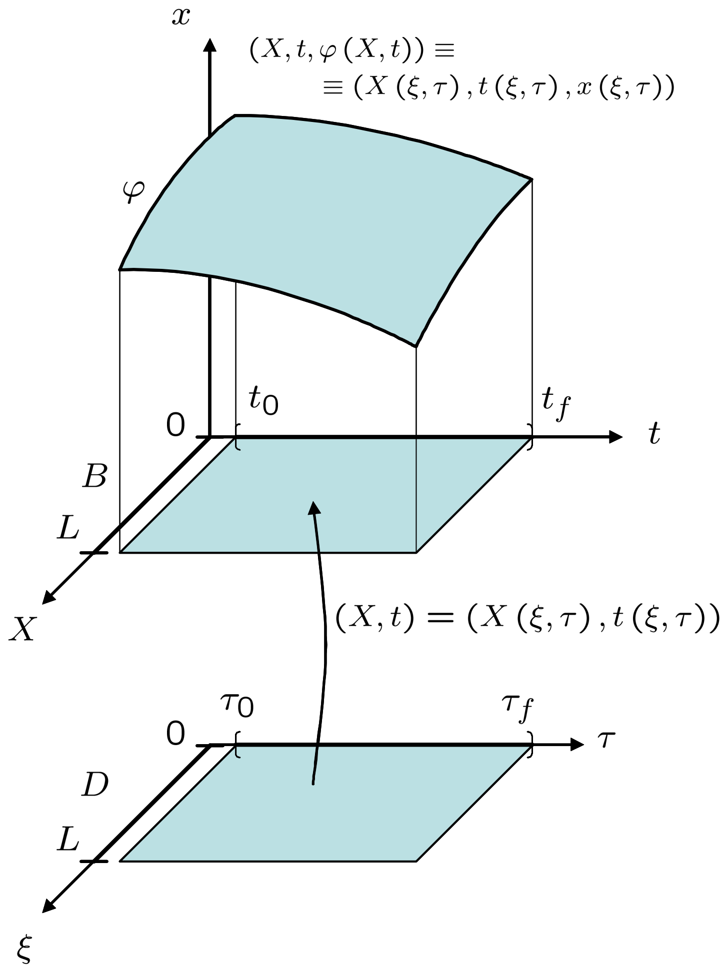

Figure 2.4: Graph of the motion $\varphi(X,t)$ of a one-dimensional body B and change of parametrization of its base space, i.e., the space-time subset $B \times [t_0, t_f]$.

in parametrization of the base space (see figure 2.4)

$$(X,t) = \boldsymbol{\psi}(\xi,\tau) = (X(\xi,\tau), t(\xi,\tau))$$

that maps every pair (ξ,τ) in the set $D \times [\tau_0, \tau_f]$ into the space-time domain $B \times [t_0, t_f]$ where (ξ,τ) are new space-time coordinates as depicted in figure 2.4 . We shall refer to the set $D \times [\tau_0, \tau_f]$ as the parameter space, or parametric configuration. Let

$$x = \varphi \circ \boldsymbol{\psi}$$

or

$$x(\xi,\tau) = \varphi(X(\xi,\tau), t(\xi,\tau))$$

be the composition mapping. Differentiating the latter with respect to the space and time parameters ξ and τ we find

$$\begin{pmatrix} \frac{\partial x}{\partial \xi} \\ \frac{\partial x}{\partial \tau} \end{pmatrix} = \mathbf{J}(\xi,\tau) \begin{pmatrix} D\varphi \\ \dot{\varphi} \end{pmatrix} \circ \boldsymbol{\psi} \tag{2.27}$$

where $\mathbf{J}$ is the Jacobian matrix of the space-time reparametrization mapping

$$\mathbf{J}(\xi,\tau) = \begin{bmatrix} \frac{\partial X}{\partial \xi} & \frac{\partial t}{\partial \xi} \\ \frac{\partial X}{\partial \tau} & \frac{\partial t}{\partial \tau} \end{bmatrix}$$

We next refer the action functional to the parameter configuration to find

$$\begin{aligned} S &= \int_{t_0}^{t_f} \int_0^L \mathcal{L}(X, t, \varphi, (D\varphi, \dot{\varphi}))\, dX dt = \\ &= \int_{\tau_0}^{\tau_f} \int_0^L \mathcal{L}\left(X(\xi,\tau), t(\xi,\tau), x(\xi,\tau), \left(\frac{\partial x}{\partial \xi}, \frac{\partial x}{\partial \tau} \right) \mathbf{J}^{-T} \right) \det(\mathbf{J})\, d\xi d\tau = \\ &= S[X, t, x] \end{aligned}$$

Horizontal variations of the action $S[X,t,x]$ are those corresponding to variations in the parametrization of the base space $\delta\boldsymbol{\psi}(\xi,\tau) = (\delta X(\xi,\tau), \delta t(\xi,\tau))$. To compute these variations we switch to indicial notation and write

$$\begin{aligned} X &= \psi_1 \\ t &= \psi_2 \\ \xi &= Z_1 \\ \tau &= Z_2 \end{aligned}$$

whereupon the change of parametrization is reexpressed as

$$\begin{aligned} \boldsymbol{\psi}(\mathbf{Z}) &= (\psi_1(Z_1, Z_2), \psi_2(Z_1, Z_2)) = \\ &= (X(\xi,\tau), t(\xi,\tau)) \end{aligned}$$

and the Jacobian relation (2.27) shall be rewritten as

$$x_{,\alpha} = \left(\varphi_{,A} \circ \boldsymbol{\psi} \right) \psi_{A,\alpha} \tag{2.28}$$

with Jacobian

$$J_{A\alpha} = \psi_{A,\alpha}$$

Here and in what follows we will use Latin indices $(A, B, \cdots)$ for physical space-time coordinates

(X,t) and Greek indices $(\alpha,\beta,\cdots)$ for the space-time parametric coordinates (ξ,τ). Using this notation the action might be reexpressed as

$$S[\boldsymbol{\psi},x]=\int_{t_0}^{t_f}\int_0^L \mathcal{L}\left(Z_A,x,x_{,\alpha}\psi^{-1}_{\alpha,A}\circ\boldsymbol{\psi}\right)\det\left(\psi_{A,\alpha}\right)d\xi d\tau$$

Noticing then that

$$\begin{aligned}
\frac{d}{d\varepsilon}\det\left(\psi_{A,\alpha}+\varepsilon\delta\psi_{A,\alpha}\right)\Big|_{\varepsilon=0} &= \delta\psi_{A,\alpha}\psi^{-1}_{\alpha,A}\\
\frac{d}{d\varepsilon}\left(\psi_{A,\alpha}+\varepsilon\delta\psi_{A,\alpha}\right)^{-1}\Big|_{\varepsilon=0} &= \delta\psi_{B,\beta}\frac{\partial}{\partial\psi_{B,\beta}}\left(\psi_{\alpha,A}+\varepsilon\delta\psi_{\alpha,B}\right)\Big|_{\varepsilon=0}=\\
&= -\psi^{-1}_{\alpha,B}\delta\psi_{B,\beta}\psi^{-1}_{\beta A}
\end{aligned}$$

the horizontal variations evaluate to

$$\begin{aligned}
\langle\delta S,\delta\boldsymbol{\psi}\rangle &= \frac{d}{d\varepsilon}\left(S[\boldsymbol{\psi}+\varepsilon\delta\boldsymbol{\psi},x]\right)\Big|_{\varepsilon=0}=\\
&= \int_{\tau_0}^{\tau_f}\int_0^L\left(\delta\psi_A\frac{\partial\mathcal{L}}{\partial Z_A}+\mathcal{L}\delta\psi_{A,\alpha}\psi^{-1}_{\alpha,A}-\frac{\partial\mathcal{L}}{\partial\varphi_{,A}}x_{,\alpha}\psi^{-1}_{\alpha,B}\delta\psi_{B,\beta}\psi^{-1}_{\beta A}\right)\circ\boldsymbol{\psi}\det\left(\psi_{A,B}\right)d\xi d\tau=\\
&= \int_{\tau_0}^{\tau_f}\int_0^L\left(\delta\psi_A\frac{\partial\mathcal{L}}{\partial Z_A}+\delta\psi_{B,\beta}\psi^{-1}_{\beta,A}\left(\mathcal{L}\delta_{AB}-\frac{\partial\mathcal{L}}{\partial\varphi_{,A}}x_{,\alpha}\psi^{-1}_{\alpha,B}\right)\right)\circ\boldsymbol{\psi}\det\left(\psi_{A,B}\right)d\xi d\tau=\\
&= \int_{\tau_0}^{\tau_f}\int_0^L\left(\delta\psi_A\frac{\partial\mathcal{L}}{\partial Z_A}+\delta\psi_{B,\beta}\psi^{-1}_{\beta,A}\left(\mathcal{L}\delta_{AB}-\frac{\partial\mathcal{L}}{\partial\varphi_{,A}}\varphi_{,B}\right)\right)\circ\boldsymbol{\psi}\det\left(\psi_{A,B}\right)d\xi d\tau
\end{aligned}$$

where relation (2.28) has been invoked. Referring now the previous integral back to the space-time reference configuration $[0,L]\times[t_0,t_f]$ we obtain

$$\langle\delta S,\delta\boldsymbol{\psi}\rangle=\int_{t_0}^{t_f}\int_0^L\left(\left(\delta\psi_A\circ\boldsymbol{\psi}^{-1}\right)\frac{\partial\mathcal{L}}{\partial Z_A}+\left(\delta\psi_B\circ\boldsymbol{\psi}^{-1}\right)_{,A}\left(\mathcal{L}\delta_{AB}-\frac{\partial\mathcal{L}}{\partial\varphi_{,A}}\varphi_{,B}\right)\right)dX\,dt$$

where we have made use of the identity

$$\left(\delta\psi_B\circ\boldsymbol{\psi}^{-1}\right)_{,A}=\left(\delta\psi_{B,\beta}\circ\boldsymbol{\psi}^{-1}\right)\psi^{-1}_{\beta,A}$$

Integrating by parts in the second term and assuming that horizontal variations vanish in the boundary of the space-time domain we finally obtain

$$\langle\delta S,\delta\boldsymbol{\psi}\rangle=\int_{t_0}^{t_f}\int_0^L\left(\delta\psi_A\circ\boldsymbol{\psi}^{-1}\right)\left(\frac{\partial\mathcal{L}}{\partial Z_A}-\left(\mathcal{L}\delta_{AB}-\frac{\partial\mathcal{L}}{\partial\varphi_{,A}}\varphi_{,B}\right)_{,A}\right)dX\,dt$$

which rewritten in terms of the component functions $(\psi_1(Z_1,Z_2), \psi_2(Z_1,Z_2)) = (X(\xi,\tau), t(\xi,\tau))$ takes the form

$$\begin{aligned}\langle \delta S, \delta \boldsymbol{\psi} \rangle &= \int_{t_0}^{t_f}\int_0^L \left(\left(\frac{\partial \mathcal{L}}{\partial X}, \frac{\partial \mathcal{L}}{\partial t} \right) \cdot \begin{pmatrix} \delta X \\ \delta t \end{pmatrix} \circ \boldsymbol{\psi}^{-1} + \right. \\ &\left. - \left(\frac{\partial}{\partial X}, \frac{\partial}{\partial t} \right) \cdot \left[\mathcal{L} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \begin{pmatrix} \frac{\partial \mathcal{L}}{\partial F} \\ \frac{\partial \mathcal{L}}{\partial V} \end{pmatrix} (D\varphi, \dot{\varphi}) \right] \cdot \begin{pmatrix} \delta X \\ \delta t \end{pmatrix} \circ \boldsymbol{\psi}^{-1} \right) dX dt\end{aligned}$$

Horizontal Euler-Lagrange equations follow by demanding the stationarity of the action functional with respect to admissible horizontal variations,

$$\langle \delta S, \delta \boldsymbol{\psi} \rangle = 0$$

which implies under appropriate smoothness conditions on the integrand the space-time equations

$$\left(\frac{\partial \mathcal{L}}{\partial X}, \frac{\partial \mathcal{L}}{\partial t} \right) - \left(\frac{d}{dX}, \frac{d}{dt} \right) \cdot \left(\mathcal{L} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \begin{pmatrix} \frac{\partial \mathcal{L}}{\partial F} \\ \frac{\partial \mathcal{L}}{\partial V} \end{pmatrix} (D\varphi, \dot{\varphi}) \right) = (0,0) \tag{2.29}$$

with space and time components

$$\frac{\partial \mathcal{L}}{\partial X} + \frac{d}{dX}\left(-\left(\mathcal{L} - \frac{\partial \mathcal{L}}{\partial F} F \right) \right) - \frac{d}{dt}\left(-\frac{\partial \mathcal{L}}{\partial V} F \right) = 0 \tag{2.30}$$

$$\frac{\partial \mathcal{L}}{\partial t} + \frac{d}{dX}\left(\frac{\partial \mathcal{L}}{\partial F} V \right) + \frac{d}{dt}\left(-\left(\mathcal{L} - \frac{\partial \mathcal{L}}{\partial V} V \right) \right) = 0 \tag{2.31}$$

The magnitude

$$\begin{aligned}\mathbf{C} &= -\left(\mathcal{L} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \begin{pmatrix} \frac{\partial \mathcal{L}}{\partial F} \\ \frac{\partial \mathcal{L}}{\partial V} \end{pmatrix} (F, V) \right) = \\ &= - \begin{bmatrix} \mathcal{L} - \frac{\partial \mathcal{L}}{\partial F} F & -\frac{\partial \mathcal{L}}{\partial F} V \\ -\frac{\partial \mathcal{L}}{\partial V} F & \mathcal{L} - \frac{\partial \mathcal{L}}{\partial V} V \end{bmatrix}\end{aligned} \tag{2.32}$$

which represents the space-time analog of

$$E = -\left(L - \frac{\partial L}{\partial \dot{q}} \dot{q} \right)$$

(see §2.1.3, equation (2.6)) is the *space-time energy-(material) momentum tensor* or *space-time Eshelby stress tensor* ([6], [7], [29],[30], [63]) and equation (2.29) is the *equation of balance of energy-(material) momentum.*

The magnitude

$$C = -\left(\mathcal{L} - \frac{\partial \mathcal{L}}{\partial F} F\right)$$

which corresponds to the *space-space* component of the *space-time Eshelby stress tensor* defined in (2.32) will be referred to as the *dynamic Eshelby stress tensor*. The space component (2.30) of equation (2.29) is the *equation of balance of material momentum* or equation of *balance of dynamic configurational forces* while its time component (2.31) is the equation of *balance of mechanical energy*.

For Lagrangian densities of the form

$$\mathcal{L} = \frac{1}{2} R V^2 - W\left(X, t, \varphi, F\right)$$

the space-time Eshelby stress tensor evaluates to

$$\mathbf{C} = \begin{bmatrix} \left(W - \frac{1}{2} R V^2\right) - PF & -PV \\ RVF & \frac{1}{2} R V^2 + W \end{bmatrix}$$

and equations (2.30) and (2.31) reduce to

$$\frac{\partial \mathcal{L}}{\partial X} + \frac{\partial C}{\partial X} - \frac{\partial}{\partial t}\left(-RVF\right) = 0 \tag{2.33}$$

$$\frac{\partial \mathcal{L}}{\partial t} + \frac{\partial}{\partial X}\left(-PV\right) + \frac{\partial}{\partial t}\left(\frac{1}{2} R V^2 + W\right) = 0 \tag{2.34}$$

where

$$\begin{aligned} C &= -\frac{1}{2} R V^2 + W - PF \\ P &= \frac{\partial W}{\partial F} \end{aligned}$$

are, respectively, the dynamic Eshelby stress tensor and first Piolla-Kirchhoff stress tensor.

As we shall explain shortly, we will particularize the variational adaptivity framework to space adaption only. It follows that the equations of interest in our formulation will be the vertical Euler-Lagrange equation (2.25) and the horizontal Euler-Lagrange equation in the direction of space (2.30), i.e., the equations of motion and the equation of balance of dynamic configurational forces. We shall rewrite these equations jointly in a column vector equation as

$$\begin{pmatrix} \frac{\partial \mathcal{L}}{\partial X} \\ \frac{\partial \mathcal{L}}{\partial \varphi} \end{pmatrix} + \frac{d}{dX} \begin{pmatrix} -\left(\mathcal{L} - \frac{\partial \mathcal{L}}{\partial F} F\right) \\ -\frac{\partial \mathcal{L}}{\partial F} \end{pmatrix} - \frac{d}{dt} \begin{pmatrix} -\frac{\partial \mathcal{L}}{\partial V} F \\ \frac{\partial \mathcal{L}}{\partial V} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

or alternatively as

$$\begin{pmatrix} \frac{\partial \mathcal{L}}{\partial X} \\ \frac{\partial \mathcal{L}}{\partial \varphi} \end{pmatrix} + \frac{d}{dX}\begin{pmatrix} -\left(\mathcal{L} - \frac{\partial \mathcal{L}}{\partial F} F\right) \\ -\frac{\partial \mathcal{L}}{\partial F} \end{pmatrix} - \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial V}\begin{pmatrix} -F \\ 1 \end{pmatrix}\right) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

2.2.3 Equivalence of vertical and horizontal Euler-Lagrange equations

As was demonstrated in the case of finite degree-of-freedom Lagrangian systems (see §2.1.3), for conservative systems, horizontal and vertical Euler-Lagrange equations are equivalent in the sense that if the vertical equation is satisfied, both horizontal Euler-Lagrange equations will be automatically satisfied. This can be directly verified in complete analogy to what was done in the finite-dimensional case, by defining the following Euler-Lagrange operators (left hand side of the vertical and horizontal Euler-Lagrange equations (2.25), (2.30), and (2.31))

$$\begin{aligned} \mathcal{F}_x(\varphi) &= \frac{\partial \mathcal{L}}{\partial \varphi} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial V} - \frac{d}{dX}\frac{\partial \mathcal{L}}{\partial F} \\ \mathcal{F}_X(\varphi) &= \frac{\partial \mathcal{L}}{\partial X} + \frac{d}{dX}\left(-\left(\mathcal{L} - \frac{\partial \mathcal{L}}{\partial F}F\right)\right) - \frac{d}{dt}\left(-\frac{\partial \mathcal{L}}{\partial V}F\right) \\ \mathcal{F}_t(\varphi) &= \frac{\partial \mathcal{L}}{\partial t} + \frac{d}{dX}\left(\frac{\partial \mathcal{L}}{\partial F}V\right) + \frac{d}{dt}\left(-\left(\mathcal{L} - \frac{\partial \mathcal{L}}{\partial V}V\right)\right) \end{aligned}$$

whereupon the balance equations reduce to

$$\begin{aligned} \mathcal{F}_x(\varphi) &= 0 \\ \mathcal{F}_X(\varphi) &= 0 \\ \mathcal{F}_t(\varphi) &= 0 \end{aligned}$$

Then it is straightforward to prove the *identities* (compare with identity (2.7), see §3.3.3 for a formal proof in the multidimensional setting)

$$\begin{aligned} \mathcal{F}_X &= -F\mathcal{F}_x \\ \mathcal{F}_t &= -V\mathcal{F}_x \end{aligned}$$

where

$$\begin{aligned} F &= D\varphi \\ V &= \dot{\varphi} \end{aligned}$$

which implies

$$\mathcal{F}_x = 0 \Leftrightarrow \mathcal{F}_X = 0 \Leftrightarrow \mathcal{F}_t = 0$$

As will be illustrated as we proceed and as happened in finite dimensional Lagrangians systems, this is not the case when the system has been *discretized*. Indeed, requiring then satisfaction of the discrete counterparts of the horizontal Euler-Lagrange equations by rendering the *discrete* action stationarity with respect to the horizontal discrete reparametrization will give a new set of equations that can be used to solve for the discrete base space, i.e., for the space-time mesh. Both time and space adaptivity could be eventually be driven by this set of equations.

2.2.4 Mixed Lagrangian formulation for elastodynamics

Following the same ideas that led to the formulation of the mixed Hamilton's principle in finite-dimensional (time-only-dependent) Lagrangian systems, we proceed to present a mixed variational formulation for continuous (space-time-dependent) bodies. To this end we assume that $\dot{\varphi}$ and V are different fields and impose the compatibility condition $\dot{\varphi} - V = 0$ by making use of a Lagrange multiplier $p(X,t)$, that is taken itself as independent variable. The (three-field) mixed action functional follows then as

$$S[\varphi, V, p] = \int_{t_0}^{t_f} \int_0^L \left(\mathcal{L}(X, t, \varphi, V, D\varphi) + p(\dot{\varphi} - V)\right) dX dt$$

The previous functional might be contrasted with the well-known "De-Beubeke-Hu-Washizu" mixed variational principle for elasto-statics (see for example [9], [62]) that in the context of one-dimensional elasticity and for zero-traction boundary conditions, takes the form

$$I[\varphi, F, P] = \int_0^L \left(W(X, \varphi, F) + P(D\varphi - F)\right) dX$$

The variations of the mixed action functional with respect to each of its arguments are

$$\begin{aligned}
\langle \delta S, \delta\varphi \rangle &= \int_{t_0}^{t_f} \int_0^L \left(\frac{\partial \mathcal{L}}{\partial \varphi} \delta\varphi + p\delta\dot{\varphi} + \frac{\partial \mathcal{L}}{\partial F} D\delta\varphi \right) dX dt \\
\langle \delta S, \delta V \rangle &= \int_{t_0}^{t_f} \int_0^L \left(\frac{\partial \mathcal{L}}{\partial V} - p \right) \delta V dX dt \\
\langle \delta S, \delta p \rangle &= \int_{t_0}^{t_f} \int_0^L (\dot{\varphi} - V) \delta p dX dt
\end{aligned}$$

Invoking next the stationarity of the mixed action $S[\varphi, V, p]$ with respect to variations of each of its arguments implies

$$\begin{aligned}
\langle \delta S, \delta\varphi \rangle &= 0 \\
\langle \delta S, \delta V \rangle &= 0 \\
\langle \delta S, \delta p \rangle &= 0
\end{aligned}$$

The corresponding Euler-Lagrange equations are

$$\begin{aligned}\frac{\partial\mathcal{L}}{\partial\varphi}-\frac{d}{dt}p-\frac{d}{dX}\left(\frac{\partial\mathcal{L}}{\partial F}\right) &= 0\\ \frac{\partial\mathcal{L}}{\partial V}-p &= 0\\ \dot{\varphi}-V &= 0\end{aligned}$$

that are equivalent to the Euler-Lagrange equations associated to the stationarity of the standard action $S[\varphi]$ given in (2.25). For the Lagrangian density of the form (2.23), the previous yields

$$\begin{aligned}B-\frac{d}{dt}p+\frac{dP}{dX} &= 0\\ RV-p &= 0\\ \dot{\varphi}-V &= 0\end{aligned}$$

that correspond to the equations of balance of mechanical forces.

Using now the second Euler-Lagrange equation to eliminate the Lagrange multiplier p, the following two-field mixed action is obtained:

$$S[\varphi,V]=\int_{t_0}^{t_f}\int_0^L\left(\mathcal{L}(X,t,\varphi,V,D\varphi)+\left.\frac{\partial\mathcal{L}}{\partial V}\right|_{(X,t,\varphi,V,D\varphi)}(\dot{\varphi}-V)\right)dX\,dt \tag{2.35}$$

The previous should be compared with the deformation-strain dual of the Hellinger-Reissner variational principle for statics which for one dimensional elasticity and zero Dirichlet and traction boundary conditions takes the form

$$I[\varphi,F]=\int_0^L\left(W(X,\varphi,F)+\left.\frac{\partial W}{\partial F}\right|_{(X,t,\varphi,F)}(D\varphi-F)\right)dX$$

The variations of the mixed action with respect to each of its arguments yield

$$\begin{aligned}\langle\delta S,\delta\varphi\rangle &= \int_{t_0}^{t_f}\int_0^L\left(\frac{\partial\mathcal{L}}{\partial\varphi}\delta\varphi+\frac{\partial\mathcal{L}}{\partial F}D\delta\varphi+\frac{\partial\mathcal{L}}{\partial V}\delta\dot{\varphi}+\frac{\partial^2\mathcal{L}}{\partial\varphi\partial V}(\dot{\varphi}-V)\,\delta\varphi\right)dX\,dt\\ \langle\delta S,\delta V\rangle &= \int_{t_0}^{t_f}\int_0^L\frac{\partial^2\mathcal{L}}{\partial V^2}(\dot{\varphi}-V)\,\delta V\,dX\,dt\end{aligned}$$

Stationarity of the mixed (two-field) action demands

$$\langle\delta S,\delta\varphi\rangle = 0 \tag{2.36}$$

$$\langle\delta S,\delta V\rangle = 0 \tag{2.37}$$

The corresponding Euler-lagrange equations are

$$\begin{aligned}\frac{\partial \mathcal{L}}{\partial \varphi} - \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial V}\right) - \frac{d}{dX}\left(\frac{\partial \mathcal{L}}{\partial F}\right) + \frac{\partial^2 \mathcal{L}}{\partial \varphi \partial V}\left(\dot{\varphi} - V\right) &= 0 \\ \frac{\partial^2 \mathcal{L}}{\partial V^2}\left(\dot{\varphi} - V\right) &= 0\end{aligned}$$

As in the case of finite-dimensional Lagrangians, this equation is equivalent to the Euler-Lagrange equations corresponding to the standard, single-field Hamilton's principle. For the particular Lagrangian density (2.23) the mixed Lagrangian reduces to

$$S\left[\varphi, V\right] = \int_{t_0}^{t_f} \int_0^L \left(\frac{1}{2} R V^2 - W\left(X, t, \varphi, D\varphi\right) + RV\left(\dot{\varphi} - V\right)\right) dX\, dt \tag{2.38}$$

their variations to

$$\langle \delta S, \delta \varphi \rangle = \int_{t_0}^{t_f} \int_0^L \left(-\frac{\partial W}{\partial \varphi}\delta\varphi - \frac{\partial W}{\partial F} D\delta\varphi + RV\delta\dot{\varphi}\right) dX\, dt \tag{2.39}$$

$$\langle \delta S, \delta V \rangle = \int_{t_0}^{t_f} \int_0^L R\left(\dot{\varphi} - V\right)\delta V\, dX\, dt \tag{2.40}$$

and their corresponding Euler-Lagrange equation to

$$\begin{aligned}B + \frac{dP}{dX} - \frac{d}{dt}\left(RV\right) &= 0 \\ R\left(\dot{\varphi} - V\right) &= 0\end{aligned}$$

with

$$\begin{aligned}B &= -\frac{\partial W}{\partial \varphi} \\ P &= \frac{\partial W}{\partial F}\end{aligned}$$

In this way the (two-field) mixed variational formulation operates as a variational principle equivalent to the mechanical force balance equations and the compatibility (in time) condition $V = \dot{\varphi}$.

2.2.5 Finite element discretization and variational mesh adaption

We focus now on the discretization (in space and time) of the boundary-value problem (2.26). As was outlined in Chapter 1, the main idea behind the *variational* approach to mesh adaption is to use the principle of stationary action (Hamilton's principle) to determine not only the unknown of the problem (the motion φ) but the discretization, i.e., *the finite element mesh is chosen in such a way as to render the discretized action stationary.*

To motivate the idea and as a background for the upcoming developments we review the concept of variational adaptivity as it applies to *static* problems. Within the context of solid statics the idea of variational adaptivity and its connection with configurational forces has been studied by a number of authors, see for example [24], [25], [35], [36], [37], [59], [60].

We proceed next to present the *space-time* generalization of this idea and its implementation in terms of space-time isoparametric finite elements. An essential problem related to this approach is the issue of solvability of the time step, which is involved in a highly non-linear way. As a result we study the restriction of this methodology to *space adaption only*, which results in a particular class of space-time elements where the same time step is used for all nodes in the mesh, i.e., space-time is discretized with a *homogeneous time step*. We will show that for this particular class of space-time finite elements there is no need to resort to the machinery and formalism of space-time finite elements since, as we shall prove, this discretization is *equivalent* to effect the space-time discretization in two separated and *uncoupled* stages, the first stage (semidiscretization in space) where the space variable is discretized keeping the time continuous and *over a continuously deforming spatial mesh*, followed by a second stage in which the time is discretized using an appropriate time integrator. Since during the first stage the time is kept continuous and since time adaption is no longer pursued there is no need to use the theoretical space-time framework. By contrast a *space-space* picture becomes more appropriate and provides more insight. We finally present a semidiscrete *mixed* formulation based on independent interpolations for motion φ and velocities V and the use of the mixed Hamilton's principle presented in the previous subsection. This mixed interpolation is proposed as an approach to overcome instability problems arising when consistent velocity interpolations are used with continuously evolving spatial meshes.

2.2.6 Review of Variational Mesh Adaption for statics

In static, non-linear elastic problems the operative variational principle is the principle of minimum potential energy, which states that the stable configurations $\varphi(X)$ of the body B are those for which the potential energy $I[\varphi]$ is minimized:

$$\inf_{\varphi} I[\varphi]$$

The total potential energy (assuming zero traction boundary conditions) is given by

$$I[\varphi] = \int_B W(X, \varphi, D\varphi)\, dX$$

where

$$W(X, \varphi, F) = A(X, F) - B(X)\, \varphi$$

is the total potential energy density per unit of length of the body.

The standard (displacement-based) finite element method (see for example [17]) proposes then to discretize the energy functional $I[\varphi]$ by the introduction of a triangulation $\mathcal{T}_h$ of the domain B and approximating the deformation $\varphi(X)$ with the finite element interpolation

$$\varphi_h(X) = \sum_a N_a(X)\, x_a$$

where $N_a(X)$ are the nodal shape functions and x_a are the nodal coordinates in the deformed configuration. The discretized potential energy I_h follows by evaluating the continuous potential energy in the discretized deformation

$$I_h(\cdots, x_a, \cdots) = I[\varphi_h]$$

and the finite element solution φ_h is found by minimizing the discretized energy I_h with respect to the parameters that define the finite element interpolation, i.e., nodal coordinates x_a

$$\inf_{x_a} I_h(\cdots, x_a, \cdots)$$

It is observed next (see for example [59]) that the minimum attained by this minimization problem depends not only on the spatial nodal coordinates x_a but also on the choice of the mesh. In particular it will depend on the reference coordinates of nodes X_a

$$I_h(\cdots, X_a, x_a, \cdots)$$

It has been then proposed (see for example Thoutireddy and Ortiz, [59]) to use the energy as a measure of mesh quality and to regard as *better* mesh the particular one that produces a lower potential energy. We therefore formulate the extended minimization problem

$$\inf_{X_a, x_a} I_h(\cdots, X_a, x_a, \cdots)$$

which implies

$$\langle \delta I_h, \delta X_a \rangle = \sum_a \frac{\partial I_h}{\partial X_a} \delta X_a = 0 \tag{2.41}$$

$$\langle \delta I_h, \delta x_a \rangle = \sum_a \frac{\partial I_h}{\partial x_a} \delta x_a = 0 \tag{2.42}$$

i.e., the potential energy is minimized not only with respect to nodal spatial coordinates x_a, but with respect to the node referential placements X_a. In this way the underlying variational principle of the problem, the principle of minimum potential energy, is used to supply both the finite element solution and the optimal mesh. Energy minimization with respect to the spatial positions x_a has the effect of equilibrating the mechanical nodal forces, while minimization with respect to referential nodal coordinates has the effect of equilibrating the nodal *configurational forces* induced by the discretization.

2.2.7 Relation with static configurational forces

Within the context of static applications, the idea of using the underlying variational principle (the principle of minimum potential energy) as an optimality criterion to find a "better" mesh (and therefore to minimize the energy with respect to both nodal referential and spatial coordinates (X_a, x_a)) enjoys a long tradition in the finite element literature and traces back at least to [33], [10], [11]. At that moment the calculation of the analytic derivatives of the discretized energy I_h with respect to the X_a variables was thought to be "a hopeless task in the case of arbitrary two and three dimensional grids" (see [10]) and only optimization techniques based on energy *evaluation* (and without computing the energy derivatives with respect to X_a) were studied. For high dimensionality problems those optimization techniques proved to be too costly and prohibitive for the computational resources available at the time.

By contrast, the connection between derivatives of the energy I_h with respect to node referential coordinates X_a and *configurational or material forces* has been recognized only recently [24], [35], [**?**]. The analytic differentiation of the energy I_h with respect to X_a can be computed directly and the forces conjugate to changes in node placements $F_a = \frac{\partial I_h}{\partial X_a}$ can be interpreted as *discrete configurational forces.*

We recall from §2.2.2 that the equation of balance of dynamic configurational forces for one-dimensional elasticity is given by (see equation (2.30))

$$\frac{\partial \mathcal{L}}{\partial X} + \frac{d}{dX}\left(-\left(\mathcal{L} - F\frac{\partial \mathcal{L}}{\partial F}\right)\right) - \frac{d}{dt}\left((-F)\,\frac{\partial \mathcal{L}}{\partial V}\right) = 0 \tag{2.43}$$

For Lagrangian densities of the form

$$\begin{aligned} \mathcal{L} &= \frac{RV^2}{2} - W\left(X, \varphi, F\right) = \\ &= \frac{RV^2}{2} - A\left(X, F\right) + B\varphi \end{aligned}$$

this balance equation reduces to

$$\frac{\partial}{\partial X}\left(B + \frac{RV^2}{2}\right) + \frac{d}{dX}\left(\left(W - \frac{RV^2}{2}\right) - FP\right) - \frac{d}{dt}\left(\left(-F\right)RV\right) = 0 \tag{2.44}$$

and in the static case (no inertia) to

$$\frac{\partial B}{\partial X}+\frac{d}{dX}\left(W-FP\right)=0$$

We recall also that the magnitude

$$C=-\left(\mathcal{L}-F\frac{\partial\mathcal{L}}{\partial F}\right)$$

is the *Eshelby stress tensor* ([6], [7], see also Chapter 3) which for Lagrangian densities of the form (2.23) (and in 1D) is given by

$$C=\left(W-\frac{RV^2}{2}\right)-FP$$

and in the static case it reduces to

$$C=W-FP$$

A straightforward computation ([59], appendix A) that mirrors that developed in §2.2.2 for the derivation of the continuous configurational force balance equation in the space-time setting, shows that the derivative of the discretized energy I_h with respect to the reference coordinate X_a corresponds to the *nodal (static) configurational force* associated to node a given by

$$F_a=\frac{\partial I_h}{\partial X_a}=\int_B C_h\frac{\partial N_a}{\partial X}dX+\int_B\frac{\partial B}{\partial X}N_a dX$$

where C_h is the static Eshelby stress tensor evaluated in the discretized deformation φ_h, i.e.,

$$C_h=W_h-F_hP_h$$

with

$$\begin{aligned}
W_h &= W\left(X,\varphi_h,D\varphi_h\right)= \\
&= W\Big|_{\left(X,\sum_a N_a x_a,\sum_a \frac{\partial N_a}{\partial X}x_a\right)} \\
F_h &= D\varphi_h=\sum_a\frac{\partial N_a}{\partial X}x_a \\
P_h &= \left.\frac{\partial W}{\partial F}\right|_{(X,\varphi_h,D\varphi_h)}= \\
&= \left.\frac{\partial W}{\partial F}\right|_{\left(X,\sum_a N_a x_a,\sum_a \frac{\partial N_a}{\partial X}x_a\right)}
\end{aligned}$$

The derivative of the discretized energy I_h with respect to nodal spatial coordinates x_a is the nodal mechanical nodal force given by (see for example [17])

$$f_a = \frac{\partial I_h}{\partial x_a} = \int_B (P_h) \frac{\partial N_a}{\partial X} dX + \int_B B N_a dX$$

where P_h is the (Piolla-Kirchhoff) stress evaluated in the discretized deformation φ_h and given above. Then the system of equations (2.41, 2.42) arranged jointly in a column array evaluates to

$$\begin{pmatrix} F_a \\ f_a \end{pmatrix} = \begin{pmatrix} \frac{\partial I_h}{\partial X_a} \\ \frac{\partial I_h}{\partial x_a} \end{pmatrix} = \int_B \begin{pmatrix} W_h - F_h P_h \\ P_h \end{pmatrix} \frac{\partial N_a}{\partial X} dX + \int_B \begin{pmatrix} \frac{\partial B}{\partial X} \\ B \end{pmatrix} N_a dX = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{2.45}$$

As we have explained in §2.2.3, the continuous counterpart of the previous equations, namely the equations of balance of mechanical forces (2.25, 2.26) and configurational forces (2.43, 2.44) are *equivalent* in the sense that if one equation is satisfied, the other is automatically satisfied. In the discrete setting however this equivalence is broken. The discretization induces *discrete* configurational forces that are not balanced in general, even in homogeneous materials where no configurational forces are expected. The joint system (2.45) is therefore and, in general, a non-degenerate, non-singular system of equations with a unique solution (X_a, x_a). In many situations however the solution is not unique, the system is ill-posed, or even non-convex (as reported in [49]). In those cases regularization techniques are required to find an admissible solution for (2.45).

Within the context of static applications, the variational mesh adaption framework suggests then to minimize the discretized energy I_h with respect to referential nodal placements X_a along with the standard minimization with respect to nodal spatial coordinates x_a. Minimization with respect to X_a has the effect of equilibrating the nodal configurational forces that are unbalanced in general, even when the continuous counterpart are automatically balanced. In the upcoming subsections we analyze possible extensions of this concept to dynamic applications.

2.2.8 Space-time finite elements

We proceed in this subsection to generalize to solid dynamics applications the previous spatial mesh adaption method for statics and its time adaption analog considered in §2.1.7 within the context of finite degree-of-freedom Lagrangian systems. The *direct* generalization is obtained by making use of *space-time finite elements* supported on a space-time mesh that is not prescribed at the outset but *computed* using Hamilton's principle. More precisely, we discretize the action functional $S[\varphi]$ by introducing a triangulation $\mathcal{T}_h$ *of the space-time domain* $B \times [t_0, t_f]$, as depicted in figure 2.5, and approximating the motion $\varphi(X, t)$ with a space-time finite element interpolation φ_h given by

$$\varphi_h(X, t) = \sum_{ak} N_{ak}(X, t)\, x_{ak} \tag{2.46}$$

where $N_{ak}(X,t)$ are the space-time shape functions, x_{ak} are the spatial coordinates of the space-time node ak, and where the index "ak" is used to enumerate nodes in the space-time element. Figure

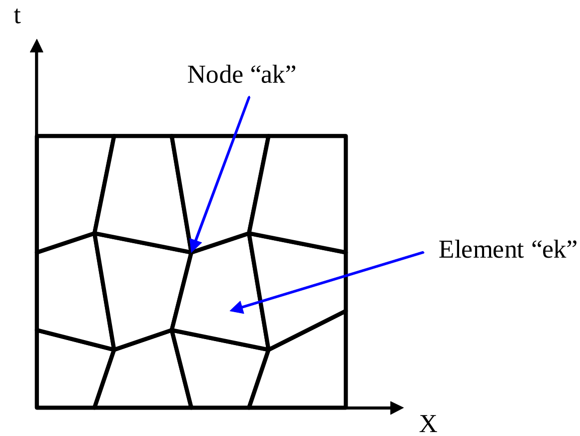

Figure 2.5: General triangulation of the space-time domain $B \times [t_0, t_f]$.

(2.6) sketches the discretization for the motion and the space time mesh. Compare with figure 2.4. The discrete action functional S_d follows then by evaluating the continuous action functional $S[\varphi]$

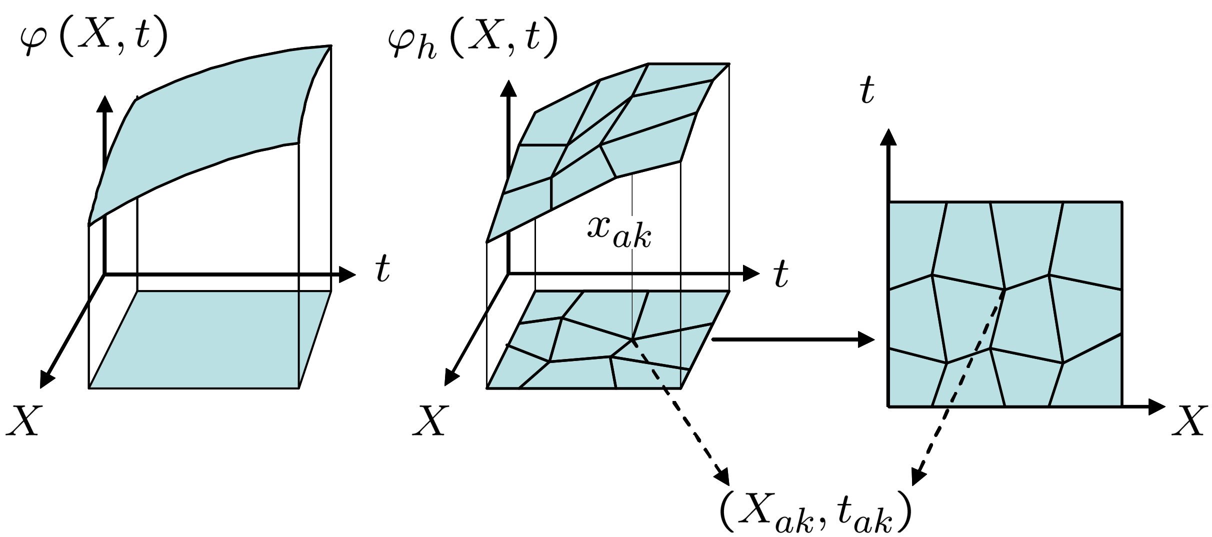

Figure 2.6: Discretization of the motion $\varphi(X,t)$ with space-time finite elements. The space-time placements (X_{ak}, t_{ak}) and the nodal deformation x_{ak} represent, respectively, horizontal and vertical coordinates of points on the graph of the discretized motion $(X, t\varphi_h(X,t))$

in the discretized motion

$$S_d(\cdots, x_{ak}, \cdots) = S[\varphi_h]$$

and the finite element solution for the motion $\varphi_h(X,t)$ is found by rendering the discrete action S_d stationary with respect to x_{ak}

$$\langle \delta S_d, \delta x_{ak} \rangle = \sum_{ak} \frac{\partial S_h}{\partial x_{ak}} \delta x_{ak} = 0 \tag{2.47}$$

Let (X_{ak}, t_{ak}) be the space-time coordinates of each space-time node "ak" in each space-time element "ek", where the index "ek" is used to enumerate the space-time elements in the space-time mesh (figure 2.7). In complete analogy to the static case where we recognized that the discretized

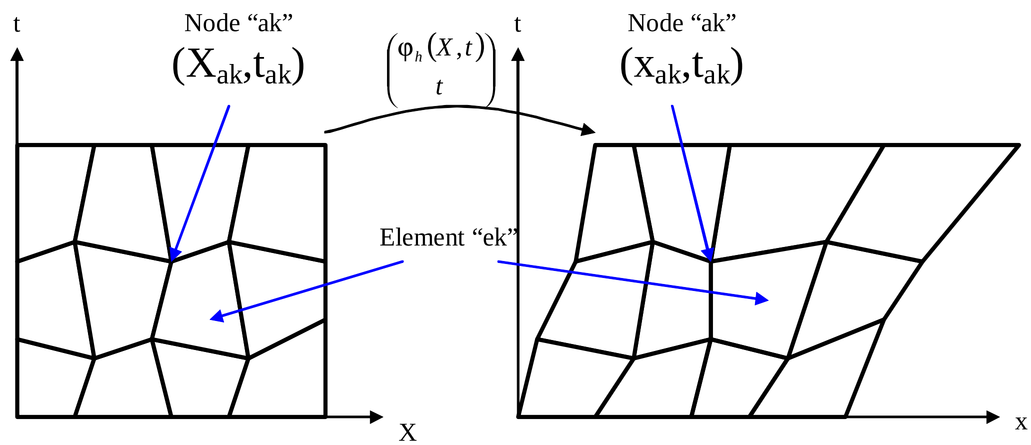

Figure 2.7: Space-time discretization. Reference (left) and spatial (right) space-time domain. Notice that for different times t (spatial) mesh change (space-adaption). Notice also that for different particles X, the time step change (time-adaption).

action I_h was-dependent not only on nodal spatial coordinates x_a but on nodal referential placements X_a and in complete analogy with the finite degree-of-freedom case where the discrete action sum was dependent on the discrete time set (see section §2.1.7), we observe now that the discrete space-time action S_d, and therefore the solution of (2.47), will depend on the space-time mesh. In particular it will depend on the space-time reference coordinates (X_{ak}, t_{ak}) of each space-time element

$$S_d = S_d(\cdots, X_{ak}, t_{ak}, x_{ak}, \cdots)$$

Motivated by the methodology presented in the static case in §2.2.6 and by the variational time integrators with horizontal variations developed in [20] (see §2.1.7), we assume now that the previous discrete action *should be rendered stationary with respect to all of its arguments.* This results in a system of equations to be solved not only for the finite element parameters x_{ak} but for the space-time nodal placements (X_{ak}, t_{ak})

$$\frac{\partial S_h}{\partial X_{ak}}(\cdots, X_{ak}, t_{ak}, x_{ak}, \cdots) = 0 \quad (2.48)$$

$$\frac{\partial S_h}{\partial t_{ak}}(\cdots, X_{ak}, t_{ak}, x_{ak}, \cdots) = 0 \quad (2.49)$$

$$\frac{\partial S_h}{\partial x_{ak}}(\cdots, X_{ak}, t_{ak}, x_{ak}, \cdots) = 0 \quad (2.50)$$

It is then conjectured that the space-time mesh nodal placements (X_{ak}, t_{ak}) obtained by solving the previous system are *optimal* since they are obtained by invoking the stationarity of the action functional, which is the operative variational principle for the problem under study. It bear emphasis that the previous is a *conjecture* and not a self-evident or obvious fact. One of the objectives of this thesis is indeed to explore its validity and scope.

2.2.9 Relation with space-time configurational forces

We recall from §2.2.2 that the equations of balance of dynamic configurational forces (2.30) and balance of energy (2.31) are the *horizontal* Euler-Lagrange equations, i.e., the Euler-Lagrange equations corresponding to the stationarity of the action functional S with respect to horizontal variations. We notice also that nodal placements (X_{ak}, t_{ak}) represent horizontal coordinates of nodal points of the discretized motion $\varphi_h(X,t)$ (see figure 2.6) and that therefore variations of (X_{ak}, t_{ak}) will induce variations on the base space, i.e., the space-time domain. It follows that the derivatives of the discretized action S_h with respect to the nodal placements (X_{ak}, t_{ak}) will correspond to the discrete space-time *nodal* configurational forces and that demanding the stationarity of the discrete action with respect to the horizontal nodal coordinates will be equivalent to enforcing discrete configurational force balance and discrete balance of energy.

The proof of this statement is straightforward and follows the lines of the procedure developed in §2.2.2 to compute horizontal variations of the continuous action and horizontal Euler-Lagrange equations. Consider the particular case of *isoparametric* space-time elements (figure 2.8) For this class of elements the space-time shape functions $N_{ak}(X,t)$ are given by

$$N_{ak} \circ \begin{pmatrix} X(\xi,\tau) \\ t(\xi,\tau) \end{pmatrix} = \hat{N}_{ak}(\xi,\tau)$$

where (ξ,τ) are parametric coordinates defined over the space-time standard domain $\hat{\Omega}$, $\hat{N}_{ak}(\xi,\tau)$ are the isoparametric space-time shape functions and the pair $(X(\xi,\tau), t(\xi,\tau))$ is the space-time

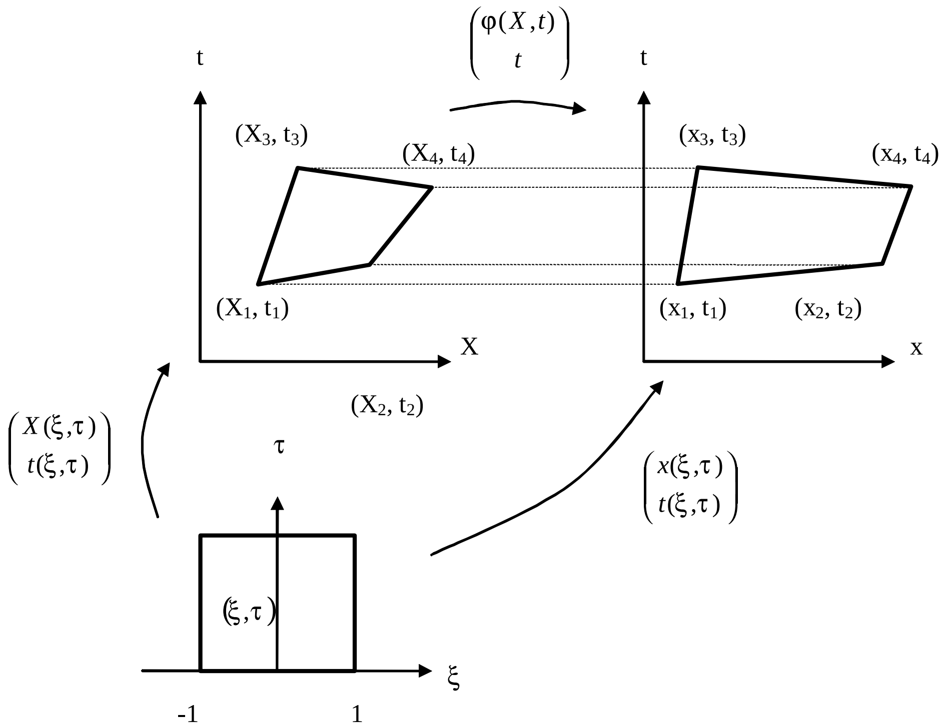

Figure 2.8: Isoparametric space-time element. The isoparametric "standard" domain $(\xi, \tau) \in \hat{\Omega}$ is mapped to each space-time element Ω^{ek} with the isoparametric space-time mapping $(X(\xi,\tau), t(\xi,\tau))$.

isoparametric mapping given by

$$\begin{pmatrix} X(\xi,\tau) \\ t(\xi,\tau) \end{pmatrix} = \sum_{ak} \hat{N}_{ak}(\xi,\tau) \begin{pmatrix} X_{ak} \\ t_{ak} \end{pmatrix} \tag{2.51}$$

The interpolation for the motion φ_h written in terms of the parametric coordinates follows then as

$$\begin{aligned} x(\xi,\tau) &= \varphi_h \circ \begin{pmatrix} X(\xi,\tau) \\ t(\xi,\tau) \end{pmatrix} = \\ &= \sum_{ak} \left(N_{ak} \circ \begin{pmatrix} X(\xi,\tau) \\ t(\xi,\tau) \end{pmatrix} \right) x_{ak} \\ &= \sum_{ak} \hat{N}_{ak}(\xi,\tau)\, x_{ak} \end{aligned} \tag{2.52}$$

For example, for linear spatial elements (two nodes) and linear time interpolation the space-time isoparametric shape functions are given by

$$\begin{aligned}
N_1(\xi,\tau) &= \frac{1}{2}(1-\xi)(1-\tau)\\
N_2(\xi,\tau) &= \frac{1}{2}(1+\xi)(1-\tau)\\
N_3(\xi,\tau) &= \frac{1}{2}(1-\xi)(\tau)\\
N_4(\xi,\tau) &= \frac{1}{2}(1+\xi)(\tau)
\end{aligned}$$

and the space-time standard element is

$$(\xi,\tau) \in \hat{\Omega} = [-1,1] \times [0,1]$$

We focus next in the discretization of the action functional, given in the continuos case by

$$S[\varphi] = \int_{t_0}^{t_f} \left(\frac{R}{2}\dot{\varphi}^2 - W(X,t,\varphi,D\varphi) \right) dX dt \tag{2.53}$$

The discrete action S_d is built by evaluating the continuous action $S[\varphi]$ on the discretization φ_h. This requires the computation of interpolations for the material velocity $V = \dot{\varphi}$ and deformation gradient $F = D\varphi$, which might be obtained by differentiating the interpolation for the motion (2.46) φ_h with respect to time

$$V_h(X,t) = \dot{\varphi}_h(X,t) = \sum_{ak} \frac{\partial N_{ak}}{\partial t}(X,t)\, x_{ak} \tag{2.54}$$

$$F_h(X,t) = D\varphi_h(X,t) = \sum_{ak} \frac{\partial N_{ak}}{\partial X}(X,t)\, x_{ak} \tag{2.55}$$

For the particular case of isoparametric space-time elements, the space and time derivatives of the shape functions $\frac{\partial N_{ak}}{\partial t}$ and $\frac{\partial N_{ak}}{\partial \mathbf{X}}$ are computed by making use of the (inverse of the) Jacobian of the (space-time) isoparametric mapping $(X(\xi,\tau), t(\xi,\tau))$

$$\mathbf{J}(\xi,\tau) = \begin{bmatrix} \frac{\partial t}{\partial \tau} & \frac{\partial X}{\partial \tau} \\ \frac{\partial t}{\partial \xi} & \frac{\partial X}{\partial \xi} \end{bmatrix}$$

in the form

$$\mathbf{J} \begin{pmatrix} \frac{\partial N_{ak}}{\partial t} \\ \frac{\partial N_{ak}}{\partial X} \end{pmatrix} = \begin{pmatrix} \frac{\partial \hat{N}_{ak}}{\partial \tau} \\ \frac{\partial \hat{N}_{ak}}{\partial \xi} \end{pmatrix}$$

which implies along with definition (2.52) for $x(\xi,\tau)$

$$\mathbf{J}\begin{pmatrix} V_h \\ F_h \end{pmatrix} = \begin{pmatrix} \frac{\partial x}{\partial \tau} \\ \frac{\partial x}{\partial \xi} \end{pmatrix} \tag{2.56}$$

Inserting the approximation V_h and F_h in the action functional (2.53) we obtain the discretized action as

$$\begin{aligned} S_d &= \sum_{ek} L_h^{ek} \\ L_d^{ek} &= \iint_{\Omega_{ek}} \left\{ \frac{1}{2} R \left(\sum_{ak} \frac{\partial N_{ak}}{\partial t} x_{ak} \right)^2 - W\left(X, t, \sum_{ak} N_{ak} x_{ak}, \sum_{am} \frac{\partial N_{ak}}{\partial X} x_{ak} \right) \right\} dX dt \end{aligned}$$

where L_d^{ek} is the discrete Lagrangian, and where the index "ek" ranges over all space-time elements Ω_{ek}. Different discrete Lagrangians L_d^{ek} follow then by choosing an appropriate quadrature rule to approximate the integrals over each space-time element Ω_{ek}. Since the space-time mesh (and therefore the space-time shape functions N_{ak} and the space-time element domains Ω_{ek}) depend on the space-time nodal coordinates (X_{ak}, t_{ak}), then the discrete action S_d itself will depend explicitly on (X_{ak}, t_{ak}).

$$S_d = S_d(\cdots, X_{ak}, t_{ak}, x_{ak}, \cdots)$$

Rendering now the discrete action sum S_d stationary with respect to all of its arguments equations for the computation of all variables are obtained. Differentiation of the previous discrete action sum with respect to x_{ak} yields

$$\frac{\partial S_d}{\partial x_{ak}} = \sum_{ek} \iint_{\Omega_{ek}} \left\{ RV_h \frac{\partial N_{ak}}{\partial t} - P_h \frac{\partial N_{ak}}{\partial X} + BN_{ak} \right\} dX dt$$

where P_h is the discretized stress. Differentiation of S_h with respect to (X_{ak}, t_{ak}) might look prohibitive at first sight. However, following a methodology similar to that presented in §2.2.2, it can be computed analytically and as we anticipated before, correspond to the *space-time* nodal configurational forces. For a Lagrangian density of the form (2.23) these are given by (see §2.2.2)

$$\begin{pmatrix} \frac{\partial S_d}{\partial X_{ak}} \\ \frac{\partial S_d}{\partial t_{ak}} \end{pmatrix} = \sum_{ek} \iint_{\Omega_{ek}} \left\{ -\mathbf{C}_h \begin{pmatrix} \frac{\partial N_{ak}}{\partial X} \\ \frac{\partial N_{ak}}{\partial t} \end{pmatrix} + \begin{pmatrix} \frac{\partial \mathcal{L}}{\partial X} \\ \frac{\partial \mathcal{L}}{\partial t} \end{pmatrix} N_{ak} \right\} dX dt$$

where $\mathbf{C}_h$ is the discretized space-time Eshelby tensor (or energy-(material) momentum tensor)

$$\mathbf{C}_h = \begin{bmatrix} \left(W_h - \frac{RV_h^2}{2} \right) - F_h P_h & F_h R V_h \\ -V_h P_h & \frac{RV_h^2}{2} + W_h \end{bmatrix}$$

discrete counterpart of (2.32). The system of equations to solve for the unknowns (X_{ak}, t_{ak}, x_{ak}) is therefore

$$\begin{aligned}
\frac{\partial S_d}{\partial X_{ak}} &= \sum_{ek} \iint_{\Omega_{ek}} \left\{ -F_h R V_h \frac{\partial N_{ak}}{\partial t} - \left(W_h - \frac{R V_h^2}{2} - F_h P_h \right) \frac{\partial N_{ak}}{\partial X} + \frac{\partial \mathcal{L}}{\partial X} N_{ak} \right\} dX dt = 0 \\
\frac{\partial S_d}{\partial t_{ak}} &= \sum_{ek} \iint_{\Omega_{ek}} \left\{ -\left(\frac{R V_h^2}{2} + W_h \right) \frac{\partial N_{ak}}{\partial t} + V_h P_h \frac{\partial N_{ak}}{\partial X} + \frac{\partial \mathcal{L}}{\partial t} N_{ak} \right\} dX dt = 0 \\
\frac{\partial S_d}{\partial x_{ak}} &= \sum_{ek} \iint_{\Omega_{ek}} \left\{ R V_h \frac{\partial N_{ak}}{\partial t} - P_h \frac{\partial N_{ak}}{\partial X} + B N_{ak} \right\} dX dt = 0
\end{aligned}$$

which represent the discretization of equations (2.33), (2.34), and (2.26).

As happens in the static and finite-dimensional cases, in the continuous setting, the Euler-Lagrange equations corresponding to horizontal variations are equivalent to those corresponding to vertical variations. This is not the case when the system has been discretized. Requiring then stationarity of the discrete action S_d with respect to horizontal variations gives independent equations that can be used to *solve* for the space-time mesh. Enforcing the satisfaction of these equations results in a discretization that exactly preserves energy and exactly satisfies discrete balance of dynamic configurational forces.

2.2.10 Space-time elements with homogeneous time steps

An essential problem related to the space-time generalization and its implementation in terms of space-time finite elements is the issue of solvability for the time step. It has been noticed (see for example [20], [29], [30]) that the energy equation involves the unknown discrete time in a highly non-linear way and that it is not always possible to find admissible solutions. It was then suggested ([60]) to restrict the methodology *to space adaption only* by regarding only the spatial mesh as unknown while providing the discrete times at the outset.

An implementation of this approach based on the space-time framework was attempted in ([60]). The approach in this case was to adopt a particular class of space-time finite elements where the same time step was used for all nodes in the mesh, i.e., space-time is discretized with a *homogeneous time step*. In this section we will show that for this particular class of space-time finite elements there is no need to resort to the machinery and formalism of space-time finite elements since, as we shall prove, this discretization is equivalent to effect the space-time discretization in two separated and uncoupled stages, the first stage (semidiscretization in space) where the space variable is discretized keeping the time continuous, followed by a second stage in which the time is discretized using an appropriate time integrator.

To prove this equivalence, consider the particular class of isoparametric space-time elements obtained by making use of isoparametric shape functions of the form

$$\hat{N}_{ak}(\xi,\tau) = \hat{N}_a^{space}(\xi)\,\hat{N}_k^{time}(\tau) \tag{2.57}$$

where $N_a^{space}(\xi)$ and $N_a^{time}(\tau)$ are *uncoupled* space and time shape functions and where two separated indexes a and k instead of a single index "ak" are used. We recall that the isoparametric space-time interpolation is

$$\begin{aligned} X(\xi,\tau) &= \sum_{ak} \hat{N}_{ak}(\xi,\tau)\,X_{ak} \\ t(\xi,\tau) &= \sum_{ak} \hat{N}_{ak}(\xi,\tau)\,t_{ak} \\ x(\xi,\tau) &= \sum_{ak} \hat{N}_{ak}(\xi,\tau)\,x_{ak} \end{aligned}$$

where $x(\xi,\tau)$ is given by

$$x(\xi,\tau) = \varphi_h \circ \begin{pmatrix} X(\xi,\tau) \\ t(\xi,\tau) \end{pmatrix} \tag{2.58}$$

with $\varphi_h(X,t)$ the discretized motion (2.46). Inserting (2.57) in the isoparametric interpolation we find

$$\begin{aligned} X(\xi,\tau) &= \sum_k \sum_a \hat{N}_a^{space}(\xi)\,\hat{N}_k^{time}(\tau)\,X_a^k \\ t(\xi,\tau) &= \sum_k \sum_a \hat{N}_a^{space}(\xi)\,\hat{N}_k^{time}(\tau)\,t_a^k \\ x(\xi,\tau) &= \sum_k \sum_a \hat{N}_a^{space}(\xi)\,\hat{N}_k^{time}(\tau)\,x_a^k \end{aligned}$$

that might be split in two staggered interpolations: a first interpolation in the ξ variable,

$$\begin{aligned} X(\xi,\tau) &= \sum_a \hat{N}_a^{space}(\xi)\,X_a(\tau) \\ t(\xi,\tau) &= \sum_a \hat{N}_a^{space}(\xi)\,t_a(\tau) \\ x(\xi,\tau) &= \sum_a \hat{N}_a^{space}(\xi)\,x_a(\tau) \end{aligned}$$

and a second interpolation in the τ variable

$$\begin{aligned} X_a(\tau) &= \sum_k \hat{N}_k^{time}(\tau)\,X_a^k \\ t_a(\tau) &= \sum_k \hat{N}_k^{time}(\tau)\,t_a^k \\ x_a(\tau) &= \sum_k \hat{N}_k^{time}(\tau)\,x_a^k \end{aligned}$$

Assume also that we make use of *homogeneous time steps in each space-time element*, i.e., that the isoparametric function $t(\xi,\tau)$ is not a function of ξ but only of τ

$$t(\xi,\tau) = t(\tau) \tag{2.59}$$

For space-time shape functions of the form in (2.57) the previous condition will be satisfied provided that the time component of the space-time nodal coordinates $(X_{ak}, t_{ak}) = \left(X_a^k, t_a^k\right)$ is chosen such that

$$t_a^k = t^k \tag{2.60}$$

independent on the index a and for all k (see figure 2.9, compare with figure 2.8). This can be directly verified by observing that (2.57) and (2.60) imply

$$\begin{aligned}
t(\xi,\tau) &= \sum_k \sum_a \hat{N}_a^{space}(\xi)\, \hat{N}_k^{time}(\tau)\, t_a^k = \\
&= \sum_k \sum_a \hat{N}_a^{space}(\xi)\, \hat{N}_k^{time}(\tau)\, t^k = \\
&= \left(\sum_k \hat{N}_k^{time}(\tau)\, t^k\right)\left(\sum_a \hat{N}_a^{space}(\xi)\right) = \\
&= \sum_k \hat{N}_k^{time}(\tau)\, t^k = \\
&= t(\tau)
\end{aligned}$$

where we have assumed that the shape functions for the space N_a^{space} satisfy the partition of unity property

$$\sum_a \hat{N}_a^{space}(\xi) = 1$$

Figure 2.9 illustrates condition (2.60) for a one-dimensional (in-space) mesh.

Using the particular class of space-time shape functions (2.57) in combination with "homogeneous time steps" (assumptions (2.59) and (2.60)) we obtain

$$\begin{aligned}
X(\xi,\tau) &= \textstyle\sum_a \hat{N}_a^{space}(\xi)\, X_a(\tau) \\
t(\xi,\tau) &= t(\tau) = t_a(\tau) \\
x(\xi,\tau) &= \textstyle\sum_a \hat{N}_a^{space}(\xi)\, x_a(\tau)
\end{aligned}$$

Furthermore, since the time t and the time parameter τ are in a one-to-one correspondence, we may eliminate the latter (using for that the inverse of $t(\tau)$) and regard X_a and x_a as functions of t to

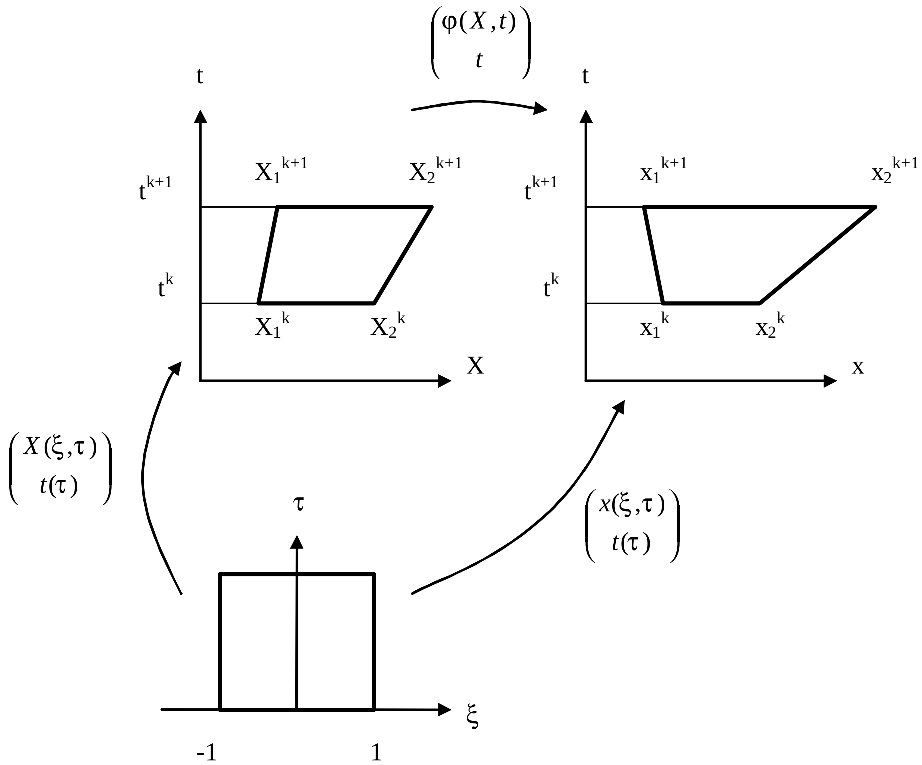

Figure 2.9: Isoparametric mapping in 1D using a time step that is independent of the spatial parameter ξ. All the grid points in the element are sampled at the same time t^k.

obtain

$$\begin{aligned} X(\xi,t) &= \sum_a \hat{N}_a^{space}(\xi)\, X_a(t) \\ x(\xi,t) &= \sum_a \hat{N}_a^{space}(\xi)\, x_a(t) \end{aligned}$$

We thus arrive to the *same interpolation used in static isoparametric finite elements but with node referential and spatial coordinates regarded as continuous functions of time.*

By way of example consider as in the previous section the case of linear shape functions in space and time:

$$\begin{aligned} N_{11}(\xi,\tau) &= \frac{1}{2}(1-\xi)(1-\tau) \\ N_{21}(\xi,\tau) &= \frac{1}{2}(1+\xi)(1-\tau) \\ N_{12}(\xi,\tau) &= \frac{1}{2}(1-\xi)(\tau) \\ N_{22}(\xi,\tau) &= \frac{1}{2}(1+\xi)(\tau) \end{aligned}$$

where we are now using two indices to label the functions. Consider also a particular space-time element with four nodes, two nodes at time t^k and the other two at time t^{k+1} as depicted in figure 2.10 (homogeneous time step)

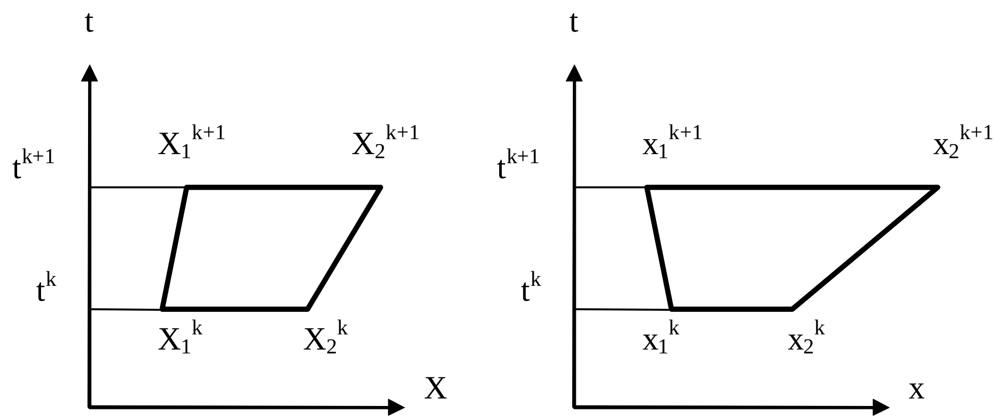

Figure 2.10: Space-time linear finite element with two nodes sampled at time t^k and the other two sampled at time t^{k+1} (homogeneous time step). For this particular space-time nodal arrangement the time part of the isoparametric space-time mapping is independent of the space parameter $t(\xi,\tau) = t(\tau)$.

In this case the space-time isoparametric mapping reduces to

$$\begin{aligned}
X(\xi,\tau) &= N_{11}(\xi,\tau)\,X_1^k + N_{21}(\xi,\tau)\,X_2^k + N_{12}(\xi,\tau)\,X_1^{k+1} + N_{22}(\xi,\tau)\,X_2^{k+1} = \\
&= \left(\frac{1}{2}(1-\xi)\,X_1^k + \frac{1}{2}(1+\xi)\,X_2^k\right)(1-\tau) + \left(\frac{1}{2}(1-\xi)\,X_1^{k+1} + \frac{1}{2}(1+\xi)\,X_2^{k+1}\right)(\tau) = \\
&= \frac{1}{2}(1-\xi)\left((1-\tau)\,X_1^k + (\tau)\,X_1^{k+1}\right) + \frac{1}{2}(1+\xi)\left((1-\tau)\,X_2^k + (\tau)\,X_2^{k+1}\right) \\
t(\xi,\tau) &= N_{11}(\xi,\tau)\,t^k + N_{21}(\xi,\tau)\,t^k + N_{12}(\xi,\tau)\,t^{k+1} + N_{22}(\xi,\tau)\,t^{k+1} = \\
&= \left(\frac{1}{2}(1-\xi)\,t^k + \frac{1}{2}(1+\xi)\,t^k\right)(1-\tau) + \left(\frac{1}{2}(1-\xi)\,t^{k+1} + \frac{1}{2}(1+\xi)\,t^{k+1}\right)(\tau) = \\
&= t^k(1-\tau) + (\tau)\,t^{k+1}
\end{aligned}$$

and the motion referred to the isoparametric domain becomes

$$\begin{aligned}
x(\xi,\tau) &= N_{11}(\xi,\tau)\,x_1^k + N_{21}(\xi,\tau)\,x_2^k + N_{12}(\xi,\tau)\,x_1^{k+1} + N_{22}(\xi,\tau)\,x_2^{k+1} = \\
&= \left(\frac{1}{2}(1-\xi)\,x_1^k + \frac{1}{2}(1+\xi)\,x_2^k\right)(1-\tau) + \left(\frac{1}{2}(1-\xi)\,x_1^{k+1} + \frac{1}{2}(1+\xi)\,x_2^{k+1}\right)(\tau) = \\
&= \frac{1}{2}(1-\xi)\left((1-\tau)\,x_1^k + (\tau)\,x_1^{k+1}\right) + \frac{1}{2}(1+\xi)\left((1-\tau)\,x_2^k + (\tau)\,x_2^{k+1}\right)
\end{aligned}$$

Therefore, the time component of the space-time mapping $t(\xi,\tau)$ becomes only a function of τ.

Inverting we get

$$\tau = \frac{t - t^k}{t^{k+1} - t^k}$$

Composing the mappings $X(\xi,\tau)$ and $t(\xi,\tau)$ with the previous we find

$$\begin{aligned}
X(\xi,t) &= \left(\frac{1-\xi}{2}X_1^k + \frac{1+\xi}{2}X_2^k\right)\frac{t^{k+1}-t}{t^{k+1}-t^k} + \left(\frac{1-\xi}{2}X_1^{k+1} + \frac{1+\xi}{2}X_2^{k+1}\right)\frac{t-t^k}{t^{k+1}-t^k} = \\
&= \frac{1-\xi}{2}\left(\frac{t^{k+1}-t}{t^{k+1}-t^k}X_1^k + \frac{t-t^k}{t^{k+1}-t^k}X_1^{k+1}\right) + \frac{1+\xi}{2}\left(\frac{t^{k+1}-t}{t^{k+1}-t^k}X_2^k + \frac{t-t^k}{t^{k+1}-t^k}X_2^{k+1}\right) \\
x(\xi,t) &= \left(\frac{1-\xi}{2}x_a^k + \frac{1+\xi}{2}x_{a+1}^k\right)\frac{t^{k+1}-t}{t^{k+1}-t^k} + \left(\frac{1-\xi}{2}x_a^{k+1} + \frac{1+\xi}{2}x_{a+1}^{k+1}\right)\frac{t-t^k}{t^{k+1}-t^k} = \\
&= \frac{1-\xi}{2}\left(\frac{t^{k+1}-t}{t^{k+1}-t^k}x_1^k + \frac{t-t^k}{t^{k+1}-t^k}x_1^{k+1}\right) + \frac{1+\xi}{2}\left(\frac{t^{k+1}-t}{t^{k+1}-t^k}x_2^k + \frac{t-t^k}{t^{k+1}-t^k}x_2^{k+1}\right)
\end{aligned}$$

which might be written as

$$X(\xi,t) = \frac{1-\xi}{2}X_1(t) + \frac{1+\xi}{2}X_2(t) \tag{2.61}$$

$$x(\xi,t) = \frac{1-\xi}{2}x_1(t) + \frac{1+\xi}{2}x_2(t) \tag{2.62}$$

along with

$$\begin{aligned}
X_a(t) &= \frac{t^{k+1}-t}{t^{k+1}-t^k}X_a^k + \frac{t-t^k}{t^{k+1}-t^k}X_a^{k+1} \\
x_a(t) &= \frac{t^{k+1}-t}{t^{k+1}-t^k}x_a^k + \frac{t-t^k}{t^{k+1}-t^k}x_a^{k+1}
\end{aligned}$$

for $a = 1$ and 2. Furthermore, solving for ξ in (2.61) we find

$$\xi = \frac{X - \frac{X_1(t)+X_2(t)}{2}}{\frac{X_2(t)-X_1(t)}{2}}$$

which implies

$$\begin{aligned}
\frac{1-\xi}{2} &= \frac{X_2(t) - X}{X_2(t) - X_1(t)} \\
\frac{1+\xi}{2} &= \frac{X - X_1(t)}{X_2(t) - X_1(t)}
\end{aligned}$$

Equation (2.62) becomes

$$x = \varphi_h(X,t) = \frac{X_2(t) - X}{X_2(t) - X_1(t)}x_1(t) + \frac{X_2(t) - X}{X_2(t) - X_1(t)}x_2(t)$$

which results in the same interpolation used in static finite elements but with nodal positions in the reference and spatial configurations (X_a, x_a) regarded as continuous functions of time.

We therefore conclude that in space-time finite elements with uncoupled space and time shape functions and homogeneous time steps the time parameter τ and the physical time t result in one-to-one correspondence and the time parametrization might be thus eliminated at the element level. The machinery of space-time finite elements, which involves the computation of the space-time Jacobian and its inverse, is no longer needed and might be sidestepped. Consider for example the computation of *material velocities* V_h. We recall that in a general space-time finite element the velocity is given by (2.56) which requires the inversion of the Jacobian of the space-time isoparametric mapping. Notice now that if the time is homogeneous (and uncoupled space/time shape functions are used) we have

$$\begin{aligned} X(\xi,\tau) &= \sum_a \hat{N}_a^{space}(\xi)\, X_a(\tau) \\ t(\xi,\tau) &= t(\tau) \end{aligned}$$

whereupon relation (2.56) for material velocity V_h and deformation gradient F_h reduces to (2.51)

$$\begin{bmatrix} \frac{\partial t}{\partial \tau} & \frac{\partial X}{\partial \tau} \\ 0 & \frac{\partial X}{\partial \xi} \end{bmatrix} \begin{pmatrix} V_h \\ F_h \end{pmatrix} = \begin{pmatrix} \frac{\partial x}{\partial \tau} \\ \frac{\partial x}{\partial \xi} \end{pmatrix}$$

The inverse of the Jacobian might be thus computed *analytically* and evaluates to

$$\begin{aligned} \begin{pmatrix} V_h \\ F_h \end{pmatrix} &= \frac{1}{\frac{\partial t}{\partial \tau}\frac{\partial X}{\partial \xi}} \begin{bmatrix} \frac{\partial X}{\partial \xi}\frac{\partial x}{\partial \tau} - \frac{\partial X}{\partial \tau}\frac{\partial x}{\partial \xi} \\ \frac{\partial t}{\partial \tau}\frac{\partial x}{\partial \xi} \end{bmatrix} = \\ &= \begin{bmatrix} \frac{\frac{\partial x}{\partial \tau}}{\frac{\partial t}{\partial \tau}} - \frac{\frac{\partial x}{\partial \xi}}{\frac{\partial X}{\partial \xi}} \frac{\frac{\partial X}{\partial \tau}}{\frac{\partial t}{\partial \tau}} \\ \frac{\frac{\partial x}{\partial \xi}}{\frac{\partial X}{\partial \xi}} \end{bmatrix} \end{aligned}$$

or more compactly to

$$\begin{aligned} V_h &= \dot{x} - F_h \dot{X} \\ F_h &= \frac{\frac{\partial x}{\partial \xi}}{\frac{\partial X}{\partial \xi}} \end{aligned} \tag{2.63}$$

where

$$\begin{aligned} \dot{x} &= \frac{\frac{\partial x}{\partial \tau}}{\frac{\partial t}{\partial \tau}} \\ \dot{X} &= \frac{\frac{\partial X}{\partial \tau}}{\frac{\partial t}{\partial \tau}} \end{aligned}$$

2.2.11 Space semidiscretization and mesh adaption in "Space-Space"

The key observation that results from the developments of the previous subsection is that when time adaption is no longer pursued there is no need to resort to the formalism of the space-time framework and its implementation using the machinery of space-time finite elements. The particular class of space-time finite elements based on uncoupled space and time shape functions (assumption (2.57)) and homogeneous time steps (assumption (2.59)) is equivalent to an *uncoupled* spatial and time interpolations that may be completed in two separated stages: a *spatial discretization*, keeping the time continuous and leading to the formulation of a differential problem with unknowns $(X_a(t), x_a(t))$, and a second *time-discretization* stage where the latter is integrated. Since the time variable is kept continuous during the first stage of the discretization process, the expanded space-time framework that serves as the theoretical basis for the analysis of variational space-time mesh adaption and its implementation in terms of space-time finite elements is not advantageous. By contrast, much more insight can be gained by adopting a *space-space* point of view.

Within the framework just outlined, consider a spatial semidiscretization with an isoparametric interpolation of the form

$$\begin{aligned} X(\xi, t) &= \sum_a \hat{N}_a(\xi) X_a(t) \\ x(\xi, t) &= \sum_a \hat{N}_a(\xi) x_a(t) \end{aligned}$$

where $\hat{N}_a(\xi)$ are the isoparametric shape functions for space (previously denoted as $N_a^{space}(\xi)$) and $x(\xi, t)$ is the motion referred to the isoparametric domain ξ, i.e.,

$$x(\xi, t) = \varphi_h(X(\xi, t), t)$$

As was demonstrated in the previous subsection, this interpolation is equivalent to that resulting from space-time isoparametric finite elements with homogeneous time steps where the time parameter has been eliminated at the element level and the time is regarded as a continuous variable. Let $N_a(X, t)$ be the global shape functions given for the case of isoparametric elements such that

$$N_a(X(\xi, t), t) = \hat{N}_a(\xi) \tag{2.64}$$

and let $\varphi_h(X, t)$ be the (semidiscretized) motion

$$\varphi_h(X, t) = \sum_a N_a(X, t) x_a(t) \tag{2.65}$$

The proposed interpolation is illustrated from a *space-space* point of view in figure 2.11 where the approximation for the motion φ_h for two successive times t and $t+\Delta t$ is shown when the same mesh is used for every time (standard semidiscrete interpolation, figure 2.11(a)) and when the nodes are allowed to move (figure 2.11(b)) It may be also illustrated from a *space-time* point of view as

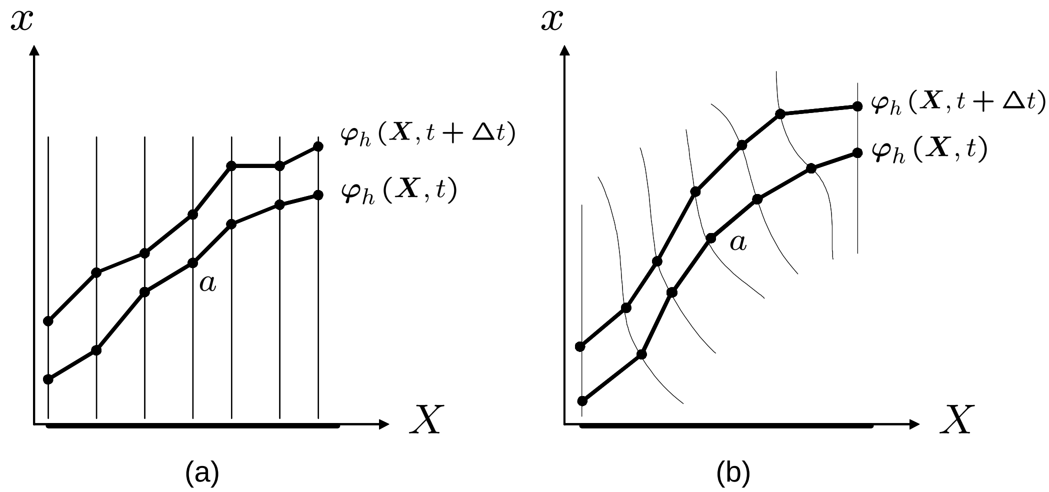

Figure 2.11: Approximation for the motion φ at two different time steps, t and $t+\Delta t$, using the same mesh at every time (a) and a mesh supported on a node set that moves continuously in time (b)

depicted in figure (**??**) where the spatial mesh for two successive times t and $t+\Delta t$ is shown for both a fixed and a moving mesh. From figure 2.11 we observe that the unknown of the problem, the motion $\varphi(X,t)$, *might be reinterpreted as an continuously evolving curve* $(X, \varphi(X,t))$ *imbedded in the* space-space *bundle* $[0,L]\times\ \mathbb{R}$. This curve is the *graph of the deformation mapping* and the proposed interpolation is just a piecewise continuous approximation for this curve, the graph, with its two-dimensional nodal positions (X_a, x_a) all treated as unknowns.

2.2.12 Semidiscrete action functional and discrete action sum

In the *space-time* finite element approach a discrete action S_d was built by inserting the space-time interpolation for the motion φ_h into the continuous action $S[\varphi]$. We then invoked the stationarity of the discrete action sum with respect to the parameters that define the discrete motion, namely (X_{ak}, t_{ak}, x_{ak}) to obtain a joint system of equations to solve not only for the spatial coordinates x_{ak} but for the space-time nodal placements (X_{ak}, t_{ak}) (equations (2.48), (2.49), (2.50)). We proceed now to build a discrete action S_h for the current interpolation. This will be accomplished in two stages: First a *semidiscrete* action $S_{sd}(X_a(t), x_a(t))$ will be built by inserting the semidiscrete interpolation (2.65) into the continuous action $S[\varphi]$. Then a discrete action S_d will be constructed by discretizing the semidiscrete action in time by an appropriate time interpolation of the nodal trajectories $(X_a(t), x_a(t))$.

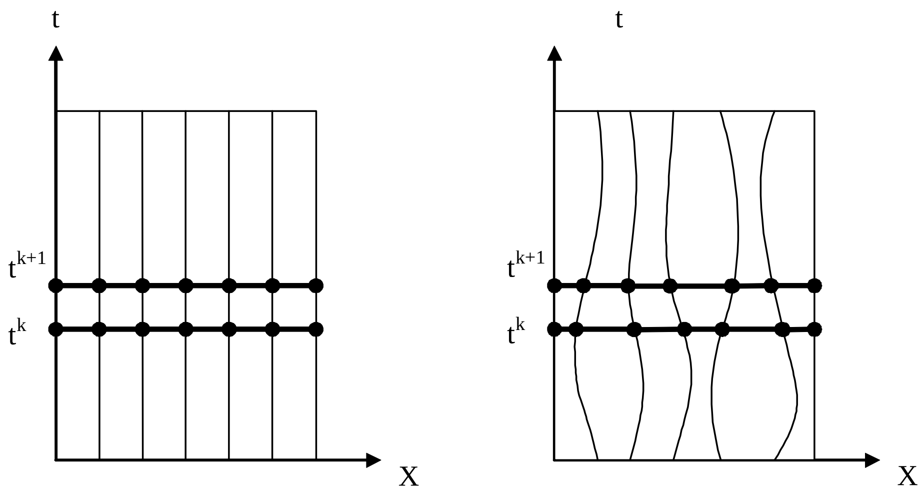

Figure 2.12: Spatial mesh for two successive times t^k and t^{k+1}. (a) The same mesh is used for every time (no adaption), (b) a mesh with time-dependent nodal placements $X_a(t)$.

The continuous action functional is given by

$$\begin{aligned} S[\varphi] &= \int_{t_0}^{t_f}\int_0^L \left(\frac{R}{2}\dot{\varphi}^2 - W(X,\varphi,D\varphi)\right) dX dt = \\ &= \int_{t_0}^{t_f}\int_0^L \left(\frac{R}{2}\dot{\varphi}^2 - A(X,D\varphi) + B\varphi\right) dX dt \end{aligned}$$

We would like now to insert the interpolation for the motion φ (2.65) into the previous. To this end we first need to provide appropriate interpolations for velocities and deformation gradients $V = \dot{\varphi}$ and $F = D\varphi$. At first sight it seems natural to take

$$\begin{aligned} V_h &= \dot{\varphi}_h = \frac{d}{dt}\left(\sum_a N_a(X,t)\, x_a(t)\right) \\ &= \sum_a N_a \dot{x}_a + \dot{N}_a x_a \end{aligned} \tag{2.66}$$

$$\begin{aligned} F_h &= D\varphi_h = \frac{d}{dX}\left(\sum_a N_a(X,t)\, x_a(t)\right) \\ &= \sum_a \frac{\partial N_a}{\partial X} x_a \end{aligned} \tag{2.67}$$

However, and as will be illustrated in Chapter 6, the natural (or consistent) velocity interpolation $V_h = \dot{\varphi}_h$ is usually a very poor approximation for V_h. Therefore independent (inconsistent) velocity interpolations are needed. In the next section we will explore interpolations of the form

$$V_h = \sum_a N_a(X,t)\, V_a(t)$$

where $V_a(t)$ are new parameters that must be taken as unknowns along with the nodal referential and spatial trajectories $(X_a(t), x_a(t))$.

For the duration of this subsection, consider the consistent velocity interpolation (2.66). For this particular case of isoparametric elements (elements supported on moving meshes), the derivative $\dot{N}_a$ can be directly computed. This can be accomplished by differentiating relation (2.65) with respect to time to find

$$\frac{\partial N_a}{\partial X}\dot{X}(\xi,t) + \dot{N}_a = 0$$

with

$$\dot{X}(\xi,t) = \sum_a \hat{N}_a(\xi)\, \dot{X}_a(t)$$

Composing the previous with the inverse of $X(\cdot,t)$ and rearranging we obtain

$$\dot{N}_a = -\frac{\partial N_a}{\partial X}\sum_a N_a \dot{X}_a(t)$$

The suggested interpolation for the velocity field thus becomes

$$\begin{aligned}
V_h &= \dot{\varphi}_h = \sum_a N_a \dot{x}_a + \dot{N}_a x_a = \\
&= \sum_a N_a \dot{x}_a + \left(-\frac{\partial N_a}{\partial X}\sum_b N_b \dot{X}_b\right) x_a = \\
&= \sum_a N_a \dot{x}_a - \left(\frac{\partial N_a}{\partial X} x_a\right)\sum_b N_b \dot{X}_b = \\
&= \sum_a N_a \left(\dot{x}_a - F_h \dot{X}_b\right)
\end{aligned}$$

As was illustrated in the example of §2.2.10 (see equation (2.63)) this formula can also be obtained by inverting analytically the Jacobian of the space-time isoparametric mapping.

Inserting now the obtained interpolations for V_h and F_h into the continuous action, we obtain the semidiscrete action S_{sd} as

$$\begin{aligned}
S_{sd}(X_a, x_a) &= S[\varphi_h] = \\
&= \int_{t_0}^{t_f}\int_B \left(\frac{R}{2}\left(\sum_a N_a\left(\dot{x}_a - F_h\dot{X}_b\right)\right)^2 - W\left(X, t, \sum_a N_a x_a, \sum_a \frac{\partial N_a}{\partial X} x_a\right)\right) dX dt
\end{aligned}$$

The previous can be compactly expressed as

$$S_{sd}\left(\cdots,X_a,x_a,\cdots\right)=\int_{t_0}^{t_f}\left(\frac{1}{2}\left(\dot{X}_a,\dot{x}_a\right)m_{ab}\begin{pmatrix}\dot{X}_b\\ \dot{x}_b\end{pmatrix}-I_h\left(X_a,x_a\right)\right)dt \tag{2.68}$$

where m_{ab} is a configuration-dependent extended mass matrix (space-space mass) given by

$$m_{ab}=\int_B RN_aN_b\begin{pmatrix}F_hF_h & -F_h\\ -F_h & 1\end{pmatrix}dX$$

and I_h is the discrete potential energy given as in the static case as

$$I_h=\int_B W\left(X,t,\sum_a N_a x_a\left(t\right),\sum_a\frac{\partial N_a}{\partial X}x_a\left(t\right)\right)dX$$

We invoke next the stationarity of the semidiscrete action functional with respect to all of its arguments $\left(X_a\left(t\right),x_a\left(t\right)\right)$.

$$\begin{aligned}\langle\delta S_{sd},\delta X_a\rangle &= 0\\ \langle\delta S_{sd},\delta x_a\rangle &= 0\end{aligned}$$

Computing the variations of the semidiscrete action S_{sd} with respect to $x_a\left(t\right)$ yields

$$\langle\delta S_{sd},\delta x_a\rangle=\int_{t_0}^{t_f}\int_B\left(R\dot{\varphi}_hN_b\left(\delta\dot{x}_b-\left(\tfrac{\partial N_c}{\partial X}\delta x_c\right)\dot{X}_b\right)-P_h\tfrac{\partial N_c}{\partial X}+BN_a\right)dX\,dt$$

To compute the variations with respect to $X_a\left(t\right)$ we follow the same procedure developed in §2.2.2 to compute variations in the continuous space-time setting (see also next chapter and Chapter 6) to find

$$\langle\delta S_{sd},\delta X_a\rangle=\int_{t_0}^{t_f}\int_B\left(R\dot{\varphi}_hN_b\left(-F_h\right)\left(\delta\dot{X}_b-\left(\tfrac{\partial N_c}{\partial X}\delta X_c\right)\dot{X}_b\right)-C_h\tfrac{\partial N_a}{\partial X}+\left(\tfrac{\partial B}{\partial X}+\frac{1}{2}\tfrac{\partial R}{\partial X}V^2\right)N_a\right)dX\,dt$$

where

$$C_h=\left(W_h-\frac{RV_h^2}{2}\right)-F_hP_h$$

is the (semi) discrete dynamic Eshelby stress tensor. As happens in the static case and in the case of space-time finite elements, variations of the action functional with respect to nodal referential placements correspond to the nodal configurational forces. The corresponding Euler-Lagrange equations might be written as

$$\frac{d}{dt}\left(m_{ab}\begin{pmatrix}\dot{X}_b\\ \dot{x}_b\end{pmatrix}\right)-\begin{pmatrix}\frac{\partial}{\partial X_a}\\ \frac{\partial}{\partial x_a}\end{pmatrix}\left(\frac{1}{2}\left(\dot{X}_a,\dot{x}_a\right)m_{ab}\begin{pmatrix}\dot{X}_b\\ \dot{x}_b\end{pmatrix}-I_h\left(X_a,x_a\right)\right)=\begin{pmatrix}0\\ 0\end{pmatrix} \tag{2.69}$$

which represents a system of two differential equations for the joint unknown $(X_a(t), x_a(t))$. As was explained before, we conjecture that the nodal instantaneous referential placements $X_a(t)$ obtained by solving the previous system are optimal for every time t since they follow by invoking the stationarity of the action functional, which is the operative variational principle for dynamics.

We finally discretize in time the semidiscrete system of ordinary differential equations (2.69) for the unknowns $(X_a(t), x_a(t))$. To this end an appropriate time integrator needs to be formulated. Since the system of equations to integrate derive from a Lagrangian, and to avoid any ad-hoc time-stepping device that ignores this particular structure of the equations, we shall make use in particular of a *variational* integrator.

This is simply accomplished by discretizing in time the *semidiscrete* action integral S_{sd} to build a *discrete* action sum S_d by interpolating in time the nodal trajectories $(X_a(t), x_a(t))$. The time-stepping algorithm follows then by invoking the stationarity of the latter with respect to discrete trajectories to obtain the *discrete* Euler-Lagrange equations. The construction of the *discrete* action sum follows exactly the same procedure presented in §2.1.3 to formulate variational integrators for finite-dimensional systems with generalized coordinates $q(t)$. Indeed, after discretizing the space variable (while keeping the time continuous) the *continuous* Lagrangian system becomes a *finite* dimensional dynamical system with generalized coordinates given by $\mathbf{q}(t) = (\cdots, X_a(t), x_a(t), \cdots)$. More precisely, the *semidiscrete* Lagrangian (2.68) can be rewritten as

$$S_{sd}(\mathbf{q}) = \int_{t_0}^{t_f}\left(\frac{1}{2}\dot{\mathbf{q}}_a m_{ab}(\mathbf{q})\dot{\mathbf{q}}_b - I_h(\mathbf{q})\right)dt$$

which is the class of Lagrangians studied in the first section of this chapter (Notice that the extended mass matrix is configuration-dependent). If for example, piecewise linear (continuous) interpolation (in time) is used for $q_a(t)$, i.e., for both $X_a(t)$ and $x_a(t)$ and if a single quadrature point for the time integral is used (as was assumed in §2.1.3, equation 2.11), then the following *discrete* action sum S_d is obtained

$$S_d\left(\cdots, X_a^k, x_a^k, X_a^{k+1}, x_a^{k+1}, \cdots\right) =$$
$$=\sum_{k=0}^{K}\left(\sum_{ab}\frac{1}{2}\left(\frac{X_a^{k+1}-X_a^k}{t^{k+1}-t^k},\frac{x_a^{k+1}-x_a^k}{t^{k+1}-t^k}\right)m_{ab}^{k+\alpha}\begin{pmatrix}\frac{X_a^{k+1}-X_a^k}{t^{k+1}-t^k}\\ \frac{x_a^{k+1}-x_a^k}{t^{k+1}-t^k}\end{pmatrix}-I_h\left(X_a^{k+\alpha},x_a^{k+\alpha}\right)\right)$$

with

$$m_{ab}^{k+\alpha} = m_{ab}\left((1-\alpha)\,\mathbf{q}^{k} + (\alpha)\,\mathbf{q}^{k+1}\right)$$

Invoking the stationarity of the previous with respect to all of its argument demands

$$\begin{aligned}\frac{\partial S_h}{\partial X_a^k}\left(\cdots, X_a^k, x_a^k, X_a^{k+1}, x_a^{k+1}, \cdots\right) &= 0\\ \frac{\partial S_h}{\partial x_a^k}\left(\cdots, X_a^k, x_a^k, X_a^{k+1}, x_a^{k+1}, \cdots\right) &= 0\end{aligned}$$

The previous represents a system of two equations for the unknowns $\mathbf{q}^{k+1} = \left(\cdots, X_a^{k+1}, x_a^{k+1}, \cdots\right)$ to be solved given the configuration at the preceding time $\mathbf{q}^{k} = \left(\cdots, X_a^{k}, x_a^{k}, \cdots\right)$ and represents therefore a time stepping algorithm for the integration of the semidiscrete system of equations (2.69).

2.2.13 Velocity interpolation

As was briefly mentioned in the previous subsection, an important difficulty that arises when we make use of the semidiscrete interpolation (2.65) is the problem of how to interpolate the material velocities $V = \dot{\varphi}$. The consistent approximation is obtained by differentiating the interpolation for the motion φ_h with respect to time, i.e., by choosing $V_h \equiv \dot{\varphi}_h$. This results in

$$\dot{\varphi}(X,t) \simeq \dot{\varphi}_h(X,t) = \sum_a \Big(N_a(X,t)\,\dot{x}_a(t) + \dot{N}_a(X,t)\,x_a(t)\Big)$$

which, as was proved in the previous section, for isoparametric elements reduces to

$$\dot{\varphi}(X,t) \simeq \dot{\varphi}_h(X,t) = \sum_a N_a(X,t)\Big(\dot{x}_a(t) - F_h(X,t)\,\dot{X}_a(t)\Big)$$

with

$$F_h = \sum_a \frac{\partial N_a}{\partial X}(X,t)\,x_a$$

Notice that the consistent velocity field will be discontinuous across element boundaries, since it is a function of the deformation gradient that in standard finite element interpolations is only elementwise continuous. Although this approximation looks natural and appealing (in fact it was initially adopted in the process of this investigation), our experience showed (as will be illustrated in Chapter 6) that it becomes very poor in many situations and leads to instability problems and meaningless solutions. To overcome this difficulty we propose the use of an *independent* velocity approximation of the form

$$V_h = \sum_a N_a(X,t)\,V_a(t)$$

that differs pointwise from the consistent velocity field, i.e., $V_h \neq \dot{\varphi}_h$ but approximates it *globally* or in a *weak sense*. This global approximation will be accomplished by making use of the *mixed* variational formulation presented in §2.2.4. that was precisely designed to allow for the use of independent interpolations for V_h and $\dot{\varphi}_h$. More precisely, and as we will show in detail in the following subsection, inserting independent interpolations for φ_h and V_h into the *mixed* action functional (2.38), a semidiscrete *mixed* action $S_{sd}^{mix}\left(X_a\left(t\right), x_a\left(t\right), V_a\left(t\right)\right)$ is obtained. This *mixed* functional will depend not only on referential and spatial coordinates $\left(X_a\left(t\right), x_a\left(t\right)\right)$ but also on the velocities parameters $V_a\left(t\right)$. Invoking the stationarity of this semidiscrete *mixed* action (see relations (2.39) and (2.40)) we will find differential equations to solve for the complete set of unknowns (X_a, x_a, V_a).

Figure 2.13 illustrates the difference between these two velocity interpolations. Assume we have a mesh with two elements. Figure 2.13(a) shows the interpolated displacement $u_h = \varphi_h - X$ at two different times t^k and t^{k+1}. Notice that both the displacements and the and mesh change from time k to time $k+1$. Figure 2.13(b) shows an approximation for the velocity obtained using a finite difference between the two consecutive displacement fields $V_h = \frac{\varphi^{k+1}-\varphi^k}{t^{k+1}-t^k}$. This approximation exhibit a kink inside an element and is difficult to handle. 2.13(c) shows the consistent velocity approximation $\dot{\varphi}_h$. Since the latter is a function of F_h, the approximated deformation gradient, and since F_h exhibits jumps across elements, then the consistent velocity itself will be discontinuous across elements. As was mentioned before, we have found that this is not a good approximation and brings instability problems. 2.13(d) shows the independent (inconsistent but continuous) approximation for the velocity. We will use this (continuous) approximation that differs pointwise from the (discontinuous) consistent velocity interpolation but approximates it in a global or averaged sense.

2.2.14 Semidiscrete *mixed* Interpolation

We consider then independent semidiscrete interpolations for the motion $\varphi\left(X,t\right)$ and the material velocity field $V\left(X,t\right)$ of the form

$$\varphi_h\left(X,t\right) = \sum_a N_a\left(X,t\right) x_a\left(t\right) \tag{2.70}$$

$$V_h\left(X,t\right) = \sum_a N_a\left(X,t\right) V_a\left(t\right) \tag{2.71}$$

where the shape functions $N_a\left(X,t\right)$ satisfy the isoparametric relation

$$N_a \circ X\left(\xi,t\right) = \hat{N}_a\left(\xi\right) \tag{2.72}$$

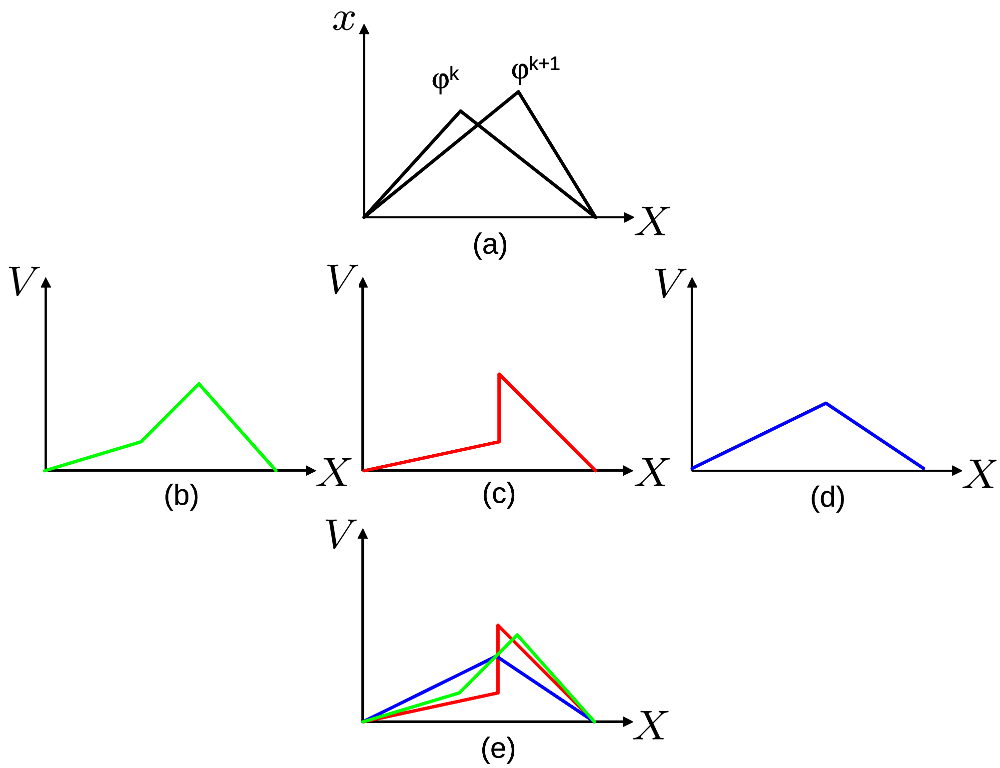

Figure 2.13: Possible approximations for the velocity field: (a) approximated displacement for two successive times t^k and t^{k+1}. (b) Finite-difference approximation for the velocity. (c) Consistent velocity approximation. (d) Independent velocity interpolation. (e) The three alternative velocity interpolations.

with $\hat{N}_a(\xi)$ the isoparametric shape functions referred to the standard domain $\xi \in [-1, 1]$, and $X(\xi, t)$ the isoparametric (time-dependent) mapping

$$X(\xi, t) = \sum_a \hat{N}_a(\xi) X_a(t)$$

The consistent velocity interpolation is given by

$$\dot{\varphi}_h = \sum_a N_a \left(\dot{x}_a - F_h \dot{X}_a \right) \tag{2.73}$$

where

$$F_h = \sum_a \frac{\partial N_a}{\partial X} x_a \tag{2.74}$$

is the (consistent) interpolation for the deformation gradient $F = D\varphi$. As was illustrated in the previous subsection, the consistent velocity field $\dot{\varphi}_h$ is discontinuous across element boundaries, the assumed (inconsistent) velocity interpolation V_h is continuous, and the two differ pointwise: $\dot{\varphi}_h(X, t) \neq V_h(X, t)$.

In this formulation we will regard as unknowns to the complete set $(X_a(t), x_a(t), V_a(t))$ and will make use of the *mixed* Hamilton's principle (2.36, 2.37) to find the differential equations for the evolution of these unknowns. A *semidiscrete-mixed action functional* $S_{sd}(X_a(t), x_a(t), V_a(t))$ will be built by inserting the mixed interpolation into the mixed action (2.35). The differential equations for $(X_a(t), x_a(t), V_a(t))$ will follow then by invoking the stationarity of the semidiscrete-mixed action with respect to each of its arguments. As happened in the static, space-time and semidiscrete (with consistent velocities) cases, the Euler-Lagrange equations corresponding to the stationarity of the action functional with respect to x_a and X_a will correspond, respectively, to the equations of balance of nodal mechanical forces and nodal configurational forces. In addition, the Euler-Lagrange equation corresponding to the stationarity of S_{sd} with respect to V_a will correspond to the weak statement of the compatibility equation between the assumed V_h and consistent $\dot{\varphi}_h$ velocity interpolations. The Euler-Lagrange equations will then be discretized in time using a *mixed* variational integrator of the class studied in §2.1.7.

2.2.15 Semidiscrete *mixed* action and discrete *mixed* action sum

Following the program just outlined, we proceed to discretize first in space the mixed action $S[\varphi, V]$ (2.38) with *independent* interpolations for φ and V to obtain a *semidiscrete-mixed action* functional $S_{sd}(X_a(t), x_a(t), V_a(t))$. We next discretize the latter in time to obtain a *discrete-mixed action sum* S_h using a *mixed* variational integrator. We recall that for Lagrangian densities of the form (2.23), the mixed (two-field) action functional is given by

$$S[\varphi, V] = \int_{t_0}^{t_f} \int_B L^{mix}(X, t, \varphi, D\varphi, V, \dot{\varphi})\, dX dt$$

with

$$L^{mix}(X, t, \varphi, F, V, \dot{\varphi}) = \frac{R}{2} V^2 - W(X, t, \varphi, F) + RV(\dot{\varphi} - V)$$

Inserting the semidiscrete-mixed interpolation (2.70, 2.71) with consistent velocity and deformation gradient interpolations (2.73, 2.74) we obtain the semidiscrete-mixed action in the form

$$\begin{aligned} S_{sd}(X_a(t), x_a(t), V_a(t)) &= S[\varphi_h, V_h] = \\ &= \int_{t_0}^{t_f} \int_B \left(\frac{R}{2} \left(\sum_a N_a V_a \right)^2 - W\left(X, t, \sum_a N_a x_a, \sum_a \frac{\partial N_a}{\partial X} x_a \right) \right. \\ &\quad \left. + \sum_{ab} R V_a N_a N_b \left(\dot{x}_b - F_h \dot{X}_b - V_b \right) \right) dX dt \end{aligned}$$

The previous may be compactly rewritten as

$$S_{sd}\left(\cdots, X_a, x_a, V_a, \cdots\right) = \int_{t_0}^{t_f} \left(\frac{1}{2} V_a m_{ab} V_b - I_h\left(X_a, x_a\right) + V_a \left(m_{ab}\left(\dot{x}_b - V_b\right) + M_{ab}\dot{X}_b \right) \right) dt \tag{2.75}$$

where m_{ab} and M_{ab} are the mass matrices

$$\begin{pmatrix} M_{ab} \\ m_{ab} \end{pmatrix} = \int_B R N_a N_b \begin{pmatrix} -F_h \\ 1 \end{pmatrix} dX$$

and I_h is the discrete potential energy given as in the static case as

$$I_h = -\int_B W\left(X, t, \sum_a N_a x_a\left(t\right), \sum_a \frac{\partial N_a}{\partial X} x_a\left(t\right) \right) dX$$

or, using the notation $\mathbf{q} = \left(\cdots, X_a, x_a, \cdots\right)$, $\mathbf{V} = \left(\cdots, V_a, \cdots\right)$ as

$$S_{sd}\left(\mathbf{q}, \mathbf{V}\right) = \int_{t_0}^{t_f} \left(\frac{1}{2} V_a m_{ab}\left(\mathbf{q}\right) V_b - I_h\left(\mathbf{q}\right) + V_a\left(\left(M_{ab}, m_{ab}\right)\mathbf{q}_b - m_{ab}V_b\right) \right) dt$$

The semidiscrete-mixed action (2.75) might be contrasted with the semidiscrete (standard) action (2.68) obtained when a consistent interpolation $\dot{\varphi}_h$ instead an independent assumed interpolation V_h is used to approximate velocities.

Invoking next the stationarity of the semidiscrete *mixed* action functional with respect to all of its arguments $\left(X_a\left(t\right), x_a\left(t\right), V_a\left(t\right)\right)$ implies

$$\begin{aligned} \langle \delta S_{sd}, \delta X_a \rangle &= 0 \\ \langle \delta S_{sd}, \delta x_a \rangle &= 0 \\ \langle \delta S_{sd}, \delta V_a \rangle &= 0 \end{aligned}$$

Variations of the semidiscrete action S_{sd} with respect to $x_a\left(t\right)$ yield

$$\langle \delta S_{sd}, \delta x_a \rangle = \int_{t_0}^{t_f} \int_B \left(R V_h N_b \left(\delta \dot{x}_b - \left(\tfrac{\partial N_c}{\partial X} \delta x_c \right) \dot{X}_b \right) - P_h \tfrac{\partial N_c}{\partial X} + B N_a \right) dX dt$$

The variations with respect to $X_a\left(t\right)$ are given by

$$\langle \delta S_{sd}, \delta X_a \rangle = \int_{t_0}^{t_f} \int_B \left(R V_h N_b \left(-F_h\right) \left(\delta \dot{X}_b - \left(\tfrac{\partial N_c}{\partial X} \delta X_c \right) \dot{X}_b \right) - C_h^{mix} \tfrac{\partial N_a}{\partial X} + B_h^{mix} N_a \right) dX dt$$

where

$$\begin{aligned} C_h^{mix} &= \left(W_h - \frac{RV_h^2}{2} - RV_h \left(\dot{\varphi}_h - V_h \right) \right) - F_h P_h \\ B_h^{mix} &= \frac{\partial B}{\partial X} + \frac{\partial R}{\partial X} \frac{V_h^2}{2} + \frac{\partial R}{\partial X} V_h \left(\dot{\varphi}_h - V_h \right) \end{aligned}$$

is the (semi)discrete (mixed) Eshelby stress tensor. Finally, variations of the semidiscrete action with respect to V_h yield

$$\int_{t_0}^{t_f} \int_B R \delta V_a N_a N_b \left(\dot{x}_b - F_h \dot{X}_b - V_b \right) = 0$$

The corresponding Euler-Lagrange equations might be written as

$$\begin{aligned} \begin{pmatrix} 0 \\ 0 \end{pmatrix} &= \frac{d}{dt} \left(m_{ab} V_b \right) \\ &\quad - \begin{pmatrix} \frac{\partial}{\partial X_a} \\ \frac{\partial}{\partial x_a} \end{pmatrix} \left(\frac{1}{2} V_a m_{ab} V_b - I_h \left(X_a, x_a \right) + V_a \left(m_{ab} \left(\dot{x}_b - V_b \right) + M_{ab} \dot{X}_b \right) \right) \quad (2.76) \\ 0 &= m_{ab} \dot{x}_b + M_{ab} \dot{X}_b - m_{ab} V_b \quad (2.77) \end{aligned}$$

which represent a system of three differential equations for the joint unknown $(X_a(t), x_a(t), V_a(t))$ (compare with the system (2.69)).

We finally establish an appropriate time integrator to discretize (in time) the previous system of ordinary differential equations. This is accomplished by making use of the *mixed* variational integrators studied in §2.1.7. Recall that these integrators are built by discretizing in time the curves $X_a(t)$ $x_a(t)$ and $V_a(t)$ using suitable (time) interpolation spaces (not necessarily coincident) to build a *discrete-mixed action sum* S_d. Following the example of §2.1.7 (see equations (2.16) and (2.17)) we use piecewise linear time interpolation for nodal referential and spatial trajectories

$$\begin{aligned} X_a(t) &= (1-\alpha) X_a^k + (\alpha) X_a^{k+1} \\ x_a(t) &= (1-\alpha) x_a^k + (\alpha) x_a^{k+1} \end{aligned}$$

and piecewise constant interpolation for nodal velocity parameters

$$V_a(t) = V_a^{k+\beta} = const$$

Inserting this interpolation in the semidiscrete-mixed action (2.75) and integrating the resulting time integral with a single quadrature point located at $t^{k+\alpha}$, the following discrete-mixed action sum is obtained:

$$S_d\left(\cdots, X_a^k, x_a^k, V_a^{k+\beta}, \cdots\right) = \sum_{k=0}^{K} L_d^{mix}\left(X^k, X^{k+1}, x^k, x^{k+1}, V^{k+\beta}, t^k, t^{k+1}\right)$$

with

$$\begin{aligned} L_d^{mix} &= \left(t^{k+1} - t^k\right)\left(\frac{1}{2}V_a^{k+\beta} m_{ab}^{k+\alpha} V_b^{k+\beta} - I_h^{k+\alpha} + \right. \\ &\left. + V_a^{k+\beta}\left(m_{ab}^{k+\alpha}\left(\frac{x_b^{k+1} - x_b^k}{t^{k+1} - t^k} - V_b^{k+\beta}\right) + M_{ab}^{k+\alpha}\frac{X_b^{k+1} - X_b^k}{t^{k+1} - t^k}\right)\right) \end{aligned}$$

The integration of the semidiscrete system of equations (2.76, 2.77) follows then by invoking the stationarity of the previous discrete-mixed action with respect to all of its arguments.

$$\begin{aligned} \frac{\partial S_d}{\partial X_a^k} &= 0 \\ \frac{\partial S_d}{\partial x_a^k} &= 0 \\ \frac{\partial S_d}{\partial V_a^{k+\beta}} &= 0 \end{aligned}$$

The previous represent a non-linear system of equations for the determination of $\left(X_a^{k+1}, x_a^{k+1}, V_a^{k+\beta}\right)$ given $\left(X_a^k, x_a^k, V_a^{k-1+\beta}\right)$ and defines therefore a time stepping algorithm.

2.3 Concluding remarks

We have presented in this chapter the salient features of the variational methods developed in this thesis. The main objective is to formulate a mesh adaption framework for non-linear solid dynamic applications for which the *mesh itself is taken as unknown*. We then conjecture that *this unknown might be found using the same variational principle that governs the evolution of the main unknown* (the motion of the body under study), namely Hamilton's principle. The discretized action functional S_d is therefore rendered stationary with respect to all the parameters that define the discretization, namely, nodal spatial coordinates $\mathbf{x}_h$, and nodal space-time referential placements $(\mathbf{X}_h, \mathbf{t}_h)$. After the theoretical conceptualization of this space-time approach it was observed that effecting space and time adaption simultaneously was too costly since the time unknown was involved in the resulting equations in a highly non-linear way. It was thus suggested to pursue only variational space adaption while providing the discrete time steps from the outset. This led to the development of the particular class of space-time meshes with *homogeneous time steps*, i.e., the same time step is chosen everywhere in the (spatial) mesh. We have proved that for this particular space-time finite element interpolation the time parametrization might be eliminated at the element level and all the machinery required to formulate general space-time finite elements, i.e., space-time isoparametric mappings and Jacobians, becomes thus unnecessary. We might simplify notably the formulation, implementation, and analysis by *performing the space-time discretization in two separated stages*, a semidiscrete (in space) initial stage where the space is discretized keeping the time continuous and leading to the construction of a semidiscrete action S_{sd} and Lagrangian L_{sd}, and a second time integration stage where a discrete action S_d and discrete Lagrangian L_d are built by discretizing the semidiscrete action S_{sd} and semidiscrete Lagrangian L_{sd} in time. Since the time is kept continuous and homogeneous during the first stage, *a space-space*, as opposed to a space-time, picture becomes more appropriate. Within this space-space framework, nodal referential and spatial coordinates $\mathbf{X}_h$ and $\mathbf{x}_h$ are reinterpreted as horizontal and vertical components of a position vector $\mathbf{q}_h = (\mathbf{X}_h, \mathbf{x}_h)$ in a higher dimensional space, the space-space bundle. When both nodal referential coordinates $\mathbf{X}_h$ and spatial coordinates $\mathbf{x}_h$ are assumed to evolve continuously in time, particular care must be taken in the *velocity interpolation*. It was proved that the natural (or *consistent*) interpolation for the velocity is given by $\dot{\boldsymbol{\varphi}}_h = \sum_a N_a \left(\dot{\mathbf{x}}_a - F_h \dot{\mathbf{X}}_a \right)$ which is *discontinuous* across element boundaries because of its dependence on $\mathbf{F}_h$. If this interpolation is used to approximate velocities, then very poor solutions are obtained. To overcome this problem, we proposed to use an independent, or *assumed* velocity interpolation $\mathbf{V}_h = \sum_a N_a \mathbf{V}_a$, which as opposed to the consistent velocity interpolation, is *continuous* across elements. This implies that we are required to accommodate for the use of a continuous velocity interpolation that differs pointwise with the consistent (and discontinuous) velocity field, namely $\mathbf{V}_h \neq \dot{\boldsymbol{\varphi}}_h$. Motivated by the well-known De-Beuveke-Hu-Washizu mixed variational principle for statics that allows for independent interpolations for deformation gradient $\mathbf{F}_h$, and deformation mapping $\boldsymbol{\varphi}_h$, and for which the (space) compatibility condition $\mathbf{F}_h = D\boldsymbol{\varphi}_h$ is imposed by recourse of a Lagrange multiplier $\mathbf{P}_h$ we formulate the analogous version for dynamics by replacing space by time. More precisely, we formulate a mixed variational principle for dynamics (the mixed Hamilton's principle) that allows for independent interpolations of velocities $\mathbf{V}_h$ and deformations $\boldsymbol{\varphi}_h$ and for which the (time) compatibility condition $\mathbf{V}_h = \dot{\boldsymbol{\varphi}}_h$ is imposed by means of a Lagrange multiplier $\mathbf{p}_h$. Using independent (semidiscrete) interpolations for velocities and deformations, we arrive at the construction of a *mixed semidiscrete action* S_h *and mixed semidiscrete Lagrangian* L_h^{mix} with two independent unknown variables, configurations $\mathbf{q}_h$ and velocities $\mathbf{V}_h$. Appropriate time integration of their corresponding Euler-Lagrange equations might be accomplished by making use of a new family of time integrators, the so-called mixed variational integrators, that allow for the use of *independent time interpolations* of both variables and possible independent (or selective) quadrature rules.

In the following we proceed to develop this formulation in the more general setting of three-dimensional elasticity with possibly viscous, thermal, and inelastic processes.

Chapter 3

Configurational forces in elastic materials with viscosity

In this chapter we study different aspects of the theory of configurational forces. We begin by presenting the Lagrangian formulation of dynamics in the context of non-linear elasticity and the Lagrange-d'Alembert principle to account for viscous behavior. Hamilton's principle is then rephrased in a more general way to render simultaneously the equations of motion and the equations of balance of configurational forces. We review and further develop the geometrical interpretation of this variational framework for which the motion is regarded as a time-dependent family of sections evolving in the higher dimensional space, the space-space bundle. We also develop an extended version of Lagrange-d'Alembert principle that accounts properly for viscous effects both in the spatial (vertical) and material (horizontal) manifolds. In this chapter we focus on isothermal hyperelastic materials with viscosity. Temperature and internal process will be studied in the next chapter.

3.1 Lagrangian formulation of elastodynamics

We consider a body occupying at some arbitrary reference time a region B of ambient space $\mathbb{R}^n$. The set $B \subset \mathbb{R}^n$ is the reference (material or undeformed) configuration of the body. We will use the usual convention of labeling material particles of the body by their position in the reference configuration B. Let $\boldsymbol{\varphi} : B \times I \rightarrow \mathbb{R}^n$ be a smooth motion over the time interval $I = [t_0, t_f] \subset \mathbb{R}$. The set $B_t = \boldsymbol{\varphi}(B, t) \subset \mathbb{R}^n$ is the deformed (spatial or current) configuration of the body at time t and the sets $B_0 = \boldsymbol{\varphi}(B, t_0)$ and $B_f = \boldsymbol{\varphi}(B, t_f)$ are the initial and final configurations, not necessarily coincident with the reference configuration B. For a fixed time t the motion $\boldsymbol{\varphi}$ maps material particles $\mathbf{X} \in B$ in the reference configuration with their position $\mathbf{x} = \boldsymbol{\varphi}(\mathbf{X}, t)$ in the deformed configuration at time t. In Cartesian coordinates we shall write

$$x_i = \varphi_i \left(X_I, t \right)$$

Here and in what follows we will use upper (respectively, lower) case indices to denote components of vector and tensor fields over the reference (respectively, deformed) configuration. The deformation gradient and material velocity fields are given by

$$\begin{aligned} \mathbf{F} &= D\boldsymbol{\varphi} \left(\mathbf{X}, t \right) \\ \mathbf{V} &= \dot{\boldsymbol{\varphi}} \left(\mathbf{X}, t \right) \end{aligned}$$

where $D\varphi$ and $\dot{\varphi}$ denote, respectively, differentiation with respect to $\mathbf{X}$ and t. The Jacobian of the deformation is given by

$$J = \det \left(\mathbf{F} \right)$$

In Cartesian components we shall write

$$\begin{aligned} F_{iJ} &= \frac{\partial \varphi_i}{\partial X_I} \\ V_i &= \frac{\partial \varphi_i}{\partial t} \end{aligned}$$

We will consider in this section a (possibly inhomogeneous) non-linear hyperelastic material, i.e., a material for which the constitutive behavior can be described with a Helmholtz free energy density per unit of undeformed volume of the form

$$A \left(\mathbf{X}, \mathbf{F} \right)$$

such that the constitutive relation takes the form

$$P_{iJ} = \frac{\partial A}{\partial F_{iJ}}$$

where $\mathbf{P}$ is the first Piola-Kirchhoff stress tensor. It should be noticed that to account for the inhomogeneity of the material, the free energy is assumed to depend explicitly on $\mathbf{X}$ along with its implicit dependence through $\mathbf{F} \left(\mathbf{X}, t \right)$. In this section we will assume that the free energy is independent of temperature (isothermal hyperelasticity).

For every material particle $\mathbf{X} \in B$ the total potential energy $\mathbf{W}$ may be defined as

$$W \left(\mathbf{X}, t, \boldsymbol{\varphi}, \mathbf{F} \right) = A \left(\mathbf{X}, \mathbf{F} \right) - \mathbf{B} \left(\mathbf{X}, t \right) \boldsymbol{\varphi}$$

where $\mathbf{B}$ is the body force density per unit mass (possibly dependent on $\mathbf{X}$ and t). It follows from this definition that

$$P_{iJ} = \frac{\partial W}{\partial F_{iJ}} \tag{3.1}$$

$$B_i = -\frac{\partial W}{\partial \varphi_i} \tag{3.2}$$

To formulate an initial-boundary-value problem we assume that the boundary ∂B of B can be divided disjointly in two parts, the traction part ∂B_1 and the Dirichlet or deformation part ∂B_2:

$$\begin{aligned} \partial B &= \partial B_1 \cup \partial B_2 \\ \emptyset &= \partial B_1 \cap \partial B_2 \end{aligned}$$

and that the motion $\boldsymbol{\varphi}$ must satisfy the following boundary conditions:

$$\begin{aligned} P_{iJ} N_J &= \bar{T}_i \qquad \text{on } \partial B_1 \text{ and } \forall t \in I \\ \varphi_i &= \bar{\varphi}_i \qquad \text{on } \partial B_2 \text{ and } \forall t \in I \end{aligned}$$

where N_J is the outer unit normal to the boundary of the reference configuration B and $\bar{\mathbf{T}}$ and $\bar{\boldsymbol{\varphi}}$ are the applied tractions and prescribed deformation mapping. To simplify the exposition, we will consider zero deformation and traction boundary conditions, i.e., $\bar{\varphi}_i = 0$ and $\bar{T}_i = 0$. Also the motion must satisfy the following initial conditions:

$$\begin{aligned} \boldsymbol{\varphi} &= \boldsymbol{\varphi}_0(\mathbf{X}) \qquad \text{at } t = t_0 \text{ and } \forall \mathbf{X} \in B \\ \mathbf{V} &= \mathbf{V}_0(\mathbf{X}) \qquad \text{at } t = t_0 \text{ and } \forall \mathbf{X} \in B \end{aligned}$$

where $\boldsymbol{\varphi}_0(\mathbf{X})$ is the initial deformation mapping and $\mathbf{V}_0(\mathbf{X})$ is the initial material velocities. The initial configuration is then given by $B_0 = \boldsymbol{\varphi}(B, t_0) = \boldsymbol{\varphi}_0(B)$.

Within the framework of the Lagrangian field theory [34], we regard the body B undergoing a spatial motion as a Lagrangian system whose Lagrangian is defined in terms of a density. For elastic materials the Lagrangian density may be defined as

$$\mathcal{L}(\mathbf{X}, t, \boldsymbol{\varphi}, \mathbf{V}, \mathbf{F}) = \frac{1}{2} R \|\mathbf{V}\|^2 - W(\mathbf{X}, t, \boldsymbol{\varphi}, \mathbf{F}) \tag{3.3}$$

where R is the mass density per unit of undeformed volume (also assumed to depend possibly on

X). The action functional follows as

$$S[\boldsymbol{\varphi}] = \int_{t_0}^{t_f} \int_B \mathcal{L}(\mathbf{X}, t, \boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}, D\boldsymbol{\varphi})\, dV dt \tag{3.4}$$

or, using definition (3.3), as

$$S[\boldsymbol{\varphi}] = \int_{t_0}^{t_f} \int_B \left(\frac{1}{2} R \|\dot{\boldsymbol{\varphi}}\|^2 - W(\mathbf{X}, t, \boldsymbol{\varphi}, D\boldsymbol{\varphi})\right) dV dt \tag{3.5}$$

The corresponding variations with respect to the argument $\boldsymbol{\varphi}$ are

$$\langle \delta S, \delta\varphi_i \rangle = \int_{t_0}^{t_f} \int_B \left(\frac{\partial \mathcal{L}}{\partial \varphi_i} \delta\varphi_i + \frac{\partial \mathcal{L}}{\partial V_i} \delta\dot{\varphi}_i + \frac{\partial \mathcal{L}}{\partial F_{iJ}} \delta\varphi_{i,J}\right) dV dt \tag{3.6}$$

that upon integration by parts in time for the first term and in space for the second term yield[1]

$$\begin{aligned} \langle \delta S, \delta\varphi_i \rangle \quad &= \quad \int_{t_0}^{t_f} \int_B \left(\frac{\partial \mathcal{L}}{\partial \varphi_i} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial V_i} - \frac{d}{dX_J}\frac{\partial \mathcal{L}}{\partial F_{iJ}}\right) \delta\varphi_i dV dt + \\ &+ \left(\int_B \frac{\partial \mathcal{L}}{\partial V_i} \delta\varphi_i dV\right)_{t_o}^{t_f} + \int_{t_0}^{t_f} \int_{\partial B} \left(\delta\varphi_i \frac{\partial \mathcal{L}}{\partial F_{iJ}} N_J\right) dS dt \end{aligned} \tag{3.7}$$

Hamilton's principle postulates that the actual motion $\boldsymbol{\varphi}(X, t)$ of the body from its initial configuration B_0 at time t_0 to its final configuration at time t_f corresponds to that motion that renders the action functional S stationary with respect to all admissible variations, i.e., variations $\delta\boldsymbol{\varphi}$ vanishing at the initial and final times and satisfying the essential boundary conditions on ∂B_2. This may be written in the form

$$\langle \delta S, \delta\boldsymbol{\varphi} \rangle = 0$$

[1] Here, and in what follows, the notations $\frac{d}{dX}$ and $\frac{d}{dt}$ shouldn't be confused with the standard notation $\frac{\partial}{\partial X}$ and $\frac{\partial}{\partial t}$ for partial differentiation. We recall that we are considering the possibility of inhomogeneities that are taken into account by assuming an explicit dependence of W (and hence on $\mathcal{L}$ and $\frac{\partial \mathcal{L}}{\partial F_{iJ}}$) on the position X_I along with its implicit dependence through F_{iJ} and φ_i. We also assume an explicit dependence on time. For functions that exhibit such an explicit/implicit dependence we will use the notation $\frac{d}{dX_J}$ (respectively $\frac{d}{dt}$) for the derivative with respect to the total (explicit and implicit) dependence on X_J (resp. t) while the notation $\frac{\partial}{\partial X_J}$ (or alternatively $\frac{\partial}{\partial X_J}\Big|_{\exp}$ (resp. $\frac{\partial}{\partial t}\Big|_{\exp}$)) will be restricted to the derivative with respect to the explicit dependence. More precisely if $W = W(X_I, t, \varphi_i, F_{iJ})$ then

$$\begin{aligned} \frac{dW}{dX_I} \quad &= \quad \frac{\partial W}{\partial X_I} + \frac{\partial W}{\partial \varphi_i}\frac{\partial \varphi_i}{\partial X_I} + \frac{\partial W}{\partial F_{iJ}}\frac{\partial F_{iJ}}{\partial X_I} \\ \frac{\partial W}{\partial X_I} \quad &= \quad \frac{\partial W}{\partial X_I}\Big|_{\exp} = \frac{\partial W}{\partial X_I}\Big|_{\varphi_i, F_{iJ}} \end{aligned}$$

Consistently we will use the notation $\frac{d}{dt}$ and $\frac{\partial}{\partial t}$ for the total and explicit dependence on time. Then

$$\begin{aligned} \frac{dW}{dt} \quad &= \quad \frac{\partial W}{\partial \varphi_i}\frac{\partial \varphi_i}{\partial t} + \frac{\partial W}{\partial F_{iJ}}\frac{\partial F_{iJ}}{\partial t} \\ \frac{\partial W}{\partial t} \quad &= \quad \frac{\partial W}{\partial t}\Big|_{\exp} = \frac{\partial W}{\partial X_I}\Big|_{\varphi_i, F_{iJ}} \end{aligned}$$

for every admissible variation $\delta\boldsymbol{\varphi}$. Under appropriate smoothness conditions on the integrand in (3.7) this implies the well-known Euler-Lagrange equations

$$\frac{\partial \mathcal{L}}{\partial \varphi_i} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial V_i} - \frac{d}{dX_J}\frac{\partial \mathcal{L}}{\partial F_{iJ}} = 0 \qquad \text{in } B \text{ and } \forall t \in I \tag{3.8}$$

along with the traction boundary conditions

$$\frac{\partial \mathcal{L}}{\partial F_{iJ}} N_J = 0 \qquad \text{in } \partial B_1 \text{ and } \forall t \in I \tag{3.9}$$

On account of (3.1), (3.2) and (3.3), equation (3.7) gives

$$\begin{aligned} \langle \delta S, \delta\varphi_i \rangle \quad = \quad & \int_{t_0}^{t_f} \int_B \left(B_i - \frac{d}{dt}\left(R\dot{\varphi}_i\right) + \frac{dP_{iJ}}{dX_J} \right) \delta\varphi_i dV dt + \\ & + \int_B R\dot{\varphi}_i \delta\varphi_i dV \Big|_{t_o}^{t_f} - \int_{t_0}^{t_f} \int_{\partial B} \left(-\delta\varphi_i P_{iJ} N_J\right) dS dt \end{aligned}$$

and the Euler-Lagrange equations (3.8) and boundary conditions (3.9) reduce to

$$B_i - \frac{d}{dt}\left(R\dot{\varphi}_i\right) + \frac{dP_{iJ}}{dX_J} = 0 \qquad \text{in } B \text{ and } \forall t \in I \tag{3.10}$$

$$-P_{iJ}N_J = 0 \qquad \text{in } \partial B_1 \text{ and } \forall t \in I$$

or, written in invariant notation, to

$$\mathbf{B} - \frac{d}{dt}\left(R\dot{\boldsymbol{\varphi}}\right) + \mathrm{DIV}\left(\mathbf{P}\right) = \mathbf{0} \tag{3.11}$$

$$-\mathbf{PN} = \mathbf{0}$$

that corresponds to the equations of motion.

3.2 Viscosity and Lagrange-d'Alembert principle

We shall also consider elastic materials exhibiting viscous effects, i.e., materials for which the total state of stress depends not only on $\mathbf{F}$ but also on the rate of deformation $\dot{\mathbf{F}}$ in the form

$$\mathbf{P} = \mathbf{P}^e\left(\mathbf{F}\right) + \mathbf{P}^v\left(\mathbf{F}, \dot{\mathbf{F}}\right)$$

where $\mathbf{P}^e\left(\mathbf{F}\right)$ is the equilibrium or elastic part of the stress given by

$$\mathbf{P}^e = -\frac{\partial \mathcal{L}}{\partial \mathbf{F}} = \frac{\partial W}{\partial \mathbf{F}}$$

and $\mathbf{P}^v\left(\mathbf{F},\dot{\mathbf{F}}\right)$ is the viscous stress. We shall study in particular Newtonian viscosity for which the viscous stress is assumed to be of the form

$$\mathbf{P}^v\left(\mathbf{F},\dot{\mathbf{F}}\right) = J\boldsymbol{\sigma}^v\mathbf{F}^{-T} \tag{3.12}$$

where σ^v is the Cauchy viscous stress given by

$$\boldsymbol{\sigma}^v = 2\mu\,\mathrm{sym}\left(\dot{\mathbf{F}}\mathbf{F}^{-1}\right)^{\mathrm{dev}} \tag{3.13}$$

with μ the (shear) viscosity, $\mathbf{d} = \dot{\mathbf{F}}\mathbf{F}^{-1}$ the rate of deformation spatial tensor and sym and dev the symmetric and deviatoric operators, namely,

$$\begin{aligned} \mathrm{sym}\left(\mathbf{d}\right) &= \frac{1}{2}\left(\mathbf{d}+\mathbf{d}^T\right) \\ \mathbf{d}^{\mathrm{dev}} &= \mathbf{d} - \frac{\mathrm{tr}\left(\mathbf{d}\right)}{3}\mathbf{i} \end{aligned}$$

In the presence of viscosity the equations of motion (3.11) with their corresponding boundary conditions (3.9) become

$$\mathbf{B} - R\ddot{\boldsymbol{\varphi}} + \mathrm{DIV}\left(\mathbf{P}^e + \mathbf{P}^v\right) = \mathbf{0} \qquad \text{in } B \text{ and } \forall t \in I \tag{3.14}$$

$$-\left(\mathbf{P}^e + \mathbf{P}^v\right)\mathbf{N} = \mathbf{0} \qquad \text{in } \partial B_1 \text{ and } \forall t \in I$$

that for systems with a Lagrangian density of the form (3.3) may be rewritten as

$$\frac{\partial L}{\partial \boldsymbol{\varphi}} - \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \mathbf{V}}\right) - \mathrm{DIV}\left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right) + \mathrm{DIV}\left(\mathbf{P}^v\right) = \mathbf{0} \qquad \text{in } B \text{ and } \forall t \in I \tag{3.15}$$

$$\left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}} - \mathbf{P}^v\right)\mathbf{N} = \mathbf{0} \qquad \text{in } \partial B_1 \text{ and } \forall t \in I$$

We notice next that unlike in the case of elastic materials, these equations cannot be obtained directly from Hamilton's principle. They may be established instead from the *Lagrange-d'Alembert* principle, namely,

$$\begin{aligned} &\langle \delta S, \delta\boldsymbol{\varphi}\rangle + \int_{t_0}^{t_f}\int_B \left(\delta\boldsymbol{\varphi}\,\mathrm{DIV}\left(\mathbf{P}^v\right)\right) dV\,dt \\ &+ \int_{t_0}^{t_f}\int_{\partial B_1} \left(\delta\boldsymbol{\varphi}\left(-\mathbf{P}^v\right)\mathbf{N}\right) dS dt = \mathbf{0} \end{aligned}$$

where S is the action and $\langle \delta S, \delta\boldsymbol{\varphi}\rangle$ are its corresponding variation. Integrating by parts the viscosity terms and making use of the divergence theorem the Lagrange-d'Alembert principle reads

$$\langle \delta S, \delta \boldsymbol{\varphi} \rangle - \int_{t_0}^{t_f} \int_B \left(\mathbf{P}^v \cdot \frac{\partial \delta \varphi}{\partial \mathbf{X}} \right) dV dt = \mathbf{0} \tag{3.16}$$

or, in Cartesian coordinates,

$$\langle \delta S, \delta \boldsymbol{\varphi}_i \rangle - \int_{t_0}^{t_f} \int_B \left(P^v_{iJ} \frac{\partial \delta \varphi_i}{\partial X_J} \right) dV dt = 0$$

3.3 Elastic configurational forces and configurational force balance

Configurational forces, also known as material forces, arise in applications involving the evolution of defects within the material. As opposed to standard (Newtonian or mechanical) forces that drive the motion of material particles in space, configurational forces drive the motion of entities that migrate relative to the material. Examples include dislocations, cracks, inclusions, voids, vacancies, or evolving interfaces.

The concept was introduced in the context of elasticity and continuum mechanics by Eshelby [6],[7]. Since then several approaches have been proposed to elucidate their true nature and to formulate the equations of configurational force balance. Without claiming completeness we mention 1) the "pull-back" approach ([40], [41], [42], [43]) in which configurational force balance is regarded as the projection (pull-back) of the mechanical force balance equations onto the material manifold and configurational forces are related to the concept of material uniformity and homogeneity (as defined in [51] or [58]) as the forces behind continuous distribution of inhomogeneities ([4], [5], [8], [39], [46]). 2) the "basic primitive objects" approach of Gurtin ([2], [15], [16], [18]), where configurational forces are postulated as primitive physical entities, independent of mechanical forces, and their balance is derived using invariance arguments. 3) the "Noether's theorem" approach ([23], [29], [31], [34]), where conservation (lack of conservation) of configurational forces arises as the conservation law associated to material translational symmetry (lack of symmetry) of the Lagrangian density, 4) the "inverse motion" approach ([38], [40], [53], [56]) for which the equations of balance of configurational forces follow from the stationarity of the energy (or action) functional with respect to the reference configuration keeping the current configuration fixed, and 5) very closely related to the previous two, what we refer to as the "variational approach" ([24], [26], [29], [30], [31]) where, in addition to the reference (or material) configuration B and the deformed (or spatial) configuration B_t, a new configuration is introduced (the "parameter configuration" D) as a fixed reference for the motion of defects with respect to the material manifold, in analogy to the material configuration that acts as a reference for the motion of material particles in space. The equations of balance of configurational forces follow then as those energetically conjugate to variations with respect to the material configuration B keeping fixed the new reference D.

The "variational approach" admits an important geometrical interpretation originally suggested in [29], [30]: The deformation mapping $\boldsymbol{\varphi} : B \to R^n$ may be reinterpreted as a section $(\mathbf{X}, \boldsymbol{\varphi}(\mathbf{X}))$ of the configuration bundle $B \times R^n$ that may be conceptually represented in two axes, the horizontal axis for the reference configuration B and the vertical axis for the space R^n. Variations of the energy functional with respect to the deformed configuration B_t, keeping the reference configuration B fixed, can be interpreted as *vertical* variations, while variations of the reference configuration B keeping the deformed configuration B_t fixed may be regarded as *horizontal* variations. Hence mechanical and configurational forces may be described as those forces associated to vertical and horizontal variations of the energy (or action) functional.

In this work we will follow the variational approach, with a formulation similar to that of [29], [30], [31], but using a "space-space" (as opposed to a "space-time-space") configuration bundle, i.e., using the body B (instead of the space-time body $B \times [t_0, t_f]$) as the base for the bundle. We will extend the geometrical interpretation by regarding the motion $\boldsymbol{\varphi}(\mathbf{X}, t)$ as a family of sections of the space-space bundle parametrized by time, analyzing "normal" and "tangential" variations (in addition to horizontal and vertical variations) and reexpressing the joint system of configurational and mechanical force balance as a single equation for the evolution of the time-dependent section $(\mathbf{X}, \boldsymbol{\varphi}(\mathbf{X}, t))$ in the space-space bundle. The resulting system of equations will exhibit a structure that will be preserved in the discrete setting.

3.3.1 Defect motion and Defect reference configuration

In his original papers on configurational forces [6], [7], Eshelby considered solids with "defects or imperfections capable of altering their configuration in a crystal" and observed that the total energy of the body will be function not only of the applied external forces but of the "set of parameters required to specify the configuration of the defects." Therefore he defined "force on the defect" as the negative gradient (or variation) of the total energy with respect to the position of the imperfections.

With this picture in mind we shall consider a continuous body B with *defects* undergoing two simultaneous and independent kinematic processes: the motion of material particles with respect to the ambient space $\mathbb{R}^n$ and the motion of "defects" within the material. We will refer to the first motion as the *material motion* or *mechanical motion*, and to the second as the *defect motion* or *defect rearrangement*.

In the mathematical description of the material motion, the body is identified with its reference configuration B, and the (material) motion is defined as a time-dependent family of smooth mappings $\boldsymbol{\varphi} : B \to \mathbb{R}^n$ from the reference configuration $B \subseteq \mathbb{R}^n$ onto space $\mathbb{R}^n$. Analogously we may describe the "defect motion" by introducing a "reference configuration for the defect rearrangement" $D \subseteq B$

and a family of smooth mappings from this new configuration D onto the reference configuration B. We will refer to this new configuration D as the "defect reference configuration" or as the "parameter configuration."

Within the context just outlined, we consider a new configuration D, an open bounded subset of the reference configuration B, the elements of which will be called "continuous defects." We label continuous defects with their position vector $\boldsymbol{\xi}$ relative to some convenient reference frame as shown in figure 3.1.

A "defect motion" or "defect rearrangement" may be described by considering a time-dependent family of smooth mapping $\boldsymbol{\psi}$, (independent and coexisting with the deformation mapping $\boldsymbol{\varphi}$) that maps the "defect reference configuration" D onto the reference configuration B, i.e.,

$$\boldsymbol{\psi} : D \times I \rightarrow B$$

such that, for every time t of the interval $I = [t_0, t_f]$ the instantaneous defect rearrangement map $\boldsymbol{\psi}(\cdot, t)$ is bijective.

The particle $\mathbf{X} = \boldsymbol{\psi}(\boldsymbol{\xi}, t) \in B$ is the particle on which the continuous defect $\boldsymbol{\xi} \in D$ is sitting at time t. For a given fixed continuous defect $\boldsymbol{\xi}$ the set $\mathbf{X}(t) = \boldsymbol{\psi}(\boldsymbol{\xi}, t)$ is the collection of different material particles visited by the defect during its migration within the material. In coordinates we shall write

$$X_I = \psi_I(\xi_\alpha, t)$$

Here and in what follows, we will use greek indexes to denote components of coordinates and vector and tensor fields in D.

Let $\boldsymbol{\phi} = \boldsymbol{\varphi} \circ \boldsymbol{\psi}$ be the composition mapping between the deformation and the defect rearrangement mappings. Then the map $\boldsymbol{\phi}$ maps the defect reference configuration D onto the deformed configuration. In coordinates we shall write

$$\phi_i(\xi_\alpha, t) = \varphi_i(\psi_I(\xi_\alpha, t), t) \tag{3.17}$$

Figure (3.1) sketches the three configurations (defect reference configuration D, body reference configuration B, and deformed configuration at time t $\varphi_t(B)$), and the relation between the three mappings $\boldsymbol{\varphi}, \boldsymbol{\psi}$, and $\boldsymbol{\phi}$.

The set D is also known in the literature as the "space of reference labels" and the coordinates $\xi_\alpha \in D$ as "reference labels," see Gurtin [15] and Kalpakides & Dascalu [18]. For a given neighborhood P of $\boldsymbol{\xi} \in D$ the set $\boldsymbol{\psi}(P, t)$ is regarded as a migrating control volume within the reference configuration B. The set D is also known as the "referential configuration" and the maps $\boldsymbol{\psi}$ and $\boldsymbol{\phi} = \boldsymbol{\varphi} \circ \boldsymbol{\psi}$ as "the referential maps" ([26], [24]). Epstein & Maugin ([4], , [5], [39]) and Epstein [8]

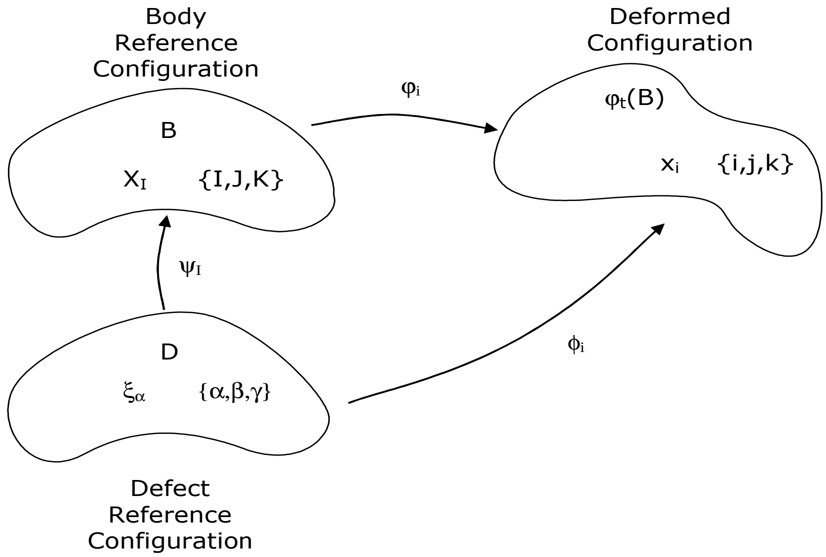

Figure 3.1: Reference configuration, deformed configuration, defect reference (or parametric) configuration, and composition mappings.

consider "local rearrangements" that bring a "reference or stress-free crystal" into the neighborhood of each particle, the local rearrangement need not to be integrable to a global rearrangement $\boldsymbol{\psi}$. Maugin & Trimarco [38] choose the defect reference configuration D coincident with the deformed configuration B_t and spatial positions as instantaneous reference labels for the defect configuration, the map $\boldsymbol{\psi}$ becoming in this case the inverse motion $\boldsymbol{\varphi}^{-1}$, see also [27], [40], [53], [56]. The defect rearrangement $\boldsymbol{\psi} : D \to B$ may be also interpreted as a change of parametrization of the reference configuration ([29], [30], [31]) and the set D is referred to as the "parameter space" or "parametric configuration," or, more generally, the space projection of a change of parametrization of space-time $B \times [t_0, t_f]$.

On account of the existence of two simultaneous and independent motions, we next regard the action as a functional that depends on both mappings $\boldsymbol{\phi}$ and $\boldsymbol{\psi}$ independently. To do this we make use of the following relations, which are obtained by direct differentiation with respect to $\boldsymbol{\xi}$ and t of (3.17):

- Relation between mappings

$$\boldsymbol{\varphi} = \boldsymbol{\phi} \circ \boldsymbol{\psi}^{-1}$$

- Relation for the deformation gradients

$$\mathbf{F} = D\boldsymbol{\phi} \left(D\boldsymbol{\psi}\right)^{-1} \tag{3.18}$$

- Relation between velocities

$$\begin{aligned} \dot{\boldsymbol{\varphi}} &= \dot{\boldsymbol{\phi}} - D\boldsymbol{\phi}\,(D\boldsymbol{\psi})^{-1}\,\dot{\boldsymbol{\psi}} \\ &= \dot{\boldsymbol{\phi}} - \mathbf{F}\dot{\boldsymbol{\psi}} \end{aligned} \tag{3.19}$$

Here $D\boldsymbol{\phi}$, $D\boldsymbol{\psi}$, $\dot{\boldsymbol{\phi}}$, and $\dot{\boldsymbol{\psi}}$ are the derivatives of $\phi_i(\xi_\alpha, t)$ and $\psi_J(\xi_\alpha, t)$ with respect to the parameter $\boldsymbol{\xi}$ and time t, i.e.,

$$\begin{aligned} (D\boldsymbol{\phi})_{i\alpha} &= \phi_{i,\alpha} = \frac{\partial \phi_i}{\partial \xi_\alpha} \\ (D\boldsymbol{\psi})_{I\alpha} &= \psi_{I,\alpha} = \frac{\partial \psi_I}{\partial \xi_\alpha} \\ \dot{\phi}_i &= \frac{\partial \phi_i}{\partial t} \\ \dot{\psi}_I &= \frac{\partial \psi_I}{\partial t} \end{aligned}$$

Referring the action functional (3.4) to the parametric configuration D and making use of the the deformation gradient and velocity relations (3.18) and (3.19) we obtain:

$$\begin{aligned} S[\boldsymbol{\psi}, \boldsymbol{\phi}] &= \int_{t_0}^{t_f} \int_D \mathcal{L} \circ \boldsymbol{\psi} \det(D\boldsymbol{\psi})\, d\boldsymbol{\xi} dt \\ &= \int_{t_0}^{t_f} \int_D \mathcal{L}\left(\boldsymbol{\psi}, t, \boldsymbol{\phi}, \dot{\boldsymbol{\phi}} - D\boldsymbol{\phi}\,(D\boldsymbol{\psi})^{-1}\,\dot{\boldsymbol{\psi}}, D\boldsymbol{\phi}\,(D\boldsymbol{\psi})^{-1}\right) \det(D\boldsymbol{\psi})\, d\boldsymbol{\xi} dt \end{aligned} \tag{3.20}$$

In coordinates the previous reads

$$S[\psi_I, \varphi_i] = \int_{t_0}^{t_f} \int_D \mathcal{L}\left(\psi_I, t, \phi_i, \dot{\phi}_i - \frac{\partial \phi_i}{\partial \xi_\alpha}\left(\frac{\partial \psi_\alpha^{-1}}{\partial X_I}\right)\dot{\psi}_I, \frac{\partial \phi_i}{\partial \xi_\alpha}\left(\frac{\partial \psi_\alpha^{-1}}{\partial X_I}\right)\right) \det\left(\frac{\partial \psi_I}{\partial X_\alpha}\right) d\boldsymbol{\xi}_\alpha dt$$

3.3.2 Variations and Euler-Lagrange equations

Hamilton's principle states that the actual (particle) motion renders the action functional S stationary with respect to all admissible variations. In keeping with this principle we invoke the stationarity of the action $S[\boldsymbol{\psi}, \boldsymbol{\phi}]$ with respect to admissible variations of both arguments:

$$\begin{aligned} \langle \delta S, \delta \phi_i \rangle &= 0 \\ \langle \delta S, \delta \psi_I \rangle &= 0 \end{aligned}$$

The variation of the action functional $S[\boldsymbol{\psi}, \boldsymbol{\phi}]$ with respect to $\boldsymbol{\phi}$ (keeping $\boldsymbol{\psi}$ fixed) is

$$\langle \delta S, \delta \phi_i \rangle = \int_{t_0}^{t_f} \int_D \left(\frac{\partial \mathcal{L}}{\partial \varphi_i}\delta\phi_i + \frac{\partial \mathcal{L}}{\partial V_i}\left(\delta\dot{\phi}_i - \left(\delta\phi_{i,\alpha}\psi_{\alpha,J}^{-1}\right)\dot{\psi}_J\right) + \frac{\partial \mathcal{L}}{\partial F_{iJ}}\left(\delta\phi_{i,\alpha}\psi_{\alpha,J}^{-1}\right)\right) \det(D\boldsymbol{\psi})\, d\boldsymbol{\xi} dt \tag{3.21}$$

Referring the integral back to the reference configuration B we find

$$\langle \delta S, \delta\phi_i \rangle = \int_{t_0}^{t_f} \int_B \left(\frac{\partial \mathcal{L}}{\partial \varphi_i} \left(\delta\phi_i \circ \boldsymbol{\psi}^{-1}\right) + \frac{\partial \mathcal{L}}{\partial V_i} \frac{d}{dt} \left(\delta\phi_i \circ \boldsymbol{\psi}^{-1}\right) + \frac{\partial \mathcal{L}}{\partial F_{iJ}} \frac{d}{dX_J} \left(\delta\phi_i \circ \boldsymbol{\psi}^{-1}\right) \right) dV dt \quad (3.22)$$

where the following identities have been used:

$$\frac{d}{dt} \left(\delta\phi_i \circ \boldsymbol{\psi}^{-1}\right) = \left(\delta\dot{\phi}_i \circ \boldsymbol{\psi}^{-1}\right) - \left(\delta\phi_{i,\alpha} \circ \boldsymbol{\psi}^{-1}\right) \psi^{-1}_{\alpha,J} \left(\dot{\psi}_J \circ \boldsymbol{\psi}^{-1}\right) \quad (3.23)$$

$$\frac{d}{dX_J} \left(\delta\phi_i \circ \boldsymbol{\psi}^{-1}\right) = \left(\delta\phi_{i,\alpha} \circ \boldsymbol{\psi}^{-1}\right) \psi^{-1}_{\alpha,J} \quad (3.24)$$

Integrating by parts in (3.22) yields the identity

$$\begin{aligned} \langle \delta S, \delta\phi_i \rangle &= \int_{t_0}^{t_f} \int_B \left(\frac{\partial \mathcal{L}}{\partial \varphi_i} - \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial V_i}\right) - \frac{d}{dX_J}\left(\frac{\partial \mathcal{L}}{\partial F_{iJ}}\right) \right) \left(\delta\phi_i \circ \boldsymbol{\psi}^{-1}\right) dV dt \\ &+ \int_B \frac{\partial \mathcal{L}}{\partial V_i} \left(\delta\phi_i \circ \boldsymbol{\psi}^{-1}\right) dV \Big|_{t_o}^{t_f} + \int_{t_0}^{t_f} \int_{\partial B} \left(\left(\delta\phi_i \circ \boldsymbol{\psi}^{-1}\right) \frac{\partial \mathcal{L}}{\partial F_{iJ}} N_J \right) dS dt \quad (3.25) \end{aligned}$$

We next compute the variations with respect to $\boldsymbol{\psi}$ (keeping $\boldsymbol{\phi}$ fixed). Notice first that since $S[\phi, \psi] = \int_{t_0}^{t_f} \int_D (\mathcal{L} \circ \boldsymbol{\psi}) \det(D\boldsymbol{\psi}) \, d\xi dt$ then there are two contributions for this variation, namely

$$\langle \delta \{\mathcal{L} \circ \boldsymbol{\psi} \det(D\boldsymbol{\psi})\}, \delta\psi_I \rangle = \langle \delta(\mathcal{L} \circ \boldsymbol{\psi}), \delta\psi_I \rangle \det(D\boldsymbol{\psi}) + (\mathcal{L} \circ \boldsymbol{\psi}) \langle \delta \det(D\boldsymbol{\psi}), \delta\psi_I \rangle$$

Notice also that

$$\begin{aligned} \langle \delta \det(D\boldsymbol{\psi}), \delta\psi_I \rangle &= \frac{d}{d\varepsilon} \det(D\boldsymbol{\psi} + \varepsilon D\delta\boldsymbol{\psi})\big|_{\varepsilon=0} = \\ &= \delta\psi_{I,\beta} \frac{\partial \det(D\psi)}{\partial \psi_{I,\beta}} = \\ &= \delta\psi_{I,\beta} \psi^{-1}_{\beta,I} \det(D\boldsymbol{\psi}) \quad (3.26) \end{aligned}$$

and

$$\begin{aligned} \left\langle \delta\psi^{-1}_{\alpha,J} \circ \boldsymbol{\psi}, \delta\psi_I \right\rangle &= \frac{d}{d\varepsilon} \left(\boldsymbol{\psi} + \varepsilon\delta\boldsymbol{\psi}\right)^{-1}_{\alpha,J} \Big|_{\varepsilon=0} = \\ &= -\left(\psi^{-1}_{\alpha,I} \circ \boldsymbol{\psi}\right) \delta\psi_{I,\beta} \left(\psi^{-1}_{\beta,J} \circ \boldsymbol{\psi}\right) \quad (3.27) \end{aligned}$$

Hence, the variation with respect to $\boldsymbol{\psi}$ gives

$$\begin{aligned} \langle \delta S, \delta\psi_I \rangle &= \int_{t_0}^{t_f} \int_D \left(\frac{\partial \mathcal{L}}{\partial X_I} \delta\psi_I + \frac{\partial \mathcal{L}}{\partial V_i} \left(-\phi_{i,\alpha}\psi^{-1}_{\alpha,I}\right) \left(\delta\dot{\psi}_I - \left(\delta\psi_{I,\beta}\psi^{-1}_{\beta,J}\right) \dot{\psi}_J\right) + \right. \\ &+ \left. \left(\mathcal{L}\delta_{IJ} - \frac{\partial \mathcal{L}}{\partial F_{iJ}} \left(\phi_{i,\alpha}\psi^{-1}_{\alpha,I}\right)\right) \left(\delta\psi_{I,\beta}\psi^{-1}_{\beta,J}\right) \right) \det(D\boldsymbol{\psi}) \, d\boldsymbol{\xi} dt \quad (3.28) \end{aligned}$$

Referring the integral back to the reference configuration B, the previous takes the form

$$\begin{aligned}\langle \delta S, \delta\psi_I\rangle &= \int_{t_0}^{t_f}\int_B \left(\frac{\partial \mathcal{L}}{\partial X_I}\left(\delta\psi_I\circ\boldsymbol{\psi}^{-1}\right)+\frac{\partial \mathcal{L}}{\partial V_i}\left(-F_{iI}\right)\frac{d}{dt}\left(\delta\psi_I\circ\boldsymbol{\psi}^{-1}\right)+\right.\\ &\quad\left.+\left(\mathcal{L}\delta_{IJ}-\frac{\partial \mathcal{L}}{\partial F_{iJ}}F_{iI}\right)\frac{d}{dX_J}\left(\delta\psi_I\circ\boldsymbol{\psi}^{-1}\right)\right)dV dt \qquad (3.29)\end{aligned}$$

where the following identities have been used:

$$\frac{d}{dX_J}\left(\delta\psi_I\circ\boldsymbol{\psi}^{-1}\right) = \left(\delta\psi_{I,\beta}\circ\boldsymbol{\psi}^{-1}\right)\psi^{-1}_{\beta,J} \qquad (3.30)$$

$$\frac{d}{dt}\left(\delta\psi_I\circ\boldsymbol{\psi}^{-1}\right) = \left(\delta\dot{\psi}_I\circ\boldsymbol{\psi}^{-1}\right)-\left[\left(\delta\psi_{I,\beta}\circ\boldsymbol{\psi}^{-1}\right)\psi^{-1}_{\beta,J}\right]\left(\dot{\psi}_J\circ\boldsymbol{\psi}^{-1}\right) \qquad (3.31)$$

Integrating by parts in (3.29) gives the variations in the form

$$\begin{aligned}\langle \delta S, \delta\psi_I\rangle &= \int_{t_0}^{t_f}\int_B \left(\frac{\partial \mathcal{L}}{\partial X_I}-\frac{d}{dt}\left(-F_{iI}\frac{\partial \mathcal{L}}{\partial V_i}\right)-\frac{d}{dX_J}\left(\mathcal{L}\delta_{IJ}-\frac{\partial \mathcal{L}}{\partial F_{iJ}}F_{iI}\right)\right)\left(\delta\psi_I\circ\boldsymbol{\psi}^{-1}\right)+\\ &\quad+\int_B\left(\frac{\partial \mathcal{L}}{\partial V_i}\left(-F_{iI}\right)\right)\left(\delta\psi_I\circ\boldsymbol{\psi}^{-1}\right)dV\Big|_{t_o}^{t_f}\\ &\quad+\int_{t_0}^{t_f}\int_{\partial B}\left(\left(\delta\psi_I\circ\boldsymbol{\psi}^{-1}\right)\left(\mathcal{L}\delta_{IJ}-\frac{\partial \mathcal{L}}{\partial F_{iJ}}F_{iI}\right)N_J\right)dSdt \qquad (3.32)\end{aligned}$$

We next obtain the corresponding Euler-Lagrange equations. Stationarity of the action with respect to admissible variations $\delta\phi$, i.e., mappings $\delta\boldsymbol{\phi}$ such that $\left(\delta\boldsymbol{\phi}\circ\boldsymbol{\psi}^{-1}\right)$ vanishes on the Dirichlet boundary ∂B_2 $\forall t\in I=[t_0,t_f]$ and everywhere in B at t_o and t_f, yields the Euler-Lagrange equation

$$\frac{\partial \mathcal{L}}{\partial \varphi_i}-\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial V_i}\right)-\frac{d}{dX_J}\left(\frac{\partial \mathcal{L}}{\partial F_{iJ}}\right)=0 \qquad \text{in } B \text{ and } \forall t\in I \qquad (3.33)$$

along with the boundary condition

$$\frac{\partial \mathcal{L}}{\partial F_{iJ}}N_J=0 \qquad \text{in } \partial B_1 \text{ and } \forall t\in I$$

that, as was shown in the previous section, corresponds to the equation of motion (3.10).

Stationarity of the action with respect to admissible variations $\delta\boldsymbol{\psi}$, i.e., mappings $\delta\boldsymbol{\psi}$ such that $\left(\delta\boldsymbol{\psi}\circ\boldsymbol{\psi}^{-1}\right)$ vanishes in the complete boundary ∂B $\forall t\in I=[t_0,t_f]$ and everywhere in B at t_o and t_f, yields the Euler-Lagrange equation

$$\frac{\partial \mathcal{L}}{\partial X_I}-\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial V_i}\left(-F_{iI}\right)\right)-\frac{d}{dX_J}\left(\mathcal{L}\delta_{IJ}-\frac{\partial \mathcal{L}}{\partial F_{iJ}}F_{iI}\right)=0 \qquad \text{in } B \text{ and } \forall t\in I \qquad (3.34)$$

The magnitude

$$C_{IJ}=-\left(\mathcal{L}\delta_{IJ}-\frac{\partial \mathcal{L}}{\partial F_{iJ}}F_{iI}\right)$$

is the dynamic Eshelby tensor or (or space-space component of the space-time energy-momentum tensor) and equation (3.34) is the equation of balance of Configurational Forces. The magnitude

$$j_I = \frac{\partial \mathcal{L}}{\partial V_i} \left(-F_{iI}\right) \tag{3.35}$$

is the "material momentum" [34], or pseudomomentum ([40], [41], [42], [44], [45], [46]). The term

$$B_I^{inh} = \frac{\partial \mathcal{L}}{\partial X_I} = \left.\frac{\partial \mathcal{L}}{\partial X_I}\right|_{\exp}$$

is a source resulting from the assumption that the Lagrangian density is inhomogeneous. Equation (3.34) is also referred to as the equation of balance of pseudomomentum. For a Lagrangian density $\mathcal{L}$ of the form (3.3), the material momentum, dynamic Eshelby stress tensor, and inhomogeneity source term yield

$$\begin{aligned} j_I &= -RV_iF_{iI} \\ C_{IJ} &= \left(W - \frac{1}{2}R\left\|\dot{\boldsymbol{\varphi}}\right\|^2\right)\delta_{IJ} - P_{iJ}F_{iI} \\ B_I^{inh} &= \left.\frac{\partial}{\partial X_I}\left\{\frac{1}{2}R\left\|\dot{\boldsymbol{\varphi}}\right\|^2 - W\left(X_i, \varphi_i, F_{iJ}\right)\right\}\right|_{\exp} \end{aligned}$$

and the equations of balance of configurational forces read

$$B_I^{inh} - \frac{d}{dt}\left(-F_{iI}R\dot{\varphi}_i\right) + \frac{dC_{IJ}}{dX_J} = 0 \qquad \text{in } B \text{ and } \forall t \in I \tag{3.36}$$

that resemble the equations of motion

$$B_i - \frac{d}{dt}\left(R\dot{\varphi}_i\right) + \frac{dP_{iJ}}{dX_J} = 0 \qquad \text{in } B \text{ and } \forall t \in I$$

The Euler-Lagrange equations written in invariant notation yield

$$\begin{aligned} \mathbf{B} - \frac{d}{dt}\left(R\mathbf{V}\right) + DIV\left(\mathbf{P}\right) &= \mathbf{0} \\ \mathbf{B}^{inh} - \frac{d}{dt}\left(-\mathbf{F}^T\frac{\partial L}{\partial \mathbf{V}}\right) + DIV\left(\mathbf{C}\right) &= \mathbf{0} \end{aligned}$$

3.3.3 Equivalence between mechanical and configurational force balance

We notice now that the action functional (3.20) does not depend on the two mappings $(\boldsymbol{\psi}, \boldsymbol{\phi})$ independently, but only on the combination $\boldsymbol{\varphi} = \boldsymbol{\phi} \circ \boldsymbol{\psi}^{-1}$. It follows then that the equations of configurational and mechanical force balance are equivalent in the sense that if equation (3.33) is satisfied, then equation (3.34) will be automatically satisfied. More precisely, let $\mathcal{F}_{\boldsymbol{\phi}}\left(\boldsymbol{\varphi}\right)$ and $\mathcal{F}_{\boldsymbol{\psi}}\left(\boldsymbol{\varphi}\right)$

be the left hand sides of the Euler-Lagrange equations (3.33) and (3.34), namely

$$\left(\mathcal{F}_{\boldsymbol{\phi}}\left(\boldsymbol{\varphi}\right)\right)_i = \frac{\partial L}{\partial \varphi_i} - \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial V_i}\right) - \frac{d}{dX_J}\left(\frac{\partial \mathcal{L}}{\partial F_{iJ}}\right) \tag{3.37}$$

$$\left(\mathcal{F}_{\boldsymbol{\psi}}\left(\boldsymbol{\varphi}\right)\right)_I = \frac{\partial v}{\partial X_I} - \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial V_i}\left(-F_{iI}\right)\right) - \frac{d}{dX_J}\left(\mathcal{L}\delta_{IJ} - \frac{\partial \mathcal{L}}{\partial F_{iJ}}F_{iI}\right) \tag{3.38}$$

Then we have

$$\mathcal{F}_{\boldsymbol{\phi}}\left(\boldsymbol{\varphi}\right) = 0 \Leftrightarrow \mathcal{F}_{\boldsymbol{\psi}}\left(\boldsymbol{\varphi}\right) = 0$$

To prove this equivalence observe that

$$\begin{aligned}\frac{d\mathcal{L}}{dX_I} &= \frac{\partial \mathcal{L}}{\partial \mathbf{X}} + \frac{\partial \mathcal{L}}{\partial \varphi_i}\frac{\partial \varphi_i}{\partial X_I} + \frac{\partial \mathcal{L}}{\partial V_i}\frac{\partial \dot{\varphi}_i}{\partial X_I} + \frac{\partial \mathcal{L}}{\partial F_{iJ}}\frac{\partial F_{iJ}}{\partial X_I} = \\ &= \frac{\partial \mathcal{L}}{\partial X_I} + \frac{\partial \mathcal{L}}{\partial \varphi_i}F_{iI} + \frac{\partial \mathcal{L}}{\partial \dot{\varphi}_i}\frac{\partial F_{iI}}{\partial t} + \frac{\partial \mathcal{L}}{\partial F_{iJ}}\frac{\partial F_{iJ}}{\partial X_I}\end{aligned} \tag{3.39}$$

where we have made use of the relation between mixed partial derivatives $\frac{\partial \dot{\varphi}_i}{\partial X_I} = \frac{\partial F_{iI}}{\partial t}$. Substituting equation (3.33) in the previous we find

$$\begin{aligned}\frac{d\mathcal{L}}{dX_I} &= \frac{\partial \mathcal{L}}{\partial \mathbf{X}} + \left(\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial V_i}\right) + \frac{d}{dX_J}\left(\frac{\partial \mathcal{L}}{\partial F_{iJ}}\right)\right)F_{iI} + \frac{\partial \mathcal{L}}{\partial V_i}\frac{\partial F_{iI}}{\partial t} + \frac{\partial \mathcal{L}}{\partial F_{iJ}}\frac{\partial F_{iJ}}{\partial X_I} = \\ &= \frac{\partial L}{\partial \mathbf{X}} + \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial V_i}F_{iI}\right) + \frac{d}{dX_J}\left(\frac{\partial \mathcal{L}}{\partial F_{iJ}}F_{iI}\right)\end{aligned}$$

that, using the identity

$$\frac{d\mathcal{L}}{dX_I} = \frac{d}{dX_I}\left(\mathcal{L}\delta_{IJ}\right) \tag{3.40}$$

may be reexpresed in the form (3.34).

Alternatively, the equivalence between (3.33) and (3.34) may be proved as follows: multiplying $\mathcal{F}_{\boldsymbol{\phi}}\left(\boldsymbol{\varphi}\right)$ by $\left(-\mathbf{F}^T\right)$ and rearranging terms yields

$$\begin{gathered}-F_{iI}\left(\frac{\partial \mathcal{L}}{\partial \varphi_i} - \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial V_i}\right) - \frac{d}{dX_J}\left(\frac{\partial \mathcal{L}}{\partial F_{iJ}}\right)\right) = \\ -F_{iI}\frac{\partial \mathcal{L}}{\partial \varphi_i} - \frac{d}{dt}\left(-F_{iI}\frac{\partial \mathcal{L}}{\partial V_i}\right) - \frac{\partial F_{iI}}{\partial t}\frac{\partial \mathcal{L}}{\partial V_i} - \frac{d}{dX_J}\left(-F_{iI}\frac{\partial \mathcal{L}}{\partial F_{iJ}}\right) - \frac{\partial F_{iI}}{\partial X_J}\frac{\partial \mathcal{L}}{\partial F_{iJ}}\end{gathered}$$

Making use of the identities (3.39) and (3.40) we then find

$$\begin{gathered}-F_{iI}\left(\frac{\partial \mathcal{L}}{\partial \varphi_i} - \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial V_i}\right) - \frac{d}{dX_J}\left(\frac{\partial \mathcal{L}}{\partial F_{iJ}}\right)\right) = \\ \frac{\partial \mathcal{L}}{\partial X_I} - \frac{d}{dt}\left(-F_{iI}\frac{\partial \mathcal{L}}{\partial V_i}\right) - \frac{d}{dX_J}\left(\mathcal{L}\delta_{IJ} - F_{iI}\frac{\partial \mathcal{L}}{\partial F_{iJ}}\right)\end{gathered} \tag{3.41}$$

that may be compactly expressed, using the notation (3.37) and (3.38) as

$$-\mathbf{F}^T \mathcal{F}_{\boldsymbol{\phi}}(\boldsymbol{\varphi}) = \mathcal{F}_{\boldsymbol{\psi}}(\boldsymbol{\varphi}) \tag{3.42}$$

Therefore the left hand side of the equations of configurational force balance is identically equal to the left hand side of the equations of mechanical force balance multiplied by $-\mathbf{F}^T$. The operation of multiplying equations (3.33) by $-\mathbf{F}^T$ may be interpreted as a pull-back or projection of this balance law onto the material manifold, thus the terms "material" momentum and forces, see Maugin [40], [43], [46].

Of fundamental importance for understanding the finite element method studied in this work is the following remark: While in the continuum setting the mechanical and configurational force balance equations are equivalent, in the discrete setting this equivalence does not hold. The discrete (nodal) configurational force system computed from the finite element discretization is unbalanced in general, even in homogeneous materials where configurational forces are not expected. These discrete configurational forces will be used as driving forces for the motion of the finite element mesh.

3.3.4 Noether's theorem and material translational symmetry

We also notice that if the material is homogeneous, i.e., the Lagrangian density L is independent of $\mathbf{X}$, and if $\boldsymbol{\varphi}$ is a solution of the Euler-Lagrange equations (3.33), then the equation of balance of configurational forces (3.34) becomes the local conservation law

$$\frac{d}{dt}\left(-F_{iI}\frac{\partial \mathcal{L}}{\partial V_i}\right) + \frac{d}{dX_J}\left(\mathcal{L}\delta_{IJ} - F_{iI}\frac{\partial \mathcal{L}}{\partial F_{iJ}}\right) = 0 \tag{3.43}$$

with momentum given by $j_I = -F_{iI}\frac{\partial L}{\partial V_i}$ (the material momentum) and with the Eshelby stress tensor $C_{IJ} = -\left(\mathcal{L}\delta_{IJ} - F_{iI}\frac{\partial \mathcal{L}}{\partial F_{iJ}}\right)$ acting as the momentum flux. This result may be also obtained as a direct application of Noether's theorem to elasticity ([40], [43], [22], [29], [30], [31], [34]).

Assume that for fixed $(\boldsymbol{\psi}, \boldsymbol{\phi})$ the action (3.34) is symmetric (or invariant) with respect to a one-parameter family of transformations in their variables, i.e., the action functional remains invariant

$$S[\boldsymbol{\psi}, \boldsymbol{\phi}] = S[\boldsymbol{\psi}_\varepsilon, \boldsymbol{\phi}_\varepsilon] \tag{3.44}$$

under the influence of a family of maps $\boldsymbol{\psi}_\varepsilon(\boldsymbol{\xi}, t)$ and $\boldsymbol{\phi}_\varepsilon(\boldsymbol{\xi}, t)$ such that

$$\begin{aligned}\boldsymbol{\psi}_0 &= \boldsymbol{\psi} \\ \boldsymbol{\phi}_0 &= \boldsymbol{\phi}\end{aligned}$$

Denoting by

$$\begin{aligned}\mathbf{Y} &= \left.\frac{d\boldsymbol{\psi}_\varepsilon}{d\varepsilon}\right|_{\varepsilon=0} \\ \mathbf{y} &= \left.\frac{d\boldsymbol{\phi}_\varepsilon}{d\varepsilon}\right|_{\varepsilon=0}\end{aligned}$$

the infinitesimal generators of the symmetries and differentiating the identity (3.44) with S given by (3.20) with respect to the parameter ε gives

$$\begin{aligned}0 = & \int_{t_0}^{t_f}\int_D \left\{ \frac{\partial \mathcal{L}}{\partial X_I} Y_I \circ \boldsymbol{\psi}^{-1} + \frac{\partial \mathcal{L}}{\partial \varphi_i} y_i \circ \boldsymbol{\psi}^{-1} + \right. \\ & + \frac{\partial \mathcal{L}}{\partial V_i}\left(\dot{y}_i - y_{i,\alpha}\psi^{-1}_{\alpha,J}\dot{\psi}_J \right) + \\ & + \frac{\partial \mathcal{L}}{\partial V_i}\left(-\phi_{i,\alpha}\psi^{-1}_{\alpha,I} \right)\left(\dot{Y}_I - Y_{I,\beta}\psi^{-1}_{\beta,J}\dot{\psi}_J \right) + \\ & + \frac{\partial \mathcal{L}}{\partial F_{iI}}\left(y_{i,\alpha}\psi^{-1}_{\alpha,I} - \phi_{i,\alpha}\psi^{-1}_{\alpha,J} Y_{J,\beta}\psi^{-1}_{\beta,I} \right) + \\ & \left. + \mathcal{L} Y_{I,\alpha}\psi^{-1}_{\alpha,I} \right\} \det\left(\frac{\partial \psi_I}{\partial \xi_\alpha} \right) d\boldsymbol{\xi} dt \end{aligned} \tag{3.45}$$

where we have made use of the following equalities:

$$\begin{aligned}\left.\frac{d}{d\varepsilon}\det\left(D\boldsymbol{\psi}_\varepsilon\right)\right|_{\varepsilon=0} &= \det\left(D\boldsymbol{\psi}_\varepsilon\right)\psi^{-1}_{\alpha,I} Y_{I,\alpha} \\ \left.\frac{d}{d\varepsilon}\left(D\boldsymbol{\psi}_\varepsilon\right)^{-1}\right|_{\varepsilon=0} &= -\psi^{-1}_{\alpha,I} Y_{I,\beta}\psi^{-1}_{\beta,J}\end{aligned}$$

Referring the previous integral back to the reference configuration B equation (3.45) gives the local symmetry condition as

$$\begin{aligned}0 = & \int_{t_0}^{t_f}\int_B \left\{ \frac{\partial \mathcal{L}}{\partial X_I} Y_I \circ \boldsymbol{\psi}^{-1} + \frac{\partial \mathcal{L}}{\partial \varphi_i} y_i \circ \boldsymbol{\psi}^{-1} + \right. \\ & + \left(\frac{\partial \mathcal{L}}{\partial V_i} \right)\left(\frac{d}{dt}\left(y_i \circ \boldsymbol{\psi}^{-1} \right) - F_{iI}\frac{d}{dt}\left(Y_I \circ \boldsymbol{\psi}^{-1} \right) \right) \\ & + \left(\frac{\partial \mathcal{L}}{\partial F_{iI}} \right)\left(\frac{d}{dX_I}\left(y_i \circ \boldsymbol{\psi}^{-1} \right) - F_{iJ}\frac{d}{dX_I}\left(Y_J \circ \boldsymbol{\psi}^{-1} \right) \right) + \\ & \left. + \mathcal{L}\frac{d}{dX_I}\left(Y_I \circ \boldsymbol{\psi}^{-1} \right) \right\} d\mathbf{X} dt \end{aligned}$$

where we have made use of the identities

$$\begin{aligned}\frac{d}{dt}\left(Y_I \circ \boldsymbol{\psi}^{-1} \right) &= \left(\dot{Y}_I \circ \boldsymbol{\psi}^{-1} \right) - \left(Y_{I,\alpha} \circ \boldsymbol{\psi}^{-1} \right)\psi^{-1}_{\alpha,J}\left(\dot{\psi}_J \circ \boldsymbol{\psi}^{-1} \right) \\ \frac{d}{dX_J}\left(Y_I \circ \boldsymbol{\psi}^{-1} \right) &= \left(Y_{I,\alpha} \circ \boldsymbol{\psi}^{-1} \right)\psi^{-1}_{\alpha,J}\end{aligned}$$

$$\begin{aligned}\frac{d}{dt}\left(y_i\circ\boldsymbol{\psi}^{-1}\right) &= \left(\dot{y}_i\circ\boldsymbol{\psi}^{-1}\right)-\left(y_{i,\alpha}\circ\boldsymbol{\psi}^{-1}\right)\psi^{-1}_{\alpha,J}\left(\dot{\psi}_J\circ\boldsymbol{\psi}^{-1}\right)\\ \frac{d}{dX_J}\left(y_i\circ\boldsymbol{\psi}^{-1}\right) &= \left(y_{i,\alpha}\circ\boldsymbol{\psi}^{-1}\right)\psi^{-1}_{\alpha,J}\end{aligned}$$

On account of equation (3.39), the symmetry condition may be written as

$$\begin{aligned}0 &= \int_{t_0}^{t_f}\int_B \Big\{\left(\mathcal{F}_{\boldsymbol{\phi}}\left(\boldsymbol{\varphi}\right)\right)_i\left(y_i-F_{iJ}Y_J\right)+\\ &+\frac{d}{dt}\left(\left(y_i-F_{iJ}Y_J\right)\frac{\partial\mathcal{L}}{\partial V_i}\right)+\frac{d}{dX_I}\left(\left(y_i-F_{iJ}Y_J\right)\frac{\partial\mathcal{L}}{\partial F_{iI}}+\mathcal{L}Y_I\right)\Big\}\,d\mathbf{X}dt\end{aligned}$$

where $\mathcal{F}_{\boldsymbol{\phi}}\left(\boldsymbol{\varphi}\right)$ is the Euler-Lagrange operator defined in (3.37). Therefore, if $\boldsymbol{\varphi}$ is a solution of the Euler-Lagrange equations (3.33), i.e., if $\mathcal{F}_{\boldsymbol{\phi}}\left(\boldsymbol{\varphi}\right)=\mathbf{0}$, and if the action (3.20) is symmetric with respect to the flows $\left(\boldsymbol{\psi}_\varepsilon,\boldsymbol{\phi}_\varepsilon\right)$ then the following local conservation law is satisfied:

$$\frac{d}{dt}\left(\left(y_i-F_{iJ}Y_J\right)\frac{\partial\mathcal{L}}{\partial V_i}\right)+\frac{d}{dX_I}\left(\left(y_i-F_{iJ}Y_J\right)\frac{\partial\mathcal{L}}{\partial F_{iI}}+\mathcal{L}Y_I\right)=0$$

or in global form

$$\int_P\left(y_i-F_{iJ}Y_J\right)\frac{\partial\mathcal{L}}{\partial V_i}dV\Big|_{t_0}^{t_f}+\int_{t_0}^{t_f}\int_{\partial P}\left(\left(y_i-F_{iJ}Y_J\right)\frac{\partial\mathcal{L}}{\partial F_{iI}}+\mathcal{L}Y_I\right)N_I dS dt=0$$

where $P\subseteq B$ is any open subset of B. This result is the statement of Noether's theorem. In particular, if the action is symmetric with respect to material (or horizontal) translations $\left(\boldsymbol{\psi}_\varepsilon,\boldsymbol{\phi}_\varepsilon\right)=\left(\boldsymbol{\xi}+\varepsilon\mathbf{Y},\boldsymbol{\phi}\right)$ with $\mathbf{Y}$ a constant vector, as happens when the Lagrangian density L is independent of $\mathbf{X}$ (homogeneous materials), Noether's theorem yields the conservation law

$$Y_J\left(\frac{d}{dt}\left(\left(-F_{iJ}\right)\frac{\partial\mathcal{L}}{\partial V_i}\right)+\frac{d}{dX_I}\left(\mathcal{L}\delta_{IJ}-F_{iJ}\frac{\partial\mathcal{L}}{\partial F_{iI}}\right)\right)=0$$

or in global form

$$Y_J\left(\int_P\left(-F_{iJ}\right)\frac{\partial\mathcal{L}}{\partial V_i}dV\Big|_{t_0}^{t_f}+\int_{t_0}^{t_f}\int_{\partial P}\left(\mathcal{L}\delta_{IJ}-F_{iJ}\frac{\partial\mathcal{L}}{\partial F_{iI}}\right)N_I dS dt\right)=0$$

that implies the conservation law (3.34). The equations of conservation (lack of) of mechanical forces may be thus reinterpreted as the conservation (balance) law associated to material translational symmetry (lack of symmetry) of the action functional.

The global form of this conservation law may alternatively be written as

$$\mathbf{Q}\left(t_f\right)-\mathbf{Q}\left(t_0\right)=\int_{t_0}^{t_f}\mathbf{J}\left(t\right)dt$$

or equivalently as

$$\mathbf{J} - \dot{\mathbf{Q}} = \mathbf{0}$$

where

$$Q_J(t) = \int_P (-F_{iJ}) \frac{\partial L}{\partial V_i} dV$$

is the total material momentum or total pesudomentum (see the definition of material momentum density in (3.35)) of the subbody $P \subseteq B$ and

$$\begin{aligned} J_J(t) &= \int_{\partial P} -\left(\mathcal{L}\delta_{IJ} - F_{iJ}\frac{\partial \mathcal{L}}{\partial F_{iI}}\right) N_I dS = \\ &= \int_{\partial P} C_{IJ} N_I dS \end{aligned}$$

is the total configurational force within the subbody $P \subseteq B$. The magnitude

$$\mathbf{J}^{dyn} = \mathbf{J} - \dot{\mathbf{Q}}$$

is the dynamic **J**-integral (see [12], [50]). For a Lagrangian density of the form (3.3) it reduces to

$$\begin{aligned} J_J^{dyn} &= \int_{\partial P} \left(\left(W - \frac{R\left\|\mathbf{V}\right\|^2}{2} \right) \delta_{IJ} - F_{iJ} \frac{\partial W}{\partial F_{iI}} \right) N_I dS - \int_P \frac{d}{dt} \left(-F_{iJ} R V_i \right) dV = \\ &= \int_{\partial P} \left(\left(W + \frac{R\left\|\mathbf{V}\right\|^2}{2} \right) \delta_{IJ} - F_{iJ} \frac{\partial W}{\partial F_{iI}} \right) N_I dS + \int_P R \left(F_{iJ} \dot{V}_i - V_i V_{i,J} \right) dV \end{aligned}$$

In the context of Noether's theorem and the established relation between material symmetry and conservation of material momentum, we may restate the remark of the previous subsection in the following way: While in the continuous setting and for homogeneous materials the material momentum is conserved, in the discrete setting and for arbitrary meshes, the discrete material momentum will not be conserved in general. The discretization breaks the material translational symmetry in general and the material momentum may not be conserved even when the mechanical momentum is conserved. The out of balance discrete configurational forces that preclude the conservation of the discrete material momentum will be used as driving forces for the evolution of the moving mesh.

3.3.5 Energy release rate and dynamic J-integral

So far we have focused attention in the kinematics of defect motion given by the mapping $\boldsymbol{\psi}(\boldsymbol{\xi}, t)$ and on what are the consequences of demanding the stationarity of an action functional that was built with a Lagrangian and energy densities that depend *implicitly* on $\boldsymbol{\psi}$, i.e., depend on $\boldsymbol{\psi}$ only through $\boldsymbol{\varphi} = \boldsymbol{\phi} \circ \boldsymbol{\psi}^{-1}$. In this section we will analyze materials for which the energy density A depends explicitly on the defect parameter $\boldsymbol{\xi}$. We recall that the parameter $\boldsymbol{\xi}$ specifies one particular configuration of the defects, namely the defect reference configuration. Just as the parameter $\mathbf{X}$, which is used to label particles but coincides with the spatial position $\mathbf{x}$ occupied by the material particle $\mathbf{X}$ at a reference time t_{ref}, i.e., $\mathbf{x} = \boldsymbol{\varphi}(\mathbf{X}, t_{ref})$, the defect parameter $\boldsymbol{\xi}$, used to label continuous defects, is in one-to-one correspondence with the material particle on which the defect is sitting at the reference time t_{ref}, i.e., $\mathbf{X} = \boldsymbol{\psi}(\boldsymbol{\xi}, t_{ref})$. It follows then that assuming that A is function of $\boldsymbol{\xi}$ implies that the material has a memory of where the defect was at the reference time t_{ref} just as do elastic materials that "remember" the reference position of particles. Since $\boldsymbol{\xi} = \boldsymbol{\psi}^{-1}(\mathbf{X}, t)$, an explicit dependence of A on $\boldsymbol{\xi}$ implies an explicit dependence on the defect motion $\boldsymbol{\psi}$.

We shall therefore assume in this section that the free energy depends *explicitly* on the parameters $\boldsymbol{\xi}$ required to specify the reference configuration of the defects, i.e.,

$$A = A(\boldsymbol{\xi}, \mathbf{X}, \mathbf{F})$$

This results, since $\boldsymbol{\xi} = \boldsymbol{\psi}^{-1}(\mathbf{X}, t)$. in a free energy density A, Lagrangian density $\mathcal{L}$, and action functional S that depend explicitly on the the defect motion $\boldsymbol{\psi}$, namely,

$$\begin{aligned} A &= A\left(\boldsymbol{\psi}^{-1}(\mathbf{X}, t), \mathbf{X}, \mathbf{F}\right) \\ \mathcal{L} &= \mathcal{L}\left(\boldsymbol{\psi}^{-1}(\mathbf{X}, t), \mathbf{X}, t, \varphi, \mathbf{V}, \mathbf{F}\right) \\ S &= S(\boldsymbol{\varphi}, \boldsymbol{\psi}) = \int_{t_0}^{t_f} \int_B \mathcal{L}\left(\boldsymbol{\psi}^{-1}(\mathbf{X}, t), \mathbf{X}, t, \boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}, D\boldsymbol{\varphi}\right) dV dt \end{aligned}$$

Notice that the free energy density and Lagrangian density become therefore explicit functions of position $\mathbf{X}$ through two different sources, namely, those that are a consequence of the explicit dependence on $\boldsymbol{\xi}$ and those that are a consequence of the explicit dependence on $\mathbf{X}$. To distinguish between these two sources we will use the notation

$$\begin{aligned} \left.\frac{\partial \mathcal{L}}{\partial \mathbf{X}}\right|_1 &= \frac{\partial \mathcal{L}}{\partial \boldsymbol{\xi}} \frac{\partial\left(\boldsymbol{\psi}^{-1}\right)}{\partial \mathbf{X}} \\ \left.\frac{\partial \mathcal{L}}{\partial \mathbf{X}}\right|_2 &= \frac{\partial \mathcal{L}}{\partial \mathbf{X}} \end{aligned}$$

and the explicit derivative of the Lagrangian with respect to $\mathbf{X}$ becomes

$$\begin{aligned} \left.\frac{\partial \mathcal{L}}{\partial \mathbf{X}}\right|_{\exp} &= \left.\frac{\partial \mathcal{L}}{\partial \mathbf{X}}\right|_1 + \left.\frac{\partial \mathcal{L}}{\partial \mathbf{X}}\right|_2 = \\ &= \frac{\partial \mathcal{L}}{\partial \boldsymbol{\xi}} \frac{\partial\left(\boldsymbol{\psi}^{-1}\right)}{\partial \mathbf{X}} + \frac{\partial \mathcal{L}}{\partial \mathbf{X}} \end{aligned}$$

It follows that the pull-back relation (3.41) reduces in this case to

$$-\mathbf{F}^T\left(\frac{\partial\mathcal{L}}{\partial\boldsymbol{\varphi}}-\frac{d}{dt}\left(\frac{\partial\mathcal{L}}{\partial\mathbf{V}}\right)-\frac{d}{d\mathbf{X}}\left(\frac{\partial\mathcal{L}}{\partial\mathbf{F}}\right)\right)=$$
$$\left.\frac{\partial\mathcal{L}}{\partial\mathbf{X}}\right|_1+\left.\frac{\partial\mathcal{L}}{\partial\mathbf{X}}\right|_2-\frac{d}{dt}\left(-\mathbf{F}^T\frac{\partial\mathcal{L}}{\partial\mathbf{V}}\right)-\frac{d}{d\mathbf{X}}\left(\mathcal{L}\mathbf{I}-\mathbf{F}^T\frac{\partial\mathcal{L}}{\partial\mathbf{F}}\right)\tag{3.46}$$

We notice also that the free energy becomes in this case an explicit function of time. As we will see shortly this implies energy dissipation.

We observe next that when the free energy of the material A depends explicitly on $\boldsymbol{\xi}$, we cannot demand the stationarity of the action with respect to variations in the defect motion $\boldsymbol{\psi}$. This can directly be verified by taking variations of the action functional $S(\boldsymbol{\varphi},\boldsymbol{\psi})$ with respect to each of its arguments to find

$$\begin{aligned}\langle\delta S,\delta\boldsymbol{\varphi}\rangle &= \int_{t_0}^{t_f}\int_B\left(\frac{\partial\mathcal{L}}{\partial\boldsymbol{\varphi}}\delta\boldsymbol{\varphi}+\frac{\partial\mathcal{L}}{\partial\mathbf{V}}\delta\dot{\boldsymbol{\varphi}}+\frac{\partial\mathcal{L}}{\partial\mathbf{F}}\delta D\boldsymbol{\varphi}\right)dV\,dt=\\ &= \int_{t_0}^{t_f}\int_B\left(\left(\frac{\partial\mathcal{L}}{\partial\boldsymbol{\varphi}}-\frac{d}{dt}\left(\frac{\partial\mathcal{L}}{\partial\mathbf{V}}\right)-\frac{d}{d\mathbf{X}}\frac{\partial\mathcal{L}}{\partial\mathbf{F}}\right)\delta\boldsymbol{\varphi}\right)dV\,dt\\ &\quad+\int_B\frac{\partial\mathcal{L}}{\partial\mathbf{V}}\delta\boldsymbol{\varphi}\Big|_{t_0}^{t_f}dV+\int_{t_0}^{t_f}\int_{\partial B}\delta\boldsymbol{\varphi}\frac{\partial\mathcal{L}}{\partial\mathbf{F}}\mathbf{N}dS dt\\ \langle\delta S,\delta\boldsymbol{\psi}\rangle &= \int_{t_0}^{t_f}\int_B\frac{\partial\mathcal{L}}{\partial\boldsymbol{\xi}}\delta\left(\boldsymbol{\psi}^{-1}\right)dV\,dt\end{aligned}$$

Using the identity

$$\delta\left(\boldsymbol{\psi}^{-1}\right)=\left|\frac{\partial}{\partial\varepsilon}\left(\boldsymbol{\psi}+\varepsilon\delta\boldsymbol{\psi}\right)^{-1}\right|_{\varepsilon=0}=-\frac{\partial\left(\boldsymbol{\psi}\right)^{-1}}{\partial\mathbf{X}}\left(\delta\boldsymbol{\psi}\circ\boldsymbol{\psi}^{-1}\right)$$

the variation with respect to $\boldsymbol{\psi}$ (keeping $\boldsymbol{\varphi}$ constant) can be rewritten as

$$\begin{aligned}\langle\delta S,\delta\boldsymbol{\psi}\rangle &= \int_{t_0}^{t_f}\int_B-\frac{\partial\mathcal{L}}{\partial\boldsymbol{\xi}}\frac{\partial\left(\boldsymbol{\psi}\right)^{-1}}{\partial\mathbf{X}}\left(\delta\boldsymbol{\psi}\circ\boldsymbol{\psi}^{-1}\right)dV\,dt=\\ &= \int_{t_0}^{t_f}\int_B\left(-\left.\frac{\partial\mathcal{L}}{\partial\mathbf{X}}\right|_1\right)\left(\delta\boldsymbol{\psi}\circ\boldsymbol{\psi}^{-1}\right)dV\,dt\end{aligned}$$

Invoking then the stationarity of the action functional with respect to admissible variations of $\boldsymbol{\varphi}$, and keeping constant $\boldsymbol{\psi}$, requires

$$\langle\delta S,\delta\boldsymbol{\varphi}\rangle=0$$

with corresponding Euler-Lagrange equation

$$\frac{\partial\mathcal{L}}{\partial\boldsymbol{\varphi}}-\frac{d}{dt}\left(\frac{\partial\mathcal{L}}{\partial\mathbf{V}}\right)-\frac{d}{d\mathbf{X}}\frac{\partial\mathcal{L}}{\partial\mathbf{F}}=0\tag{3.47}$$

However for our original assumption of an energy that depends exclusively on $\boldsymbol{\xi}=\boldsymbol{\psi}^{-1}$ to remain true, we cannot invoke also the stationarity of the action functional with respect to $\boldsymbol{\psi}$ since in that case we would obtain the Euler-Lagrange equation

$$\left.\frac{\partial \mathcal{L}}{\partial \mathbf{X}}\right|_1 = \frac{\partial \mathcal{L}}{\partial \boldsymbol{\xi}} \frac{\partial (\boldsymbol{\psi})^{-1}}{\partial \mathbf{X}} = 0$$

which contradicts the aforementioned assumption.

We can also consider variations of the action with respect to $\boldsymbol{\psi}$ keeping constant $\boldsymbol{\phi} = \boldsymbol{\varphi} \circ \boldsymbol{\psi}$ instead of keeping constant $\boldsymbol{\varphi}$ as before. This can be accomplished by referring the action integral S to the defect reference configuration to obtain

$$S[\boldsymbol{\phi}, \boldsymbol{\psi}] = \int_{t_0}^{t_f} \int_D \mathcal{L}\left(\boldsymbol{\xi}, \boldsymbol{\psi}, t, \boldsymbol{\phi}, \dot{\boldsymbol{\phi}} - D\boldsymbol{\phi} D\boldsymbol{\psi}^{-1} \dot{\boldsymbol{\psi}}, D\boldsymbol{\phi} D\boldsymbol{\psi}^{-1}\right) \det(D\boldsymbol{\psi})\, d\boldsymbol{\xi} dt$$

The variations of this action with respect to $\boldsymbol{\psi}$ keeping $\boldsymbol{\phi}$ follow then as

$$\begin{aligned} \langle \delta S, \delta \psi_I \rangle &= \int_{t_0}^{t_f} \int_B \left(\left.\frac{\partial \mathcal{L}}{\partial X_I}\right|_2 \left(\delta \psi_I \circ \boldsymbol{\psi}^{-1}\right) + \frac{\partial \mathcal{L}}{\partial V_i} \left(-F_{iI}\right) \frac{d}{dt} \left(\delta \psi_I \circ \boldsymbol{\psi}^{-1}\right) + \right. \\ &\left. + \left(\mathcal{L} \delta_{IJ} - \frac{\partial \mathcal{L}}{\partial F_{iJ}} F_{iI}\right) \frac{d}{dX_J} \left(\delta \psi_I \circ \boldsymbol{\psi}^{-1}\right) \right) dV dt \end{aligned}$$

where now only the derivative with respect to the second kind of inhomogeneity $\left.\frac{\partial L}{\partial X_I}\right|_2$ is involved in the integrand. However, and as happened with variations of S with respect to $\boldsymbol{\psi}$ and keeping $\boldsymbol{\varphi}$ constant, we shall not demand

$$\langle \delta S, \delta \boldsymbol{\psi} \rangle = 0$$

since this contradicts the original hypothesis of a Lagrangian-dependent explicitly on $\boldsymbol{\xi}$.

We define now the total (internal) energy of a portion P of the body B as

$$E(t) = \int_P \left(-\mathcal{L}\left(\boldsymbol{\psi}^{-1}(\mathbf{X}, t), \mathbf{X}, t, \boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}, D\boldsymbol{\varphi}\right) + \frac{\partial \mathcal{L}}{\partial \mathbf{V}} \dot{\boldsymbol{\varphi}} + \frac{\partial \mathcal{L}}{\partial \boldsymbol{\varphi}} \boldsymbol{\varphi} \right) dV$$

Notice that for a Lagrangian density of the form $\mathcal{L} = \frac{1}{2} R \|\mathbf{V}\|^2 - A + \mathbf{B}\boldsymbol{\varphi}$ the previous takes the form

$$\begin{aligned} E(t) &= \int_P \left(W - \frac{1}{2} R \|\dot{\boldsymbol{\varphi}}\|^2 - \mathbf{B} \cdot \boldsymbol{\varphi} + R \dot{\boldsymbol{\varphi}} \cdot \dot{\boldsymbol{\varphi}} + \mathbf{B} \cdot \boldsymbol{\varphi} \right) dV = \\ &= \int_P \left(A + \frac{1}{2} R \|\dot{\boldsymbol{\varphi}}\|^2 \right) dV \end{aligned}$$

which corresponds the standard definition of total (internal) energy of a subbody P. Differentiating the total energy with respect to time we find

$$\begin{aligned}\dot{E}(t) &= \int_P \left(-\frac{\partial \mathcal{L}}{\partial \boldsymbol{\xi}}\frac{d}{dt}\left(\boldsymbol{\psi}^{-1}\right) - \frac{\partial \mathcal{L}}{\partial t} - \frac{\partial \mathcal{L}}{\partial \boldsymbol{\varphi}}\dot{\boldsymbol{\varphi}} - \frac{\partial \mathcal{L}}{\partial \mathbf{V}}\ddot{\boldsymbol{\varphi}} - \frac{\partial \mathcal{L}}{\partial \mathbf{F}}D\dot{\boldsymbol{\varphi}} + \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \mathbf{V}}\dot{\boldsymbol{\varphi}} + \frac{\partial \mathcal{L}}{\partial \varphi}\boldsymbol{\varphi}\right)\right) dV = \\ &= \int_P \left(-\frac{\partial \mathcal{L}}{\partial \boldsymbol{\xi}}\frac{d}{dt}\left(\boldsymbol{\psi}^{-1}\right) - \frac{\partial \mathcal{L}}{\partial t} - \frac{\partial \mathcal{L}}{\partial \mathbf{F}}D\dot{\boldsymbol{\varphi}} + \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \mathbf{V}}\right)\dot{\boldsymbol{\varphi}} + \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \varphi}\right)\boldsymbol{\varphi}\right) dV\end{aligned}$$

Integrating by parts in the third factor and on account of the identity

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{\xi}}\frac{d}{dt}\left(\boldsymbol{\psi}^{-1}\right) = -\frac{\partial \mathcal{L}}{\partial \boldsymbol{\xi}}D\boldsymbol{\psi}^{-1}\left(\dot{\boldsymbol{\psi}} \circ \boldsymbol{\psi}^{-1}\right) = -\left.\frac{\partial \mathcal{L}}{\partial \mathbf{X}}\right|_1 \left(\dot{\boldsymbol{\psi}} \circ \boldsymbol{\psi}^{-1}\right)$$

the rate of change of total energy $\dot{E}$ can be rewritten as

$$\begin{aligned}\dot{E}(t) &= \int_P \left(-\left.\frac{\partial \mathcal{L}}{\partial \mathbf{X}}\right|_1 \left(\dot{\boldsymbol{\psi}} \circ \boldsymbol{\psi}^{-1}\right) - \left(\frac{\partial \mathcal{L}}{\partial t} - \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \varphi}\right)\boldsymbol{\varphi}\right)\right) dV \\ &+ \int_P -\dot{\boldsymbol{\varphi}}\left(\frac{\partial \mathcal{L}}{\partial \boldsymbol{\varphi}} - \frac{d}{d\mathbf{X}}\left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right) - \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \mathbf{V}}\right)\right) dV \\ &+ \int_{\partial P} \dot{\boldsymbol{\varphi}}\left(-\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)\mathbf{N}dS + \int_{\partial B} \dot{\boldsymbol{\varphi}}\left(\frac{\partial \mathcal{L}}{\partial \varphi}\right) dV\end{aligned}$$

Assuming also that for every time t the Euler-Lagrange equations (3.46) are satisfied, we finally obtain

$$\begin{aligned}\dot{E}(t) &= \int_P \left(-\left.\frac{\partial \mathcal{L}}{\partial \mathbf{X}}\right|_1 \left(\dot{\boldsymbol{\psi}} \circ \boldsymbol{\psi}^{-1}\right) - \left(\frac{\partial L}{\partial t} - \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \varphi}\right)\boldsymbol{\varphi}\right)\right) dV \\ &+ \int_{\partial B} \dot{\boldsymbol{\varphi}}\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\mathbf{N}dS + \int_{\partial B} \dot{\boldsymbol{\varphi}}\frac{\partial \mathcal{L}}{\partial \boldsymbol{\varphi}} dV\end{aligned}$$

In particular, for Lagrangian densities of the form

$$\mathcal{L} = \frac{1}{2}R\left\|\mathbf{V}\right\|^2 - A\left(\boldsymbol{\xi}, \mathbf{X}, \mathbf{F}\right) + \mathbf{B}\boldsymbol{\varphi}$$

we have

$$\frac{\partial L}{\partial t} - \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \varphi}\right)\boldsymbol{\varphi} = \dot{\mathbf{B}}\boldsymbol{\varphi} - \dot{\mathbf{B}}\boldsymbol{\varphi} = \mathbf{0}$$

and the rate of change of energy follows in this case as

$$\dot{E}(t) = \int_P -\left.\frac{\partial \mathcal{L}}{\partial \mathbf{X}}\right|_1 \left(\dot{\boldsymbol{\psi}} \circ \boldsymbol{\psi}^{-1}\right) dV + \int_{\partial B} \dot{\boldsymbol{\varphi}}\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\mathbf{N}dS + \int_{\partial B} \dot{\boldsymbol{\varphi}}\frac{\partial \mathcal{L}}{\partial \boldsymbol{\varphi}} dV$$

We can see therefore that for materials with explicit dependence of A on $\boldsymbol{\xi}$ and Lagrangian densities of the form $\mathcal{L} = \frac{1}{2}R\left\|\mathbf{V}\right\|^2 - A + \mathbf{B}\boldsymbol{\varphi}$, the rate of change of the total energy of a portion P of the body depends not only on the power of external forces $\mathbf{P} = -\frac{\partial \mathcal{L}}{\partial \mathbf{F}}$ and $\mathbf{B} = \frac{\partial \mathcal{L}}{\partial \boldsymbol{\varphi}}$ but also on the evolution of the defects evolving within this portion P. We thus define energy release rate as

$$G(t) = \int_P -\left.\frac{\partial \mathcal{L}}{\partial \mathbf{X}}\right|_1 \left(\dot{\boldsymbol{\psi}} \circ \boldsymbol{\psi}^{-1}\right) dV$$

Using the pull-back relation (3.46) we have the identity

$$G(t) = \int_P \left(\left.\frac{\partial \mathcal{L}}{\partial \mathbf{X}}\right|_2 - \frac{d}{dt}\left(-\mathbf{F}^T \frac{\partial \mathcal{L}}{\partial \mathbf{V}}\right) - \frac{d}{d\mathbf{X}}\left(\mathcal{L}\mathbf{I} - \mathbf{F}^T \frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)\right) \left(\dot{\boldsymbol{\psi}} \circ \boldsymbol{\psi}^{-1}\right) dV$$

We finally define the dynamic $\mathbf{J}-$integral $\mathbf{J}^{dyn}$ as

$$\begin{aligned} \mathbf{J}^{dyn}(t) &= \int_P \left(\left.\frac{\partial \mathcal{L}}{\partial \mathbf{X}}\right|_2 - \frac{d}{dt}\left(-\mathbf{F}^T \frac{\partial \mathcal{L}}{\partial \mathbf{V}}\right) - \frac{d}{d\mathbf{X}}\left(\mathcal{L}\mathbf{I} - \mathbf{F}^T \frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right)\right) dV = \\ &= \int_P \left(\left.\frac{\partial \mathcal{L}}{\partial \mathbf{X}}\right|_2 - \frac{d}{dt}\left(-\mathbf{F}^T \frac{\partial \mathcal{L}}{\partial \mathbf{V}}\right)\right) dV - \int_{\partial P} \left(\mathcal{L}\mathbf{I} - \mathbf{F}^T \frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right) \mathbf{N} dS \end{aligned}$$

Then if the defects move at uniform velocity, i.e., if the field $\mathbf{W} = \dot{\boldsymbol{\psi}} \circ \boldsymbol{\psi}^{-1}$ is not a function of $\mathbf{X}$, then we have the result

$$G(t) = \mathbf{J}^{dyn}(t) \cdot \mathbf{W}(t)$$

3.3.6 Space-space bundle

The variational formulation outlined in the previous subsections admits the following geometrical interpretation: consider the "space-space" bundle, i.e., the set $E = B \times S$ where $S = \mathbb{R}^n$ is the ambient space, figure 3.2. Local coordinates for this bundle are $\left(X^I, x^i\right)$ and its projection map is $\boldsymbol{\pi} : E \to B$ given in coordinates by $\pi^I\left(X^I, x^i\right) = X^I$. For a fixed time t we consider the graph $\mathbf{f}_t(\mathbf{X}) = (\mathbf{X}, \boldsymbol{\varphi}(\mathbf{X}, t))$ of the deformation mapping $\boldsymbol{\varphi}$ at time t. This graph is an n-dimensional manifold immersed in $2n$-dimensional space, the space-space bundle, and is one of its sections, i.e., $\pi \circ \mathbf{f}_t = Id : B \to B$, the identity map in B. Therefore, rather than looking at the motion $\varphi(X, t)$ as a time-dependent family of mappings from B to S we shall regard it as an evolving manifold or section in the space-space bundle $B \times S$.

We next notice that for a one-dimensional body undergoing one-dimensional deformations, i.e., when $B \subset \mathbb{R}$ and $S = \mathbb{R}$, the graph $\mathbf{f}_t(X) = (X, \varphi(X, t))$ becomes a curve in $B \times S = \mathbb{R}^2$ with X acting as parameter (figure(3.2)). For this curve the tangent vector will be given by

$$\mathbb{T} = \frac{d\mathbf{f}_t}{dX} = \begin{pmatrix} 1 \\ F \end{pmatrix}$$

where $F = \frac{\partial \varphi}{\partial X}$ is the deformation gradient at time t. Furthermore, if the standard euclidean inner

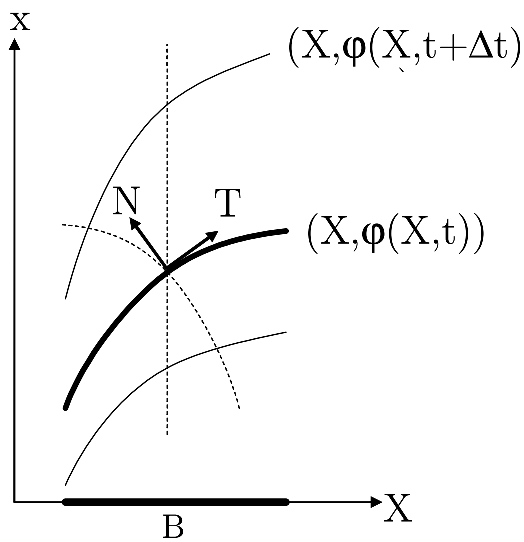

Figure 3.2: The graph of the deformation mapping as a manifold (section) of the space-space bundle. Finding the motion is equivalent to finding the evolution of this manifold.

product in $\mathbb{R}^2$ is used, then a vector in the normal direction will be

$$\mathbb{N}^* = (-F, 1)$$

since

$$\mathbb{N}^* \cdot \mathbb{T} = (-F, 1) \begin{pmatrix} 1 \\ F \end{pmatrix} = 0$$

Analogously, for an n-dimensional body immersed and deforming in n-dimensional space we may define the tangent vectors to the manifold $\mathbf{f}_t(\mathbf{X})$ as

$$\mathbb{T}_J = \frac{\partial \mathbf{f}_t}{\partial X_J} = \begin{pmatrix} \delta^I{}_J \\ F^i{}_J \end{pmatrix} = \begin{pmatrix} \mathbf{I} \\ \mathbf{F} \end{pmatrix} \tag{3.48}$$

and a (co)vectors in the normal direction as

$$\mathbb{N}^* = \left(-F^i{}_J, \delta^i{}_j\right) = (-\mathbf{F}, \mathbf{i}) \tag{3.49}$$

where $\mathbf{I}$ and $\mathbf{i}$ are, respectively, the metric tensors in B and S. Also, the tangent covector may be defined as

$$\mathbb{T}^* = \left(\delta_I{}^J, F_i{}^J\right) = \left(\mathbf{I}, \mathbf{F}^T\right) \tag{3.50}$$

and a normal vector as

$$\mathbb{N} = \begin{pmatrix} -F_i{}^J \\ \delta_i{}^j \end{pmatrix} = \begin{pmatrix} -\mathbf{F}^T \\ \mathbf{i} \end{pmatrix} \tag{3.51}$$

We have

$$\begin{aligned} \mathbb{N}^* \cdot \mathbb{T} &= \left(-F^i{}_J, \delta^i{}_j\right) \cdot \begin{pmatrix} \delta^J{}_K \\ F^j{}_K \end{pmatrix} = -F^i{}_K + F^i{}_K = \mathbf{0} \\ \mathbb{T}^* \cdot \mathbb{N} &= \left(\delta_J{}^I, F_j{}^I\right) \cdot \begin{pmatrix} -F_k{}^J \\ \delta_k{}^j \end{pmatrix} = -F_k{}^I + F_k{}^I = -\left(\mathbf{F}^T\right)^I{}_k + \left(\mathbf{F}^T\right)^I{}_k = \mathbf{0} \end{aligned}$$

where we are using the following inner product in $B \times S$ to define orthogonality:

$$\begin{aligned} \mathbb{A}^* \cdot \mathbb{B} &= (A_J, a_j) \cdot \begin{pmatrix} B^K \\ b^k \end{pmatrix} \\ &= (A_J, a_j) \begin{pmatrix} \delta^J_K & 0 \\ 0 & \delta^j_k \end{pmatrix} \begin{pmatrix} B^K \\ b^k \end{pmatrix} = \\ &= A_J \delta^J_K B^K + a_j \delta^j_k b^k = \\ &= A_J B^J + a_j b^j \end{aligned}$$

We now observe that $\mathbf{f}_t(\mathbf{X}) = (\mathbf{X}, \boldsymbol{\varphi}(\mathbf{X}, t))$ is only a particular parametrization of the manifold at time t, i.e., a parametrization with parameter $\mathbf{X}$. Consider any alternative parametrization $\mathbf{g}_t(\boldsymbol{\xi}) = (\boldsymbol{\psi}(\boldsymbol{\xi}, t), \boldsymbol{\phi}(\boldsymbol{\xi}, t))$ of the *same* manifold, where $\boldsymbol{\xi} \in D$ is a new parameter and D is the parameter set. For $\mathbf{f}_t(\mathbf{X})$ and $\mathbf{g}_t(\boldsymbol{\xi})$ to be two different parametrizations of the same manifold, the component functions must be related by

$$\boldsymbol{\varphi}(\boldsymbol{\psi}(\boldsymbol{\xi}, t), t) = \boldsymbol{\phi}(\boldsymbol{\xi}, t) \tag{3.52}$$

that corresponds to equation (3.17). The velocity of the parametrized points on the manifold will be given by

$$\frac{d}{dt}\mathbf{f}_t(\mathbf{X}) = (0, \dot{\boldsymbol{\varphi}})$$

when the manifold is parametrized using $\mathbf{f}_t(\mathbf{X})$, and by

$$\frac{d}{dt}\mathbf{g}_t(\boldsymbol{\xi}) = \left(\dot{\boldsymbol{\psi}}, \dot{\boldsymbol{\phi}}\right)$$

when parametrized using $\mathbf{g}_t(\boldsymbol{\xi})$. Differentiating identity (3.52) with respect to time and rearranging yields

$$\begin{aligned} \dot{\boldsymbol{\varphi}} &= \dot{\boldsymbol{\phi}} - \mathbf{F}\dot{\boldsymbol{\psi}} = \\ &= (-\mathbf{F}, \mathbf{i}) \cdot \begin{pmatrix} \dot{\boldsymbol{\psi}} \\ \dot{\boldsymbol{\phi}} \end{pmatrix} = \\ &= \mathbb{N}^* \cdot \begin{pmatrix} \dot{\boldsymbol{\psi}} \\ \dot{\boldsymbol{\phi}} \end{pmatrix} \end{aligned} \tag{3.53}$$

which may be rewritten as

$$\mathbf{V} = \mathbb{N}^* \cdot \begin{pmatrix} 0 \\ \dot{\boldsymbol{\varphi}} \end{pmatrix} = \mathbb{N}^* \cdot \begin{pmatrix} \dot{\boldsymbol{\psi}} \\ \dot{\boldsymbol{\phi}} \end{pmatrix}$$

where $\mathbf{V}$ is the material velocity and $\mathbb{N}$ is the (co)normal to the manifold. This identity has the following geometrical interpretation (3.3). The normal projection of the manifold velocity onto the normal direction to the manifold is independent of the parametrization and coincident with the material velocity $\mathbf{V}$. Different parametrizations of the manifold will render different manifold velocities, however with identical normal component.

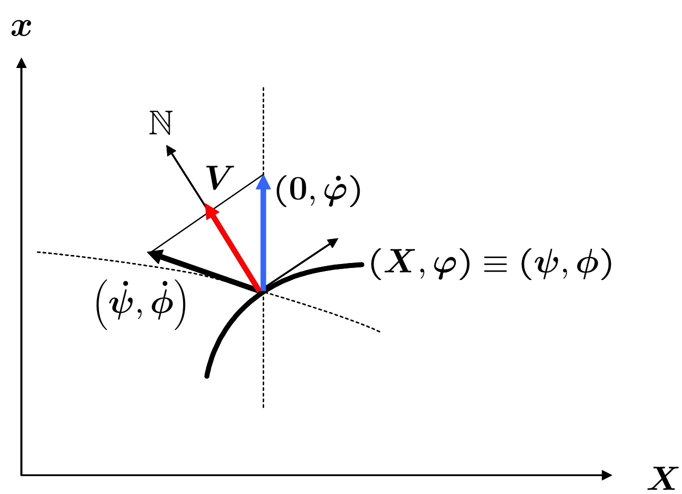

Figure 3.3: Representation of the relation between the *graph* velocities ($(\mathbf{0}, \dot{\boldsymbol{\varphi}})$ when the graph is parametrized with parameter $\mathbf{X}$ and $\left(\dot{\boldsymbol{\psi}}, \dot{\boldsymbol{\phi}}\right)$ when it is parametrized with parameter $\boldsymbol{\xi}$) and the material velocity $\mathbf{V}$. The latter is the projection of the graph velocity onto the normal $\mathbb{N}$ to the graph.

3.3.7 Horizontal-Vertical Variations—Tangential-Normal variations

We have reinterpreted each configuration parametrized either as $(\mathbf{X}, \boldsymbol{\varphi}(\mathbf{X}))$ or as $(\boldsymbol{\psi}(\boldsymbol{\xi}), \boldsymbol{\phi}(\boldsymbol{\xi}))$ as a manifold in the space-space bundle $B \times S$. This space can be conceptually represented (see reference [29]) in two axes, the horizontal axis for the body B and the vertical axis for the ambient space S. From this representation, variations with respect to $\boldsymbol{\psi}$ and $\boldsymbol{\phi}$ may be easily interpreted as follows: A variation $(\mathbf{0}, \delta\boldsymbol{\phi})$ can be regarded as a vertical perturbation of the surface $(\boldsymbol{\psi}, \boldsymbol{\phi})$ and a variation $(\delta\boldsymbol{\psi}, \mathbf{0})$ as an horizontal perturbation (Figure (3.4)). Therefore variations on $\boldsymbol{\psi}$ are also called *horizontal* variations while variations $\delta\boldsymbol{\phi}$ are named *vertical* variations.We notice that for

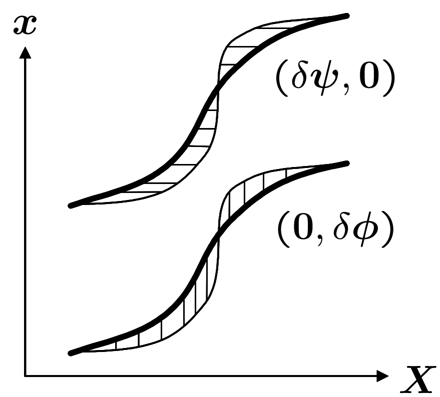

Figure 3.4: Horizontal and vertical variations. Every horizontal variation might be interpreted as a vertical variation and reciprocally. Therefore variations of the action with respect to horizontal and vertical variations are equivalent.

smooth configurations $(\boldsymbol{\psi}, \boldsymbol{\phi})$, every vertical variation can be interpreted as a horizontal variation and conversely, every horizontal variation can be regarded as a vertical variation. This provides a geometrical justification of the fact that variations of the action functional (3.20) with respect to horizontal and vertical variations are equivalent in the absence of singular defects.

Alternatively we may illustrate this equivalence by considering *tangential* and *normal* variations as shown in figure 3.5. For smooth configurations, an admissible variation $\delta\mathbf{T}$ in the tangent direction

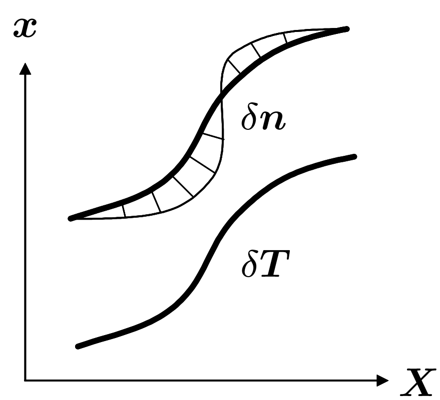

Figure 3.5: Tangential and normal variations. For smooth configurations, variations in the tangential direction and vanishing at the end points leave the configuration unperturbed.

(a variation in the tangent direction that vanishes in the boundary of the body B) will leave the configuration unperturbed. Therefore the action will remain itself unperturbed (symmetric) with respect to tangential variations if it is only a function of the configuration $\boldsymbol{\varphi} = \boldsymbol{\phi} \circ \boldsymbol{\psi}^{-1}$, namely,

$$\langle \delta S, \delta \mathbf{T} \rangle = 0 \qquad \forall \delta \mathbf{T}$$

This statement may be easily verified by computing tangential and normal variations and making use of the pull-back property (3.42). To do this notice first that on account of (3.25) and (3.32) and by making use of the notation (3.37) and (3.38), horizontal and vertical (admissible) variations can be written as

$$\begin{aligned} \langle \delta S, \delta \boldsymbol{\phi} \rangle &= \int_{t_0}^{t_f} \int_B \left(\delta \boldsymbol{\phi}^T \cdot \mathcal{F}_{\boldsymbol{\phi}} \left(\boldsymbol{\varphi} \right) \right) dV dt \\ \langle \delta S, \delta \boldsymbol{\psi} \rangle &= \int_{t_0}^{t_f} \int_B \left\{ \delta \boldsymbol{\psi}^T \cdot \mathcal{F}_{\boldsymbol{\psi}} \left(\boldsymbol{\varphi} \right) \right\} dV dt \end{aligned}$$

where the boundary terms of (3.25) and (3.32) vanish if $(\delta \boldsymbol{\psi}, \delta \boldsymbol{\phi})$ are admissible. Combining both we find

$$\begin{aligned} \langle \delta S, \delta \boldsymbol{\psi} \rangle + \langle \delta S, \delta \boldsymbol{\phi} \rangle &= \int_{t_0}^{t_f} \int_B \left\{ \delta \boldsymbol{\psi}^T \cdot \mathcal{F}_{\boldsymbol{\psi}} \left(\boldsymbol{\varphi} \right) + \delta \boldsymbol{\phi}^T \cdot \mathcal{F}_{\boldsymbol{\phi}} \left(\boldsymbol{\varphi} \right) \right\} dV dt = \\ &= \int_{t_0}^{t_f} \int_B \left\{ \left(\delta \boldsymbol{\psi}^T, \delta \boldsymbol{\phi}^T \right) \cdot \begin{pmatrix} \mathcal{F}_{\boldsymbol{\psi}} \left(\boldsymbol{\varphi} \right) \\ \mathcal{F}_{\boldsymbol{\phi}} \left(\boldsymbol{\varphi} \right) \end{pmatrix} \right\} dV dt \end{aligned} \tag{3.54}$$

Tangential and normal variations $(\delta \mathbf{T}, \delta \mathbf{n})$ are defined as components on the tangential and normal directions $\mathbb{T}$ and $\mathbb{N}$ of horizontal and vertical variations $\left(\delta \boldsymbol{\psi}^T, \delta \boldsymbol{\phi}^T \right)$, namely,

$$\begin{aligned} \left(\delta \boldsymbol{\psi}^T, \delta \boldsymbol{\phi}^T \right) &= \delta \mathbf{n}^T \cdot \mathbb{N}^* + \delta \mathbf{T}^T \cdot \mathbb{T}^* = \\ &= \delta \mathbf{n}^T \cdot (-\mathbf{F}, \mathbf{i}) + \delta \mathbf{T}^T \cdot \left(\mathbf{I}, \mathbf{F}^T \right) \\ &= \left(\delta \mathbf{T}^T - \delta \mathbf{n}^T \cdot \mathbf{F}, \delta \mathbf{n}^T + \delta \mathbf{T}^T \cdot \mathbf{F}^T \right) \end{aligned}$$

In coordinates the previous yields

$$\begin{aligned} \left(\delta \psi_J, \delta \phi_j \right) &= \delta n_i \left(-F^i{}_J, \delta^i{}_j \right) + \delta T_I \left(\delta_J{}^I, F_j{}^I \right) \\ &= \left(\delta T_J - F^i{}_J \delta n_i, \delta n_j + F_j{}^I \delta T_I \right) \end{aligned}$$

Substituting this definition in the combined variations (3.54) we find

$$\begin{aligned} \langle \delta S, \delta \boldsymbol{\psi} \rangle + \langle \delta S, \delta \boldsymbol{\phi} \rangle &= \int_{t_0}^{t_f} \int_B \left\{ \delta \mathbf{n}^T \cdot (-\mathbf{F}, \mathbf{i}) \cdot \begin{pmatrix} \mathcal{F}_{\boldsymbol{\psi}} \left(\boldsymbol{\varphi} \right) \\ \mathcal{F}_{\boldsymbol{\phi}} \left(\boldsymbol{\varphi} \right) \end{pmatrix} + \delta \mathbf{T}^T \cdot \left(\mathbf{I}, \mathbf{F}^T \right) \cdot \begin{pmatrix} \mathcal{F}_{\boldsymbol{\psi}} \left(\boldsymbol{\varphi} \right) \\ \mathcal{F}_{\boldsymbol{\phi}} \left(\boldsymbol{\varphi} \right) \end{pmatrix} \right\} dV dt = \\ &= \langle \delta S, \delta \mathbf{n} \rangle + \langle \delta S, \delta \mathbf{T} \rangle \end{aligned}$$

Therefore, tangential and normal variations will be given by

$$\begin{aligned}
\langle \delta S, \delta \mathbf{T} \rangle &= \int_{t_0}^{t_f} \int_B \delta \mathbf{T}^T \cdot \left(\mathbf{I}, \mathbf{F}^T \right) \cdot \begin{pmatrix} \mathcal{F}_{\boldsymbol{\psi}}(\boldsymbol{\varphi}) \\ \mathcal{F}_{\boldsymbol{\phi}}(\boldsymbol{\varphi}) \end{pmatrix} dV\, dt = \\
&= \int_{t_0}^{t_f} \int_B \delta \mathbf{T}^T \cdot \mathbb{T}^* \cdot \begin{pmatrix} \mathcal{F}_{\boldsymbol{\psi}}(\boldsymbol{\varphi}) \\ \mathcal{F}_{\boldsymbol{\phi}}(\boldsymbol{\varphi}) \end{pmatrix} dV\, dt = \\
&= \int_{t_0}^{t_f} \int_B \delta \mathbf{T}^T \cdot \left(\mathcal{F}_{\boldsymbol{\psi}}(\boldsymbol{\varphi}) + \mathbf{F}^T \mathcal{F}_{\boldsymbol{\phi}}(\boldsymbol{\varphi}) \right) dV\, dt
\end{aligned}$$

$$\begin{aligned}
\langle \delta S, \delta \mathbf{n} \rangle &= \int_{t_0}^{t_f} \int_B \delta \mathbf{n}^T \cdot (-\mathbf{F}, \mathbf{i}) \cdot \begin{pmatrix} \mathcal{F}_{\boldsymbol{\psi}}(\boldsymbol{\varphi}) \\ \mathcal{F}_{\boldsymbol{\phi}}(\boldsymbol{\varphi}) \end{pmatrix} dV\, dt = \\
&= \int_{t_0}^{t_f} \int_B \delta \mathbf{n}^T \cdot \mathbb{N}^* \cdot \begin{pmatrix} \mathcal{F}_{\boldsymbol{\psi}}(\boldsymbol{\varphi}) \\ \mathcal{F}_{\boldsymbol{\phi}}(\boldsymbol{\varphi}) \end{pmatrix} dV\, dt = \\
&= \int_{t_0}^{t_f} \int_B \delta \mathbf{n}^T \cdot \left(-\mathbf{F} \mathcal{F}_{\boldsymbol{\psi}}(\boldsymbol{\varphi}) + \mathcal{F}_{\boldsymbol{\phi}}(\boldsymbol{\varphi}) \right) dV\, dt
\end{aligned}$$

with corresponding tangential and normal Euler-Lagrange equations

$$\begin{aligned}
\mathcal{F}_{\mathbf{T}}(\boldsymbol{\varphi}) &= \mathbb{T}^* \cdot \begin{pmatrix} \mathcal{F}_{\boldsymbol{\psi}}(\boldsymbol{\varphi}) \\ \mathcal{F}_{\boldsymbol{\phi}}(\boldsymbol{\varphi}) \end{pmatrix} = \\
&= \mathcal{F}_{\boldsymbol{\psi}}(\boldsymbol{\varphi}) + \mathbf{F}^T \mathcal{F}_{\boldsymbol{\phi}}(\boldsymbol{\varphi}) = \mathbf{0} \\
\mathcal{F}_{\mathbf{n}}(\boldsymbol{\varphi}) &= \mathbb{N}^* \cdot \begin{pmatrix} \mathcal{F}_{\boldsymbol{\psi}}(\boldsymbol{\varphi}) \\ \mathcal{F}_{\boldsymbol{\phi}}(\boldsymbol{\varphi}) \end{pmatrix} = \\
&= -\mathbf{F} \mathcal{F}_{\boldsymbol{\psi}}(\boldsymbol{\varphi}) + \mathcal{F}_{\boldsymbol{\phi}}(\boldsymbol{\varphi}) = \mathbf{0}
\end{aligned}$$

We now recall that from the pull-back relation (3.42) we have

$$\begin{aligned}
\begin{pmatrix} \mathcal{F}_{\boldsymbol{\psi}}(\boldsymbol{\varphi}) \\ \mathcal{F}_{\boldsymbol{\phi}}(\boldsymbol{\varphi}) \end{pmatrix} &= \begin{pmatrix} -\mathbf{F}^T \\ \mathbf{i} \end{pmatrix} \mathcal{F}_{\boldsymbol{\phi}}(\boldsymbol{\varphi}) = \\
&= \mathbb{N} \mathcal{F}_{\boldsymbol{\phi}}(\boldsymbol{\varphi})
\end{aligned}$$

Therefore tangential and normal variations reduce to

$$\begin{aligned}
\langle \delta S, \delta \mathbf{T} \rangle &= \int_{t_0}^{t_f} \int_B \delta \mathbf{T}^T \cdot \left(\mathbf{I}, \mathbf{F}^T \right) \cdot \begin{pmatrix} -\mathbf{F}^T \\ \mathbf{i} \end{pmatrix} \mathcal{F}_{\boldsymbol{\phi}}(\boldsymbol{\varphi})\, dV\, dt = \\
&= \int_{t_0}^{t_f} \int_B \delta \mathbf{T}^T \cdot \left(\mathbb{T}^* \cdot \mathbb{N} \right) \mathcal{F}_{\boldsymbol{\phi}}(\boldsymbol{\varphi})\, dV\, dt \\
&= \mathbf{0}
\end{aligned}$$

$$\begin{aligned}
\langle \delta S, \delta \mathbf{n} \rangle &= \int_{t_0}^{t_f} \int_B \delta \mathbf{n}^T \cdot (-\mathbf{F}, \mathbf{i}) \cdot \begin{pmatrix} -\mathbf{F}^T \\ \mathbf{i} \end{pmatrix} \mathcal{F}_{\boldsymbol{\phi}} (\boldsymbol{\varphi}) \, dV dt = \\
&= \int_{t_0}^{t_f} \int_B \delta \mathbf{n}^T \cdot (\mathbb{N}^* \cdot \mathbb{N}) \, \mathcal{F}_{\boldsymbol{\phi}} (\boldsymbol{\varphi}) \, dV dt = \\
&= \int_{t_0}^{t_f} \int_B \delta \mathbf{n}^T \cdot \|\mathbb{N}\|^2 \, \mathrm{el} (\boldsymbol{\varphi}) \, dV dt
\end{aligned}$$

where

$$\begin{aligned}
\|\mathbb{N}\|^2 &= (\mathbb{N}^* \cdot \mathbb{N}) = \\
&= (-\mathbf{F}, \mathbf{i}) \cdot \begin{pmatrix} -\mathbf{F}^T \\ \mathbf{i} \end{pmatrix} \\
&= \mathbf{i} + \mathbf{F}\mathbf{F}^T
\end{aligned}$$

In coordinates

$$\begin{aligned}
\left\langle \delta S, \delta T^I \right\rangle &= 0 \\
\left\langle \delta S, \delta n^i \right\rangle &= \int_{t_0}^{t_f} \int_B \delta n_i \left(\|\mathbb{N}\|^2 \right)^i{}_j \left(\mathcal{F}_{\boldsymbol{\phi}} (\boldsymbol{\varphi}) \right)^j dV dt = \\
&= \int_{t_0}^{t_f} \int_B \delta n^i \left(\|\mathbb{N}\|^2 \right)_i{}^j \left(\mathcal{F}_{\boldsymbol{\phi}} (\boldsymbol{\varphi}) \right)^j dV dt
\end{aligned}$$

where

$$\begin{aligned}
\left(\|\mathbb{N}\|^2 \right)^i{}_j &= \delta^i{}_j + F^i{}_J F_j{}^J \\
\left(\|\mathbb{N}\|^2 \right)_i{}^j &= \delta_i{}^j + F_i{}^J F^j{}_J
\end{aligned}$$

Summarizing, tangential variations vanish identically for materials with no singular defects, and the Euler-Lagrange equations corresponding to normal variations are equal to the Euler-Lagrange equation corresponding to vertical variations multiplied by the spatial tensor $\|\mathbb{N}\|^2 = \mathbf{i} + \mathbf{F}\mathbf{F}^T$.

3.3.8 Equations of motion in "Space-Space"

The equations of balance of configurational and mechanical forces (3.34) and (3.33) are therefore the Euler-Lagrange equations corresponding to the horizontal and vertical components of variations in the configuration regarded as subset of the space-space bundle $B \times S$. Being components in a higher dimensional combined space it is useful to write them jointly as a single $2n$-dimensional equation rather than two separately n-dimensional equations. We thus obtain

$$\begin{aligned}\begin{pmatrix} (\mathcal{F}_{\boldsymbol{\psi}}(\boldsymbol{\varphi}))_I \\ (\mathcal{F}_{\boldsymbol{\phi}}(\boldsymbol{\varphi}))_i \end{pmatrix} &= \begin{pmatrix} \frac{\partial \mathcal{L}}{\partial X_I} \\ \frac{\partial \mathcal{L}}{\partial \varphi_i} \end{pmatrix} - \frac{d}{dt}\left(\begin{pmatrix} -F^j{}_I \\ \delta^j{}_i \end{pmatrix} \frac{\partial \mathcal{L}}{\partial V_j}\right) - \frac{d}{dX_J}\begin{pmatrix} \mathcal{L}\delta^J_I - \frac{\partial \mathcal{L}}{\partial F^i{}_J} F^i{}_I \\ \frac{\partial \mathcal{L}}{\partial F^i{}_J} \end{pmatrix} \\ &= \begin{pmatrix} 0 \\ 0 \end{pmatrix}\end{aligned}$$

or in invariant notation

$$\begin{aligned}\begin{pmatrix} \mathcal{F}_{\boldsymbol{\psi}}(\boldsymbol{\varphi}) \\ \mathcal{F}_{\boldsymbol{\phi}}(\boldsymbol{\varphi}) \end{pmatrix} &= \begin{pmatrix} \frac{\partial}{\partial \mathbf{X}} \\ \frac{\partial}{\partial \boldsymbol{\varphi}} \end{pmatrix} \mathcal{L} - \frac{d}{dt}\left(\begin{pmatrix} -\mathbf{F}^T \\ \mathbf{i} \end{pmatrix} \frac{\partial \mathcal{L}}{\partial \mathbf{V}}\right) + \mathrm{DIV}\begin{pmatrix} \mathbf{C} \\ \mathbf{P} \end{pmatrix} \\ &= \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \end{pmatrix}\end{aligned}$$

where

$$\begin{pmatrix} \mathbf{C} \\ \mathbf{P} \end{pmatrix} = -\begin{pmatrix} \mathcal{L}\mathbf{I} - \mathbf{F}^T \frac{\partial \mathcal{L}}{\partial \mathbf{F}} \\ \frac{\partial \mathcal{L}}{\partial \mathbf{F}} \end{pmatrix}$$

are the Eshelby tensor and the Piolla-Kirchhoff stress tensors regarded as a tensor on $B \times S$ and

$$\mathbf{V} = \dot{\boldsymbol{\varphi}}$$

is the material velocity at time t, related to the manifold velocity $\left(\dot{\boldsymbol{\psi}}, \dot{\boldsymbol{\phi}}\right)$ by (3.53). For a Lagrangian density of the form (3.3) the above reads

$$\begin{pmatrix} \mathbf{B}^{inh} \\ \mathbf{B} \end{pmatrix} - \frac{d}{dt}\left(\begin{pmatrix} -\mathbf{F}^T \\ \mathbf{i} \end{pmatrix} R\mathbf{V}\right) + \mathrm{DIV}\begin{pmatrix} \mathbf{C} \\ \mathbf{P} \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \end{pmatrix}$$

with

$$\mathbf{B}^{inh} = \left.\frac{\partial \mathcal{L}}{\partial \mathbf{X}}\right|_{\exp} = \left(\frac{1}{2}\frac{\partial R}{\partial \mathbf{X}} |\mathbf{V}|^2 - \left.\frac{\partial W}{\partial \mathbf{X}}\right|_{\exp}\right)$$

Combining with (3.53) and rearranging we obtain the differential system

$$\begin{aligned}\frac{d}{dt}\left(\begin{pmatrix} -\mathbf{F}^T \\ \mathbf{i} \end{pmatrix} R\mathbf{V}\right) &= \mathrm{DIV}\begin{pmatrix} \mathbf{C} \\ \mathbf{P} \end{pmatrix} + \begin{pmatrix} \mathbf{B}^{inh} \\ \mathbf{B} \end{pmatrix} \\ \mathbf{V} &= (-\mathbf{F}, \mathbf{i}) \cdot \begin{pmatrix} \dot{\boldsymbol{\psi}} \\ \dot{\boldsymbol{\phi}} \end{pmatrix}\end{aligned}$$

that may be rewritten as

$$\frac{d}{dt}\left(\begin{pmatrix} -\mathbf{F}^T \\ \mathbf{i} \end{pmatrix} R\left(-\mathbf{F},\mathbf{i}\right)\cdot\begin{pmatrix} \dot{\boldsymbol{\psi}} \\ \dot{\boldsymbol{\phi}} \end{pmatrix}\right) = \mathrm{DIV}\begin{pmatrix} \mathbf{C} \\ \mathbf{P} \end{pmatrix} + \begin{pmatrix} \mathbf{B}^{inh} \\ \mathbf{B} \end{pmatrix}$$

or more compactly as

$$\frac{d}{dt}\left(\mathbb{N}R\mathbb{N}^*\cdot\begin{pmatrix} \dot{\boldsymbol{\psi}} \\ \dot{\boldsymbol{\phi}} \end{pmatrix}\right) = \mathrm{DIV}\begin{pmatrix} \mathbf{C} \\ \mathbf{P} \end{pmatrix} + \begin{pmatrix} \mathbf{B}^{inh} \\ \mathbf{B} \end{pmatrix}$$

where $\mathbb{N}$ is a vector in the normal direction to the configuration at time t defined in (3.51). The above may be further simplified as

$$\frac{d}{dt}\left(\mathbb{M}\cdot\dot{\mathbf{q}}\right) = \mathrm{DIV}\left(\mathbb{P}\right) + \mathbb{B} \tag{3.55}$$

were $\mathbb{M}$ is the mass matrix in $B \times S$ given by

$$\begin{aligned} \mathbb{M} &= \mathbb{N}R\mathbb{N}^* = \\ &= \begin{pmatrix} -\mathbf{F}^T \\ \mathbf{i} \end{pmatrix} R\left(-\mathbf{F},\mathbf{i}\right) = \\ &= R\begin{pmatrix} \mathbf{F}^T\mathbf{F} & -\mathbf{F}^T \\ -\mathbf{F} & \mathbf{i} \end{pmatrix} \end{aligned} \tag{3.56}$$

the vector $\mathbf{q} \in B \times S$ is the array of combined horizontal/vertical coordinates

$$\begin{aligned} \mathbf{q} &= \begin{pmatrix} \boldsymbol{\psi} \\ \boldsymbol{\phi} \end{pmatrix} \\ \dot{\mathbf{q}} &= \begin{pmatrix} \dot{\boldsymbol{\psi}} \\ \dot{\boldsymbol{\phi}} \end{pmatrix} \end{aligned}$$

and

$$\begin{aligned} \mathbb{P} &= \begin{pmatrix} \mathbf{C} \\ \mathbf{P} \end{pmatrix} = -\begin{pmatrix} \mathcal{L}\mathbf{I} - \mathbf{F}^T\frac{\partial\mathcal{L}}{\partial\mathbf{F}} \\ \frac{\partial\mathcal{L}}{\partial\mathbf{F}} \end{pmatrix} \\ \mathbb{B} &= \begin{pmatrix} \mathbf{B}^{inh} \\ \mathbf{B} \end{pmatrix} = \begin{pmatrix} \frac{\partial\mathcal{L}}{\partial\mathbf{X}}\Big|_{\exp} \\ \frac{\partial\mathcal{L}}{\partial\boldsymbol{\varphi}} \end{pmatrix} \end{aligned}$$

are, respectively, the combined (horizontal/vertical) stress tensor and combined (horizontal/vertical) body forces. Equation (3.55) is thus an equation for the evolution of the manifold with coordinates

$\mathbf{q} = (\boldsymbol{\psi}, \boldsymbol{\phi})$ within the space-space bundle $B \times S$.

3.4 Configurational forces in the presence of viscosity

We recall from §3.2 (equation 3.59) that the equations of balance of mechanical forces in the presence of viscosity can be written as

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{\varphi}} - \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \mathbf{V}}\right) - \mathrm{DIV}\left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right) + \mathrm{DIV}\left(\mathbf{P}^v\right) = \mathbf{0} \qquad \text{in } B \text{ and } \forall t \in I$$

Using the Euler-Lagrange operator (3.37) the previous can be compactly written as

$$\mathcal{F}_{\boldsymbol{\phi}}\left(\boldsymbol{\varphi}\right) + \mathrm{DIV}\left(\mathbf{P}^v\right) = 0$$

We recall also that these equations do not derive from Hamilton's principle, but they can be established instead from the Lagrange-d'Alembert principle (3.16). Using vertical variations $\delta\boldsymbol{\phi}$ instead of full variations $\delta\boldsymbol{\varphi}$ in the previous, the following "vertical" version of Lagrange-d'Alembert principle is obtained

$$\begin{aligned}\langle \delta S, \delta \boldsymbol{\phi}\rangle &+ \int_{t_0}^{t_f}\int_B \left(\left(\delta\boldsymbol{\phi}^T \circ \boldsymbol{\psi}^{-1}\right) \mathrm{DIV}\left(\mathbf{P}^v\right)\right) dV dt \\ &+ \int_{t_0}^{t_f}\int_{\partial B_1} \left(\left(\delta\boldsymbol{\phi}^T \circ \boldsymbol{\psi}^{-1}\right)\left(-\mathbf{P}^v\right)\mathbf{N}\right) dS dt = \mathbf{0}\end{aligned}$$

where S is the action and $\langle \delta S, \delta \boldsymbol{\phi}\rangle$ are its vertical variations. Integrating by parts the viscosity terms and making use of the divergence theorem the (vertical) Lagrange-d'Alembert principle becomes

$$\langle \delta S, \delta \boldsymbol{\phi}\rangle - \int_{t_0}^{t_f}\int_B \left(\mathbf{P}^v \cdot \frac{\partial}{\partial \mathbf{X}}\left(\delta\boldsymbol{\phi} \circ \boldsymbol{\psi}^{-1}\right)\right) dV dt = \mathbf{0} \tag{3.57}$$

or, in Cartesian coordinates,

$$\langle \delta S, \delta \phi_i\rangle - \int_{t_0}^{t_f}\int_B \left(P^v_{iJ}\frac{\partial}{\partial X_J}\left(\delta\phi_i \circ \boldsymbol{\psi}^{-1}\right)\right) dV dt = 0$$

We turn now the equations of balance of configurational forces in the presence of viscosity. Following the approach of Maugin for materials with a general dissipative behavior [44], since we cannot use a direct variational principle (Hamilton's principle) as we did in the elastic case, we are required to establish the balance of configurational forces by a *direct* method, namely by multiplying (or pulling back) the equations of balance of mechanical forces with $\mathbf{F}^T$. On account of the identity

(3.41), multiplying equations (3.15) by $-\mathbf{F}^T$ yields

$$\frac{\partial \mathcal{L}}{\partial \mathbf{X}} - \frac{d}{dt}\left(\left(-\mathbf{F}^T\right)\frac{\partial \mathcal{L}}{\partial \mathbf{V}}\right) - \mathrm{DIV}\left(\mathcal{L}\mathbf{I} - \mathbf{F}^T\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right) + \left(-\mathbf{F}^T\right)\mathrm{DIV}\left(\mathbf{P}^v\right) = \mathbf{0} \qquad \text{in } B \text{ and } \forall t \in I \quad (3.58)$$

or using the Euler-Lagrange operator (3.38)

$$\mathcal{F}_{\boldsymbol{\psi}}\left(\boldsymbol{\varphi}\right) + \left(-\mathbf{F}^T\right)\mathrm{DIV}\left(\mathbf{P}^v\right) = 0$$

For a Lagrangian density of the form (3.3) the previous yields

$$\mathbf{B}^{inh} - \frac{d}{dt}\left(\left(-\mathbf{F}^T\right)R\mathbf{V}\right) + \mathrm{DIV}\left(\mathbf{C}\right) + \left(-\mathbf{F}^T\right)\mathrm{DIV}\left(\mathbf{P}^v\right) = \mathbf{0} \qquad \text{in } B \text{ and } \forall t \in I \qquad (3.59)$$

Equations (3.58) and (3.59) are thus the equations of balance of configurational forces in the presence of viscous effects.

In analogy to the equations of mechanical (vertical) force balance with viscous effects (3.14) (3.15), the configurational (horizontal) balance (3.58) (3.59) cannot be derived from a direct variational principle (Hamilton's principle with horizontal variations), but can instead be established from the following (horizontal) Lagrange-d'Alembert principle:

$$\langle \delta S, \delta\boldsymbol{\psi}\rangle + \int_{t_0}^{t_f}\int_B \left(\left(\delta\boldsymbol{\psi}^T \circ \boldsymbol{\psi}^{-1}\right)\left(-\mathbf{F}^T\right)\mathrm{DIV}\left(\mathbf{P}^v\right)\right) dV dt = \mathbf{0}$$

Integrating by parts the previous reads

$$\langle \delta S, \delta\boldsymbol{\psi}\rangle - \int_{t_0}^{t_f}\int_B \left(\mathbf{P}^v \cdot \frac{\partial}{\partial \mathbf{X}}\left(-\mathbf{F}\left(\delta\boldsymbol{\psi} \circ \boldsymbol{\psi}^{-1}\right)\right)\right) dV dt = \mathbf{0} \qquad (3.60)$$

In Cartesian coordinates

$$\langle \delta S, \delta\psi_I\rangle - \int_{t_0}^{t_f}\int_B \left(P^v_{iJ}\frac{\partial}{\partial X_J}\left(F_{iI}\delta\psi_I \circ \boldsymbol{\psi}^{-1}\right)\right) dV dt = 0$$

Finally we combine horizontal and vertical Lagrange-d'Alembert principle to establish a variational principle in the space-space bundle $B \times S$. The equations of balance of mechanical and configurational forces in the presence of viscosity are

$$\begin{aligned} \mathcal{F}_{\boldsymbol{\psi}}\left(\boldsymbol{\varphi}\right) + \left(-\mathbf{F}^T\right)\mathrm{DIV}\left(\mathbf{P}^v\right) &= 0 \\ \mathcal{F}_{\boldsymbol{\phi}}\left(\boldsymbol{\varphi}\right) + \mathrm{DIV}\left(\mathbf{P}^v\right) &= 0 \end{aligned}$$

These equations may be written jointly as an equation in the space-space bundle $B \times S$ as

$$\begin{pmatrix} \mathcal{F}_{\psi}(\boldsymbol{\varphi}) \\ \mathcal{F}_{\phi}(\boldsymbol{\varphi}) \end{pmatrix} + \begin{pmatrix} -\mathbf{F}^T \\ \mathbf{i} \end{pmatrix} \mathrm{DIV}\left(\mathbf{P}^v\right) = 0 \tag{3.61}$$

or alternatively as

$$\begin{pmatrix} \mathcal{F}_{\psi}(\boldsymbol{\varphi}) \\ \mathcal{F}_{\phi}(\boldsymbol{\varphi}) \end{pmatrix} + \mathbb{N}\,\mathrm{DIV}\left(\mathbf{P}^v\right) = 0 \tag{3.62}$$

where $\mathbb{N}$ is a normal vector to the configuration as regarded as a manifold in the space-space bundle. The weak form of this equations (combined horizontal-vertical Lagrange-d'Alembert principle) is therefore

$$\langle \delta S, \delta \boldsymbol{\psi} \rangle + \langle \delta S, \delta \boldsymbol{\phi} \rangle + \int_{t_0}^{t_f} \int_B \left(\delta \boldsymbol{\psi}^T, \delta \boldsymbol{\phi}^T \right) \begin{pmatrix} -\mathbf{F}^T \\ \mathbf{i} \end{pmatrix} \mathrm{DIV}\left(\mathbf{P}^v\right) dV dt +$$
$$+ \int_{t_0}^{t_f} \int_{\partial B_1} \left(\delta \boldsymbol{\psi}^T, \delta \boldsymbol{\phi}^T \right) \begin{pmatrix} -\mathbf{F}^T \\ \mathbf{i} \end{pmatrix} \left(\mathbf{P}^v \mathbf{N}\right) dS dt = \mathbf{0}$$

or, more compactly

$$\langle \delta S, \delta \boldsymbol{\psi} \rangle + \langle \delta S, \delta \boldsymbol{\phi} \rangle + \int_{t_0}^{t_f} \int_B \left(\delta \boldsymbol{\phi}^T - \delta \boldsymbol{\psi}^T \mathbf{F}^T \right) \mathrm{DIV}\left(\mathbf{P}^v\right) dV dt +$$
$$+ \int_{t_0}^{t_f} \int_{\partial B_1} \left(\delta \boldsymbol{\phi}^T - \delta \boldsymbol{\psi}^T \mathbf{F}^T \right) \left(\mathbf{P}^v \mathbf{N}\right) dS dt = \mathbf{0} \tag{3.63}$$

Integrating by parts and making use of the divergence theorem the (combined horizontal-vertical) Lagrange-d'Alembert principle takes the form

$$\langle \delta S, \delta \boldsymbol{\psi} \rangle + \langle \delta S, \delta \boldsymbol{\phi} \rangle - \int_{t_0}^{t_f} \int_B \mathbf{P}^v \frac{\partial}{\partial \mathbf{X}} \left(\delta \boldsymbol{\phi} - \mathbf{F} \delta \boldsymbol{\psi} \right) dV dt = 0 \tag{3.64}$$

In Cartesian coordinates

$$\langle \delta S, \delta \psi_I \rangle + \langle \delta S, \delta \phi_i \rangle - \int_{t_0}^{t_f} \int_B P^v_{iJ} \frac{\partial}{\partial X_J} \left(\delta \phi_i - F_{iI} \delta \psi_I \right) dV dt = 0$$

with horizontal and vertical components given by (3.60) and (3.57).

Chapter 4

Configurational forces in materials with viscous, thermal, and internal processes

In this chapter we study a Lagrange-d'Alembert formulation for materials with coupled thermomechanical and internal processes, and derive the equations of configurational force balance in the presence of the new sources of dissipation, namely, thermal and internal effects. Thermal processes are incorporated by making use of the approach of Green and Naghdi's (c.f. [13]) of considering as primitive thermal variables the so-called *thermal displacements* instead of the temperature. Thermal displacements $\alpha\left(X,t\right)$ are defined as the time integral of the temperature, i.e., $\alpha\left(X,t\right)=\int_{t_0}^{t}T\left(X,\tau\right)d\tau$ or equivalently, as the scalar quantity such that $\dot{\alpha}=T$. The reinterpretation of temperature as a rate suggests that the entropy N given by the relation $RN=\frac{\partial L}{\partial T}$ where $\mathcal{L}$ is the (temperature-dependent) Lagrangian, and the heat flux $\mathbf{H}$ given by a generalized Fourier's law $\mathbf{H}=\mathbf{H}\left(DT\right)$, *should be reinterpreted, respectively, as a momentum and as a viscous stress*, in complete analogy to the velocity $RV=\frac{\partial\mathcal{L}}{\partial\dot{\varphi}}$ and viscous force $\mathbf{P}^{v}=\mathbf{P}^{v}\left(D\dot{\boldsymbol{\varphi}}\right)$. Once this analogy is established, a Lagrange-d'Alembert formulation for all balance equations and the equations of balance of configurational forces for materials with thermal processes follow by mirroring the procedure developed for elastic materials with viscosity in the previous chapter.

The main consequence of introducing thermal displacements α as primitive variables is that a *correspondence* or *analogy* between mechanical variables and thermal variables can be established. For each quantity in the equation of mechanical force balance, there are parallel or analogues in the equation of entropy balance. For example, to the (elastic part of the) mechanical stress $\mathbf{P}=\frac{\partial W}{\partial D\boldsymbol{\varphi}}$ corresponds the (conservative or dissipationless part of the) entropy flux $\frac{\mathbf{H}}{T}=\frac{\partial W}{\partial D\alpha}$. Direct attempts to exploit this analogy have been explored for example in [47] and [48], where Lagrangian and Hamiltonian formulations of (dissipationless) thermoelasticity were investigated, see also [19]. Furthermore, using Noether's theorem with a Lagrangian expressed in terms of the "direct motion and thermal displacements" $(\boldsymbol{\varphi}, \alpha)$, or alternatively, invoking the stationarity of the Lagrangian expressed in terms of the inverse motion and inverse thermal displacements $\left(\boldsymbol{\varphi}^{-1}, \alpha^{-1}\right)$ a (dissipationless) thermoelastic configurational force balance equation was obtained (c.f. [47], [48]). The extension of the latter for the dissipative case was studied for example in [3]. This extension was obtained by "pulling-back" or "projecting" both balance equations (mechanical force balance and entropy balance) onto the material manifold as was suggested in [44] as a general or "direct" method to establish the configurational force balance equation in general dissipative materials. The same equation was later obtained using Gurtin's approach to configurational forces (see [15], [16]) in [18].

The objective of this chapter is to take this analogy or parallelism further. We propose an additive decomposition for the heat flux $\mathbf{H} = \mathbf{H}^e + \mathbf{H}^v$ into a conservative (or equilibrium or dissipationless) heat $\mathbf{H}^e$ and a non-conservative (or non-equilibrium or dissipative) heat $\mathbf{H}^v$ in complete analogy to the decomposition of the mechanical stress $\mathbf{P}$ into elastic (or equilibrium or conservative) part and viscous (on non-equilibrium) parts $\mathbf{P} = \mathbf{P}^e + \mathbf{P}^v$. The dissipationless part of the heat $\mathbf{H}^e$ derives from the energy (or Lagrangian density) in the form $\frac{\mathbf{H}^e}{T} = \frac{\partial W}{\partial D\alpha} = -\frac{\partial \mathcal{L}}{\partial D\alpha}$ while the dissipative part $\mathbf{H}^v$ derives from a kinetic potential Φ in the form $\frac{\mathbf{H}^v}{T} = \frac{\partial \Phi}{\partial D\dot{\alpha}} = \frac{\partial \Phi}{\partial DT}$ in perfect parallelism with the elastic and viscous parts of the mechanical stress $P^e = \frac{\partial W}{\partial D\boldsymbol{\varphi}}$ and $\mathbf{P}^v = \frac{\partial \Phi}{\partial D\dot{\boldsymbol{\varphi}}} = \frac{\partial \Phi}{\partial \dot{\mathbf{F}}}$. We shall furthermore pursue equivalent decompositions for the thermodynamic stresses conjugate to the internal variables $\mathbf{Y} = \mathbf{Y}^e + \mathbf{Y}^v$ and for the mechanical body forces $\mathbf{B} = \mathbf{B}^e + \mathbf{B}^v$ and heat sources per unit of reference volume $S = S^e + S^v$.

A thermomechanical Lagrangian and thermomechanical action is considered. The independent thermomechanical variables are taken to be the motion $\boldsymbol{\varphi}$, the thermal displacements α, and the collection of internal variables $\mathbf{Q}$. The thermomechanical Lagrangian is assumed to depend on the independent variables, their rates, and their gradients. Derivatives of the Lagrangian with respect to the rates define *momenta*. Derivatives of the Lagrangian with respect to gradients define *equilibrium stresses*, and derivatives of the Lagrangian with respect to the thermomechanical variables define *equilibrium forces*. We also define *non-equilibrium stresses* and *non-equilibrium body forces* for all the processes. All these are assumed to derive from a kinetic potential as derivatives with respect to the rates of each independent variables and their gradients. Non-equilibrium stresses are obtained as derivatives with respect to the gradient rates, namely $\left(\dot{\mathbf{Q}}, D\dot{\boldsymbol{\varphi}}, D\dot{\alpha}\right)$. Non-equilibrium forces are obtained as derivatives with respect to the rate of the independent variables $(\dot{\boldsymbol{\varphi}}, \dot{\alpha})$. Adding the equilibrium and non-equilibrium parts of stresses we obtain the total stresses. Adding equilibrium and non-equilibrium parts of the forces we obtain total forces. The Euler-Lagrange equations associated to the stationarity of the thermomechanical action with respect to each variable will give the *equilibrium part* of the "mechanical force balance," "entropy balance," and "internal force balance" equations. Each equation will have also a *non-equilibrium part* that unlike the "equilibrium" part cannot be obtained from the stationarity of the thermomechanical action. The *total* balance can be established instead from a "thermomechanical" Lagrange-d'Alembert principle.

4.1 Balance equations and constitutive assumptions

We begin this chapter by reviewing the balance laws and constitutive assumptions that govern the motion and thermodynamic processes of a deformable body with reference configuration $B \subseteq \mathbb{R}^n$. The local form of the balance equations written in Lagrangian coordinates are:

- Conservation of mass

$$\dot{R} = 0$$

- Balance of mechanical forces (or balance of linear momentum)

$$\frac{d}{dt}(R\mathbf{V}) - DIV(\mathbf{P}) - \mathbf{B} = 0$$

- Balance of energy

$$\frac{d}{dt}\left(\frac{1}{2}R\|\mathbf{V}\|^2 + A + RTN\right) - DIV(\mathbf{PV} - \mathbf{H}) - S - \mathbf{B}\cdot\mathbf{V} = 0$$

- Clausius-Duhem inequality

$$\frac{d}{dt}(RN) + DIV\left(\frac{\mathbf{H}}{T}\right) - \frac{S}{T} \geq 0$$

where $\boldsymbol{\varphi}(\mathbf{X}, t)$ is the motion, $\mathbf{V}(\mathbf{X}, \mathbf{t}) = \dot{\boldsymbol{\varphi}}(\mathbf{X}, t)$ is the material velocity, $R(\mathbf{X})$ (independent of t by conservation of mass) is the mass density per unit of undeformed volume, $\mathbf{P}(\mathbf{X}, t)$ is the total stress tensor (force per unit of undeformed area or Piolla-Kirchhoff stress tensor), $\mathbf{B}(\mathbf{X}, t)$ are body forces per unit of undeformed volume, $A(\mathbf{X}, t)$ is the free energy, $N(\mathbf{X}, t)$ is the entropy density per unit mass, $T(\mathbf{X}, t)$ is the temperature, $U(\mathbf{X}, t) = A + RTN$ is the internal energy per unit of undeformed volume, $S(\mathbf{X}, t)$ is the heat source (per unit of undeformed volume), and $\mathbf{H}(\mathbf{X}, t)$ is the heat flux per unit of undeformed area.

We shall be interested in the treatment of thermal variables and mechanical variables in an equal footing. To this end we split the Clausius-Duhem inequality into an *entropy balance equation*,

$$\dot{\Gamma} = \frac{d}{dt}(RN) - DIV\left(\frac{\mathbf{H}}{T}\right) - \frac{S}{T}$$

and the inequality

$$\dot{\Gamma} \geq 0$$

where $\dot{\Gamma}$ is the *internal entropy production.* Entropy balance and mechanical force balance will become the main objects of the upcoming developments. More precisely these two balance equations will be considered as the Euler-Lagrange equations of the Lagrangian and Lagrange-d'Alembert formulation of the next section.

Let $\mathcal{F}_p$, $\mathcal{F}_N$ and $\mathcal{F}_t$ be the left hand side of the three balance equations (mechanical momentum balance, entropy balance and energy balance), i.e.,

$$\begin{aligned}
\mathcal{F}_p &= \frac{d}{dt}(R\mathbf{V}) - DIV(\mathbf{P}) - \mathbf{B} \\
\mathcal{F}_N &= \frac{d}{dt}(RN) + DIV\left(\frac{\mathbf{H}}{T}\right) - \frac{S}{T} - \dot{\Gamma} \\
\mathcal{F}_t &= \frac{d}{dt}\left(\frac{1}{2}R\|\mathbf{V}\|^2 + A + RTN\right) - DIV(\mathbf{PV} - \mathbf{H}) - S - \mathbf{B}\cdot\mathbf{V}
\end{aligned}$$

Then it is straightforward to prove the *identity*

$$\mathcal{F}_t - \mathbf{V}\mathcal{F}_p - T\mathcal{F}_N = \dot{A} + R\dot{T}N + T\dot{\Gamma} - \mathbf{P}D\mathbf{V} + \frac{\mathbf{H}}{T}DT$$

Combining this identity with the balance equations ($\mathcal{F}_p = 0$, $\mathcal{F}_N = 0$ and $\mathcal{F}_t = 0$) the following relation is obtained:

$$\dot{A} + R\dot{T}N + T\dot{\Gamma} - \mathbf{P}D\mathbf{V} + \frac{\mathbf{H}}{T}DT = 0 \tag{4.1}$$

which is usually regarded as another statement of energy conservation.

In addition to the balance equations, the following constitutive assumptions are made:

- The local thermodynamic state is assumed to depend on $(\mathbf{F}, T, \mathbf{Q})$ where $\mathbf{F} = D\boldsymbol{\varphi}$ is the deformation gradient, T is the temperature, and $\mathbf{Q}$ is a set of internal additional variables. Each material particle with reference coordinates $\mathbf{X}$ is regarded as a thermodynamic system in equilibrium undergoing a thermodynamic process defined completely by the curve $(\mathbf{F}(\mathbf{X},t), T(\mathbf{X},t), Q(\mathbf{X},t))$

- The stress is split additively into an "equilibrium" part $\mathbf{P}^e$ (or "elastic" or "conservative" part) and a non-equilibrium part (or viscous or non-conservative part)

$$\mathbf{P} = \mathbf{P}^e + \mathbf{P}^v$$

The total stress $\mathbf{P}$ is assumed to depend on the local thermodynamic state $(\mathbf{F}, T, \mathbf{Q})$ and on the rate of deformation $\dot{\mathbf{F}}$, i.e., $\mathbf{P} = \mathbf{P}\left(\dot{\mathbf{F}}, \mathbf{F}, T, \mathbf{Q}\right)$ and the equilibrium part satisfies the relation

$$\mathbf{P}^e = \mathbf{P}\left(\dot{\mathbf{F}} = 0, \mathbf{F}, T, \mathbf{Q}\right)$$

- The internal energy of each material point is assumed to depend on the local thermodynamic state, namely on $(\mathbf{X}, \mathbf{F}, T, \mathbf{Q})$, i.e.,

$$A = A\left(\mathbf{X}, \mathbf{F}, T, \mathbf{Q}\right)$$

- The equilibrium stresses and thermodynamic forces conjugate to the internal variables are defined as

$$\begin{aligned} \mathbf{P}^e &= \frac{\partial A}{\partial \mathbf{F}}\left(\mathbf{X}, \mathbf{F}, T, \mathbf{Q}\right) \\ \mathbf{Y} &= -\frac{\partial A}{\partial \mathbf{Q}}\left(\mathbf{X}, \mathbf{F}, T, \mathbf{Q}\right) \end{aligned}$$

  and the entropy N is given by the relation

$$RN = -\frac{\partial A}{\partial T}\left(\mathbf{X}, \mathbf{F}, T, \mathbf{Q}\right)$$

Under these assumptions we have

$$\begin{aligned} \dot{A} &= \frac{\partial A}{\partial \mathbf{F}}\dot{\mathbf{F}} + \frac{\partial A}{\partial T}\dot{T} + \frac{\partial A}{\partial \mathbf{Q}}\dot{\mathbf{Q}} = \\ &= \mathbf{P}^e\dot{\mathbf{F}} + RN\dot{T} - \mathbf{Y}\dot{\mathbf{Q}} \end{aligned}$$

and the identity (4.1) reduces then to

$$T\dot{\Gamma} - \mathbf{Y}\dot{\mathbf{Q}} - \mathbf{P}^v\dot{\mathbf{F}} + \frac{\mathbf{H}}{T}DT = 0$$

which implies that the viscous power $\mathbf{P}^v\dot{\mathbf{F}}$, heat flux against thermal gradients $\frac{\mathbf{H}}{T}DT$, and power of internal processes $\mathbf{Y}\dot{\mathbf{Q}}$ contribute additively to the internal entropy production

$$T\dot{\Gamma} = \mathbf{Y}\dot{\mathbf{Q}} + \mathbf{P}^v\dot{\mathbf{F}} - \frac{\mathbf{H}}{T}DT$$

The entropy balance equation becomes then

$$\frac{d}{dt}\left(RN\right) - DIV\left(\frac{\mathbf{H}}{T}\right) - \frac{S}{T} - \frac{1}{T}\left(\mathbf{Y}\dot{\mathbf{Q}} + \mathbf{P}^v\dot{\mathbf{F}} - \frac{\mathbf{H}}{T}DT\right) = 0$$

Finally the set of balance equations and constitutive relations need to be complemented with appropriate kinetic relations that enable the determination of $(\mathbf{Y}, \mathbf{P}^v, \mathbf{H})$. They usually assume the general form

$$\begin{aligned}
\mathbf{P}^v &= \mathbf{P}^v\left(\mathbf{X}, \mathbf{F}, \mathbf{Q}, T, \dot{\mathbf{F}}, \dot{\mathbf{Q}}, DT\right) \\
\mathbf{Y} &= \mathbf{Y}\left(\mathbf{X}, \mathbf{F}, \mathbf{Q}, T, \dot{\mathbf{F}}, \dot{\mathbf{Q}}, DT\right) \\
\frac{\mathbf{H}}{T} &= \frac{\mathbf{H}}{T}\left(\mathbf{X}, \mathbf{F}, \mathbf{Q}, T, \dot{\mathbf{F}}, \dot{\mathbf{Q}}, DT\right)
\end{aligned}$$

Furthermore we shall assume that the previous functions derive from a kinetic potential

$$\Phi = \Phi\left(\mathbf{X}, \mathbf{F}, \mathbf{Q}, T, \dot{\mathbf{F}}, \dot{\mathbf{Q}}, DT\right) \tag{4.2}$$

such that

$$\begin{aligned}
\mathbf{P}^v &= \frac{\partial \Phi}{\partial \dot{\mathbf{F}}} \\
\mathbf{Y} &= \frac{\partial \Phi}{\partial \dot{\mathbf{Q}}} \\
\frac{\mathbf{H}}{T} &= -\frac{\partial \Phi}{\partial (DT)}
\end{aligned}$$

4.2 Restatement of the balance laws in terms of thermal displacements.

We next proceed to study how the previous equations and constitutive assumptions are reframed in a more general context when we assume that the local thermodynamic state is specified by $(\mathbf{F}, \mathbf{Q})$ and the *thermal displacement* α instead of the temperature T. Thermal displacements α are defined as

$$\alpha(\mathbf{X}, t) = \int_{t_0}^{t} T(\mathbf{X}, \tau)\, d\tau$$

or equivalently as the scalar field such that

$$\dot{\alpha} = T$$

The reinterpretation of T as a rate has the following two fundamental consequences:

1. If the free energy is assumed to be dependent on $(\mathbf{F}, T, \mathbf{Q}) = (\mathbf{F}, \dot{\alpha}, \mathbf{Q})$ then the relation for the entropy becomes

$$RN = -\frac{\partial A}{\partial \dot{\alpha}}$$

or, using the Lagrangian density defined as

$$\begin{aligned}\mathcal{L} &= \frac{R}{2}\|\mathbf{V}\|^2 - A(\mathbf{F}, T, \mathbf{Q}) = \\ &= \frac{R}{2}\|\dot{\boldsymbol{\varphi}}\|^2 - A(\mathbf{F}, \dot{\alpha}, \mathbf{Q})\end{aligned}$$

the entropy result

$$RN = \frac{\partial \mathcal{L}}{\partial \dot{\alpha}}$$

This relation is in perfect analogy to

$$RV = \frac{\partial \mathcal{L}}{\partial \dot{\boldsymbol{\varphi}}}$$

which states that $R\mathbf{V}$ is a (mechanical) momentum for the particular Lagrangian $\mathcal{L}$ defined above. We thus reinterpret RN as a *thermal momentum* and consider A not as an energy but as a *Lagrangian*, or more precisely, as a Lagrangian excluding the kinetic energy term.

2. Let $\boldsymbol{\beta} = D\alpha$ be the *thermal displacement gradient* and assume now that the free energy depends not only on deformation gradient $\mathbf{F}$ but also on thermal displacements gradients $\boldsymbol{\beta}$, i.e.,

$$A = A(\mathbf{F}, T, \mathbf{Q}, \boldsymbol{\beta})$$

In analogy to the equilibrium stress $\mathbf{P}^e$ defined as

$$\mathbf{P}^e = \frac{\partial A}{\partial \mathbf{F}}$$

and the viscous or non-equilibrium part of the stress $\mathbf{P}^v$ defined such that

$$\mathbf{P} = \mathbf{P}^e + \mathbf{P}^v$$

we may define the *equilibrium part of the heat flux* $\mathbf{H}^e$ such that

$$\frac{\mathbf{H}^e}{T} = -\frac{\partial A}{\partial \boldsymbol{\beta}}$$

and the *viscous* or *non-equilibrium part of the heat flux* $\mathbf{H}^v$ such that

$$\mathbf{H} = \mathbf{H}^e + \mathbf{H}^v$$

It follows then that

$$\begin{aligned}\dot{A} &= \frac{\partial A}{\partial \mathbf{F}}\dot{\mathbf{F}} + \frac{\partial A}{\partial T}\dot{T} + \frac{\partial A}{\partial \mathbf{Q}}\dot{\mathbf{Q}} + \frac{\partial \mathbf{A}}{\partial \boldsymbol{\beta}}\dot{\boldsymbol{\beta}} = \\ &= \mathbf{P}^e\dot{\mathbf{F}} + RN\dot{T} - \mathbf{Y}\dot{\mathbf{Q}} + \frac{\mathbf{H}^e}{T}DT\end{aligned}$$

whereupon the identity (4.1) reduces to

$$T\dot{\Gamma} - \mathbf{Y}\dot{\mathbf{Q}} - \mathbf{P}^v\dot{\mathbf{F}} + \frac{\mathbf{H}^v}{T}DT = 0$$

or equivalently to

$$T\dot{\Gamma} = \mathbf{Y}\dot{\mathbf{Q}} + \mathbf{P}^v\dot{\mathbf{F}} - \frac{\mathbf{H}^v}{T}DT$$

The previous suggests that only the "non-equilibrium" part of the heat flux $\mathbf{H}^v$ will contribute to internal entropy production $\dot{\Gamma}$ and only this part will be related with the temperature gradient $DT = \dot{\beta}$ through a kinetic relation

$$\begin{aligned}\frac{\mathbf{H}^v}{T} &= -\frac{\partial \Phi}{\partial \dot{\boldsymbol{\beta}}} \\ &= -\frac{\partial \Phi}{\partial DT}\end{aligned}$$

in complete analogy with the non-equilibrium part of the mechanical stress

$$\mathbf{P}^v = \frac{\partial \Phi}{\partial \dot{\mathbf{F}}}$$

Materials for which $\mathbf{H}^v = 0$ and $\mathbf{H}^e \neq 0$ are referred to as thermoelastic materials with dissipationless thermal conduction.

Motivated by the decomposition

$$\mathbf{H} = \mathbf{H}^e + \mathbf{H}^v$$

we proceed now to pursue an equivalent decomposition for the thermodynamic forces conjugate to the internal processes $\mathbf{Y}$, namely

$$\mathbf{Y} = \mathbf{Y}^e + \mathbf{Y}^v$$

To this end we recall first that for these forces we have defined

$$\mathbf{Y} = -\frac{\partial A}{\partial \mathbf{Q}} = \frac{\partial \mathcal{L}}{\partial \mathbf{Q}} \tag{4.3}$$

and assumed a kinetic relation of the form

$$\mathbf{Y} = \frac{\partial \Phi}{\partial \dot{\mathbf{Q}}} \tag{4.4}$$

We notice next that the notation adopted in the first of these relations seems not to be in agreement with the adopted for the mechanical stress $\mathbf{P}$ and heat flux $\mathbf{H}$ for which we have interpreted

$$\begin{aligned} \mathbf{P}^e &= \frac{\partial A}{\partial \mathbf{F}} = -\frac{\partial \mathcal{L}}{\partial \mathbf{F}} \\ \frac{\mathbf{H}^e}{T} &= -\frac{\partial A}{\partial \boldsymbol{\beta}} = \frac{\partial \mathcal{L}}{\partial \boldsymbol{\beta}} \end{aligned}$$

as a definition for the equilibrium parts of the total stress $\mathbf{P}$ and flux $\mathbf{H}$ and therefore used the supraindex e. It seems then natural to change the notation in (4.3) to

$$\mathbf{Y}^e = -\frac{\partial A}{\partial \mathbf{Q}} = \frac{\partial \mathcal{L}}{\partial \mathbf{Q}}$$

Equation (4.4) can then be rewritten as

$$\mathbf{Y}^e - \frac{\partial \Phi}{\partial \dot{\mathbf{Q}}} = 0 \tag{4.5}$$

Defining now the non-equilibrium part of the thermodynamic forces $\mathbf{Y}^v$ as

$$\mathbf{Y}^v = -\frac{\partial \Phi}{\partial \dot{\mathbf{Q}}}$$

(in complete analogy to $\mathbf{P}^v$ and $\mathbf{H}^v$) relation (4.5) becomes

$$\mathbf{Y} = \mathbf{Y}^e + \mathbf{Y}^v = \mathbf{0}$$

which might be now reinterpreted as a *balance equation* for the thermodynamic forces conjugate to the internal processes.

In light of the previous assumptions and observations, the mechanical force balance equation, entropy balance equations, and balance equations for the internal processes may be rewritten as

$$\begin{pmatrix} DIV\left(\mathbf{P}^e + \mathbf{P}^v\right) \\ -DIV\left(\frac{\mathbf{H}^e + \mathbf{H}^v}{T}\right) \\ \mathbf{Y}^e + \mathbf{Y}^v \end{pmatrix} - \begin{pmatrix} \frac{d}{dt}\left(R\dot{\boldsymbol{\varphi}}\right) \\ \frac{d}{dt}\left(RN\right) \\ \mathbf{0} \end{pmatrix} + \begin{pmatrix} \mathbf{B} \\ \frac{S}{T} + \dot{\Gamma} \\ \mathbf{0} \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ 0 \\ \mathbf{0} \end{pmatrix} \tag{4.6}$$

where in the first column we have grouped the "stresses," in the second the "momenta," and in the third the "sources," and where the "equilibrium-stresses" are given by

$$\begin{pmatrix} \mathbf{P}^e \\ \frac{\mathbf{H}^e}{T} \\ \mathbf{Y}^e \end{pmatrix} = \begin{pmatrix} \frac{\partial A}{\partial \mathbf{F}} \\ -\frac{\partial A}{\partial \boldsymbol{\beta}} \\ -\frac{\partial A}{\partial \mathbf{Q}} \end{pmatrix} = \begin{pmatrix} -\frac{\partial \mathcal{L}}{\partial \mathbf{F}} \\ \frac{\partial \mathcal{L}}{\partial \boldsymbol{\beta}} \\ \frac{\partial \mathcal{L}}{\partial \mathbf{Q}} \end{pmatrix} \tag{4.7}$$

"non-equilibrium stresses" by

$$\begin{pmatrix} \mathbf{P}^v \\ \frac{\mathbf{H}^v}{T} \\ \mathbf{Y}^v \end{pmatrix} = \begin{pmatrix} \frac{\partial \Phi}{\partial \dot{\mathbf{F}}} \\ -\frac{\partial \Phi}{\partial \dot{\boldsymbol{\beta}}} \\ -\frac{\partial \Phi}{\partial \dot{\mathbf{Q}}} \end{pmatrix} \tag{4.8}$$

and the internal entropy production follows as

$$T\dot{\Gamma} = -\mathbf{Y}^v \dot{\mathbf{Q}} + \mathbf{P}^v \dot{\mathbf{F}} - \frac{\mathbf{H}^v}{T} DT \tag{4.9}$$

or, written in terms of the kinetic potential Φ, as

$$\dot{\Gamma} = \frac{1}{\dot{\alpha}} \left(\frac{\partial \Phi}{\partial \dot{\mathbf{Q}}} \dot{\mathbf{Q}} + \frac{\partial \Phi}{\partial \dot{\mathbf{F}}} \dot{\mathbf{F}} + \frac{\partial \Phi}{\partial \dot{\boldsymbol{\beta}}} \dot{\boldsymbol{\beta}} \right)$$

Having established equivalent decompositions for mechanical stresses $\mathbf{P}$, heat fluxes $\mathbf{H}$ and internal forces $\mathbf{Y}$ we now proceed to assume similar decompositions for the *body* forces $\mathbf{B}$ and heat sources S. We shall consider therefore

$$\begin{aligned} \mathbf{B} &= \mathbf{B}^e + \mathbf{B}^v \\ \frac{S}{T} &= \frac{S^e}{T} + \frac{S^v}{T} \end{aligned}$$

where $(\mathbf{B}^e, S^e)$ and $(\mathbf{B}^v, S^v)$ are, respectively, the equilibrium (or conservative or potential) and non-equilibrium (or non-conservative or viscous) parts of the body force and heat source. The equilibrium part is assumed to derive from a potential $I(\boldsymbol{\varphi}, \alpha)$ in the form

$$\begin{pmatrix} \mathbf{B}^e \\ \frac{S^e}{T} \end{pmatrix} = \begin{pmatrix} \dfrac{\partial I}{\partial \boldsymbol{\varphi}} \\ \dfrac{\partial I}{\partial \alpha} \end{pmatrix}$$

or alternatively as

$$\begin{pmatrix} \mathbf{B}^e \\ \frac{S^e}{T} \end{pmatrix} = \begin{pmatrix} \dfrac{\partial I}{\partial \boldsymbol{\varphi}} \\ \dfrac{\partial I}{\partial \alpha} \end{pmatrix} = \begin{pmatrix} \dfrac{\partial \mathcal{L}}{\partial \boldsymbol{\varphi}} \\ \dfrac{\partial \mathcal{L}}{\partial \alpha} \end{pmatrix} \tag{4.10}$$

where we have redefined the Lagrangian density as

$$\begin{aligned}\mathcal{L} &= \frac{R}{2}\|\mathbf{V}\|^2 - A(\mathbf{X},\mathbf{F},T,\mathbf{Q},\boldsymbol{\beta}) + I(\boldsymbol{\varphi},\alpha) \\ &= \frac{R}{2}\|\dot{\boldsymbol{\varphi}}\|^2 - A(\mathbf{X},\mathbf{F},\dot{\alpha},\mathbf{Q},\boldsymbol{\beta}) + I(\boldsymbol{\varphi},\alpha)\end{aligned}$$

while the non-equilibrium parts $\mathbf{B}^v$ and $\frac{S^v}{T}$ are assumed to derive from a new kinetic potential $\phi(\dot{\boldsymbol{\varphi}},\dot{\alpha})$ in the form

$$\begin{pmatrix}\mathbf{B}^v \\ \frac{S^v}{T}\end{pmatrix} = \begin{pmatrix}\frac{\partial\phi}{\partial\dot{\boldsymbol{\varphi}}} \\ \frac{\partial\phi}{\partial\dot{\alpha}}\end{pmatrix}$$

or alternatively as

$$\begin{pmatrix}\mathbf{B}^v \\ \frac{S^v}{T}\end{pmatrix} = \begin{pmatrix}\frac{\partial\Psi}{\partial\dot{\boldsymbol{\varphi}}} \\ \frac{\partial\Psi}{\partial\dot{\alpha}}\end{pmatrix} \tag{4.11}$$

where we have combined the kinetic potential for the body sources ϕ with the kinetic potential Φ defined for the stresses in (4.2) to define a total kinetic potential

$$\Psi = \phi + \Phi$$

For example if an external body force field $\mathbf{B}^e(\mathbf{X},t)$ and an external radiation source $S^v(\mathbf{X},t)$ are applied, then we can take

$$\begin{aligned}I(\boldsymbol{\varphi},\alpha) &= \mathbf{B}^e\boldsymbol{\varphi} \\ \phi(\dot{\boldsymbol{\varphi}},\dot{\alpha}) &= S^v\log(\dot{\alpha})\end{aligned}$$

whereupon

$$\begin{aligned}\mathbf{B} &= \frac{\partial I}{\partial\boldsymbol{\varphi}} + \frac{\partial\phi}{\partial\dot{\boldsymbol{\varphi}}} = \mathbf{B}^e + \mathbf{0} \\ \frac{S}{T} &= \frac{\partial I}{\partial\alpha} + \frac{\partial\phi}{\partial\dot{\alpha}} = 0 + \frac{S^v}{\dot{\alpha}}\end{aligned}$$

On account of all the previous assumptions, the balance equations take the form

$$\begin{pmatrix}DIV(\mathbf{P}^e+\mathbf{P}^v) \\ -DIV\left(\frac{\mathbf{H}^e+\mathbf{H}^v}{T}\right) \\ \mathbf{Y}^e+\mathbf{Y}^v\end{pmatrix} - \begin{pmatrix}\frac{d}{dt}(R\dot{\boldsymbol{\varphi}}) \\ \frac{d}{dt}(RN) \\ \mathbf{0}\end{pmatrix} + \begin{pmatrix}\mathbf{B}^e+\mathbf{B}^v \\ \frac{S^e+S^v}{T} \\ \mathbf{0}\end{pmatrix} + \begin{pmatrix}\mathbf{0} \\ \dot{\Gamma} \\ \mathbf{0}\end{pmatrix} = \begin{pmatrix}\mathbf{0} \\ 0 \\ \mathbf{0}\end{pmatrix} \tag{4.12}$$

with the "equilibrium" (or conservative) and "non-equilibrium" (or non-conservative or viscous) parts of the mechanical stresses, heat fluxes, and internal stresses given, respectively, by (4.7) and

(4.8), with conservative and non-conservative parts of the body sources given, respectively, by (4.10) and (4.11), and with internal dissipation given by

$$\dot{\Gamma} = \frac{1}{\dot{\alpha}} \left(\frac{\partial \Phi}{\partial \dot{\mathbf{Q}}} \dot{\mathbf{Q}} + \frac{\partial \Phi}{\partial \dot{\mathbf{F}}} \dot{\mathbf{F}} + \frac{\partial \Phi}{\partial \dot{\boldsymbol{\beta}}} \dot{\boldsymbol{\beta}} \right)$$

4.3 Lagrange-d'Alembert formulation of the balance equations

We turn in this section to the formulation of a general Lagrangian and Lagrange-d'Alembert principle from which a generalized form of the set of balance equations stated in the previous section can be derived. To this end we take as independent thermomechanical variables

$$(\boldsymbol{\varphi}, \alpha, \mathbf{Q})$$

where $\boldsymbol{\varphi}$ is the motion, α is the thermal displacement, and $\mathbf{Q}$ are the internal variables. We envision a formulation for which the equilibrium part of the balance equations (4.12) (mechanical force balance, entropy balance, and balance of force conjugate to the internal processes) can be derived from the stationarity of an action functional defined in terms of a *thermomechanical Lagrangian density*, while the total balance equations can be defined from a thermomechanical analog to the Lagrange-d'Alembert principle.

We shall assume therefore the existence of function $\mathcal{L}$, the thermodynamical Lagrangian density, that in analogy to the mechanical Lagrangian density (3.3), is a function of the thermodynamical variables, their rates, and their spatial derivatives:

$$\mathcal{L}\left(\mathbf{X}, t, \boldsymbol{\varphi}, \alpha, \mathbf{Q}, D\boldsymbol{\varphi}, D\alpha, D\mathbf{Q}, \dot{\boldsymbol{\varphi}}, \dot{\alpha}, \dot{\mathbf{Q}}\right)$$

The Lagrangian density is also assumed to depend explicitly on the space and time variables $(\mathbf{X}, t)$. To simplify the notation we shall make use of the following new symbols for the spatial and time derivatives of $\boldsymbol{\varphi}$ and α:

$$\begin{aligned} \mathbf{V} &= \dot{\boldsymbol{\varphi}} \\ \mathbf{F} &= D\boldsymbol{\varphi} \\ T &= \dot{\alpha} \\ \boldsymbol{\beta} &= D\alpha \end{aligned}$$

which implies the compatibility conditions

$$\begin{aligned} \dot{\mathbf{F}} &= D\mathbf{V} \\ \dot{\boldsymbol{\beta}} &= DT \end{aligned}$$

The Lagrangian is then assumed to depend on

$$\mathcal{L}\left(\mathbf{X}, t, \boldsymbol{\varphi}, \alpha, \mathbf{Q}, \mathbf{F}, \boldsymbol{\beta}, D\mathbf{Q}, \mathbf{V}, T, \dot{\mathbf{Q}}\right)$$

We shall restrict ourselves to the particular case of Lagrangian densities independent of $\left(\dot{\mathbf{Q}}, D\mathbf{Q}\right)$. This assumption is motivated by the following observation: In the same way as we introduced "thermal displacements" α such that $\dot{\alpha} = T$, we could have introduced "internal deformations" $\boldsymbol{\phi}$ such that

$$D\boldsymbol{\phi} = \mathbf{Q}$$

In that case the Lagrangian would have been dependent on

$$\left(\boldsymbol{\phi}, D\boldsymbol{\phi}, \dot{\boldsymbol{\phi}}\right) = \left(\boldsymbol{\phi}, \mathbf{Q}, \dot{\boldsymbol{\phi}}\right)$$

However in the particular case of plasticity and viscoplasticity, the internal variables are given by $\mathbf{Q} = \mathbf{F}^p$ which is not integrable to a global plastic deformation $\boldsymbol{\phi}$. It seems then that taking ϕ as an independent variable is not a valid assumption. We thus take $\mathbf{Q}$ as independent variable but the Lagragian is assumed to be dependent only on $\mathbf{Q}$ and not on $\dot{\mathbf{Q}}$ and $D\mathbf{Q}$, which would have implied a dependence on second derivatives and its rates $D\dot{\boldsymbol{\phi}}$ and $D^2\boldsymbol{\phi}$. The Lagrangian density L is then assumed to depend on

$$\mathcal{L}\left(\mathbf{X}, t, \boldsymbol{\varphi}, \alpha, \mathbf{F}, \boldsymbol{\beta}, \mathbf{Q}, \mathbf{V}, T\right)$$

In particular we shall consider Lagrangian densities of the form

$$\mathcal{L}\left(\mathbf{X}, t, \boldsymbol{\varphi}, \alpha, \mathbf{F}, \boldsymbol{\beta}, \mathbf{Q}, \mathbf{V}, T\right) = \frac{R\left\|\mathbf{V}\right\|^2}{2} - W\left(\mathbf{X}, t, \boldsymbol{\varphi}, \alpha, \mathbf{F}, \boldsymbol{\beta}, \mathbf{Q}, T\right)$$

with

$$W = A\left(\mathbf{X}, t, \mathbf{F}, \boldsymbol{\beta}, \mathbf{Q}, T\right) - I\left(\mathbf{X}, t, \boldsymbol{\varphi}, \alpha\right)$$

where A is the free energy density (or the kinetic-energy-free part of the Lagrangian density) and I is the potential for the body sources.

Under these assumptions it is straightforward to prove that *the equilibrium part* of the balance equations (4.12) are the Euler-Lagrange equations corresponding to the stationarity of the following *thermomechanical action*

$$
\begin{aligned}
S(\boldsymbol{\varphi}, \alpha, \mathbf{Q}) &= \int_{t_0}^{t_f} \int_B \mathcal{L}(\mathbf{X}, t, \boldsymbol{\varphi}, \alpha, D\varphi, D\alpha, \mathbf{Q}, \dot{\boldsymbol{\varphi}}, \dot{\alpha})\, dV dt = \\
&= \int_{t_0}^{t_f} \int_B \left(\frac{R \left\| \dot{\boldsymbol{\varphi}} \right\|^2}{2} - W(\mathbf{X}, t, \boldsymbol{\varphi}, \alpha, D\varphi, D\alpha, \mathbf{Q}, \dot{\alpha}) \right) dV dt
\end{aligned}
$$

with "equilibrium stresses" given by

$$
\begin{pmatrix} \mathbf{P}^e \\ \dfrac{\mathbf{H}^e}{T} \\ \mathbf{Y}^e \end{pmatrix} = \begin{pmatrix} -\dfrac{\partial \mathcal{L}}{\partial \mathbf{F}} \\ \dfrac{\partial \mathcal{L}}{\partial \boldsymbol{\beta}} \\ -\dfrac{\partial \mathcal{L}}{\partial \mathbf{Q}} \end{pmatrix} = \begin{pmatrix} \dfrac{\partial W}{\partial \mathbf{F}} \\ -\dfrac{\partial W}{\partial \boldsymbol{\beta}} \\ \dfrac{\partial W}{\partial \mathbf{Q}} \end{pmatrix} \tag{4.13}
$$

"equilibrium body forces" given by

$$
\begin{pmatrix} \mathbf{B}^e \\ \frac{S^e}{T} \end{pmatrix} = \begin{pmatrix} \dfrac{\partial \mathcal{L}}{\partial \boldsymbol{\varphi}} \\ \dfrac{\partial \mathcal{L}}{\partial \alpha} \end{pmatrix} = \begin{pmatrix} -\dfrac{\partial W}{\partial \boldsymbol{\varphi}} \\ -\dfrac{\partial W}{\partial \alpha} \end{pmatrix} \tag{4.14}
$$

and momenta given by

$$
\begin{pmatrix} R\dot{\boldsymbol{\varphi}} \\ RN \\ \mathbf{0} \end{pmatrix} = \begin{pmatrix} \dfrac{\partial \mathcal{L}}{\partial \dot{\boldsymbol{\varphi}}} \\ \dfrac{\partial \mathcal{L}}{\partial \dot{\alpha}} \\ \dfrac{\partial \mathcal{L}}{\partial \dot{\mathbf{Q}}} \end{pmatrix} \tag{4.15}
$$

Assuming now the existence of a kinetic potential Ψ that is a function of the same variables of the Lagrangian density and, in addition, of the rate of the gradients $\dot{\boldsymbol{\beta}} = D\dot{\alpha}$, $\dot{\mathbf{F}} = D\dot{\boldsymbol{\varphi}}$ and $\dot{\mathbf{Q}}$

$$
\Psi\left((\mathbf{X}, t), (\boldsymbol{\varphi}, \alpha, \mathbf{F}, \boldsymbol{\beta}, \mathbf{Q}), \left(\dot{\boldsymbol{\varphi}}, \dot{\alpha}, \dot{\mathbf{F}}, \dot{\beta}, \dot{\mathbf{Q}} \right) \right)
$$

such that the "non-equilibrium" stresses are given by

$$
\begin{pmatrix} \mathbf{P}^v \\ \dfrac{\mathbf{H}^v}{T} \\ \mathbf{Y}^v \end{pmatrix} = \begin{pmatrix} \dfrac{\partial \Psi}{\partial \dot{\mathbf{F}}} \\ -\dfrac{\partial \Psi}{\partial \dot{\boldsymbol{\beta}}} \\ -\dfrac{\partial \Psi}{\partial \dot{\mathbf{Q}}} \end{pmatrix} \tag{4.16}
$$

and "non-equilibrium body forces" given by

$$
\begin{pmatrix} \mathbf{B}^v \\ \frac{S^v}{T} \end{pmatrix} = \begin{pmatrix} \dfrac{\partial \Psi}{\partial \dot{\boldsymbol{\varphi}}} \\ \dfrac{\partial \Psi}{\partial \dot{\alpha}} \end{pmatrix} \tag{4.17}
$$

then it is straightforward to prove that *total* balance equations (4.12) follow from the Lagrange-d'Alembert principle:

$$\langle \delta S, \delta \boldsymbol{\varphi} \rangle + \langle \delta S, \delta \alpha \rangle + \langle \delta S, \delta \mathbf{Q} \rangle +$$
$$+ \int_{t_0}^{t_f} \int_B \left(\delta \boldsymbol{\varphi}^T \left(\frac{\partial \Psi}{\partial \dot{\boldsymbol{\varphi}}} + \text{DIV} \left(\frac{\partial \Psi}{\partial \dot{\mathbf{F}}} \right) \right) + \delta \alpha \left(\frac{\partial \Psi}{\partial \dot{\alpha}} + \dot{\Gamma} + \text{DIV} \left(\frac{\partial \Psi}{\partial \dot{\beta}} \right) \right) + \delta \mathbf{Q}^T \frac{\partial \Psi}{\partial \dot{\mathbf{Q}}} \right) dV dt = 0$$

that can be split in three different principles:

$$\langle \delta S, \delta \boldsymbol{\varphi} \rangle + \int_{t_0}^{t_f} \int_B \delta \boldsymbol{\varphi}^T \left(\frac{\partial \Psi}{\partial \dot{\boldsymbol{\varphi}}} + \text{DIV} \left(\frac{\partial \Psi}{\partial \dot{\mathbf{F}}} \right) \right) dV dt = 0 \tag{4.18}$$

$$\langle \delta S, \delta \alpha \rangle + \int_{t_0}^{t_f} \int_B \delta \alpha \left(\frac{\partial \Psi}{\partial \dot{\alpha}} + \dot{\Gamma} + \text{DIV} \left(\frac{\partial \Psi}{\partial \dot{\beta}} \right) \right) dV dt = 0 \tag{4.19}$$

$$\langle \delta S, \delta \mathbf{Q} \rangle + \int_{t_0}^{t_f} \int_B \delta \mathbf{Q}^T \left(\frac{\partial \Psi}{\partial \dot{\mathbf{Q}}} \right) dV dt = 0 \tag{4.20}$$

Using the kinetic relations (4.16) and (4.17) the Lagrange-d'Alembert principle can be written as

$$\langle \delta S, \delta \boldsymbol{\varphi} \rangle + \langle \delta S, \delta \alpha \rangle + \langle \delta S, \delta \mathbf{Q} \rangle +$$
$$+ \int_{t_0}^{t_f} \int_B \left(\delta \boldsymbol{\varphi}^T \left(\mathbf{B}^v + \text{DIV} \left(\mathbf{P}^v \right) \right) + \delta \alpha \left(\frac{S^v}{T} + \dot{\Gamma} - \text{DIV} \left(\frac{\mathbf{H}^v}{T} \right) \right) - \delta \mathbf{Q}^T \mathbf{Y}^v \right) dV dt = 0$$

The proof of these statements follows standard Euler-Lagrange derivation arguments: taking first variations of the thermodynamical action with respect to all of its arguments we find

$$\langle \delta S, \delta \boldsymbol{\varphi} \rangle = \int_{t_0}^{t_f} \int_B \left(\frac{\partial \mathcal{L}}{\partial \mathbf{V}} \delta \dot{\boldsymbol{\varphi}} + \frac{\partial \mathcal{L}}{\partial \mathbf{F}} D \delta \boldsymbol{\varphi} + \frac{\partial \mathcal{L}}{\partial \boldsymbol{\varphi}} \delta \boldsymbol{\varphi} \right) dV dt$$

$$\langle \delta S, \delta \alpha \rangle = \int_{t_0}^{t_f} \int_B \left(\frac{\partial \mathcal{L}}{\partial T} \delta \dot{\alpha} + \frac{\partial \mathcal{L}}{\partial \boldsymbol{\beta}} D \delta \boldsymbol{\beta} + \frac{\partial \mathcal{L}}{\partial \alpha} \delta \alpha \right) dV dt$$

$$\langle \delta S, \delta \mathbf{Q} \rangle = \int_{t_0}^{t_f} \int_B \left(\frac{\partial \mathcal{L}}{\partial \dot{\mathbf{Q}}} \delta \dot{\mathbf{Q}} + \frac{\partial \mathcal{L}}{\partial \mathbf{Q}} \delta \mathbf{Q} \right) dV dt$$

Integrating then by parts in time we obtain

$$\begin{aligned}
\langle \delta S, \delta \boldsymbol{\varphi} \rangle &= \int_{t_0}^{t_f} \int_B \left(-\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \mathbf{V}} \right) - DIV \left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}} \right) + \frac{\partial \mathcal{L}}{\partial \boldsymbol{\varphi}} \right) \delta \boldsymbol{\varphi} dV dt \\
&+ \int_B \frac{\partial \mathcal{L}}{\partial \mathbf{V}} \delta \boldsymbol{\varphi} \Big|_{t_0}^{t_f} d\mathbf{X} dt + \int_{t_0}^{t_f} \int_{\partial B} \left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}} \delta \boldsymbol{\varphi} \right) dV dt \\
\langle \delta S, \delta \alpha \rangle &= \int_{t_0}^{t_f} \int_B \left(-\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial T} \right) - DIV \left(\frac{\partial \mathcal{L}}{\partial \boldsymbol{\beta}} \right) + \frac{\partial \mathcal{L}}{\partial \alpha} \right) \delta \alpha dV dt \\
&+ \int_B \frac{\partial \mathcal{L}}{\partial T} \delta \boldsymbol{\varphi} \Big|_{t_0}^{t_f} d\mathbf{X} dt + \int_{t_0}^{t_f} \int_{\partial B} \left(\frac{\partial \mathcal{L}}{\partial \boldsymbol{\beta}} \delta \alpha \right) dV dt \\
\langle \delta S, \delta \mathbf{Q} \rangle &= \int_{t_0}^{t_f} \int_B \left(-\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{\mathbf{Q}}} \right) + \frac{\partial \mathcal{L}}{\partial \mathbf{Q}} \right) \delta \mathbf{Q} dV dt \\
&+ \int_B \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{Q}}} \delta \mathbf{Q} \Big|_{t_0}^{t_f} dV dt
\end{aligned}$$

which under appropriate admissibility assumptions for the variations (i.e., variations $(\delta\boldsymbol{\varphi}, \delta\alpha, \delta\mathbf{Q})$ that vanish in the initial and final times and on the boundary of the body B), on account of the definitions (4.13), (4.14), (4.15), (4.16), and (4.17) and in combination with the Lagrange-d'Alembert principle (4.18), (4.19), (4.20) implies the balance equations (4.12).

4.4 Configurational forces in general dissipative solids

In this section we make use of the Lagrangian and Lagrange-d'Alembert formulations stated in the last section to derive an equation of configurational force balance for deformable materials with thermal, viscous, and internal processes. To this end we follow the same procedure developed in the previous chapter to formulate the equations of configurational force balance for isothermal elastic materials with viscosity. We first establish the equation for materials with no viscous (or non-conservative) behavior by referring the thermomechanical action to the defect reference configuration and taking variations with respect to defect rearrangements (horizontal variations). We then prove that the equation obtained is the "pull-back" of the mechanical force balance equation and entropy balance equation to the material manifold and finally use this property to formulate the equations of balance of configurational forces in the dissipative (viscous) case.

To this end we begin by considering a thermomechanical action given by

$$\begin{aligned}
S(\boldsymbol{\varphi}, \alpha, \mathbf{Q}) &= \int_{t_0}^{t_f} \int_B \mathcal{L}(\mathbf{X}, t, \boldsymbol{\varphi}, \alpha, D\varphi, D\alpha, \mathbf{Q}, \dot{\boldsymbol{\varphi}}, \dot{\alpha}) \, dV dt = \\
&= \int_{t_0}^{t_f} \int_B \left(\frac{R \left\| \dot{\boldsymbol{\varphi}} \right\|^2}{2} - W(\mathbf{X}, t, \boldsymbol{\varphi}, \alpha, D\boldsymbol{\varphi}, D\alpha, \mathbf{Q}, \dot{\alpha}) \right) dV dt
\end{aligned}$$

Let D be the defect-reference configuration, as defined in the previous chapter (§3.3.1), and let

$\boldsymbol{\psi} : D \times [t_0, t_f] \to B$ be the defect rearrangement. Furthermore let

$$\boldsymbol{\phi}(\boldsymbol{\xi}, t) = \boldsymbol{\varphi}(\boldsymbol{\psi}(\boldsymbol{\xi}, t), t) \tag{4.21}$$

$$a(\boldsymbol{\xi}, t) = \alpha(\boldsymbol{\psi}(\boldsymbol{\xi}, t), t) \tag{4.22}$$

$$\mathbf{q}(\boldsymbol{\xi}, t) = \mathbf{Q}(\boldsymbol{\psi}(\boldsymbol{\xi}, t), t) \tag{4.23}$$

be the composition mappings between the motion, thermal displacement, and internal variable fields $\boldsymbol{\varphi}$, α and $\mathbf{Q}$ with the defect rearrangement $\boldsymbol{\psi}(\boldsymbol{\xi}, t)$. Differentiating the previous with respect to the parameter $\boldsymbol{\xi}$ and time t we obtain

$$\begin{aligned}
\mathbf{F} &= D\boldsymbol{\phi} D\boldsymbol{\psi}^{-1} \\
\mathbf{V} &= \dot{\boldsymbol{\phi}} - \left(D\boldsymbol{\phi} D\boldsymbol{\psi}^{-1}\right)\dot{\boldsymbol{\psi}} \\
&= \dot{\boldsymbol{\phi}} - \mathbf{F}\dot{\boldsymbol{\psi}} \\
\boldsymbol{\beta} &= DaD\boldsymbol{\psi}^{-1} \\
T &= \dot{a} - \left(DaD\boldsymbol{\psi}^{-1}\right)\dot{\boldsymbol{\psi}} \\
&= \dot{a} - \beta\dot{\boldsymbol{\psi}}
\end{aligned}$$

Referring now the action functional to the domain D we obtain

$$\begin{aligned}
S(\boldsymbol{\phi}, a, \mathbf{q}, \boldsymbol{\psi}) &= \int_{t_0}^{t_f} \int_B \mathcal{L} \circ \boldsymbol{\psi} \det(D\boldsymbol{\psi})\, d\boldsymbol{\xi} dt = \\
&= \int_{t_0}^{t_f} \int_D \mathcal{L}\left(\boldsymbol{\psi}, t, \boldsymbol{\phi}, a, D\boldsymbol{\phi} D\boldsymbol{\psi}^{-1}, DaD\boldsymbol{\psi}^{-1}, \mathbf{q},\right. \\
&\qquad \left., \dot{\boldsymbol{\phi}} - \left(D\boldsymbol{\phi} D\boldsymbol{\psi}^{-1}\right)\dot{\boldsymbol{\psi}}, \dot{a} - \left(DaD\boldsymbol{\psi}^{-1}\right)\dot{\boldsymbol{\psi}}\right) \det(D\boldsymbol{\psi})\, d\boldsymbol{\xi} dt
\end{aligned}$$

We next compute variations of the previous with respect to each of its arguments keeping the rest fixed. Taking variations with respect to $(\boldsymbol{\phi}, a, \mathbf{q})$ yields

$$\begin{aligned}
\langle \delta S, \delta\phi_i \rangle &= \int_{t_0}^{t_f} \int_D \left(\frac{\partial \mathcal{L}}{\partial \varphi_i}\delta\phi_i + \frac{\partial \mathcal{L}}{\partial F_{iJ}}\delta\phi_{i,\alpha}\psi^{-1}_{\alpha,J} + \frac{\partial \mathcal{L}}{\partial V_i}\left(\delta\dot{\phi}_i - \delta\phi_{i,\alpha}\psi^{-1}_{\alpha,J}\dot{\psi}_J\right)\right) \det(D\boldsymbol{\psi})\, d\boldsymbol{\xi} dt \\
\langle \delta S, \delta a \rangle &= \int_{t_0}^{t_f} \int_D \left(\frac{\partial \mathcal{L}}{\partial \alpha}\delta a + \frac{\partial \mathcal{L}}{\partial \beta_J}\delta a_{,\alpha}\psi^{-1}_{\alpha,J} + \frac{\partial \mathcal{L}}{\partial T}\left(\delta\dot{a} - \delta a_{,\alpha}\psi^{-1}_{\alpha,J}\dot{\psi}_J\right)\right) \det(D\boldsymbol{\psi})\, d\boldsymbol{\xi} dt \\
\langle \delta S, \delta q_A \rangle &= \int_{t_0}^{t_f} \int_D \left(\frac{\partial \mathcal{L}}{\partial Q_A}\delta q_A \right) \det(D\boldsymbol{\psi})\, d\boldsymbol{\xi} dt
\end{aligned}$$

Referring all the previous integrals back to the reference configuration B we find

$$\begin{aligned}
\langle \delta S, \delta\phi_i \rangle &= \int_{t_0}^{t_f} \int_B \left(\frac{\partial \mathcal{L}}{\partial \varphi_i} \left(\delta\phi_i \circ \boldsymbol{\psi}^{-1}\right) + \frac{\partial \mathcal{L}}{\partial F_{iJ}} \frac{d}{dX_J} \left(\delta\phi_i \circ \boldsymbol{\psi}^{-1}\right) + \frac{\partial \mathcal{L}}{\partial V_i} \frac{d}{dt} \left(\delta\phi_i \circ \boldsymbol{\psi}^{-1}\right) \right) dV dt \\
\langle \delta S, \delta a \rangle &= \int_{t_0}^{t_f} \int_B \left(\frac{\partial \mathcal{L}}{\partial \alpha} \delta a + \frac{\partial \mathcal{L}}{\partial \beta_J} \delta a_{,\alpha} \psi^{-1}_{\alpha,J} + \frac{\partial \mathcal{L}}{\partial T} \frac{d}{dt} \left(\delta a \circ \boldsymbol{\psi}^{-1}\right) \right) dV dt \\
\langle \delta S, \delta q_A \rangle &= \int_{t_0}^{t_f} \int_B \left(\frac{\partial \mathcal{L}}{\partial Q_A} \left(\delta q_A \circ \psi^{-1}\right) \right) dV dt
\end{aligned}$$

where we have used the identities

$$\begin{aligned}
\frac{d}{dt} \left(\delta\phi_i \circ \boldsymbol{\psi}^{-1}\right) &= \left(\delta\dot{\phi}_i \circ \boldsymbol{\psi}^{-1}\right) - \left(\delta\phi_{i,\alpha} \circ \boldsymbol{\psi}^{-1}\right) \psi^{-1}_{\alpha,J} \left(\dot{\psi}_J \circ \boldsymbol{\psi}^{-1}\right) \\
\frac{d}{dX_J} \left(\delta\phi_i \circ \boldsymbol{\psi}^{-1}\right) &= \left(\delta\phi_{i,\alpha} \circ \boldsymbol{\psi}^{-1}\right) \psi^{-1}_{\alpha,J} \\
\frac{d}{dt} \left(\delta a \circ \boldsymbol{\psi}^{-1}\right) &= \left(\delta\dot{a} \circ \boldsymbol{\psi}^{-1}\right) - \left(\delta a_{,\alpha} \circ \boldsymbol{\psi}^{-1}\right) \psi^{-1}_{\alpha,J} \left(\dot{\psi}_J \circ \boldsymbol{\psi}^{-1}\right) \\
\frac{d}{dX_J} \left(\delta a \circ \boldsymbol{\psi}^{-1}\right) &= \left(\delta a_{,\alpha} \circ \boldsymbol{\psi}^{-1}\right) \psi^{-1}_{\alpha,J}
\end{aligned}$$

Integrating by parts we obtain

$$\begin{aligned}
\langle \delta S, \delta\phi_i \rangle &= \int_{t_0}^{t_f} \int_B \left(\frac{\partial \mathcal{L}}{\partial \varphi_i} - \frac{d}{dX_J} \frac{\partial \mathcal{L}}{\partial F_{iJ}} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial V_i} \right) \left(\delta\phi_i \circ \boldsymbol{\psi}^{-1}\right) dV dt \\
&\quad + \int_B \left(\delta\phi_i \circ \boldsymbol{\psi}^{-1}\right) \frac{\partial \mathcal{L}}{\partial V_i} dV \Big|_{t_o}^{t_f} + \int_{t_0}^{t_f} \int_{\partial B} \left(\delta\phi_i \circ \boldsymbol{\psi}^{-1}\right) \frac{\partial \mathcal{L}}{\partial F_{iJ}} N_J dS dt \\
\langle \delta S, \delta a \rangle &= \int_{t_0}^{t_f} \int_B \left(\frac{\partial \mathcal{L}}{\partial \alpha} - \frac{d}{dX_J} \frac{\partial \mathcal{L}}{\partial \beta_J} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial T} \right) \left(\delta a \circ \boldsymbol{\psi}^{-1}\right) dV dt \\
&\quad + \int_B \left(\delta a \circ \boldsymbol{\psi}^{-1}\right) \frac{\partial \mathcal{L}}{\partial T} dV \Big|_{t_o}^{t_f} + \int_{t_0}^{t_f} \int_{\partial B} \left(\delta a \circ \boldsymbol{\psi}^{-1}\right) \frac{\partial \mathcal{L}}{\partial \beta_J} N_J dS dt \\
\langle \delta S, \delta q_A \rangle &= \int_{t_0}^{t_f} \int_B \left(\frac{\partial \mathcal{L}}{\partial Q_A} \left(\delta q_A \circ \boldsymbol{\psi}^{-1}\right) \right) dV dt
\end{aligned}$$

Taking next variations with respect to the defect rearrangement $\boldsymbol{\psi}$ keeping constant the other tree fields $(\boldsymbol{\phi}, a, \mathbf{q})$ we find

$$\begin{aligned}
\langle \delta S, \delta\psi_I \rangle &= \int_{t_0}^{t_f} \int_D \left(\frac{\partial \mathcal{L}}{\partial X_I} \delta\psi_I + \left(\frac{\partial \mathcal{L}}{\partial V_i} \left(-\phi_{i,\alpha} \psi^{-1}_{\alpha,I}\right) + \frac{\partial \mathcal{L}}{\partial T} \left(-a_{,\alpha} \psi^{-1}_{\alpha,I}\right) \right) \left(\delta\dot{\psi}_I - \left(\delta\psi_{I,\beta} \psi^{-1}_{\beta,J} \right) \dot{\psi}_J \right) + \right. \\
&\quad \left. + \left(\mathcal{L}\delta_{IJ} - \frac{\partial \mathcal{L}}{\partial F_{iJ}} \left(\phi_{i,\alpha} \psi^{-1}_{\alpha,I}\right) - \frac{\partial \mathcal{L}}{\partial \beta_J} \left(a_{,\alpha} \psi^{-1}_{\alpha,I}\right) \right) \left(\delta\psi_{I,\beta} \psi^{-1}_{\beta,J} \right) \right) \det\left(D\boldsymbol{\psi}\right) d\boldsymbol{\xi} dt
\end{aligned}$$

Notice that the first term involves the derivative of $\mathcal{L}$ with respect to the explicit dependence of X and excluding derivatives with respect to $\boldsymbol{\varphi}, \alpha, \mathbf{Q}$ and their time and spatial derivatives. Referring the integral back to the reference configuration B, the variations with respect to $\boldsymbol{\psi}$ take the form

$$\begin{aligned}\langle \delta S, \delta\psi_I \rangle &= \int_{t_0}^{t_f} \int_B \left(\frac{\partial \mathcal{L}}{\partial X_I} \left(\delta\psi_I \circ \boldsymbol{\psi}^{-1}\right) + \left(-F_{iI} \frac{\partial \mathcal{L}}{\partial V_i} - \beta_I \frac{\partial \mathcal{L}}{\partial T} \right) \frac{d}{dt} \left(\delta\psi_I \circ \boldsymbol{\psi}^{-1}\right) + \right. \\ &\quad \left. + \left(\mathcal{L}\delta_{IJ} - \frac{\partial \mathcal{L}}{\partial F_{iJ}} F_{iI} - \frac{\partial \mathcal{L}}{\partial \beta_J} \beta_I \right) \frac{d}{dX_J} \left(\delta\psi_I \circ \boldsymbol{\psi}^{-1}\right) \right) dV dt\end{aligned}$$

where identities (3.30) and (3.31) have been used. Integrating by parts in the previous gives the variations in the form

$$\begin{aligned}\langle \delta S, \delta\psi_I \rangle &= \int_{t_0}^{t_f} \int_B \left(\frac{\partial \mathcal{L}}{\partial X_I} - \frac{d}{dt} \left(-F_{iI} \frac{\partial \mathcal{L}}{\partial V_i} - \beta_I \frac{\partial \mathcal{L}}{\partial T} \right) - \frac{d}{dX_J} \left(\mathcal{L}\delta_{IJ} - F_{iI} \frac{\partial \mathcal{L}}{\partial F_{iJ}} - \beta_I \frac{\partial \mathcal{L}}{\partial \beta_J} \right) \right) \delta\psi_I \circ \boldsymbol{\psi}^{-1} + \\ &\quad + \int_B \left(-F_{iI} \frac{\partial \mathcal{L}}{\partial V_i} - \beta_I \frac{\partial \mathcal{L}}{\partial T} \right) \left(\delta\psi_I \circ \boldsymbol{\psi}^{-1}\right) dV \Big|_{t_o}^{t_f} + \\ &\quad + \int_{t_0}^{t_f} \int_{\partial B} \left(\left(\delta\psi_I \circ \boldsymbol{\psi}^{-1}\right) \left(\mathcal{L}\delta_{IJ} - F_{iI} \frac{\partial \mathcal{L}}{\partial F_{iJ}} - \beta_I \frac{\partial \mathcal{L}}{\partial \beta_J} \right) N_J \right) dS dt\end{aligned}$$

We finally invoke the stationarity of the thermomechanical action functional with respect to admissible variations of each of its arguments to obtain the Euler-Lagrange equations. Stationarity of the action functional with respect to $(\delta\boldsymbol{\phi}, \delta a, \delta\mathbf{q})$ implies the Euler-Lagrange equations

$$\begin{aligned}\frac{\partial \mathcal{L}}{\partial \boldsymbol{\varphi}} - \mathrm{DIV}\left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right) - \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \mathbf{V}}\right) &= 0 \\ \frac{\partial \mathcal{L}}{\partial \alpha} - \mathrm{DIV}\left(\frac{\partial \mathcal{L}}{\partial \boldsymbol{\beta}}\right) - \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial T}\right) &= 0 \\ \frac{\partial \mathcal{L}}{\partial \mathbf{Q}} &= \mathbf{0}\end{aligned}$$

that, using the equilibrium relations (4.13) and momenta definitions (4.15), can be rewritten as

$$\mathbf{B}^e + \mathrm{DIV}\left(\mathbf{P}^e\right) - \frac{d}{dt}\left(R\mathbf{V}\right) = \mathbf{0} \tag{4.24}$$

$$\frac{S^e}{T} - \mathrm{DIV}\left(\frac{\mathbf{H}^e}{T}\right) - \frac{d}{dt}\left(RN\right) = 0 \tag{4.25}$$

$$\mathbf{Y}^e = \mathbf{0} \tag{4.26}$$

These equations correspond to the equilibrium part of the equations of mechanical force balance, entropy balance and internal force balance (4.12).

Invoking next the stationarity of the action functional with respect to variations of $\boldsymbol{\psi}$ implies the Euler-Lagrange equation

$$\frac{\partial \mathcal{L}}{\partial X_I} - \frac{d}{dt}\left(-F_{iI} \frac{\partial \mathcal{L}}{\partial V_i} - \beta_I \frac{\partial \mathcal{L}}{\partial T} \right) - \frac{d}{dX_J}\left(\mathcal{L}\delta_{IJ} - F_{iI} \frac{\partial \mathcal{L}}{\partial F_{iJ}} - \beta_I \frac{\partial \mathcal{L}}{\partial \beta_J} \right) = 0$$

or in invariant notation

$$\frac{\partial \mathcal{L}}{\partial \mathbf{X}} - \frac{d}{dt}\left(-\mathbf{F}^T \frac{\partial \mathcal{L}}{\partial \mathbf{V}} - \boldsymbol{\beta}\frac{\partial \mathcal{L}}{\partial T}\right) - \mathrm{DIV}\left(\mathcal{L}\mathbf{I} - \mathbf{F}^T \frac{\partial \mathcal{L}}{\partial \mathbf{F}} - \boldsymbol{\beta} \otimes \frac{\partial \mathcal{L}}{\partial \boldsymbol{\beta}}\right) = 0$$

Using the equilibrium relations (4.13) and momenta definitions (4.15) the previous yield

$$\frac{\partial \mathcal{L}}{\partial \mathbf{X}} - \frac{d}{dt}\left(-\mathbf{F}^T R\dot{\boldsymbol{\varphi}} - \boldsymbol{\beta} R N\right) - \mathrm{DIV}\left(\mathcal{L}\mathbf{I} + \mathbf{F}^T \mathbf{P}^e - \boldsymbol{\beta} \otimes \frac{\mathbf{H}^e}{T}\right) = \mathbf{0} \tag{4.27}$$

Equation (4.27) has been obtained following exactly the same procedure used to derive the equation of configurational force balance (3.34), (3.36) and will therefore be regarded as the equilibrium part of the equation of configurational force balance.

We finally derive the configurational force balance equation in the presence of dissipative (or non-conservative or viscous) stresses and forces. To this end we first prove a pull-back relation analogous to the one obtained for isotropic elastic materials (3.42). We next use this relation as a rule to build the equations in the presence of both equilibrium and non-equilibrium factors. Let $\mathcal{F}_{\boldsymbol{\phi}}$, $\mathcal{F}_a$, $\mathcal{F}_{\mathbf{q}}$, and $\mathcal{F}_{\boldsymbol{\psi}}$ be the Euler-Lagrange operators

$$\begin{aligned}
\mathcal{F}_{\boldsymbol{\phi}} &= \frac{\partial \mathcal{L}}{\partial \boldsymbol{\varphi}} - \mathrm{DIV}\left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right) - \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \mathbf{V}}\right) = \\
&= \mathbf{B}^e + \mathrm{DIV}\left(\mathbf{P}^e\right) - \frac{d}{dt}\left(R\mathbf{V}\right) \\
\mathcal{F}_a &= \frac{\partial \mathcal{L}}{\partial \alpha} - \mathrm{DIV}\left(\frac{\partial \mathcal{L}}{\partial \boldsymbol{\beta}}\right) - \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial T}\right) = \\
&= \frac{S^e}{T} - \mathrm{DIV}\left(\frac{\mathbf{H}^e}{T}\right) - \frac{d}{dt}\left(RN\right) \\
\mathcal{F}_{\mathbf{q}} &= \frac{\partial \mathcal{L}}{\partial \mathbf{Q}} = \mathbf{Y}^e \\
\mathcal{F}_{\boldsymbol{\psi}} &= \frac{\partial \mathcal{L}}{\partial \mathbf{X}} - \mathrm{DIV}\left(\mathcal{L}\mathbf{I} - \mathbf{F}^T \frac{\partial \mathcal{L}}{\partial \mathbf{F}} - \boldsymbol{\beta} \otimes \frac{\partial \mathcal{L}}{\partial \boldsymbol{\beta}}\right) - \frac{d}{dt}\left(-\mathbf{F}^T \frac{\partial \mathcal{L}}{\partial \mathbf{V}} - \boldsymbol{\beta}\frac{\partial \mathcal{L}}{\partial T}\right) \\
& \frac{\partial \mathcal{L}}{\partial \mathbf{X}} - \mathrm{DIV}\left(\mathcal{L}\mathbf{I} + \mathbf{F}^T \mathbf{P}^e - \boldsymbol{\beta} \otimes \frac{\mathbf{H}^e}{T}\right) - \frac{d}{dt}\left(-\mathbf{F}^T R\mathbf{V} - \boldsymbol{\beta} RN\right)
\end{aligned}$$

i.e., the left hand side of the Euler-Lagrange equations (4.24), (4.25), (4.26), and (4.27). Then it is straightforward to prove the identity

$$-\mathbf{F}^T \mathcal{F}_{\boldsymbol{\phi}} - \boldsymbol{\beta}\mathcal{F}_a - D\mathbf{Q}\mathcal{F}_{\mathbf{q}} = \mathcal{F}_{\boldsymbol{\psi}} \tag{4.28}$$

This relation expresses that if the first three Euler-Lagrange equations $\mathcal{F}_{\boldsymbol{\phi}} = \mathbf{0}$, $\mathcal{F}_a = 0$, $\mathcal{F}_{\mathbf{q}} = \mathbf{0}$ (those corresponding to vertical variations) are satisfied, then the configurational force balance equation $\mathcal{F}_{\boldsymbol{\psi}} = \mathbf{0}$ is automatically satisfied and establishes an algebraic relation between all balance equations. We take now this property as a rule to build the configurational force balance equation in the presence of dissipative terms. The full (including non-equilibrium terms) balance equations are

$$\mathcal{F}_{\boldsymbol{\phi}} + \mathbf{B}^v + \mathrm{DIV}\left(\mathbf{P}^v\right) = \mathbf{0} \tag{4.29}$$

$$\mathcal{F}_a + \frac{S^v}{T} + \dot{\Gamma} - \mathrm{DIV}\left(\frac{\mathbf{H}^v}{T}\right) = 0 \tag{4.30}$$

$$\mathcal{F}_{\mathbf{q}} + \mathbf{Y}^v = \mathbf{0} \tag{4.31}$$

Left-multiplying these equations, respectively, by $\left(-\mathbf{F}^T, -\boldsymbol{\beta}, -D\mathbf{Q}\right)$ and using the pull-back relation (4.28) we obtain the configurational force balance equation in the form

$$\mathcal{F}_{\boldsymbol{\psi}} - \mathbf{F}^T\left(\mathbf{B}^v + \mathrm{DIV}\left(\mathbf{P}^v\right)\right) - \boldsymbol{\beta}\left(\frac{S^v}{T} + \dot{\Gamma} - \mathrm{DIV}\left(\frac{\mathbf{H}^v}{T}\right)\right) - D\mathbf{Q}\mathbf{Y}^v = \mathbf{0} \tag{4.32}$$

The previous might also be rewritten as

$$\begin{aligned} \mathbf{0} &= \mathcal{F}_{\boldsymbol{\psi}} - \mathrm{DIV}\left(\mathbf{F}^T\mathbf{P}^v - \boldsymbol{\beta}\frac{\mathbf{H}^v}{T}\right) - \mathbf{F}^T\mathbf{B}^v - \boldsymbol{\beta}\frac{S^v}{T} \\ &\quad - \left(\boldsymbol{\beta}\dot{\Gamma} - \left(\mathbf{P}^v D\mathbf{F} - \frac{\mathbf{H}^v}{T}D\boldsymbol{\beta} - \mathbf{Y}^v D\mathbf{Q}\right)\right) \end{aligned}$$

or using the relation (4.9) for the internal entropy production $\dot{\Gamma}$ and rearranging appropriately as

$$\begin{aligned} \mathbf{0} &= \mathcal{F}_{\boldsymbol{\psi}} - \mathrm{DIV}\left(\mathbf{F}^T\mathbf{P}^v - \boldsymbol{\beta}\frac{\mathbf{H}^v}{T}\right) - \mathbf{F}^T\mathbf{B}^v - \boldsymbol{\beta}\frac{S^v}{T} \\ &\quad - \left(\boldsymbol{\beta}\frac{1}{T}\left(\mathbf{P}^v\dot{\mathbf{F}} - \frac{\mathbf{H}^v}{T}\dot{\boldsymbol{\beta}} - \mathbf{Y}^v\dot{\mathbf{Q}}\right) - \left(\mathbf{P}^v D\mathbf{F} - \frac{\mathbf{H}^v}{T}D\boldsymbol{\beta} - \mathbf{Y}^v D\mathbf{Q}\right)\right) \end{aligned}$$

Finally grouping terms in the last factor we obtain

$$\begin{aligned} \mathbf{0} &= \mathcal{F}_{\boldsymbol{\psi}} - \mathrm{DIV}\left(\mathbf{F}^T\mathbf{P}^v - \boldsymbol{\beta}\frac{\mathbf{H}^v}{T}\right) - \mathbf{F}^T\mathbf{B}^v - \boldsymbol{\beta}\frac{S^v}{T} \\ &\quad - \left(\mathbf{P}^v\left(\frac{\boldsymbol{\beta}\dot{\mathbf{F}}}{T} - D\mathbf{F}\right) - \frac{\mathbf{H}^v}{T}\left(\frac{\boldsymbol{\beta}\dot{\boldsymbol{\beta}}}{T} - D\beta\right) - \mathbf{Y}^v\left(\frac{\boldsymbol{\beta}\dot{\mathbf{Q}}}{T} - D\mathbf{Q}\right)\right) \end{aligned}$$

or alternatively, using the identity $-D\left(\frac{\boldsymbol{\beta}}{T}\right) = \frac{1}{T}\left(\frac{\boldsymbol{\beta}DT}{T} - D\boldsymbol{\beta}\right) = \frac{1}{T}\left(\frac{\boldsymbol{\beta}\dot{\boldsymbol{\beta}}}{T} - D\boldsymbol{\beta}\right)$ we finally find

$$\begin{aligned} \mathbf{0} &= \mathcal{F}_{\boldsymbol{\psi}} - \mathrm{DIV}\left(\mathbf{F}^T\mathbf{P}^v - \boldsymbol{\beta}\frac{\mathbf{H}^v}{T}\right) - \mathbf{F}^T\mathbf{B}^v - \boldsymbol{\beta}\frac{S^v}{T} \\ &\quad - \left(\mathbf{P}^v\left(\frac{\boldsymbol{\beta}\dot{\mathbf{F}}}{T} - D\mathbf{F}\right) + \mathbf{H}^v D\left(\frac{\boldsymbol{\beta}}{T}\right) - \mathbf{Y}^v\left(\frac{\boldsymbol{\beta}\dot{\mathbf{Q}}}{T} - D\mathbf{Q}\right)\right) \end{aligned} \tag{4.33}$$

Equation (4.32) or its equivalent (4.33) is the equation of balance of configurational forces in the presence of dissipative behavior. Notice that for isothermic processes we have $T\left(\mathbf{X}, t\right) = \theta$ (a constant independent of space and time) and therefore $\alpha = \theta\,(t - t_0)$ and $\boldsymbol{\beta} = D\alpha = \mathbf{0}$. Assuming in addition that $\mathbf{Q}\,(\mathbf{X}, t) = \mathbf{0}$, which implies $\dot{\mathbf{Q}} = D\mathbf{Q} = 0$, then the equation of balance of configurational forces (4.32) reduces in this case (isothermal processes with no internal variables) to

$$\mathcal{F}_{\boldsymbol{\psi}} - \mathbf{F}^T\left(\mathbf{B}^v + \mathrm{DIV}\left(\mathbf{P}^v\right)\right) = \mathbf{0}$$

with

$$\mathcal{F}_{\boldsymbol{\psi}} = \frac{\partial L}{\partial \mathbf{X}} - \mathrm{DIV}\left(\mathcal{L}\mathbf{I} + \mathbf{F}^T\mathbf{P}^v\right) - \frac{d}{dt}\left(-\mathbf{F}^T R\mathbf{V}\right)$$

This equation correspond to the equations of configurational force balance for isothermal elastic materials with viscosity obtained in the pervious chapter, equations (3.58) and (3.59). Eliminating the symbol $\mathcal{F}_{\boldsymbol{\psi}}$ from equation (4.33), the configurational force balance equation adopts the final form

$$\begin{aligned}\mathbf{0} \;=\; & \frac{\partial \mathcal{L}}{\partial \mathbf{X}} - \mathrm{DIV}\left(\mathcal{L}\mathbf{I} + \mathbf{F}^T\left(\mathbf{P}^e + \mathbf{P}^v\right) - \boldsymbol{\beta}\otimes\frac{\mathbf{H}^e + \mathbf{H}^v}{T}\right) - \frac{d}{dt}\left(-\mathbf{F}^T R\mathbf{V} - \boldsymbol{\beta}RN\right) - \mathbf{F}^T\mathbf{B}^v - \boldsymbol{\beta}\frac{S^v}{T} \\ & - \left(\mathbf{P}^v\left(\frac{\boldsymbol{\beta}\dot{\mathbf{F}}}{T} - D\mathbf{F}\right) + \mathbf{H}^v D\left(\frac{\boldsymbol{\beta}}{T}\right) - \mathbf{Y}^v\left(\frac{\boldsymbol{\beta}\dot{\mathbf{Q}}}{T} - D\mathbf{Q}\right)\right)\end{aligned}$$

We end this chapter by establishing vertical, horizontal and combined vertical-horizontal versions of the Lagrange-d'Alembert principle (4.18),(4.19),(4.20) in complete analogy with what was done in the previous chapter for isothermal materials with no internal processes. The Lagrange-d'Alembert principle for the (vertical) balance equations (4.29),(4.30),(4.31) are

$$\begin{aligned}\langle \delta S, \delta\boldsymbol{\phi}\rangle + \int_{t_0}^{t_f}\int_B \left(\delta\boldsymbol{\phi}^T \circ \boldsymbol{\psi}^{-1}\right)\left(\frac{\partial \Psi}{\partial \dot{\boldsymbol{\varphi}}} + \mathrm{DIV}\left(\frac{\partial \Psi}{\partial \dot{\mathbf{F}}}\right)\right) dV\,dt &= 0 \\ \langle \delta S, \delta a\rangle + \int_{t_0}^{t_f}\int_B \left(\delta a \circ \boldsymbol{\psi}^{-1}\right)\left(\frac{\partial \Psi}{\partial \dot{\alpha}} + \dot{\Gamma} + \mathrm{DIV}\left(\frac{\partial \Psi}{\partial \dot{\beta}}\right)\right) dV\,dt &= 0 \\ \langle \delta S, \delta\mathbf{q}\rangle + \int_{t_0}^{t_f}\int_B \left(\delta\mathbf{q}^T \circ \boldsymbol{\psi}^{-1}\right)\left(\frac{\partial \Psi}{\partial \dot{\mathbf{Q}}}\right) dV\,dt &= 0\end{aligned}$$

The Lagrange-d'Alembert principle for the configurational balance equation (horizontal balance) (4.32) is

$$\begin{aligned}0 \;=\; & \langle \delta S, \delta\boldsymbol{\psi}\rangle + \\ & + \int_{t_0}^{t_f}\int_B \left(\delta\boldsymbol{\psi}^T \circ \boldsymbol{\psi}^{-1}\right)\left(-\mathbf{F}^T\left(\frac{\partial \Psi}{\partial \dot{\boldsymbol{\varphi}}} + \mathrm{DIV}\left(\frac{\partial \Psi}{\partial \dot{\mathbf{F}}}\right)\right)\right) dV\,dt \\ & + \int_{t_0}^{t_f}\int_B \left(\delta\boldsymbol{\psi}^T \circ \boldsymbol{\psi}^{-1}\right)\left(-\boldsymbol{\beta}\left(\frac{\partial \Psi}{\partial \dot{\alpha}} + \dot{\Gamma} + \mathrm{DIV}\left(\frac{\partial \Psi}{\partial \dot{\beta}}\right)\right)\right) dV\,dt \\ & + \int_{t_0}^{t_f}\int_B \left(\delta\boldsymbol{\psi}^T \circ \boldsymbol{\psi}^{-1}\right)\left(-D\mathbf{Q}\frac{\partial \Psi}{\partial \dot{\mathbf{Q}}}\right) dV\,dt\end{aligned}$$

Combining vertical and horizontal Lagrange-d'Alembert principles we finally obtain

$$
\begin{aligned}
&\langle \delta S, \delta \boldsymbol{\phi} \rangle + \langle \delta S, \delta a \rangle + \langle \delta S, \delta \mathbf{q} \rangle + \langle \delta S, \delta \boldsymbol{\psi} \rangle + \\
&+ \int_{t_0}^{t_f} \int_B \left(\left(\delta \boldsymbol{\phi} \circ \boldsymbol{\psi}^{-1} \right) - \mathbf{F} \left(\delta \boldsymbol{\psi} \circ \boldsymbol{\psi}^{-1} \right) \right)^T \left(\frac{\partial \Psi}{\partial \dot{\boldsymbol{\varphi}}} + \mathrm{DIV} \left(\frac{\partial \Psi}{\partial \dot{\mathbf{F}}} \right) \right) + \\
&+ \int_{t_0}^{t_f} \int_B \left(\left(\delta a \circ \boldsymbol{\psi}^{-1} \right) - \boldsymbol{\beta} \left(\delta \boldsymbol{\psi} \circ \boldsymbol{\psi}^{-1} \right) \right)^T \left(\frac{\partial \Psi}{\partial \dot{\alpha}} + \dot{\Gamma} + \mathrm{DIV} \left(\frac{\partial \Psi}{\partial \dot{\beta}} \right) \right) + \\
&+ \int_{t_0}^{t_f} \int_B \left(\left(\delta \mathbf{q} \circ \boldsymbol{\psi}^{-1} \right) - D\mathbf{Q} \left(\delta \boldsymbol{\psi} \circ \boldsymbol{\psi}^{-1} \right) \right)^T \left(\frac{\partial \Psi}{\partial \dot{\mathbf{Q}}} \right) dV dt = 0
\end{aligned}
$$

that using the kinetic relations (4.16) and (4.17) can be rewritten as

$$
\begin{aligned}
&\langle \delta S, \delta \boldsymbol{\phi} \rangle + \langle \delta S, \delta a \rangle + \langle \delta S, \delta \mathbf{q} \rangle + \langle \delta S, \delta \boldsymbol{\psi} \rangle + \\
&+ \int_{t_0}^{t_f} \int_B \left(\left(\delta \boldsymbol{\phi} \circ \boldsymbol{\psi}^{-1} \right) - \mathbf{F} \left(\delta \boldsymbol{\psi} \circ \boldsymbol{\psi}^{-1} \right) \right)^T \left(\mathbf{B}^v + \mathrm{DIV} \left(\mathbf{P}^v \right) \right) + \\
&+ \int_{t_0}^{t_f} \int_B \left(\left(\delta a \circ \boldsymbol{\psi}^{-1} \right) - \boldsymbol{\beta} \left(\delta \boldsymbol{\psi} \circ \boldsymbol{\psi}^{-1} \right) \right)^T \left(\frac{S^v}{T} + \dot{\Gamma} - \mathrm{DIV} \left(\frac{\mathbf{H}^v}{T} \right) \right) + \\
&+ \int_{t_0}^{t_f} \int_B \left(\left(\delta \mathbf{q} \circ \boldsymbol{\psi}^{-1} \right) - D\mathbf{Q} \left(\delta \boldsymbol{\psi} \circ \boldsymbol{\psi}^{-1} \right) \right)^T \left(-\mathbf{Y}^v \right) dV dt = 0
\end{aligned}
$$

Chapter 5

Mixed variational principles for dynamics

We turn in this section to the formulation of a mixed (two-field) variational formulation for dynamics that allows for independent variations of deformations $\boldsymbol{\varphi}$ and velocities $\mathbf{V}$. We will refer to this formulation as the mixed Hamilton's principle. The construction of this mixed variational principle follows a standard -Lagrange multiplier argument to enforce the "time-compatiblity" identity $\mathbf{V} = \dot{\boldsymbol{\varphi}}$ between "assumed" $\mathbf{V}$ and compatible $\dot{\boldsymbol{\varphi}}$ velocity fields. We next extend this formulation to account for variations with respect to defect rearrangements (horizontal variations). The resulting mixed (three-field) formulation will render simultaneously the equations of balance of mechanical forces, configurational forces, and time compatibility.

The mixed formulation for dynamics is introduced as an approach to overcome instabilities inherent to the use of the standard (single-field) Hamilton's principle with moving meshes. More specifically, as was illustrated for one-dimensional problems in the second chapter and will be further elaborated in the next chapter, the approximation for the material velocity field $\dot{\boldsymbol{\varphi}}_h$ that results from the approximation of the motion $\boldsymbol{\varphi}_h$ with finite elements interpolated over moving meshes may exhibit jump discontinuities across element boundaries. This discontinuities eventually grow unbounded rendering unstable and meaningless solutions. These instabilities are effectively controlled by making use of a continuous, assumed velocity interpolation $\mathbf{V}_h$ in lieu of the consistent interpolation $\dot{\boldsymbol{\varphi}}_h$ and the mixed Hamilton's principle as the underlying variational framework.

The mixed variational formulation presented here may be considered as the dynamic analogous to the Beuveke-Hu-Washizu mixed variational principle for statics [9]. Furthermore, both variational principles may be combined together to establish a single mixed space-time variational principle for non-linear dynamics that accounts for independent variations of all fields (deformations, velocities, strains, momentum, and stresses).

5.1 Beuveke-Hu-Washizu variational principle for statics

The Beuveke-Hu-Washizu mixed variational principle for elastostatics allows for independent variations of deformations, strains and stresses. The Beuveke-Hu-Washizu functional is

$$\begin{aligned} I[\boldsymbol{\varphi}, \mathbf{F}, \mathbf{P}] &= \int_B \left(W(\mathbf{X}, \boldsymbol{\varphi}, \mathbf{F}) + P_{iJ}\left(\varphi_{i,J} - F_{iJ}\right)\right) dV \\ &\quad - \int_{\partial B_2} \left(\varphi_i - \bar{\varphi}_i\right) P_{iJ} N_J dS - \int_{\partial B_1} \bar{T}_i \varphi_i dS \end{aligned} \tag{5.1}$$

The stress tensor $\mathbf{P}$ acts as Lagrange multiplier in B and on the traction boundary ∂B_1 to enforce the "strain-displacement" compatibility condition $\varphi_{i,J} = F_{iJ}$ and Dirichlet boundary conditions $\varphi_i = \bar{\varphi}_i$. The variations of the generalized potential I with respect to each field are

$$\begin{aligned} \langle \delta I, \delta\varphi_i \rangle &= \int_B \left(\frac{\partial W}{\partial \varphi_i}\delta\varphi_i + P_{iJ}\delta\varphi_{i,J}\right) dV + \\ &\quad - \int_{\partial B_2} \delta\varphi_i P_{iJ} N_J dS - \int_{\partial B_1} \delta\varphi_i \bar{T}_i dS \\ \langle \delta I, \delta F_{iJ} \rangle &= \int_B \left(\frac{\partial W}{\partial F_{iJ}} - P_{iJ}\right) \delta F_{iJ} dV \\ \langle \delta I, \delta F_{iJ} \rangle &= \int_B \delta P_{iJ}\left(\varphi_{i,J} - F_{iJ}\right) dV \\ &\quad - \int_{\partial B_1} \left(\varphi_i - \bar{\varphi}_i\right) \delta P_{iJ} N_J dS \end{aligned}$$

with Euler-Lagrange equations

$$\begin{aligned} -\frac{\partial W}{\partial \varphi_i} + \frac{dP_{iJ}}{dX_J} &= 0 \qquad \text{in } B \\ P_{iJ} N_J - \bar{T}_i &= 0 \qquad \text{on } \partial B_1 \\ \frac{\partial W}{\partial F_{iJ}} - P_{iJ} &= 0 \qquad \text{in } B \\ \varphi_{i,J} - F_{iJ} &= 0 \qquad \text{in } B \\ \varphi_i - \bar{\varphi}_i &= 0 \qquad \text{on } \partial B_2 \end{aligned}$$

that correspond to the field equations and boundary conditions of elastostatics. Replacing the $\mathbf{P}$ multiplier in the Beuveke-Hu-Washizu functional I with the Euler-Lagrange equation corresponding to the variations of its conjugate $\mathbf{F}$, a two-field functional in which deformations and strains are independent variables, is obtained.

$$\begin{aligned} I[\boldsymbol{\varphi}, \mathbf{F}] &= \int_B \left(W + \frac{\partial W}{\partial F_{iJ}}\left(\varphi_{i,J} - F_{iJ}\right)\right) dV \\ &\quad - \int_{\partial B_2} \left(\varphi_i - \bar{\varphi}_i\right) \frac{\partial W}{\partial F_{iJ}} N_J dS - \int_{\partial B_1} \bar{T}_i \varphi_i dS \end{aligned}$$

This potential is a (deformation-strain) dual of the well-known Hellinger-Reissner (deformation-stress) mixed variational principle and has been attributed to Beuveke [9].

5.2 Mixed Hamilton's principle and mixed Lagrangian

Motivated by the methodology that led to the Beuveke-Hu-Washizu potential for statics and its reduction to a two field "strain-deformation" potential, the following three-field "mixed action functional" for dynamics arises:

$$\begin{aligned} S[\boldsymbol{\varphi}, \mathbf{V}, \mathbf{p}] &= \int_{t_0}^{t_f} \int_B \left(\mathcal{L}(\mathbf{X}, t, \boldsymbol{\varphi}, \mathbf{V}, D\boldsymbol{\varphi}) + p_i(\dot{\varphi}_i - V_i) \right) dV dt \\ &\quad + \int_{t_0}^{t_f} \int_{\partial B_1} \bar{T}_i \varphi_i dS dt \end{aligned} \tag{5.2}$$

where (what will turn out to be) the momentum $\mathbf{p}$ acts as the Lagrange multiplier in B to enforce the "velocity-deformation" compatibility or "time-compatibility" condition $\dot{\varphi}_i = V_i$ and where the "strain-deformation" compatibility condition $\varphi_{i,J} - F_{iJ} = 0$ is accounted for strongly. Integrals are taken over the space-time domain $[t_0, t_f] \times B$. For a Lagrangian density of the form (3.3) the mixed action functional becomes

$$\begin{aligned} S[\boldsymbol{\varphi}, \mathbf{V}, \mathbf{p}] &= \int_{t_0}^{t_f} \int_B \left(\frac{1}{2} R |\mathbf{V}|^2 - W(\mathbf{X}, t, \boldsymbol{\varphi}, D\boldsymbol{\varphi}) + p_i(\dot{\varphi}_i - V_i) \right) dV dt \\ &\quad + \int_{t_0}^{t_f} \int_{\partial B_1} \bar{T}_i \varphi_i dS dt \end{aligned} \tag{5.3}$$

Unlike the Beuveke-Hu-Washizu principle, in which not only the field equations but also the Dirichlet boundary conditions are weakly enforced within the variational framework, we do not attempt to enforce *initial* conditions variationally. Therefore we maintain the restriction on the variations $\delta\boldsymbol{\varphi}$ to belong to the set of admissible variations, i.e., variations that vanish on the initial and final times and on the Dirichlet part of the boundary ∂B_2. Nevertheless the formulation of a more general mixed variational principle for dynamics that account also for initial (and final) conditions and Dirichlet boundary conditions appears to be straightforward.

The variations of the mixed action with respect to each field are

$$\begin{aligned}
\langle \delta S, \delta\varphi_i \rangle &= \int_{t_0}^{t_f} \int_B \left(\frac{\partial \mathcal{L}}{\partial \varphi_i} \delta\varphi_i + \frac{\partial \mathcal{L}}{\partial F_{iJ}} \delta\varphi_{i,J} + p_i \delta\dot{\varphi}_i \right) dV dt + \\
&\quad \int_{t_0}^{t_f} \int_{\partial B_1} \delta\varphi_i \bar{T}_i dS dt \\
\langle \delta S, \delta V_i \rangle &= \int_{t_0}^{t_f} \int_B \left(\frac{\partial \mathcal{L}}{\partial V_i} - p_i \right) \delta V_i dV dt \\
\langle \delta S, \delta p_i \rangle &= \int_{t_0}^{t_f} \int_B \delta p_i \left(\dot{\varphi}_i - V_i \right) dV dt
\end{aligned}$$

The variational principle

$$\begin{aligned}
\langle \delta S, \delta\boldsymbol{\varphi} \rangle &= \mathbf{0} \\
\langle \delta S, \delta\mathbf{V} \rangle &= \mathbf{0} \\
\langle \delta S, \delta\mathbf{p} \rangle &= \mathbf{0}
\end{aligned}$$

for every admissible variations $(\delta\boldsymbol{\varphi}, \delta\mathbf{V}, \delta\mathbf{p})$ will be referred to as the *mixed Hamilton's principle*. We will denote the mixed Lagrangian density by

$$\mathcal{L}^{mix}\left(\mathbf{X}, t, \boldsymbol{\varphi}, \mathbf{V}, \mathbf{F}, \mathbf{p}, \dot{\boldsymbol{\varphi}}\right) = \mathcal{L}\left(\mathbf{X}, t, \boldsymbol{\varphi}, \mathbf{V}, \mathbf{F}\right) + p_i \left(\dot{\varphi}_i - V_i\right) \tag{5.4}$$

The corresponding Euler-Lagrange equations are

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial \varphi_i} - \frac{d}{dX_J}\left(\frac{\partial \mathcal{L}}{\partial F_{iJ}}\right) - \frac{dp_i}{dt} &= 0 \qquad \text{in } B \text{ and } \forall t \in I \\
\frac{\partial \mathcal{L}}{\partial V_i} - p_i &= 0 \qquad \text{in } B \text{ and } \forall t \in I \\
\dot{\varphi}_i - V_i &= 0 \qquad \text{in } B \text{ and } \forall t \in I \\
\frac{\partial \mathcal{L}}{\partial F_{iJ}} + \bar{T}_i &= 0 \qquad \text{on } \partial B_1 \text{ and } \forall t \in I
\end{aligned}$$

that correspond to the equations of mechanical force balance (3.10), time compatibility $\dot{\boldsymbol{\varphi}} = \mathbf{V}$, and traction boundary conditions, the Lagrange multiplier $\mathbf{p}$ resulting coincident to the momentum $\frac{\partial L}{\partial \mathbf{V}}$.

Replacing now the $\mathbf{p}$ multiplier in the mixed action (5.2) with the Euler-Lagrange equation corresponding to variations of its conjugate $\mathbf{V}$, the following two-field action functional in which deformations and velocities are independent variables is obtained:

$$\begin{aligned}
S\left[\boldsymbol{\varphi}, \mathbf{V}\right] &= \int_{t_0}^{t_f} \int_B \left(\mathcal{L}\left(\mathbf{X}, t, \boldsymbol{\varphi}, \mathbf{V}, D\boldsymbol{\varphi}\right) + \left.\frac{\partial \mathcal{L}}{\partial V_i}\right|_{(\mathbf{X}, t, \boldsymbol{\varphi}, \mathbf{V}, D\boldsymbol{\varphi})} \left(\dot{\varphi}_i - V_i\right) \right) dV dt \\
&\quad + \int_{t_0}^{t_f} \int_{\partial B_2} \bar{T}_i \varphi_i dS dt
\end{aligned}$$

Defining the following mixed Lagrangian density

$$\mathcal{L}^{mix}\left(\mathbf{X},t,\boldsymbol{\varphi},\mathbf{V},\mathbf{F},\dot{\boldsymbol{\varphi}}\right)=\mathcal{L}\left(\mathbf{X},t,\boldsymbol{\varphi},\mathbf{V},\mathbf{F}\right)+\left.\frac{\partial\mathcal{L}}{\partial V_i}\right|_{(\mathbf{X},t,\boldsymbol{\varphi},\mathbf{V},\mathbf{F})}\left(\dot{\varphi}_i-V_i\right) \tag{5.5}$$

the two-field action takes the form

$$S\left[\boldsymbol{\varphi},\mathbf{V}\right]=\int_{t_0}^{t_f}\int_B\mathcal{L}^{mix}\left(\mathbf{X},t,\boldsymbol{\varphi},\mathbf{V},D\boldsymbol{\varphi},\dot{\boldsymbol{\varphi}}\right)dV\,dt+\int_{t_0}^{t_f}\int_{\partial B_2}\bar{T}_i\varphi_i dSdt \tag{5.6}$$

Taking variations with respect to each independent arguments yields

$$\begin{aligned}
\langle\delta S,\delta\varphi_i\rangle &= \int_{t_0}^{t_f}\int_B\left(\frac{\partial\mathcal{L}^{mix}}{\partial\varphi_i}\delta\varphi_i+\frac{\partial\mathcal{L}^{mix}}{\partial F_{iI}}\delta\varphi_{i,I}+\frac{\partial\mathcal{L}^{mix}}{\partial V_i}\delta\dot{\varphi}_i\right)dV\,dt\\
&= \int_{t_0}^{t_f}\int_B\left(\frac{\partial\mathcal{L}}{\partial\varphi_i}\delta\varphi_i+\frac{\partial\mathcal{L}}{\partial F_{iI}}\delta\varphi_{i,I}+\frac{\partial\mathcal{L}}{\partial V_i}\delta\dot{\varphi}_i+\right.\\
&\quad\left.+\left(\frac{\partial^2\mathcal{L}}{\partial\varphi_i\partial V_j}\delta\varphi_i+\frac{\partial^2\mathcal{L}}{\partial F_{iI}\partial V_j}\delta\varphi_{i,I}\right)\left(\dot{\varphi}_j-V_j\right)\right)dV\,dt+\\
&\quad+\int_{t_0}^{t_f}\int_{\partial B_2}\bar{T}_i\delta\varphi_i dSdt\\
\langle\delta S,\delta V_i\rangle &= \int_{t_0}^{t_f}\int_B\left(\frac{\partial\mathcal{L}^{mix}}{\partial V_i}\delta V_i\right)dV\,dt\\
&= \int_{t_0}^{t_f}\int_B\left(\frac{\partial^2\mathcal{L}}{\partial V_j\partial V_i}\left(\dot{\varphi}_j-V_j\right)\delta V_i\right)dV\,dt
\end{aligned}$$

The mixed (two-field) Hamilton's principle becomes

$$\begin{aligned}
\langle\delta S,\delta\boldsymbol{\varphi}\rangle &= \mathbf{0}\\
\langle\delta S,\delta\mathbf{V}\rangle &= \mathbf{0}
\end{aligned}$$

where $\delta\boldsymbol{\varphi}$ is taken over the space of admissible variations, variations vanishing in the initial and final times and on the Dirichlet boundary. The corresponding Euler-Lagrange equations follow as in this case:

$$\begin{aligned}
\frac{\partial\mathcal{L}^{mix}}{\partial\varphi_i}-\frac{d}{dX_J}\left(\frac{\partial\mathcal{L}^{mix}}{\partial F_{iJ}}\right)-\frac{d}{dt}\left(\frac{\partial\mathcal{L}^{mix}}{\partial\dot{\varphi}_i}\right) &= 0\\
\frac{\partial\mathcal{L}^{mix}}{\partial V_i} &= 0\\
\frac{\partial\mathcal{L}^{mix}}{\partial F_{iJ}}N_J+\bar{T}_i &= 0
\end{aligned}$$

or, using the definition (5.5) as

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial \varphi_i}-\frac{d}{dX_J}\left(\frac{\partial \mathcal{L}}{\partial F_{iJ}}\right)-\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial V_i}\right)+\frac{\partial^2 \mathcal{L}}{\partial \varphi_i \partial V_j}\left(\dot{\varphi}_j-V_j\right)-\frac{d}{dX_I}\left(\frac{\partial \mathcal{L}}{\partial F_{iI}\partial V_j}\left(\dot{\varphi}_j-V_j\right)\right) &= 0 \\
\frac{\partial \mathcal{L}}{\partial V_i \partial V_j}\left(\dot{\varphi}_j-V_j\right) &= 0 \\
\left(\frac{\partial \mathcal{L}}{\partial F_{iJ}}+\frac{\partial \mathcal{L}}{\partial F_{iI}\partial V_j}\left(\dot{\varphi}_j-V_j\right)\right)N_J+\bar{T}_i &= 0
\end{aligned}$$

that are equivalent to the equations of motion (3.8).

For a Lagrangian density of the form (3.3) the mixed (two-field) action takes the form

$$\begin{aligned}
S\left[\boldsymbol{\varphi},\mathbf{V}\right] &= \int_{t_0}^{t_f}\int_B\left(\frac{1}{2}R\left|\mathbf{V}\right|^2-W\left(\mathbf{X},t,\boldsymbol{\varphi},\mathbf{F}\right)+RV_i\left(\dot{\varphi}_i-V_i\right)\right)dV\,dt \\
&+\int_{t_0}^{t_f}\int_{\partial B_2}\bar{T}_i\varphi_i dSdT
\end{aligned} \tag{5.7}$$

On account of (3.1) and (3.2) the corresponding variations are

$$\begin{aligned}
\langle \delta S,\delta\varphi_i\rangle &= \int_{t_0}^{t_f}\int_B\left(B_i\delta\varphi_i-P_{iI}\delta\varphi_{i,I}+RV_i\delta\dot{\varphi}_i\right)dV\,dt+ \\
&+\int_{t_0}^{t_f}\int_{\partial B_2}\bar{T}_i\delta\varphi_i dSdt \\
\langle \delta S,\delta V_i\rangle &= \int_{t_0}^{t_f}\int_B R\left(\dot{\varphi}_i-V_i\right)\delta V_i dV\,dt
\end{aligned}$$

and the Euler-Lagrange equations become

$$\begin{aligned}
\mathbf{B}+\mathrm{DIV}\left(\mathbf{P}\right)-\frac{d}{dt}\left(R\mathbf{V}\right) &= \mathbf{0} \\
\dot{\boldsymbol{\varphi}}-\mathbf{V} &= \mathbf{0} \\
\bar{\mathbf{T}}-\mathbf{PN} &= \mathbf{0}
\end{aligned}$$

5.3 Configurational forces and configurational force balance

In analogy to the single-field Hamilton's principle, the mixed (two-field) Hamilton's principle may be reformulated in a more general way to account not only for vertical but also for horizontal variations and to render, in addition to the equations of balance of mechanical forces and time compatibility, the equations of balance of configurational forces. To this end, let D be the defect reference configuration, $\boldsymbol{\xi}\in D$ the defect parameter, $\boldsymbol{\psi}\left(\boldsymbol{\xi},t\right)$ the defect (horizontal) motion, and $\boldsymbol{\phi}\left(\boldsymbol{\xi},t\right)$ the defect (vertical) motion in the deformed configuration at time t or composition mapping between the motion $\boldsymbol{\varphi}$ and $\boldsymbol{\psi}^{-1}$ (figure 3.1). In addition, let $\boldsymbol{\nu}\left(\boldsymbol{\xi},t\right)$ be the material velocity referred to the parametric configuration D, i.e., the composition between the material velocity field $\mathbf{V}$ and

$\boldsymbol{\psi}^{-1}$, namely

$$\begin{aligned} \boldsymbol{\varphi} &= \boldsymbol{\phi} \circ \boldsymbol{\psi}^{-1} \\ \mathbf{V} &= \boldsymbol{\nu} \circ \boldsymbol{\psi}^{-1} \end{aligned}$$

or equivalently

$$\begin{aligned} \phi_i\left(\xi_\alpha, t\right) &= \varphi_i\left(\psi_I\left(\xi_\alpha, t\right), t\right) \\ \nu_i\left(\xi_\alpha, t\right) &= V_i\left(\psi_I\left(\xi_\alpha, t\right), t\right) \end{aligned}$$

We next refer the mixed (two-field) action (5.6) to the parametric configuration and regard the action as an independent functional of both defect (horizontal) and body (vertical) motion. To do this we make use of the relations between deformation gradient and velocities (3.18) and (3.19). The mixed action thus becomes

$$\begin{aligned} S\left[\boldsymbol{\psi}, \boldsymbol{\phi}, \boldsymbol{\nu}\right] &= \int_{t_0}^{t_f} \int_D \mathcal{L}^{mix} \circ \boldsymbol{\psi} \det\left(D\boldsymbol{\psi}\right) d\boldsymbol{\xi} dt = \\ &= \int_{t_0}^{t_f} \int_D \mathcal{L}^{mix}\left(\boldsymbol{\psi}, t, \boldsymbol{\phi}, \boldsymbol{\nu}, D\boldsymbol{\phi} D\boldsymbol{\psi}^{-1}, \dot{\boldsymbol{\phi}} - (D\boldsymbol{\phi} D\boldsymbol{\psi}^{-1})\dot{\boldsymbol{\psi}}\right) \det\left(D\boldsymbol{\psi}\right) d\boldsymbol{\xi} dt = \\ &= \int_{t_0}^{t_f} \int_D \left(\mathcal{L}\left(\boldsymbol{\psi}, t, \boldsymbol{\phi}, \boldsymbol{\nu}, D\boldsymbol{\phi} D\boldsymbol{\psi}^{-1}\right) + R\boldsymbol{\nu}\left(\dot{\boldsymbol{\phi}} - (D\boldsymbol{\phi} D\boldsymbol{\psi}^{-1})\dot{\boldsymbol{\psi}} - \boldsymbol{\nu}\right)\right) \det\left(D\boldsymbol{\psi}\right) d\boldsymbol{\xi} dt \end{aligned}$$

where we have assumed zero traction boundary conditions to simplify the derivation.

We now invoke the stationarity of the mixed action $S\left[\boldsymbol{\psi}, \boldsymbol{\phi}, \boldsymbol{\nu}\right]$ with respect to admissible variations of the three arguments (mixed Hamilton's principle)

$$\begin{aligned} \langle \delta S, \delta \phi_i \rangle &= 0 \\ \langle \delta S, \delta \psi_I \rangle &= 0 \\ \langle \delta S, \delta \nu_i \rangle &= 0 \end{aligned}$$

The variation of the mixed action functional $S\left[\boldsymbol{\psi}, \boldsymbol{\phi}, \boldsymbol{\nu}\right]$ with respect to $\boldsymbol{\phi}$ (keeping $\boldsymbol{\psi}$ and $\boldsymbol{\nu}$ fixed) yields

$$\begin{aligned} \langle \delta S, \delta \phi_i \rangle &= \int_{t_0}^{t_f} \int_D \left(\frac{\partial \mathcal{L}^{mix}}{\partial \varphi_i} \delta\phi_i + \frac{\partial \mathcal{L}^{mix}}{\partial F_{iI}}\left(\delta\phi_{i,\alpha}\psi^{-1}_{\alpha,I}\right) + \frac{\partial \mathcal{L}^{mix}}{\partial \dot{\varphi}_i}\left(\delta\dot{\phi}_i - \left(\delta\phi_{i,\alpha}\psi^{-1}_{\alpha,J}\right)\dot{\psi}_J\right)\right) \det\left(D\boldsymbol{\psi}\right) d\boldsymbol{\xi} dt = \\ &= \int_{t_0}^{t_f} \int_D \left(\frac{\partial \mathcal{L}}{\partial \varphi_i} \delta\phi_i + \frac{\partial \mathcal{L}}{\partial F_{iI}}\left(\delta\phi_{i,\alpha}\psi^{-1}_{\alpha,I}\right) + \frac{\partial \mathcal{L}}{\partial V_i}\left(\delta\dot{\phi}_i - \left(\delta\phi_{i,\alpha}\psi^{-1}_{\alpha,J}\right)\dot{\psi}_J\right) + \right. \\ &\quad \left. + \left(\frac{\partial^2 \mathcal{L}}{\partial \varphi_i \partial V_j} \delta\phi_i + \frac{\partial^2 \mathcal{L}}{\partial F_{iI} \partial V_j}\left(\delta\phi_{i,\alpha}\psi^{-1}_{\alpha,I}\right)\right)\left(\dot{\phi}_j - \left(\phi_{j,\alpha}\psi^{-1}_{\alpha,J}\right)\dot{\psi}_J - \nu_j\right)\right) \det\left(D\boldsymbol{\psi}\right) d\boldsymbol{\xi} dt \end{aligned}$$

Referring the integral back to the reference configuration B we obtain

$$\begin{aligned}\langle \delta S, \delta\phi_i\rangle &= \int_{t_0}^{t_f}\int_B \left(\frac{\partial \mathcal{L}^{mix}}{\partial \varphi_i}\left(\delta\phi_i\circ\boldsymbol{\psi}^{-1}\right) + \frac{\partial \mathcal{L}^{mix}}{\partial F_{iJ}}\frac{d}{dX_J}\left(\delta\phi_i\circ\boldsymbol{\psi}^{-1}\right) + \frac{\partial \mathcal{L}^{mix}}{\partial \dot{\varphi}_i}\frac{d}{dt}\left(\delta\phi_i\circ\boldsymbol{\psi}^{-1}\right)\right) dV dt = \\ &= \int_{t_0}^{t_f}\int_B \left(\frac{\partial \mathcal{L}}{\partial \varphi_i}\left(\delta\phi_i\circ\boldsymbol{\psi}^{-1}\right) + \frac{\partial \mathcal{L}}{\partial F_{iJ}}\frac{d}{dX_J}\left(\delta\phi_i\circ\boldsymbol{\psi}^{-1}\right) + \frac{\partial \mathcal{L}}{\partial V_i}\frac{d}{dt}\left(\delta\phi_i\circ\boldsymbol{\psi}^{-1}\right) + \right. \\ &\quad \left. + \left(\frac{\partial^2 \mathcal{L}}{\partial \varphi_i \partial V_j}\left(\delta\phi_i\circ\boldsymbol{\psi}^{-1}\right) + \frac{\partial^2 \mathcal{L}}{\partial F_{iI}\partial V_j}\frac{d}{dX_I}\left(\delta\phi_i\circ\boldsymbol{\psi}^{-1}\right)\right)\left(\dot{\varphi}_j - V_j\right)\right) dV dt\end{aligned}$$

where the identities (3.23) and (3.24) have been used along with the relation:

$$\begin{aligned}\frac{d}{dt}\left(\phi_i\circ\boldsymbol{\psi}^{-1}\right) &= \left(\dot{\phi}_i\circ\boldsymbol{\psi}^{-1}\right) - \left(\phi_{i,\alpha}\circ\boldsymbol{\psi}^{-1}\right)\psi^{-1}_{\alpha,J}\left(\dot{\psi}_J\circ\boldsymbol{\psi}^{-1}\right) = \\ &= \frac{d\varphi_i}{dt} = \dot{\varphi}_i\end{aligned}$$

and where the Lagrangian density $\mathcal{L}$ and its derivatives are evaluated in $(\mathbf{X}, t, \boldsymbol{\varphi}, \mathbf{V}, D\boldsymbol{\varphi})$.

We next compute the variations with respect to $\boldsymbol{\psi}$ (keeping $\boldsymbol{\phi}$ and $\boldsymbol{\nu}$ fixed). On account of relations (3.26) (3.27) we obtain

$$\begin{aligned}\langle \delta S, \delta\psi_I\rangle &= \int_{t_0}^{t_f}\int_D \left(\frac{\partial \mathcal{L}^{mix}}{\partial X_I}\delta\psi_I + \left(\mathcal{L}^{mix}\delta_{IJ} - \frac{\partial \mathcal{L}^{mix}}{\partial F_{iJ}}\left(\phi_{i,\alpha}\psi^{-1}_{\alpha,I}\right)\right)\left(\delta\psi_{I,\beta}\psi^{-1}_{\beta,J}\right) + \right. \\ &\quad \left. + \frac{\partial \mathcal{L}^{mix}}{\partial \dot{\varphi}_i}\left(-\phi_{i,\alpha}\psi^{-1}_{\alpha,I}\right)\left(\delta\dot{\psi}_I - \left(\delta\psi_{I,\beta}\psi^{-1}_{\beta,J}\right)\dot{\psi}_J\right)\right)\det\left(D\boldsymbol{\psi}\right) d\boldsymbol{\xi} dt \\ &= \int_{t_0}^{t_f}\int_D \left(\frac{\partial \mathcal{L}}{\partial X_I}\delta\psi_I + \left(\mathcal{L}\delta_{IJ} - \frac{\partial \mathcal{L}}{\partial F_{iJ}}\left(\phi_{i,\alpha}\psi^{-1}_{\alpha,I}\right)\right)\left(\delta\psi_{I,\beta}\psi^{-1}_{\beta,J}\right) + \right. \\ &\quad + \frac{\partial \mathcal{L}}{\partial V_i}\left(-\phi_{i,\alpha}\psi^{-1}_{\alpha,I}\right)\left(\delta\dot{\psi}_I - \left(\delta\psi_{I,\beta}\psi^{-1}_{\beta,J}\right)\dot{\psi}_J\right) + \\ &\quad + \left(\frac{\partial^2 \mathcal{L}}{\partial X_I \partial V_j}\delta\psi_I + \frac{\partial}{\partial V_j}\left(\mathcal{L}\delta_{IJ} - \frac{\partial \mathcal{L}}{\partial F_{iJ}}\left(\phi_{i,\alpha}\psi^{-1}_{\alpha,I}\right)\right)\left(\delta\psi_{I,\beta}\psi^{-1}_{\beta,J}\right)\right)\cdot \\ &\quad \left. \cdot\left(\dot{\phi}_j - \left(\phi_{j,\alpha}\psi^{-1}_{\alpha,J}\right)\dot{\psi}_J - \nu_j\right)\right)\det\left(D\boldsymbol{\psi}\right) d\boldsymbol{\xi} dt\end{aligned}$$

Referring the integral back to the reference configuration B, the previous takes the form

$$\begin{aligned}\langle \delta S, \delta\psi_I\rangle &= \int_{t_0}^{t_f}\int_B \left(\frac{\partial \mathcal{L}^{mix}}{\partial X_I}\left(\delta\psi_I\circ\boldsymbol{\psi}^{-1}\right) + \left(\mathcal{L}^{mix}\delta_{IJ} - \frac{\partial \mathcal{L}^{mix}}{\partial F_{iJ}}F_{iI}\right)\frac{d}{dX_J}\left(\delta\psi_I\circ\boldsymbol{\psi}^{-1}\right) + \right. \\ &\quad \left. + \frac{\partial \mathcal{L}^{mix}}{\partial \dot{\varphi}_i}\left(-F_{iI}\right)\frac{d}{dt}\left(\delta\psi_I\circ\boldsymbol{\psi}^{-1}\right)\right) dV dt \\ &= \int_{t_0}^{t_f}\int_B \left(\frac{\partial \mathcal{L}}{\partial X_I}\left(\delta\psi_I\circ\boldsymbol{\psi}^{-1}\right) + \left(\mathcal{L}\delta_{IJ} - \frac{\partial \mathcal{L}}{\partial F_{iJ}}F_{iI}\right)\frac{d}{dX_J}\left(\delta\psi_I\circ\boldsymbol{\psi}^{-1}\right) + \right. \\ &\quad + \frac{\partial \mathcal{L}}{\partial V_i}\left(-F_{iI}\right)\frac{d}{dt}\left(\delta\psi_I\circ\boldsymbol{\psi}^{-1}\right) + \\ &\quad \left. + \left(\frac{\partial^2 \mathcal{L}}{\partial X_I \partial V_j}\left(\delta\psi_I\circ\boldsymbol{\psi}^{-1}\right) + \frac{\partial}{\partial V_j}\left(\mathcal{L}\delta_{IJ} - \frac{\partial \mathcal{L}}{\partial F_{iJ}}F_{iI}\right)\frac{d}{dX_J}\left(\delta\psi_I\circ\boldsymbol{\psi}^{-1}\right)\right)\left(\dot{\varphi}_j - V_j\right)\right) dV dt\end{aligned}$$

where identities (3.31) and (3.30) have been used. Notice that for a Lagrangian Density of the form

(3.3) the mixed derivative terms $\frac{\partial L}{\partial \varphi_i \partial V_j}$ and $\frac{\partial L}{\partial F_{iI} \partial V_j}$ vanish.

Finally we compute variations of $S\left[\boldsymbol{\psi}, \boldsymbol{\phi}, \boldsymbol{\nu}\right]$ with respect to $\boldsymbol{\nu}$ keeping $(\boldsymbol{\psi}, \boldsymbol{\phi})$ fixed. We obtain

$$\begin{aligned}\langle \delta S, \delta\nu_i \rangle &= \int_{t_0}^{t_f} \int_D \frac{\partial \mathcal{L}^{mix}}{\partial V_i} \delta\nu_i \det\left(D\boldsymbol{\psi}\right) d\boldsymbol{\xi} dt = \\ &= \int_{t_0}^{t_f} \int_D \left(\frac{\partial^2 \mathcal{L}}{\partial V_j \partial V_i} \left(\dot{\phi}_j - \left(\phi_{j,\alpha} \psi^{-1}_{\alpha,I}\right) \dot{\psi}_I - \nu_j \right) \delta\nu_i \right) \det\left(D\boldsymbol{\psi}\right) d\boldsymbol{\xi} dt\end{aligned}$$

Referring the space integral in the previous variation back to the reference configuration B yields

$$\begin{aligned}\langle \delta S, \delta\nu_i \rangle &= \int_{t_0}^{t_f} \int_B \frac{\partial \mathcal{L}^{mix}}{\partial V_i} \left(\delta\nu_i \circ \boldsymbol{\psi}^{-1}\right) dV dt = \\ &= \int_{t_0}^{t_f} \int_B \left(\frac{\partial^2 \mathcal{L}}{\partial V_j \partial V_i} \left(\dot{\varphi}_j - V_j\right) \left(\delta\nu_i \circ \boldsymbol{\psi}^{-1}\right) \right) dV dt\end{aligned}$$

We now turn to the derivation of the corresponding Euler-Lagrange equations. Stationarity of the mixed action functional with respect to admissible variations on each of its arguments requires

$$\begin{aligned}\frac{\partial \mathcal{L}^{mix}}{\partial \varphi_i} - \frac{d}{dX_J}\left(\frac{\partial \mathcal{L}^{mix}}{\partial F_{iJ}}\right) - \frac{d}{dt}\left(\frac{\partial \mathcal{L}^{mix}}{\partial \dot{\varphi}_i}\right) &= 0 \\ \frac{\partial \mathcal{L}^{mix}}{\partial X_I} - \frac{d}{dX_J}\left(\mathcal{L}^{mix}\delta_{IJ} - \frac{\partial \mathcal{L}^{mix}}{\partial F_{iJ}} F_{iI}\right) - \frac{d}{dt}\left(-F_{iI}\frac{\partial \mathcal{L}^{mix}}{\partial \dot{\varphi}_i}\right) &= 0 \\ \frac{\partial \mathcal{L}^{mix}}{\partial V_i} &= 0\end{aligned}$$

that, on account of the definition (5.5), can be rewritten as

$$\begin{aligned}0 &= \frac{\partial \mathcal{L}}{\partial \varphi_i} - \frac{d}{dX_J}\left(\frac{\partial \mathcal{L}}{\partial F_{iJ}}\right) - \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial V_i}\right) + \\ &\quad + \frac{\partial^2 \mathcal{L}}{\partial \varphi_i \partial V_j}\left(\dot{\varphi}_j - V_j\right) - \frac{d}{dX_J}\left(\frac{\partial^2 \mathcal{L}}{\partial F_{iJ} \partial V_j}\left(\dot{\varphi}_j - V_j\right)\right) \\ 0 &= \frac{\partial \mathcal{L}}{\partial X_I} - \frac{d}{dX_J}\left(\mathcal{L}\delta_{IJ} - \frac{\partial \mathcal{L}}{\partial F_{iJ}} F_{iI}\right) - \frac{d}{dt}\left(-F_{iI}\frac{\partial \mathcal{L}}{\partial V_i}\right) + \\ &\quad + \frac{\partial^2 \mathcal{L}}{\partial X_I \partial V_j}\left(\dot{\varphi}_j - V_j\right) - \frac{d}{dX_J}\left(\frac{\partial}{\partial V_j}\left(\mathcal{L}\delta_{IJ} - \frac{\partial \mathcal{L}}{\partial F_{iJ}} F_{iI}\right)\left(\dot{\varphi}_j - V_j\right)\right) \\ 0 &= \frac{\partial^2 \mathcal{L}}{\partial V_i \partial V_j}\left(\dot{\varphi}_j - V_j\right)\end{aligned}$$

This equations are equivalent to the Euler-Lagrange equations (3.33) and (3.34) corresponding to the single-field Hamilton's principle.

For a Lagrangian density of the form (3.3) the variations take the form:

- Variations with respect to $\boldsymbol{\phi}$

$$\langle \delta S, \delta\phi_i \rangle = \int_{t_0}^{t_f} \int_B \left(B_i \left(\delta\phi_i \circ \boldsymbol{\psi}^{-1}\right) - P_{iJ} \frac{d}{dX_J} \left(\delta\phi_i \circ \boldsymbol{\psi}^{-1}\right) + RV_i \frac{d}{dt} \left(\delta\phi_i \circ \boldsymbol{\psi}^{-1}\right) \right) dV dt \tag{5.8}$$

- Variations with respect to $\boldsymbol{\psi}$

$$\begin{aligned}
\langle \delta S, \delta\psi_I \rangle &= \int_{t_0}^{t_f} \int_B \left(B_I^{inh-mix} \left(\delta\psi_I \circ \boldsymbol{\psi}^{-1}\right) - C_{IJ}^{mix} \frac{d}{dX_J} \left(\delta\psi_I \circ \boldsymbol{\psi}^{-1}\right) \right. \\
&\quad \left. + RV_i \left(-F_{iI}\right) \frac{d}{dt} \left(\delta\psi_I \circ \boldsymbol{\psi}^{-1}\right) \right) dV dt \\
&= \int_{t_0}^{t_f} \int_B \left(B_I^{inh} \left(\delta\psi_I \circ \boldsymbol{\psi}^{-1}\right) - C_{IJ} \frac{d}{dX_J} \left(\delta\psi_I \circ \boldsymbol{\psi}^{-1}\right) \right. \\
&\quad + RV_i \left(-F_{iI}\right) \frac{d}{dt} \left(\delta\psi_I \circ \boldsymbol{\psi}^{-1}\right) + \\
&\quad \left. \left(\frac{\partial R}{\partial X_I} \left(\delta\psi_I \circ \boldsymbol{\psi}^{-1}\right) + R \frac{d}{dX_I} \left(\delta\psi_I \circ \boldsymbol{\psi}^{-1}\right) \right) V_j \left(\dot{\varphi}_j - V_j\right) \right) dV dt \qquad (5.9) \\
&= \int_{t_0}^{t_f} \int_B \left(B_I^{inh-static} \left(\delta\psi_I \circ \boldsymbol{\psi}^{-1}\right) - C_{IJ}^{static} \frac{d}{dX_J} \left(\delta\psi_I \circ \boldsymbol{\psi}^{-1}\right) \right. \\
&\quad + RV_i \left(-F_{iI}\right) \frac{d}{dt} \left(\delta\psi_I \circ \boldsymbol{\psi}^{-1}\right) + \\
&\quad \left. \left(\tfrac{\partial R}{\partial X_I} \left(\delta\psi_I \circ \boldsymbol{\psi}^{-1}\right) + R \tfrac{d}{dX_I} \left(\delta\psi_I \circ \boldsymbol{\psi}^{-1}\right) \right) \left(\tfrac{\|\mathbf{V}\|^2}{2} + V_j \left(\dot{\varphi}_j - V_j\right) \right) \right) dV dt
\end{aligned}$$

- Variations with respect to $\boldsymbol{\nu}$

$$\langle \delta S, \delta\nu_i \rangle = \int_{t_0}^{t_f} \int_B R \left(\dot{\varphi}_i - V_i\right) \left(\delta\nu_i \circ \boldsymbol{\psi}^{-1}\right) dV dt \tag{5.10}$$

where

$$\begin{aligned}
B_i &= \frac{\partial \mathcal{L}^{mix}}{\partial \varphi_i} = \frac{\partial \mathcal{L}}{\partial \varphi_i} = -\frac{\partial W}{\partial \varphi_i} \\
P_{iJ} &= -\frac{\partial \mathcal{L}^{mix}}{\partial F_{iJ}} = -\frac{\partial \mathcal{L}}{\partial F_{iJ}} = \frac{\partial W}{\partial F_{iJ}}
\end{aligned}$$

are the mechanical body force and first Piolla-Kirchhoff stress tensor,

$$\begin{aligned}
B_I^{inh-mix} &= \left.\frac{\partial \mathcal{L}^{mix}}{\partial X_I}\right|_{\exp} = \frac{1}{2} \frac{\partial R}{\partial X_I} \left|\mathbf{V}\right|^2 - \left.\frac{\partial W}{\partial X_I}\right|_{\exp} + \frac{\partial R}{\partial X_I} V_j \left(\dot{\varphi}_j - V_j\right) \\
C_{IJ}^{mix} &= -\left(\mathcal{L}^{mix} \delta_{IJ} - \frac{\partial \mathcal{L}^{mix}}{\partial F_{iJ}} F_{iI} \right) = \left(\left(W - \frac{1}{2} R \left|\mathbf{V}\right|^2 - R\mathbf{V} \cdot \left(\dot{\boldsymbol{\varphi}} - \mathbf{V}\right) \right) \delta_{IJ} - F_{iI} P_{iJ} \right)
\end{aligned}$$

and the inhomogeneity force and Eshelby stress tensor based on the mixed Lagrangian densities

(5.5),

$$\begin{aligned} B_I^{inh} &= \left.\frac{\partial \mathcal{L}}{\partial X_I}\right|_{\exp} = \frac{1}{2}\frac{\partial R}{\partial X_I}\left|\mathbf{V}\right|^2 - \left.\frac{\partial W}{\partial X_I}\right|_{\exp} \\ C_{IJ} &= -\left(\mathcal{L}\delta_{IJ} - \frac{\partial \mathcal{L}}{\partial F_{iJ}} F_{iI}\right) = \left(\left(W - \frac{1}{2}R\left|\mathbf{V}\right|^2\right)\delta_{IJ} - F_{iI}P_{iJ}\right) \end{aligned}$$

are the inhomogeneity force and Eshelby stress tensor but based on the standard Lagrangian (3.3), and where

$$\begin{aligned} B_I^{inh-static} &= -\left.\frac{\partial W}{\partial X_I}\right|_{\exp} \\ C_{IJ}^{static} &= W\delta_{IJ} - F_{iI}P_{iJ} \end{aligned}$$

are the static parts of the inhomogeneity force and Eshelby stress tensor. The Euler-Lagrange equations become

$$\begin{aligned} \mathbf{B} + \mathrm{DIV}\left(\mathbf{P}\right) - \frac{d}{dt}\left(R\mathbf{V}\right) &= 0 \\ \mathbf{B}^{inh-mix} + \mathrm{DIV}\left(\mathbf{C}^{mix}\right) - \frac{d}{dt}\left(\left(-\mathbf{F}^T\right)R\mathbf{V}\right) &= 0 \\ \dot{\boldsymbol{\varphi}} - \mathbf{V} &= 0 \end{aligned}$$

when written in terms of the mixed Lagrangian (5.5) or alternatively

$$\mathbf{B} + \mathrm{DIV}\left(\mathbf{P}\right) - \frac{d}{dt}\left(R\mathbf{V}\right) = 0 \tag{5.11}$$

$$\mathbf{B}^{inh} + \mathrm{DIV}\left(\mathbf{C}\right) - \frac{d}{dt}\left(\left(-\mathbf{F}^T\right)R\mathbf{V}\right) - R\,\mathrm{GRAD}\left(\mathbf{V}\cdot\left(\dot{\boldsymbol{\varphi}} - \mathbf{V}\right)\right) = 0 \tag{5.12}$$

$$\dot{\boldsymbol{\varphi}} - \mathbf{V} = 0 \tag{5.13}$$

when written in terms of the standard Lagrangian density (3.3). Furthermore, making use of the identities

$$\frac{d}{dt}\left(-\mathbf{F}^T R\mathbf{V}\right) + \mathrm{DIV}\left(\frac{1}{2}R\left\|\mathbf{V}\right\|^2\mathbf{I}\right) = -\mathbf{F}^T\frac{d}{dt}\left(R\mathbf{V}\right) + R\mathbf{V}\cdot\left(\mathrm{GRAD}\,\mathbf{V} - \mathbf{F}\right) \tag{5.14}$$

$$R\,\mathrm{GRAD}\left(\mathbf{V}\cdot\left(\dot{\boldsymbol{\varphi}} - \mathbf{V}\right)\right) = R\,\mathrm{GRAD}\left(\mathbf{V}\right)\cdot\left(\dot{\boldsymbol{\varphi}} - \mathbf{V}\right) + R\mathbf{V}\cdot\mathrm{GRAD}\left(\dot{\boldsymbol{\varphi}} - \mathbf{V}\right) \tag{5.15}$$

and rearranging conveniently, the Euler-Lagrange equations may be rewritten as

$$\mathbf{B} + \mathrm{DIV}\left(\mathbf{P}\right) - \frac{d}{dt}\left(R\mathbf{V}\right) = 0 \tag{5.16}$$

$$\mathbf{B}^{inh-static} + \mathrm{DIV}\left(\mathbf{C}^{static}\right) - \left(-\mathbf{F}^T\right)\frac{d}{dt}\left(R\mathbf{V}\right) - \left(D\mathbf{V}\right)^T\cdot R\left(\dot{\boldsymbol{\varphi}} - \mathbf{V}\right) = 0 \tag{5.17}$$

$$\dot{\boldsymbol{\varphi}} - \mathbf{V} = 0 \tag{5.18}$$

Notice that the mixed Lagrangian is $\mathcal{L}^{mix}$ is the sum of three factors, namely the kinetic energy term, the potential energy term, and the Lagrange multiplier term. We can thus define body forces and stress tensors based, respectively, on $\mathcal{L}^{mix}$, $\mathcal{L}$, and W and therefore write the Euler-Lagrange equations based on these three different representations.

We finally derive a pull-back relation analogous to the one obtained in the case of a single-field variational principle (3.42). To this end, we define the following (two-field) Euler-Lagrange operators, the left hand side of the (vertical and horizontal) Euler-Lagrange equations

$$
\begin{aligned}
\left(\mathcal{F}_{\boldsymbol{\phi}}\left(\boldsymbol{\varphi},\mathbf{V}\right)\right)_i &= \frac{\partial\mathcal{L}^{mix}}{\partial\varphi_i} - \frac{d}{dX_J}\left(\frac{\partial\mathcal{L}^{mix}}{\partial F_{iJ}}\right) - \frac{d}{dt}\left(\frac{\partial\mathcal{L}^{mix}}{\partial\dot{\varphi}_i}\right) = \\
&= \frac{\partial\mathcal{L}}{\partial\varphi_i} - \frac{d}{dX_J}\left(\frac{\partial\mathcal{L}}{\partial F_{iJ}}\right) - \frac{d}{dt}\left(\frac{\partial\mathcal{L}}{\partial V_i}\right) + \\
&\quad + \frac{\partial^2\mathcal{L}}{\partial\varphi_i\partial V_j}\left(\dot{\varphi}_j - V_j\right) - \frac{d}{dX_I}\left(\frac{\partial^2\mathcal{L}}{\partial F_{iI}\partial V_j}\left(\dot{\varphi}_j - V_j\right)\right) \\
\left(\mathcal{F}_{\boldsymbol{\psi}}\left(\boldsymbol{\varphi},\mathbf{V}\right)\right)_I &= \frac{\partial\mathcal{L}^{mix}}{\partial X_I} - \frac{d}{dX_J}\left(\mathcal{L}^{mix}\delta_{IJ} - \frac{\partial\mathcal{L}^{mix}}{\partial F_{iJ}}F_{iI}\right) - \frac{d}{dt}\left(-F_{iI}\frac{\partial\mathcal{L}^{mix}}{\partial\dot{\varphi}_i}\right) = \\
&= \frac{\partial\mathcal{L}}{\partial X_I} - \frac{d}{dX_J}\left(\mathcal{L}\delta_{IJ} - \frac{\partial\mathcal{L}}{\partial F_{iJ}}F_{iI}\right) - \frac{d}{dt}\left(-F_{iI}\frac{\partial\mathcal{L}}{\partial V_i}\right) + \\
&\quad + \frac{\partial^2\mathcal{L}}{\partial X_I\partial V_j}\left(\dot{\varphi}_j - V_j\right) - \frac{d}{dX_J}\left(\frac{\partial}{\partial V_j}\left(\mathcal{L}\delta_{IJ} - \frac{\partial\mathcal{L}}{\partial F_{iJ}}F_{iI}\right)\left(\dot{\varphi}_j - V_j\right)\right)
\end{aligned}
$$

Left multiplying $\mathcal{F}_{\boldsymbol{\phi}}\left(\boldsymbol{\varphi},\mathbf{V}\right)$ by $-\mathbf{F}^T$ yields

$$
\begin{aligned}
-F_{iI}\left(\mathcal{F}_{\boldsymbol{\phi}}\left(\boldsymbol{\varphi},\mathbf{V}\right)\right)_i &= -F_{iI}\left(\frac{\partial\mathcal{L}}{\partial\varphi_i} + \frac{\partial^2\mathcal{L}}{\partial\varphi_i\partial V_j}\left(\dot{\varphi}_j - V_j\right)\right) - \frac{d}{dX_I}\left(-F_{iJ}\left(\frac{\partial\mathcal{L}}{\partial F_{iJ}} + \frac{\partial^2\mathcal{L}}{\partial F_{iJ}\partial V_j}\left(\dot{\varphi}_j - V_j\right)\right)\right) \\
&\quad -\frac{\partial F_{iJ}}{\partial X_I}\left(\frac{\partial\mathcal{L}}{\partial F_{iJ}} + \frac{\partial^2\mathcal{L}}{\partial F_{iJ}\partial V_j}\left(\dot{\varphi}_j - V_j\right)\right) - \frac{d}{dt}\left(-F_{iI}\frac{\partial\mathcal{L}}{\partial V_i}\right) - \dot{F}_{iI}\frac{\partial\mathcal{L}}{\partial V_i}
\end{aligned}
$$

Differentiating (5.5) with respect to X_I we find

$$
\begin{aligned}
\frac{d}{dX_I}\left(\mathcal{L} + \frac{\partial\mathcal{L}}{\partial V_j}\left(\dot{\varphi}_j - V_j\right)\right) &= \frac{\partial}{\partial X_i}\left(\mathcal{L} + \frac{\partial\mathcal{L}}{\partial V_j}\left(\dot{\varphi}_j - V_j\right)\right) + \\
&\quad + F_{iI}\left(\frac{\partial\mathcal{L}}{\partial\varphi_i} + \frac{\partial\mathcal{L}}{\partial\varphi_i\partial V_j}\left(\dot{\varphi}_j - V_j\right)\right) + \\
&\quad + \frac{\partial F_{iJ}}{\partial X_I}\left(\frac{\partial\mathcal{L}}{\partial F_{iJ}} + \frac{\partial\mathcal{L}}{\partial F_{iJ}\partial V_j}\left(\dot{\varphi}_j - V_j\right)\right) \\
&\quad + \frac{\partial V_i}{\partial X_I}\left(\frac{\partial\mathcal{L}}{\partial V_i} + \frac{\partial\mathcal{L}}{\partial V_i\partial V_j}\left(\dot{\varphi}_j - V_j\right)\right) \\
&\quad + \frac{\partial\mathcal{L}}{\partial V_i}\left(\dot{F}_{iI} - \frac{\partial V_i}{\partial X_I}\right)
\end{aligned}
$$

Combining the previous two we finally obtain the relation

$$
-F_{iI}\left(\mathcal{F}_{\boldsymbol{\phi}}\left(\boldsymbol{\varphi},\mathbf{V}\right)\right)_i = \left(\mathcal{F}_{\boldsymbol{\psi}}\left(\boldsymbol{\varphi},\mathbf{V}\right)\right)_I + \frac{\partial V_i}{\partial X_I}\frac{\partial^2\mathcal{L}}{\partial V_i\partial V_j}\left(\dot{\varphi}_j - V_j\right)
$$

that when evaluated on $\mathbf{V} = \dot{\boldsymbol{\varphi}}$ reduces to the single-field relation (3.42) as expected.

5.4 Full mixed action and full mixed Hamilton's principle

We combine in this section the mixed (three-field) Hamilton's principle for dynamics with the mixed (three-field) Beuveke-Hu-Washizu variational principle for statics to establish a full (five-field) space-time mixed variational formulation for dynamics that account for independent variations in all fields (motion, velocity, strain, momentum, stress). This principle may be used to formulate high performance enhanced finite element formulations with moving meshes. Since we do not attempt to enforce initial (and final) conditions weakly, variations in $\boldsymbol{\varphi}$ are required to vanish at the initial and final times. A more general mixed variational principle than the one presented here may be formulated to account for initial conditions as well. Combining (5.1) and (5.2) the following mixed action functional is obtained

$$\begin{aligned} S[\boldsymbol{\varphi}, \mathbf{V}, \mathbf{F}, \mathbf{p}, \mathbf{P}] &= \int_{t_0}^{t_f} \int_B \left(\mathcal{L}(\mathbf{X}, t, \boldsymbol{\varphi}, \mathbf{V}, \mathbf{F}) + p_i (\dot{\varphi}_i - V_i) - P_{iJ} \left(\varphi_{i,J} - F_{iJ} \right) \right) dV dt \\ &+ \int_{t_0}^{t_f} \int_{\partial B_2} P_{iJ} N_J (\varphi_i - \bar{\varphi}_i) \, dS dt + \int_{t_0}^{t_f} \int_{\partial B_1} \bar{T}_i \varphi_i dS dt \end{aligned}$$

For a Lagrangian density $L(\mathbf{X}, t, \boldsymbol{\varphi}, \mathbf{V}, \mathbf{F})$ of the form (3.3) the previous yields

$$\begin{aligned} S[\boldsymbol{\varphi}, \mathbf{V}, \mathbf{F}, \mathbf{p}, \mathbf{P}] &= \int_{t_0}^{t_f} \int_B \left(\frac{1}{2} R |\mathbf{V}|^2 - W(\mathbf{X}, \boldsymbol{\varphi}, \mathbf{F}) + p_i (\dot{\varphi}_i - V_i) - P_{iJ} \left(\varphi_{i,J} - F_{iJ} \right) \right) dV dt \\ &+ \int_{t_0}^{t_f} \int_{\partial B_2} P_{iJ} N_J (\varphi_i - \bar{\varphi}_i) \, dS dt + \int_{t_0}^{t_f} \int_{\partial B_1} \bar{T}_i \varphi_i dS dt \end{aligned}$$

Using the space-time domain $[t_0, t_f] \times B$ with coordinates (t, X_1, X_2, X_3) and space-time gradient $\left(\frac{\partial}{\partial t}, \frac{\partial}{\partial X_J} \right)$ the mixed action may be rewritten as

$$\begin{aligned} S[\boldsymbol{\varphi}, \mathbf{V}, \mathbf{F}, \mathbf{p}, \mathbf{P}] &= \int_{[t_0, t_f] \times B} \left(\mathcal{L} + (p_i, P_{iJ}) \cdot \left(\left(\begin{array}{c} \frac{\partial}{\partial t} \\ \frac{\partial}{\partial X_J} \end{array} \right) \varphi_i - \left(\begin{array}{c} V_i \\ F_{iJ} \end{array} \right) \right) \right) dt dV \\ &+ \int_{[t_0, t_f] \times \partial B_2} (\varphi_i - \bar{\varphi}_i) (p_i, P_{iJ}) \left(\begin{array}{c} 0 \\ N_J \end{array} \right) dt dS + \int_{[t_0, t_f] \times \partial B_1} \bar{T}_i \varphi_i dt dS \end{aligned}$$

Stationarity of the mixed action with respect to (admissible) variations in each field demands

$$\begin{aligned}
\langle \delta S, \delta\varphi_i \rangle &= \int_{t_0}^{t_f}\int_B \left(\frac{\partial \mathcal{L}}{\partial \varphi_i}\delta\varphi_i - P_{iJ}\delta\varphi_{i,J} + p_i \delta\dot{\varphi}_i \right) dV dt \\
&\quad + \int_{t_0}^{t_f}\int_{\partial B_1} P_{iJ} N_J \delta\varphi_i dS dt + \int_{t_0}^{t_f}\int_{\partial B_2} \bar{T}_i \delta\varphi_i dS dt \\
\langle \delta S, \delta p_i \rangle &= \int_{t_0}^{t_f}\int_B \delta p_i \left(\dot{\varphi}_i - V_i \right) dV dt \\
\langle \delta S, \delta V_i \rangle &= \int_{t_0}^{t_f}\int_B \delta V_i \left(-p_i + \frac{\partial \mathcal{L}}{\partial V_i} \right) dV dt \\
\langle \delta S, \delta P_{iJ} \rangle &= \int_{t_0}^{t_f}\int_B \left(-\delta P_{iJ} \left(\varphi_{i,J} - F_{iJ} \right) \right) dV dt + \\
&\quad + \int_{t_0}^{t_f}\int_{\partial B_1} \delta P_{iJ} N_J \left(\varphi_i - \bar{\varphi}_i \right) dS dt \\
\langle \delta S, \delta F_{iJ} \rangle &= \int_{t_0}^{t_f}\int_B \left(P_{iJ} + \frac{\partial \mathcal{L}}{\partial F_{iJ}} \right) \delta F_{iJ} dV dt
\end{aligned}$$

which are the weak restatement of the field equations of motion along with their corresponding boundary conditions

$$\begin{aligned}
\frac{\partial L}{\partial \varphi_i} + \frac{dP_{iJ}}{dX_J} - \frac{dp_i}{dt} &= 0 \qquad \text{in } B \text{ and } \forall t \in I \\
P_{iJ}N_J - T_i &= 0 \qquad \text{on } \partial B_2 \text{ and } \forall t \in I \\
\dot{\varphi}_i - V_i &= 0 \qquad \text{in } B \text{ and } \forall t \in I \\
-p_i + \frac{\partial \mathcal{L}}{\partial V_i} &= 0 \qquad \text{in } B \text{ and } \forall t \in I \\
\varphi_{i,J} - F_{iJ} &= 0 \qquad \text{in } B \text{ and } \forall t \in I \\
P_{iJ} + \frac{\partial \mathcal{L}}{\partial F_{iJ}} &= 0 \qquad \text{in } B \text{ and } \forall t \in I \\
\varphi_i - \bar{\varphi}_i &= 0 \qquad \text{on } \partial B_1 \text{ and } \forall t \in I
\end{aligned}$$

5.5 Viscosity and mixed Lagrange-d'Alembert principle

We proceed to establish in this section a *mixed* version of the Lagrange-d'Alembert principle. We recall that the *mixed* Hamilton's principle was formulated by assuming the existence of an independent velocity field $\mathbf{V}$ different from $\dot{\boldsymbol{\varphi}}$ and enforcing the identity $\mathbf{V} = \dot{\boldsymbol{\varphi}}$ in a weak sense by the introduction of a Lagrange multiplier. We also recall from Chapter 3 (see §3.4, equation 3.63) that in the presence of viscous behavior, the equations of configurational and mechanical force balance can be established from the combined horizontal-vertical Lagrange-d'Alembert principle

$$\langle \delta S, \delta \boldsymbol{\psi} \rangle + \langle \delta S, \delta \boldsymbol{\phi} \rangle + \int_{t_0}^{t_f} \int_B \mathrm{DIV}\left(\mathbf{P}^v\right)\left(\delta \boldsymbol{\phi} - \mathbf{F}\delta \boldsymbol{\psi}\right) dV dt + \\ + \int_{t_0}^{t_f} \int_{\partial B_1} \left(\mathbf{P}^v \mathbf{N}\right)\left(\delta \boldsymbol{\phi} - \mathbf{F}\delta \boldsymbol{\psi}\right) dS dt = 0$$

where

$$\mathbf{P}^v = \mathbf{P}^v\left(\mathbf{F}, \dot{\mathbf{F}}\right)$$

are the viscous forces and $\mathbf{N}$ is the outward unit normal on the traction boundary ∂B_1. To develop a mixed version of this principle we begin assuming that the viscosity depends on $D\mathbf{V}$ instead of $\dot{\mathbf{F}}$

$$\mathbf{P}^v = \mathbf{P}^v\left(\mathbf{F}, D\mathbf{V}\right)$$

We next rewrite this principle in the form

$$\langle \delta S, \delta \boldsymbol{\psi} \rangle + \langle \delta S, \delta \boldsymbol{\phi} \rangle + \int_{t_0}^{t_f} \int_B \mathbf{R}^v \left(\delta \boldsymbol{\phi} - \mathbf{F}\delta \boldsymbol{\psi}\right) dV dt + \\ + \int_{t_0}^{t_f} \int_{\partial B_1} \mathbf{T}^v \left(\delta \boldsymbol{\phi} - \mathbf{F}\delta \boldsymbol{\psi}\right) dS dt = 0$$

where $\mathbf{R}^v$ and $\mathbf{T}^v$ are the viscous force per unit of undeformed volume and the undeformed surface viscous traction, related to the viscous stress by

$$\begin{aligned} \mathbf{R}^v &= \mathrm{DIV}\left(\mathbf{P}^v\right) \\ \mathbf{T}^v &= -\mathbf{P}^v N \end{aligned}$$

We finally impose the above identities weakly using for this a new test function $\delta \boldsymbol{\varphi}$

$$\int_{t_0}^{t_f} \int_B \left(DIV\left(\mathbf{P}^v\right) - \mathbf{R}^v\right) \delta \boldsymbol{\varphi} - \int_{t_0}^{t_f} \int_{\partial B_1} \delta \boldsymbol{\varphi}^T \left(\mathbf{P}^v \mathbf{N} + \mathbf{T}^v\right) dS dt = \mathbf{0}$$

Integrating by parts, the previous yields

$$-\int_{t_0}^{t_f} \int_B \left(\mathbf{P}^v \frac{\partial \delta \boldsymbol{\varphi}}{\partial \mathbf{X}} + \mathbf{R}^v \delta \boldsymbol{\varphi}\right) - \int_{t_0}^{t_f} \int_{\partial B_1} \delta \boldsymbol{\varphi}^T \left(\mathbf{T}^v\right) dS dt = \mathbf{0}$$

Combining the previous two principles we obtain the combined principle

$$\begin{aligned}
\mathbf{0} &= \langle\delta S,\delta\boldsymbol{\psi}\rangle+\langle\delta S,\delta\boldsymbol{\phi}\rangle+\langle\delta S,\delta\boldsymbol{\nu}\rangle+\\
&+\int_t\int_B \mathbf{R}^v\left(\delta\boldsymbol{\phi}-\mathbf{F}\delta\boldsymbol{\psi}\right)dV\,dt+\int_t\int_{\partial B_1}\mathbf{T}^v\left(\delta\boldsymbol{\phi}-\mathbf{F}\delta\boldsymbol{\psi}\right)dS\,dt\\
&-\int_{t_0}^{t_f}\int_B\left(\mathbf{P}^v\frac{\partial\delta\boldsymbol{\varphi}}{\partial\mathbf{X}}+\mathbf{R}^v\delta\boldsymbol{\varphi}\right)dV\,dt-\int_{t_0}^{t_f}\int_{\partial B_1}\delta\boldsymbol{\varphi}^T\left(\mathbf{T}^v\right)dS\,dt
\end{aligned}\tag{5.19}$$

or alternatively

$$\begin{aligned}
\mathbf{0} &= \langle\delta S,\delta\boldsymbol{\psi}\rangle+\langle\delta S,\delta\boldsymbol{\phi}\rangle+\langle\delta S,\delta\boldsymbol{\nu}\rangle+\\
&+\int_{t_0}^{t_f}\int_B\left(-\mathbf{P}^v\frac{\partial\delta\boldsymbol{\varphi}}{\partial\mathbf{X}}+\mathbf{R}^v\left(\delta\boldsymbol{\phi}-\mathbf{F}\delta\boldsymbol{\psi}-\delta\boldsymbol{\varphi}\right)\right)dV\,dt+\\
&+\int_t\int_{\partial B_1}\mathbf{T}^v\left(\delta\boldsymbol{\phi}-\mathbf{F}\delta\boldsymbol{\psi}-\delta\boldsymbol{\varphi}\right)dS\,dt
\end{aligned}\tag{5.20}$$

In this principle there are four unknown fields, namely $(\boldsymbol{\phi},\boldsymbol{\psi},\boldsymbol{\nu},\mathbf{R}^v)$ and four independent variations $(\delta\boldsymbol{\phi},\delta\boldsymbol{\psi},\delta\boldsymbol{\nu},\delta\boldsymbol{\varphi})$. The established four-field variational principle will be used in the next chapter for materials with viscous behavior.

5.6 Mixed Hamilton and mixed Lagrange-d'Alembert principles for general dissipative materials

In the previous section we formulated a mixed version of Hamilton's principle and Lagrange-d'Alembert principles for isothermal materials with no internal variables. These mixed principles follow by assuming a priori $\mathbf{V}\neq\dot{\boldsymbol{\varphi}}$ and $\mathbf{R}^v\neq\mathrm{DIV}\left(\mathbf{P}^v\right)$ and imposing the constraint $\dot{\boldsymbol{\varphi}}-\mathbf{V}=\mathbf{0}$ with a Lagrange multiplier $\mathbf{p}$ (that is lately identified with the momentum $\mathbf{p}=\frac{\partial L}{\partial V}=R\mathbf{V}$) and the constraint $\mathbf{R}^v-\mathrm{DIV}\left(\mathbf{P}^v\right)=\mathbf{0}$ with an independent weight function $\delta\boldsymbol{\varphi}$. We have also studied in the previous chapter a Lagrangian formulation for general dissipative media in which the equations of balance of mechanical forces and balance of entropy are treated on an equal footing by introducing a new variable α, the thermal displacement, such that $\dot{\alpha}=T$, the temperature. In perfect analogy to what we have done to formulate a mixed variational principle for the equation of balance of mechanical forces, we proceed now to formulate a *mixed* variational principle from which not only the mechanical force balance equation but the entropy balance equation can be derived. More precisely we shall assume a priori $T\neq\dot{\alpha}$ and impose the constraint $\dot{\alpha}-T=0$ with a Lagrange multiplier η. This Lagrange multiplier will coincide with the thermal momentum $\eta=\frac{\partial L}{\partial\dot{\alpha}}=RN$ previously identified with the entropy density per unit of volume. Furthermore, we shall introduce new symbols s^v and $\mathbf{Z}^v$ for the total thermal and internal dissipative sources $s^v=\frac{S^v}{T}+\dot{\Gamma}-\mathrm{DIV}\left(\frac{\mathbf{H}^v}{T}\right)$ and $\mathbf{Z}^v=\mathbf{Y}^v$ and impose the previous identities in a weak form by making use of independent weighting functions

$\delta\alpha$ and $\delta\mathbf{Q}$.

Motivated by the previous discussion we consider the following *mixed thermomechanical action functional*:

$$S\left[\boldsymbol{\varphi},\alpha,\mathbf{Q},\mathbf{V},T,\mathbf{p},\eta\right]=\int_{t_0}^{t_f}\int_B\left(\mathcal{L}\left(\mathbf{X},t,\boldsymbol{\varphi},\alpha,D\boldsymbol{\varphi},D\alpha,\mathbf{Q},\mathbf{V},T\right)+p_i\left(\dot{\varphi}_i-V_i\right)+\eta\left(\dot{\alpha}-T\right)\right)dV\,dt$$

Taking variations of the mixed action functional with respect to all of its seven arguments we obtain

$$\begin{aligned}\langle\delta S,\delta\boldsymbol{\varphi}\rangle &= \int_{t_0}^{t_f}\int_B\left(\frac{\partial\mathcal{L}}{\partial\boldsymbol{\varphi}}\delta\boldsymbol{\varphi}+\frac{\partial\mathcal{L}}{\partial\mathbf{F}}D\delta\boldsymbol{\varphi}+\mathbf{p}\delta\dot{\boldsymbol{\varphi}}\right)dV\,dt\\ \langle\delta S,\delta\alpha\rangle &= \int_{t_0}^{t_f}\int_B\left(\frac{\partial\mathcal{L}}{\partial\alpha}\delta\alpha+\frac{\partial\mathcal{L}}{\partial\boldsymbol{\beta}}D\delta\alpha+\eta\delta\dot{\alpha}\right)dV\,dt\\ \langle\delta S,\delta\mathbf{Q}\rangle &= \int_{t_0}^{t_f}\int_B\left(\frac{\partial\mathcal{L}}{\partial Q}\delta Q\right)dV\,dt\end{aligned}$$

$$\begin{aligned}\langle\delta S,\delta\mathbf{V}\rangle &= \int_{t_0}^{t_f}\int_B\left(\frac{\partial\mathcal{L}}{\partial\mathbf{V}}-\mathbf{p}\right)\delta\mathbf{V}dV\,dt\\ \langle\delta S,\delta T\rangle &= \int_{t_0}^{t_f}\int_B\left(\frac{\partial\mathcal{L}}{\partial T}-\eta\right)\delta T dV\,dt\end{aligned}$$

$$\begin{aligned}\langle\delta S,\delta\mathbf{p}\rangle &= \int_{t_0}^{t_f}\int_B\left(\dot{\boldsymbol{\varphi}}-\mathbf{V}\right)\delta\mathbf{p}dV\,dt\\ \langle\delta S,\delta\eta\rangle &= \int_{t_0}^{t_f}\int_B\left(\dot{\alpha}-T\right)\delta\eta dV\,dt\end{aligned}$$

Invoking now the stationarity of the mixed thermomechanical action with respect to all of its arguments imply the Euler-Lagrange equations

$$\begin{aligned}\frac{\partial\mathcal{L}}{\partial\boldsymbol{\varphi}}-\mathrm{DIV}\left(\frac{\partial\mathcal{L}}{\partial\mathbf{F}}\right)-\frac{d}{dt}\mathbf{p} &= 0\\ \frac{\partial\mathcal{L}}{\partial\alpha}-\mathrm{DIV}\left(\frac{\partial\mathcal{L}}{\partial\boldsymbol{\beta}}\right)-\frac{d}{dt}\eta &= 0\\ \frac{\partial\mathcal{L}}{\partial Q} &= 0\\ \mathbf{p}-\frac{\partial\mathcal{L}}{\partial\mathbf{V}} &= \mathbf{0}\\ \eta-\frac{\partial\mathcal{L}}{\partial T} &= 0\\ \dot{\boldsymbol{\varphi}}-\mathbf{V} &= \mathbf{0}\\ \dot{\alpha}-T &= 0\end{aligned}$$

On account of the equilibrium relations and momenta definitions (see (4.13), (4.14), and (4.15)) the previous equations take the form

$$
\begin{aligned}
\mathbf{B}^e + \mathrm{DIV}\left(\mathbf{P}^e\right) - \frac{d}{dt}\mathbf{p} &= 0 \\
\frac{S^e}{T} - \mathrm{DIV}\left(\frac{\mathbf{H}^e}{T}\right) - \frac{d}{dt}\eta &= 0 \\
\mathbf{Y}^e &= 0 \\
\mathbf{p} - RV &= \mathbf{0} \\
\eta - RN &= 0 \\
\dot{\boldsymbol{\varphi}} - \mathbf{V} &= \mathbf{0} \\
\dot{\alpha} - T &= 0
\end{aligned}
$$

The stationarity of the mixed-thermomechanical action functional implies therefore the equilibrium part of the mechanical force balance, entropy balance, and internal stress balance equations (4.12) along with the compatibility conditions $\dot{\boldsymbol{\varphi}} = \mathbf{V}$ and $\dot{\alpha} = T$ and identifies also the Lagrange multipliers $\mathbf{p}$ and η with the mechanical and thermal momenta (mass times velocity and mass times entropy).

Replacing now the Lagrange multipliers $\mathbf{p}$ and η, respectively, with $R\mathbf{V}$ and RN, the following (six-field) mixed thermomechanical action is obtained

$$
S\left[\boldsymbol{\varphi}, \alpha, \mathbf{Q}, \mathbf{V}, T, N\right] = \int_{t_0}^{t_f} \int_B \left(\mathcal{L}\left(\mathbf{X}, t, \boldsymbol{\varphi}, \alpha, D\boldsymbol{\varphi}, D\alpha, \mathbf{Q}, \mathbf{V}, T\right) + R\mathbf{V}\left(\dot{\varphi}_i - V_i\right) + RN\left(\dot{\alpha} - T\right)\right) dV\, dt
$$

Their corresponding Euler-Lagrange equations are

$$
\begin{aligned}
\frac{\partial \mathcal{L}}{\partial \boldsymbol{\varphi}} - \mathrm{DIV}\left(\frac{\partial \mathcal{L}}{\partial \mathbf{F}}\right) - \frac{d}{dt}\left(R\mathbf{V}\right) &= 0 \\
\frac{\partial \mathcal{L}}{\partial \alpha} - \mathrm{DIV}\left(\frac{\partial \mathcal{L}}{\partial \boldsymbol{\beta}}\right) - \frac{d}{dt}\left(RN\right) &= 0 \\
\mathbf{Y}^e &= 0 \\
\frac{\partial \mathcal{L}}{\partial \mathbf{V}} - RV &= 0 \\
\frac{\partial \mathcal{L}}{\partial T} - RN &= 0 \\
\dot{\boldsymbol{\varphi}} - \mathbf{V} &= \mathbf{0} \\
\dot{\alpha} - T &= 0
\end{aligned}
$$

or equivalently (using the definitions (4.13), (4.14), (4.15)

$$\begin{aligned}
\mathbf{B}^e + \mathrm{DIV}\left(\mathbf{P}^e\right) - \frac{d}{dt}\left(R\mathbf{V}\right) &= 0 \\
\frac{S^e}{T} - \mathrm{DIV}\left(\frac{\mathbf{H}^e}{T}\right) - \frac{d}{dt}\left(RN\right) &= 0 \\
\mathbf{Y}^e &= 0 \\
\frac{\partial L}{\partial T} - RN &= 0 \\
\dot{\boldsymbol{\varphi}} - \mathbf{V} &= \mathbf{0} \\
\dot{\alpha} - T &= 0
\end{aligned}$$

Defining finally the following total dissipative sources

$$\begin{aligned}
\mathbf{R}^v &= \frac{\partial \Psi}{\partial \dot{\boldsymbol{\varphi}}} + \mathrm{DIV}\left(\frac{\partial \Psi}{\partial \dot{\mathbf{F}}}\right) = \\
&= \mathbf{B}^v + \mathrm{DIV}\left(\mathbf{P}^v\right) \qquad (5.21) \\
s^v &= \frac{\partial \Psi}{\partial \dot{\alpha}} + \dot{\Gamma} + \mathrm{DIV}\left(\frac{\partial \Psi}{\partial \dot{\beta}}\right) = \\
&= \frac{S^v}{T} + \dot{\Gamma} - \mathrm{DIV}\left(\frac{\mathbf{H}^v}{T}\right) \qquad (5.22) \\
\mathbf{Z}^v &= \mathbf{Y}^v \qquad (5.23)
\end{aligned}$$

it is straightforward to see that the total balance equations (including both equilibrium and non-equilibrium parts) can be derived from the following mixed version of Lagrange-d'Alembert principle:

$$\begin{aligned}
\langle \delta S, \delta \boldsymbol{\varphi} \rangle + \int_{t_0}^{t_f} \int_B \mathbf{R}^v \delta \boldsymbol{\varphi} dV dt &= 0 \\
\langle \delta S, \delta \alpha \rangle + \int_{t_0}^{t_f} \int_B s^v \delta \alpha dV dt &= 0 \\
\langle \delta S, \delta \mathbf{Q} \rangle + \int_{t_0}^{t_f} \int_B \mathbf{Z}^v \delta \mathbf{Q} dV dt &= 0
\end{aligned}$$

along with the weak restatement of the relations (5.21), (5.22), and (5.23) given by

$$\begin{aligned}
\int_{t_0}^{t_f} \int_B \left(\mathbf{B}^v + \mathrm{DIV}\left(\mathbf{P}^v\right) - \mathbf{R}^v\right) \delta \boldsymbol{\varphi} dV dt &= 0 \\
\int_{t_0}^{t_f} \int_B \left(\frac{S^v}{T} + \dot{\Gamma} - \mathrm{DIV}\left(\frac{\mathbf{H}^v}{T}\right) - s^v\right) \delta \alpha dV dt &= 0 \\
\int_{t_0}^{t_f} \int_B \left(\mathbf{Y}^v - \mathbf{Z}^v\right) \delta \mathbf{Q} dV dt &= 0
\end{aligned}$$

which after integration by parts and assuming $\delta \boldsymbol{\varphi}$ and $\delta \alpha$ vanish on the boundary ∂B might be rewritten as

$$\begin{aligned}
\int_{t_0}^{t_f} \int_B \left(\left(\mathbf{B}^v - \mathbf{R}^v\right) \delta\boldsymbol{\varphi} - \mathbf{P}^v \frac{\partial \delta\boldsymbol{\varphi}}{\partial \mathbf{X}} \right) dV dt &= 0 \\
\int_{t_0}^{t_f} \int_B \left(\left(\frac{S^v}{T} + \dot{\Gamma} - s^v \right) \delta\alpha + \frac{\mathbf{H}^v}{T} \frac{\partial \delta\alpha}{\partial \mathbf{X}} \right) dV dt &= 0 \\
\int_{t_0}^{t_f} \int_B \left(\mathbf{Y}^v - \mathbf{Z}^v\right) \delta\mathbf{Q} dV dt &= 0
\end{aligned}$$

Chapter 6

Finite element discretization

In this chapter we present the formulation of a class of Eulerian-Lagrangian finite element methods for which the finite element mesh is allowed to evolve within the reference configuration continuously in time and simultaneously with the body motion and where both motions follow jointly from the same variational framework, namely, Hamilton's principle.

The body motion $\boldsymbol{\varphi}$ will be approximated with finite elements supported on a moving mesh. Unlike traditional arbitrary-Lagrangian-Eulerian methods in which the mesh motion is arbitrary and prescribed by the user, we will regard the mesh motion as an unknown of the problem to be handled jointly with the main unknown, the body motion. A semidiscrete approach will be used with independent spatial interpolations for deformations $\boldsymbol{\varphi}_h$ and velocities $\mathbf{V}_h$, leading to the construction of a semidiscrete-mixed action functional with nodal referential trajectories $\mathbf{X}_h\left(t\right)$, nodal spatial trajectories $\mathbf{x}_h\left(t\right)$, and nodal coefficients for the spatial interpolation of velocities $\mathbf{V}_h\left(t\right)$ as unknown variables. Stationarity of the semidiscrete-mixed action with respect to each of its arguments leads to a system of differential-algebraic equations in the time variable for the three unknowns. This system of equations corresponds to the equations of nodal mechanical force balance, nodal configurational force balance, and compatibility between assumed and consistent velocities $\mathbf{V}_h$ and $\dot{\varphi}_h$.

As was explained in the third chapter, in the continuous setting the equations of configurational and mechanical force balance are equivalent in the sense that if one equation is satisfied, the other will be automatically satisfied. In the discrete setting however this equivalence does not hold. The discretization breaks the material (horizontal) translation symmetry of the action functional inducing artificial nodal configurational forces. These forces remain unbalanced in general, even when the continuum Lagrangian density is homogeneous (material invariant) and no configurational forces are expected. The motion of the mesh is thus obtained by enforcing the configurational force equilibrium simultaneously with the mechanical force equilibrium.

The use of independent interpolations for velocities and deformations is proposed as an approach to overcome instability issues that arise when convecting the deformation with the moving mesh. The compatibility between assumed and consistent velocity fields $\mathbf{V}_h$ and $\dot{\boldsymbol{\varphi}}_h$ is enforced within a unified variational framework using the mixed (deformation-velocity) Hamilton's principle discussed in the previous chapter.

The resulting semidiscrete system of equations for the three unknowns (mesh motion, material motion, and the material velocity) is integrated with a mixed variational integrator of the kind presented in the second chapter. This integrator follows from a direct discretization in time the semidiscrete-mixed Lagrangian.

6.1 Spatial discretization

6.1.1 Semidiscrete Interpolation

Let $\mathcal{T}_h(t)$ be a time-dependent family of triangulations of the reference configuration B. We shall analyze the particular family $\mathcal{T}_h(t)$ consisting of a node set that is allowed to move continuously in time within the reference configuration while the mesh topology (connectivity and number of nodes and elements) remains constant.

We consider *independent* finite element spatial interpolations for the motion $\boldsymbol{\varphi}$ and velocities $\mathbf{V}$ of the form

$$\boldsymbol{\varphi}_h(\mathbf{X},t) = \sum_a^N N_a(\mathbf{X},t)\,\mathbf{x}_a(t) = \sum_e^E\sum_a^n N_a^e(\mathbf{X},t)\,\mathbf{x}_a^e(t) \tag{6.1}$$

$$\mathbf{V}_h(\mathbf{X},t) = \sum_a^N N_a(\mathbf{X},t)\,\mathbf{V}_a(t) = \sum_e^E\sum_a^n N_a^e(\mathbf{X},t)\,\mathbf{V}_a^e(t) \tag{6.2}$$

where N is the total number of nodes, E the total number of elements, n the total number of nodes per element, $N_a(\mathbf{X},t)$ are the nodal shape functions at time t, N_a^e are the elemental shape functions (at time t), $\mathbf{x}_a(t)$ (respectively, $\mathbf{x}_a^e(t)$) are the coordinates of node a (respectively, local node a of element e) in the deformed configuration at time t, and $\mathbf{V}_a(t)$ (respectively, $\mathbf{V}_a^e(t)$) are the coefficients for the global (local) interpolation of the material velocity $\mathbf{V}_h$ at time t. Notice that the spatial shape functions N_a depend continuously on time t because the nodes are assumed to move within the reference configuration and therefore, the shape functions result supported on a moving domain. Deformations $\boldsymbol{\varphi}_h$ and velocities $\mathbf{V}_h$ are required to be globally continuous and are interpolated with the same shape functions N_a.

In particular we shall consider an isoparametric (moving) finite element interpolation for which the elemental shape functions $N_a^e(\mathbf{X},t)$ are of the form

$$N_a^e = \hat{N}_a \circ \boldsymbol{\psi}^{e-1} \tag{6.3}$$

where

$$\boldsymbol{\psi}^e(\boldsymbol{\xi},t) = \sum_a^n \hat{N}_a(\boldsymbol{\xi})\,\mathbf{X}_a^e(t) \tag{6.4}$$

is the (time-dependent) isoparametric mapping that maps the standard element domain $\hat{\Omega}$ into the element $\Omega^e = \boldsymbol{\psi}^e\left(\hat{\Omega},t\right)$ in the reference configuration B as illustrated in figure 6.1, $\boldsymbol{\xi} \in \hat{\Omega}$ are the isoparametric coordinates and $\hat{N}_a(\boldsymbol{\xi})$ are the standard shape functions defined over the standard domain $\hat{\Omega}$.

Let $\boldsymbol{\varphi}^e(\mathbf{X},t)$ and $\mathbf{V}^e(\mathbf{X},t)$ be the restrictions of the global finite element approximation $\boldsymbol{\varphi}_h$ and $\mathbf{V}_h$ to the element Ω^e, i.e.,

$$\boldsymbol{\varphi}^e(\mathbf{X},t) = \sum_a^n N_a^e(\mathbf{X},t)\,\mathbf{x}_a^e(t) \tag{6.5}$$

$$\mathbf{V}^e(\mathbf{X},t) = \sum_a^n N_a^e(\mathbf{X},t)\,\mathbf{V}_a^e(t) \tag{6.6}$$

and let $\boldsymbol{\phi}^e(\boldsymbol{\xi},t)$ and $\boldsymbol{\nu}^e(\boldsymbol{\xi},t)$ be the composition mappings

$$\begin{aligned} \boldsymbol{\phi}^e &= \boldsymbol{\varphi}^e \circ \boldsymbol{\psi}^e \\ \boldsymbol{\nu}^e &= \mathbf{V}^e \circ \boldsymbol{\psi}^e \end{aligned}$$

It follows from this definition and (6.3) that

$$\begin{aligned} \boldsymbol{\phi}^e(\boldsymbol{\xi},t) &= \sum_a^n \hat{N}_a(\boldsymbol{\xi})\,\mathbf{x}_a^e(t) \\ \boldsymbol{\nu}^e(\boldsymbol{\xi},t) &= \sum_a^n \hat{N}_a(\boldsymbol{\xi})\,\mathbf{V}_a^e(t) \end{aligned}$$

Figure (6.1) sketches the standard domain, evolving elements in the reference and deformed configurations and the corresponding mappings (compare with figure 3.1).

The class of time-dependent triangulations of the reference configuration B here considered may be interpreted as a particular triangularization of the space-time reference domain $B \times [t_0, t_f]$ as depicted in figure 6.2. Furthermore, if nodal trajectories in the reference configuration $\mathbf{X}_a(t)$ are discretized in time with isoparametric (one-dimensional) finite elements in the time variable, a particular class of *space-time* finite elements is obtained for which the space-time isoparametric shape functions are given by the product of uncoupled spatial and time factors and homogeneous

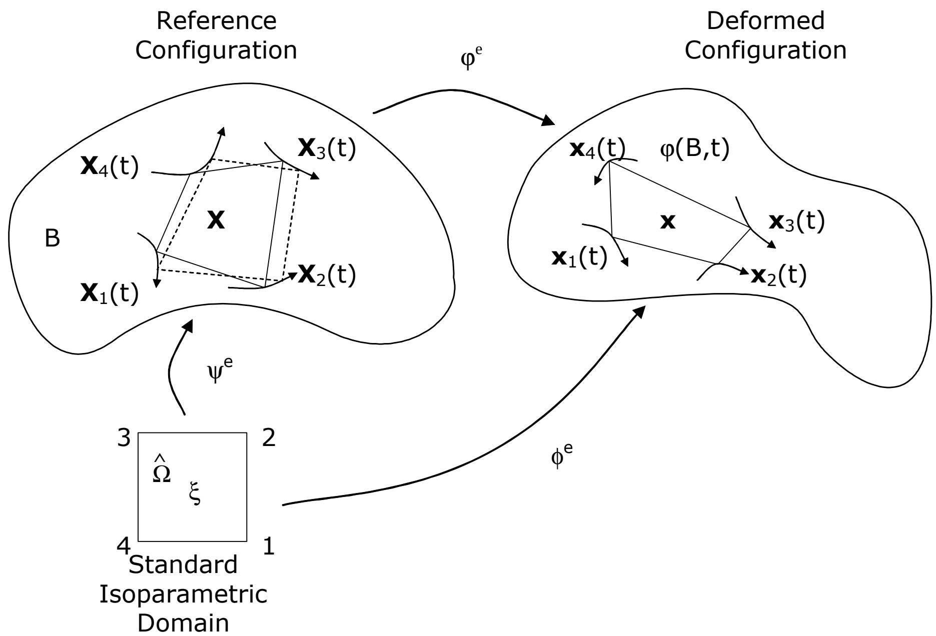

Figure 6.1: An isoparametric *moving* element and related mappings. Notice that nodes are assumed to move continuously in time within the reference configuration, simultaneously with the motion of the body.

time steps (see Chapter 2, §2.2.10 and §2.2.11). Nevertheless we will follow a semidiscrete approach and the discretization of the time variable will be postponed to a second stage.

The proposed discretization may be also understood as a time-dependent interpolation of the graphs $(\mathbf{X}, \boldsymbol{\varphi}(\mathbf{X}, t))$ and $(\mathbf{X}, \mathbf{V}(\mathbf{X}, t))$ of the deformation and velocity mappings in which both horizontal and vertical coordinates of discrete nodes on the graphs $(\mathbf{X}_a(t), \mathbf{x}_a(t))$ and $(\mathbf{X}_a(t), \mathbf{V}_a(t))$ are allowed to move continuously in time (see figure 6.3). Within this framework the space-space mappings

$$\begin{pmatrix} \boldsymbol{\psi}^e(\xi, t) \\ \boldsymbol{\phi}^e(\xi, t) \end{pmatrix} = \sum_a^n N_a^e(\boldsymbol{\xi}) \begin{pmatrix} \mathbf{X}_a^e(t) \\ \mathbf{x}_a^e(t) \end{pmatrix}$$

and

$$\begin{pmatrix} \boldsymbol{\psi}^e(\xi, t) \\ \boldsymbol{\nu}^e(\xi, t) \end{pmatrix} = \sum_a^n N_a^e(\boldsymbol{\xi}) \begin{pmatrix} \mathbf{X}_a^e(t) \\ \mathbf{V}_a^e(t) \end{pmatrix}$$

become parametrizations of the approximated graphs $(\mathbf{X}, \boldsymbol{\varphi}_h(\mathbf{X}, t))$ and $(\mathbf{X}, \mathbf{V}_h(\mathbf{X}, t))$ in the element e.

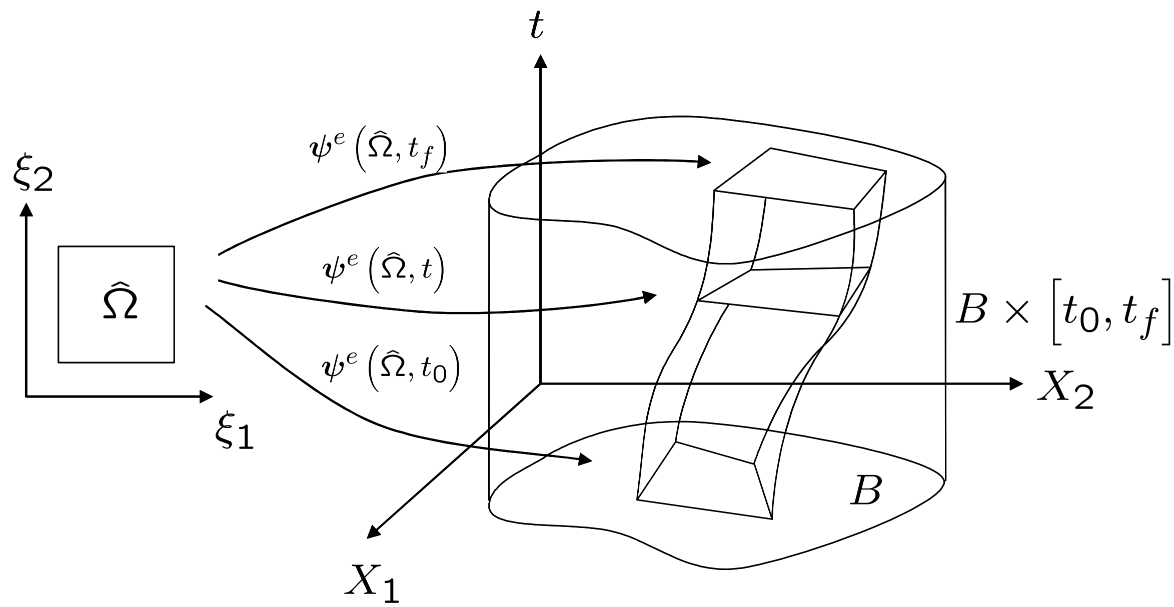

Figure 6.2: Representation of the class of finite elements considered from a space-time point of view.

6.1.2 Consistent Material velocity field for a moving isoparametric element

We next compute the consistent (discretized) material velocity field $\dot{\boldsymbol{\varphi}}_h$. Differentiating the discretized deformation mapping (6.5) with respect to time t yields

$$\dot{\boldsymbol{\varphi}}^e(\mathbf{X}, t) = \sum_a^n \left(N_a^e(\mathbf{X}, t)\, \dot{\mathbf{x}}_a^e(t) + \dot{N}_a^e(\mathbf{X}, t)\, \dot{\mathbf{x}}_a^e(t) \right) \tag{6.7}$$

In order to evaluate this expression we need to determine $\dot{N}_a^e(\mathbf{X}, t) = \frac{\partial N_a^e}{\partial t}(\mathbf{X}, t)$. To this end we first recall that in an isoparametric interpolation the shape functions must satisfy relation (6.3) that can be rewritten in the form

$$N_a^e(\boldsymbol{\psi}^e(\boldsymbol{\xi}, t), t) = \hat{N}_a(\boldsymbol{\xi})$$

Differentiating the previous with respect to time at constant $\mathbf{X}$ yields

$$\left(\frac{\partial N_a^e}{\partial t} \circ \boldsymbol{\psi}^e \right) + \left(\frac{\partial N_a^e}{\partial X_I} \circ \boldsymbol{\psi}^e \right) \dot{\psi}_I^e = 0$$

The time derivative of the isoparametric mapping (6.3) is

$$\dot{\boldsymbol{\psi}}^e(\boldsymbol{\xi}, t) = \sum_a^n \hat{N}_a(\boldsymbol{\xi})\, \dot{\mathbf{X}}_a^e(t)$$

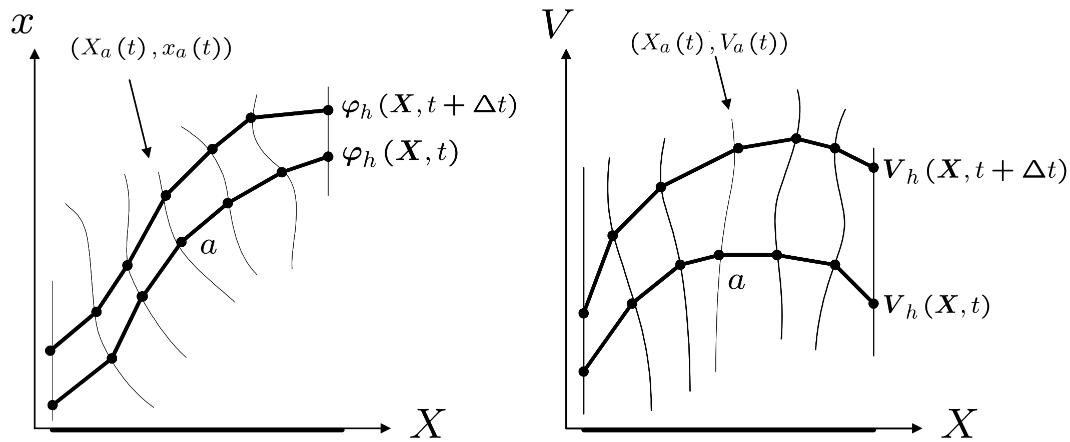

Figure 6.3: Representation of the class of finite elements considered from a space-space point of view.

Combining the previous two we find

$$\frac{\partial N_a^e}{\partial t} \circ \boldsymbol{\psi}^e = -\left(\frac{\partial N_a^e}{\partial X_I} \circ \boldsymbol{\psi}^e\right) \sum_{AA}^{n} \hat{N}_a(\boldsymbol{\xi})\, \dot{X}_{AI}^e$$

which implies after composition with $\boldsymbol{\psi}^{e-1}$ and use of relation (6.3) the sought identity

$$\frac{\partial N_a^e}{\partial t} = -\frac{\partial N_a^e}{\partial X_I} \sum_{A}^{n} N_A^e \dot{X}_{AI}^e \tag{6.8}$$

Inserting now the previous relation into (6.7) gives the consistent material velocity field as

$$\begin{aligned} \dot{\varphi}_i^e(\mathbf{X}, t) &= \sum_a^n N_a^e \dot{x}_{ai}^e - \sum_a^n \frac{\partial N_a^e}{\partial X_I} x_{ai}^e \sum_A^n N_A^e \dot{X}_{AI}^e = \\ &= \sum_a^n N_a^e \dot{x}_{ai}^e - F_{iI}^e \sum_A^n N_A^e \dot{X}_{AI}^e = \\ &= \sum_a^n N_a^e \left(\dot{x}_{ai}^e - F_{iI}^e \dot{X}_{aI}^e\right) \end{aligned} \tag{6.9}$$

where

$$F_{iI}^e(\mathbf{X}, t) = \sum_a^n \frac{\partial N_a^e}{\partial X_I} x_{ai}^e(t) \tag{6.10}$$

is the local deformation gradient field. Equation (6.9) is the discrete counterpart of relation (3.19).

Notice that the consistent velocity $\dot{\boldsymbol{\varphi}}_h$ exhibits jumps across element boundaries as a result of its dependence on the discretized deformation gradient $\mathbf{F}_h$, which is discontinuous across elements. As will be illustrated in the example of §6.1.6 these jumps may grow unbounded and the field $\dot{\boldsymbol{\varphi}}_h$ becomes a very poor approximation of the material velocity $\mathbf{V}$. The approach we follow to overcome this difficulty is to approximate the velocities with an assumed, independent, continuous interpolation $\mathbf{V}_h$ and enforce the compatibility requirement $\dot{\boldsymbol{\varphi}} = V$ in a weak sense by making use of the mixed-variational formulation introduced in Chapter 5, see also Chapter 2, §2.2.12, §2.2.14, and §2.2.15.

Relation (6.9) can be alternatively written as

$$\begin{aligned} \dot{\boldsymbol{\varphi}}^e(\mathbf{X},t) &= \sum_a^n N_a^e(\mathbf{X},t)\left(-\mathbf{F}^e,\mathbf{i}\right)\begin{pmatrix}\dot{\mathbf{X}}_a^e(t)\\ \dot{\mathbf{x}}_a^e(t)\end{pmatrix} = \\ &= \sum_a^n N_a^e(\mathbf{X},t)\,\mathbb{N}^{e*}\begin{pmatrix}\dot{\mathbf{X}}_a^e(t)\\ \dot{\mathbf{x}}_a^e(t)\end{pmatrix} \end{aligned} \tag{6.11}$$

where

$$\mathbb{N}^{e*} = \left(-\mathbf{F}^e, \mathbf{i}\right) \tag{6.12}$$

is a covector in the normal direction to the graph of the discretized deformation mapping $\boldsymbol{\varphi}_h$ in element e as depicted in figure 6.4. Relation (6.11) is the discrete counterpart of (3.53).

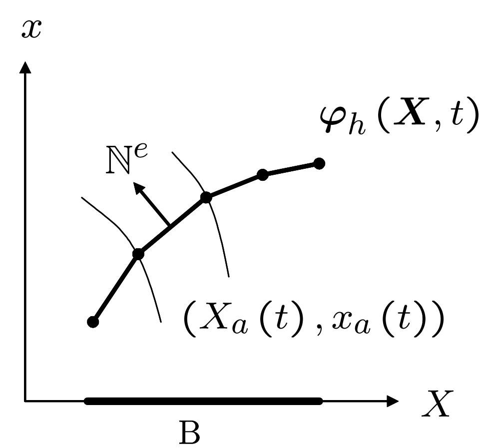

Figure 6.4: Local normal $\mathbb{N}^e$ to the graph of the discretized deformation mapping $\boldsymbol{\varphi}_h$.

6.1.3 Semidiscrete-mixed Lagrangian and semidiscrete-mixed action

We now proceed to obtain a *semidiscrete-mixed Lagrangian* by evaluating the mixed Lagrangian density $\mathcal{L}^{mix}$ on the discretized fields and integrating the latter over space. We will denote the Lagrangian (integral over space of the Lagrangian density $\mathcal{L}$) with the symbol L, namely $L = \int_B \mathcal{L}$. Inserting the deformation and velocity interpolations (6.1), (6.2) with deformation gradient (6.1) and consistent material velocity (6.9) in the mixed action functional (5.6) the following *semidiscrete-*

mixed action functional is obtained:

$$\begin{aligned} S_h\left(\mathbf{X}_h\left(t\right),\mathbf{x}_h\left(t\right),\mathbf{V}_h\left(t\right)\right) &= \int_{t_0}^{t_f} L_h^{mix}\left(\mathbf{X}_h\left(t\right),\mathbf{x}_h\left(t\right),\dot{\mathbf{X}}_h\left(t\right),\dot{\mathbf{x}}_h\left(t\right),\mathbf{V}_h\left(t\right)\right)dt = \\ &= \int_{t_0}^{t_f}\sum_e^E L^{e-mix}\left(\mathbf{X}^e\left(t\right),\mathbf{x}^e\left(t\right),\dot{\mathbf{X}}^e\left(t\right),\dot{\mathbf{x}}^e\left(t\right),\mathbf{V}^e\left(t\right)\right)dt \quad (6.13) \end{aligned}$$

where $\mathbf{x}_h\left(t\right) = \left\{\mathbf{x}_a\left(t\right),\, a=1,\cdots,N\right\}$, $\mathbf{X}_h\left(t\right) = \left\{\mathbf{X}_a\left(t\right),\, a=1,\cdots,N\right\}$ and $\mathbf{V}_h\left(t\right) = \{\mathbf{V}_a\left(t\right),$ $a=1,\cdots,N\}$ are, respectively, the global arrays of nodal coordinates in the reference and deformed configurations and velocity nodal coefficients, $\mathbf{x}^e\left(t\right) = \left\{\mathbf{x}_a^e\left(t\right),\, a=1,\cdots,n\right\}$, $\mathbf{X}^e\left(t\right) = \left\{\mathbf{X}_a^e\left(t\right),\, a=1,\cdots,n\right\}$ and $\mathbf{V}^e\left(t\right) = \left\{\mathbf{V}_a^e\left(t\right),\, a=1,\cdots,n\right\}$ the corresponding local arrays of referential and spatial coordinates and velocity coefficients of nodes in the element e, and L_h^{mix} (respectively, L^{e-mix}) are the mixed global (respectively, local) semidiscrete Lagrangians, given, respectively, by

$$L_h^{mix}\left(\mathbf{X}_h,\mathbf{x}_h,\dot{\mathbf{X}}_h,\dot{\mathbf{x}}_h,\mathbf{V}_h\right) = \sum_e^E L^{mix-e}\left(\mathbf{X}^e\left(t\right),\mathbf{x}^e\left(t\right),\dot{\mathbf{X}}^e\left(t\right),\dot{\mathbf{x}}^e\left(t\right),\mathbf{V}^e\left(t\right)\right)$$

$$L^{e-mix} = \int_{\Omega_e(t)} \mathcal{L}^{mix}\left(X_I,t,\varphi_i^e,V_i^e,F_{iI}^e,\dot{\varphi}_i^e\right)dV \quad (6.14)$$

with

$$\begin{aligned} X_I &= N_a^e X_{aI}^e \\ \varphi_i^e\left(\mathbf{X},t\right) &= N_a^e x_{ai}^e \\ \dot{\varphi}_i^e\left(\mathbf{X},t\right) &= N_a^e\left(\dot{x}_{ai}^e - F_{iI}^e\dot{X}_{aI}^e\right) \\ V_i^e\left(\mathbf{X},t\right) &= N_a^e V_{ai}^e \\ F_{iI}^e\left(\mathbf{X},t\right) &= \frac{\partial N_a^e}{\partial X_I}x_{ai}^e \end{aligned}$$

where $\mathcal{L}^{mix}\left(\mathbf{X},t,\boldsymbol{\varphi},\mathbf{V},\mathbf{F},\dot{\boldsymbol{\varphi}}\right)$ the *mixed Lagrangian density* (see equation (5.5)) defined in terms of the standard Lagrangian density $\mathcal{L}$ as

$$\mathcal{L}^{mix}\left(\mathbf{X},t,\boldsymbol{\varphi},\mathbf{V},\mathbf{F},\dot{\boldsymbol{\varphi}}\right) = \mathcal{L}\left(\mathbf{X},t,\boldsymbol{\varphi},\mathbf{V},\mathbf{F}\right) + \left.\frac{\partial\mathcal{L}}{\partial V_i}\right|_{(\mathbf{X},t,\boldsymbol{\varphi},\mathbf{V},\mathbf{F})}\left(\dot{\varphi}_i - V_i\right)$$

Here and in what follows we will use Einstein's summation convention on both nodal and coordinate indices. Referring the integrals over each element $\Omega_e\left(t\right)$ to the standard domain $\hat{\Omega}$ the local mixed Lagrangian density can be written as

$$L^{mix-e} = \int_{\hat{\Omega}_e}^{mix}\mathcal{L}^{mix}\left(\boldsymbol{\psi}^e,t,\boldsymbol{\phi}^e,\boldsymbol{\nu}^e,\left(\mathbf{F}^e\circ\boldsymbol{\psi}^e\right),\dot{\boldsymbol{\phi}}^e - \left(\mathbf{F}^e\circ\boldsymbol{\psi}^e\right)\dot{\boldsymbol{\psi}}^e\right)\det\left(D\boldsymbol{\psi}^e\right)d\boldsymbol{\xi}$$

with

$$\begin{aligned}\psi_I^e(\boldsymbol{\xi}, t) &= \hat{N}_a(\boldsymbol{\xi}) X_{aI}^e(t) \\ \phi_i^e(\boldsymbol{\xi}, t) &= \hat{N}_a(\boldsymbol{\xi}) x_{ai}^e(t) \\ \nu_i^e(\boldsymbol{\xi}, t) &= \hat{N}_a(\boldsymbol{\xi}) V_{ai}^e(t)\end{aligned}$$

and

$$\begin{aligned}F_{iI}^e \circ \boldsymbol{\psi}^e &= \varphi_{i,I}^e \circ \boldsymbol{\psi}^e = \\ &= \phi_{i,\alpha}^e \left(\psi_{\alpha,I}^{e-1} \circ \boldsymbol{\psi}^e\right) = \\ &= \left(\frac{\partial \hat{N}_a}{\partial \xi_\alpha} x_{ai}^e\right) \left(\frac{\partial \hat{N}_b}{\partial \xi_\alpha} X_{bI}^e\right)^{-1}\end{aligned}$$

For a Lagrangian density of the form (3.3) the local semidiscrete-mixed Lagrangian becomes

$$\begin{aligned}L^{mix-e} &= \int_{\Omega_e(t)} \left(\frac{R}{2}\|\mathbf{V}^e\|^2 - W\left(X_I, t, \varphi_i^e, F_{iI}^e\right) + RV_i^e\left(\dot{\varphi}_i^e - V_i^e\right)\right) dV = \\ &= \int_{\Omega_e(t)} \left(\frac{R}{2}\|N_a^e \mathbf{V}_a\|^2 - W\left(N_a^e X_{aI}^e, t, N_a^e x_{ai}^e, \frac{\partial N_a^e}{\partial X_I} x_{ai}^e\right) + \right. \\ &\qquad \left. + \sum_{a,b} R N_a^e V_{ai}^e N_b^e \left(\dot{x}_{bi}^e - F_{iI}^e \dot{X}_{bI}^e - V_{bi}^e\right)\right) dV \end{aligned} \tag{6.15}$$

that can be compactly expressed as

$$L^{mix-e} = \frac{1}{2}\mathbf{V}^{eT}\mathbf{m}^e\mathbf{V}^e - I^e + \mathbf{V}^{eT}\left(\mathbf{m}^e\dot{\mathbf{x}}^e + \mathbf{M}^e\dot{\mathbf{X}}^e - \mathbf{m}^e\mathbf{V}^e\right) \tag{6.16}$$

where

$$m_{aibj}^e = \int_{\Omega_e} R N_a^e \delta_{ij} N_b^e dV \tag{6.17}$$

$$M_{aibJ}^e = \int_{\Omega_e} R N_a^e \left(-F_{iJ}^e\right) N_b^e dV \tag{6.18}$$

are the mass matrices based on the tensors $\mathbf{i}$ and $-\mathbf{F}$ and I^e is the total potential energy over the element e

$$I^e = \int_{\Omega_e} W\left(N_a^e X_{aI}^e, t, N_a^e x_{ai}^e, \frac{\partial N_a^e}{\partial X_J} x_{ai}^e\right) dV \tag{6.19}$$

Let $\mathbf{m}_h$, $\mathbf{M}_h$ be the assembled global mass matrices and I_h the assembled global total potential energy:

$$\mathbf{m}_h = \sum_e \mathbf{m}^e \tag{6.20}$$

$$\mathbf{M}_h = \sum_e \mathbf{M}^e \tag{6.21}$$

$$I_h = \sum_e I^e \tag{6.22}$$

Notice that the global mass matrix $\mathbf{m}_h$ will be a function of the nodal global referential coordinates $\mathbf{X}_h(t)$, and that the global mass matrix $\mathbf{M}_h$ and global potential energy I_h result dependent on both nodal referential and spatial coordinates $\mathbf{X}_h(t)$ and $\mathbf{x}_h(t)$. Assembling the elemental contributions into global arrays, the semidiscrete mixed global Lagrangian becomes

$$\begin{aligned} L_h^{mix}\left(\mathbf{X}_h, \mathbf{x}_h, \dot{\mathbf{X}}_h, \dot{\mathbf{x}}_h, \mathbf{V}_h\right) &= \frac{1}{2}\mathbf{V}_h^T \mathbf{m}_h \mathbf{V}_h - I_h \\ &+ \mathbf{V}_h^T\left(\mathbf{m}_h \dot{\mathbf{x}}_h + \mathbf{M}_h \dot{\mathbf{X}}_h - \mathbf{m}_h \mathbf{V}_h\right) \end{aligned} \tag{6.23}$$

with

$$\begin{aligned} \mathbf{m}_h &= \mathbf{m}_h(\mathbf{X}_h) \\ \mathbf{M}_h &= \mathbf{M}_h(\mathbf{x}_h, \mathbf{X}_h) \\ I_h &= I_h(\mathbf{x}_h, \mathbf{X}_h) \end{aligned}$$

6.1.4 Variations and semidiscrete Euler-Lagrange equations

In analogy with the continuous case, we next compute the variations of the semidiscrete-mixed action functional (6.13) with respect to all of its arguments $\mathbf{x}_h(t)$, $\mathbf{X}_h(t)$ and $\mathbf{V}_h(t)$ and the corresponding Euler-Lagrange equations. Taking variations in (6.13) we obtain

$$\begin{aligned} \langle \delta S_h, \delta \mathbf{x}_h \rangle &= \int_{t_0}^{t_f} \sum_e \left(\frac{\partial L^{mix-e}}{\partial x^e_{ai}} \delta x^e_{ai} + \frac{\partial L^{mix-e}}{\partial \dot{x}^e_{ai}} \delta \dot{x}^e_{ai} \right) dt \\ \langle \delta S_h, \delta \mathbf{X}_h \rangle &= \int_{t_0}^{t_f} \sum_e \left(\frac{\partial L^{mix-e}}{\partial X^e_{aI}} \delta X^e_{aI} + \frac{\partial L^{mix-e}}{\partial \dot{X}^e_{aI}} \delta \dot{X}^e_{aI} \right) dt \\ \langle \delta S_h, \delta \mathbf{V}_h \rangle &= \int_{t_0}^{t_f} \sum_e \left(\frac{\partial L^{mix-e}}{\partial V^e_{ai}} \delta V^e_{aI} \right) dt \end{aligned}$$

where L^{mix-e} is the elemental mixed semidiscrete Lagrangian defined in (6.14), and (6.16). Differentiating now the latter with respect to each of its arguments, or, alternatively, substituting the semidiscrete finite element interpolations (6.5) and (6.6) with consistent velocity interpolation (6.7) and deformation gradient interpolation (6.10) into the continuous mixed variations (5.8), (5.9), and

(5.10) we obtain the variations in the form:

- Variations with respect to $\delta\mathbf{x}_h$

$$\langle \delta S, \delta x^e_{ai} \rangle = \int_{t_0}^{t_f} \sum_e \int_{\Omega^e} \left(\delta x^e_{ai} \left(N^e_a B^e_i - \frac{\partial N^e_a}{\partial X_I} P^e_{iI} \right) + R N^e_a V_{ai} \left(\delta_{ij} \right) \frac{d}{dt} \left(N^e_b \delta x^e_{bj} \right) \right) dV dt \quad (6.24)$$

- Variations with respect to $\delta\mathbf{X}_h$

$$\begin{aligned} \langle \delta S, \delta X^e_{aI} \rangle &= \int_{t_0}^{t_f} \sum_e \int_{\Omega^e} \left(\delta X^e_{aI} \left(N^e_a B^{inh-mix-e}_I - \frac{\partial N^e_a}{\partial X_J} C^{mix-e}_{IJ} \right) + \right. \\ &\quad \left. + R N^e_a V^e_{ai} \left(-F^e_{iJ} \right) \frac{d}{dt} \left(N^e_b \delta X^e_{bJ} \right) \right) dV dt \qquad (6.25) \\ &= \int_{t_0}^{t_f} \sum_e \int_{\Omega^e} \left(\delta X^e_{aI} \left(N^e_a B^{inh-e}_I - \frac{\partial N^e_a}{\partial X_J} C^e_{IJ} \right) + \right. \\ &\quad + R N^e_a V^e_{ai} \left(-F^e_{iJ} \right) \frac{d}{dt} \left(N^e_b \delta X^e_{bJ} \right) + \\ &\quad \left. + \delta X^e_{cK} \left(\frac{\partial R}{\partial X_K} N^e_c + R \frac{\partial N^e_c}{\partial X_K} \right) V^e_{ai} N^e_a \delta_{ij} \left(\frac{d}{dt} \left(N^e_b x^e_{bj} \right) - N^e_b V^e_{bj} \right) \right) dV dt \\ &\qquad (6.26) \\ &= \int_{t_0}^{t_f} \sum_e \int_{\Omega^e} \left(\delta X^e_{aI} \left(N^e_a B^{inh-static-e}_I - \frac{\partial N^e_a}{\partial X_J} C^{static-e}_{IJ} \right) + \right. \\ &\quad + R N^e_a V^e_{ai} \left(-F^e_{iJ} \right) \frac{d}{dt} \left(N^e_b \delta X^e_{bJ} \right) + \\ &\quad \left. + \delta X^e_{cK} \left(\frac{\partial R}{\partial X_K} N^e_c + R \frac{\partial N^e_c}{\partial X_K} \right) \left(\frac{\|\mathbf{V}^e\|^2}{2} + V^e_a N^e_a \delta_{ij} \left(\frac{d}{dt} \left(N^e_b x^e_{bj} \right) - N^e_b V^e_{bj} \right) \right) \right) dV dt \\ &\qquad (6.27) \end{aligned}$$

- Variations with respect to $\delta\mathbf{V}_h$

$$\langle \delta S, \delta V^e_{ai} \rangle = \int_{t_0}^{t_f} \sum_e \int_{\Omega^e} R N^e_a \delta V^e_{ai} \delta_{ij} \left(\frac{d}{dt} \left(N^e_b x^e_{bj} \right) - N^e_b V^e_{bj} \right) dV dt \quad (6.28)$$

where

$$\begin{aligned} B^e_i &= \frac{\partial \mathcal{L}^{mix-e}}{\partial \varphi_i} = \frac{\partial \mathcal{L}^e}{\partial \varphi_i} = -\frac{\partial W^e}{\partial \varphi_i} \\ P^e_{iJ} &= -\frac{\partial \mathcal{L}^{mix-e}}{\partial F_{iJ}} = -\frac{\partial \mathcal{L}^e}{\partial F_{iJ}} = \frac{\partial W^e}{\partial F_{iJ}} \end{aligned}$$

are the mechanical body force Piolla-Kirchhoff stress tensors evaluated on the discretized fields,

$$
\begin{aligned}
B_I^{inh-mix-e} &= \left.\frac{\partial \mathcal{L}^{mix}}{\partial X_I}\right|_{\exp} = \\
&= \frac{1}{2}\frac{\partial R}{\partial X_I}\|\mathbf{V}^e\|^2 - \left.\frac{\partial W}{\partial X_I}\right|_{\exp} + \frac{\partial R}{\partial X_I} V_{ai}^e N_a^e \delta_{ij} N_b^e \left(\dot{x}_{bj}^e - F_{jJ}^e \dot{X}_{bJ}^e - V_{bj}^e\right) \\
C_{IJ}^{mix-e} &= -\left(\mathcal{L}^{mix-e}\delta_{IJ} - \frac{\partial \mathcal{L}^{mix-e}}{\partial F_{iJ}} F_{iI}^e\right) = \\
&= \left(\left(W^e - \frac{1}{2}R\|\mathbf{V}^e\|^2 - RV_{ai}^e N_a^e \delta_{ij} N_b^e \left(\dot{x}_{bj}^e - F_{jJ}^e \dot{X}_{bJ}^e - V_{bj}^e\right)\right)\delta_{IJ} - F_{iI}^e P_{iJ}^e\right)
\end{aligned}
$$

are the material body force and Eshelby stress tensor constructed with $\mathcal{L}^{mix}$ (evaluated on the discretized fields),

$$
\begin{aligned}
B_i^{inh-e} &= \left.\frac{\partial \mathcal{L}^e}{\partial X_i}\right|_{\exp} = \frac{1}{2}\frac{\partial R}{\partial X_I}\|\mathbf{V}^e\|^2 - \left.\frac{\partial W^e}{\partial X_I}\right|_{\exp} \\
C_{IJ}^e &= -\left(\mathcal{L}^e\delta_{IJ} - F_{iI}^e\frac{\partial \mathcal{L}^e}{\partial F_{iJ}}\right) = \left(W^e - \frac{1}{2}R\|\mathbf{V}^e\|^2\right)\delta_{IJ} - F_{iI}^e P_{iJ}^e
\end{aligned}
$$

are the corresponding quantities computed with $\mathcal{L}$, that is to say excluding the Lagrange multiplier term (and also evaluated on the discretized fields) and

$$
\begin{aligned}
B_i^{inh-static-e} &= \left.\frac{\partial W^e}{\partial X_I}\right|_{\exp} \\
C_{IJ}^{static-e} &= W^e\delta_{IJ} - F_{iI}^e P_{iJ}^e
\end{aligned}
$$

are the static parts of the inhomogeneity force and Eshelby stress tensors. In the previous expressions $\mathcal{L}^{mix-e}$, $\mathcal{L}^e$, and W^e are, respectively, the mixed Lagrangian density (5.5), the standard Lagrangian density (3.3), and the total potential energy all evaluated on the discretized fields.

Making use of (6.8) and rearranging terms the semidiscrete variations take the compact form

$$
\langle \delta S_h, \delta x_{ai}^e \rangle = \int_{t_0}^{t_f}\left(\sum_e \delta x_{ai}^e\left(f_{ai}^e + e_{ai}^e\right) + V_{ai}^e m_{aibj}^e \delta \dot{x}_{bj}^e\right) dt \tag{6.29}
$$

$$
\langle \delta S_h, \delta X_{aI}^e \rangle = \int_{t_0}^{t_f}\left(\sum_e \delta X_{aI}^e\left(F_{aI}^e + E_{aI}^e\right) + V_{ai}^e M_{aibJ}^e \delta \dot{X}_{bJ}^e\right) dt \tag{6.30}
$$

$$
\langle \delta S_h, \delta V_{ai}^e \rangle = \int_{t_0}^{t_f}\left(\sum_e \delta V_{ai}^e\left(m_{aibj}^e \dot{x}_{bj}^e + M_{aibJ}^e \dot{X}_{bJ}^e - m_{aibj}^e V_{bj}^e\right)\right) dt \tag{6.31}
$$

where

$$
\begin{aligned}
f^e_{ai} &= -\frac{\partial I^e}{\partial x_{ai}} \\
&= -\int_{\Omega^e} \left(-B^e_i N^e_a + P^e_{iJ} \frac{\partial N^e_a}{\partial X_J} \right) dV \qquad (6.32) \\
F_{aI} &= -\frac{\partial I^e}{\partial X_{aI}} = \\
&= -\int_{\Omega^e} \left(-B^{inh-static-e}_I N^e_a + C^{static-e}_{IJ} \frac{\partial N^e_a}{\partial X_J} \right) dV \qquad (6.33)
\end{aligned}
$$

and

$$
\begin{aligned}
e^e_{ck} &= \frac{\partial}{\partial x_{ck}} \left\{ \frac{1}{2} \mathbf{V}^e \mathbf{m}^e \mathbf{V}^e + \mathbf{V}^e \left(\mathbf{m}^e \dot{\mathbf{x}}^e + \mathbf{M}^e \dot{\mathbf{X}}^e - \mathbf{m}^e \mathbf{V}^e \right) \right\} = \\
&= \int_{\Omega^e} \left(R N^e_a V^e_{ai} \left(\delta_{ik} \right) \left(-\frac{\partial N^e_c}{\partial X_J} \right) N^e_b \dot{X}^e_{bJ} \right) dV \qquad (6.34) \\
E^e_{cK} &= \frac{\partial}{\partial X_{cK}} \left\{ \frac{1}{2} \mathbf{V}^e \mathbf{m}^e \mathbf{V}^e + \mathbf{V}^e \left(\mathbf{m}^e \dot{\mathbf{x}}^e + \mathbf{M}^e \dot{\mathbf{X}}^e - \mathbf{m}^e \mathbf{V}^e \right) \right\} = \\
&= \int_{\Omega^e} \left(R N^e_a V^e_{ai} \left(-F^e_{iK} \right) \left(-\frac{\partial N^e_c}{\partial X_J} \right) N^e_b \dot{X}^e_{bJ} \right) dV \\
&\quad + \int_{\Omega^e} \left(\tfrac{\partial R}{\partial X_K} N^e_c + R \tfrac{\partial N^e_c}{\partial X_K} \right) \left(\tfrac{\|\mathbf{V}^e\|^2}{2} + V^e_a N^e_a \delta_{ij} N^e_b \left(\dot{x}^e_{bj} - F^e_{jJ} \dot{X}^e_{bJ} - V^e_{bj} \right) \right) dV \quad (6.35)
\end{aligned}
$$

The forces f^e_{ai} and F^e_{aI} are the static nodal mechanical force and nodal configurational force at node a. They are computed using body forces and stress tensors based only on the energy density W. The forces e^e_{ai} and E^e_{aI} are dynamic sources that group together all velocity-dependent terms. They arise as a consequence of the dependence of the mass matrices $\mathbf{m}^e$ and $\mathbf{M}^e$ on the configuration $(\mathbf{X}^e, \mathbf{x}^e)$.

We turn next to the derivation of the semidiscrete Euler-Lagrange equations. We will write these equations in two different forms, the first better suited for numerical implementation, and the second useful to derive simplified expressions for the tangential and normal Euler-Lagrange equations that will be computed in the next section.

6.1.4.1 Semidiscrete Euler-Lagrange equations, first form

Stationarity of the semidiscrete action S_h with respect to admissible variations of all of its arguments $\mathbf{X}_h(t)$,.$\mathbf{x}_h(t)$ and $\mathbf{V}_h(t)$ implies

$$
\begin{aligned}
\langle \delta S_h, \delta \mathbf{X}_h \rangle &= 0 \qquad \forall \delta \mathbf{X}_h \\
\langle \delta S_h, \delta \mathbf{x}_h \rangle &= 0 \qquad \forall \delta \mathbf{x}_h \\
\langle \delta S_h, \delta \mathbf{V}_h \rangle &= 0 \qquad \forall \delta \mathbf{V}_h
\end{aligned}
$$

Integrating by parts with respect to the time variable in (6.29) and (6.30) we obtain the Euler-Lagrange equations in the form

$$\begin{aligned}
\sum_e \left(\frac{d}{dt} \left(V^e_{ai} m^e_{aibj} \right) - \left(f^e_{bj} + e^e_{bj} \right) \right) &= 0 \\
\sum_e \left(\frac{d}{dt} \left(V^e_{ai} M^e_{aibJ} \right) - \left(F^e_{bJ} + E^e_{bJ} \right) \right) &= 0 \\
\sum_e \left(m^e_{aibj} \dot{x}^e_{bj} + M^e_{aibJ} \dot{X}^e_{bJ} - m^e_{aibj} V^e_{bj} \right) &= 0
\end{aligned}$$

Assembling the element contributions into global arrays, the semidiscrete Euler-Lagrange equations evaluate to the global equations

$$\frac{d}{dt} \left(\mathbf{m}_h^T \mathbf{V}_h \right) = \mathbf{e}_h + \mathbf{f}_h \tag{6.36}$$

$$\frac{d}{dt} \left(\mathbf{M}_h^T \mathbf{V}_h \right) = \mathbf{E}_h + \mathbf{F}_h \tag{6.37}$$

$$\mathbf{m}_h \dot{\mathbf{x}}_h + \mathbf{M}_h \dot{\mathbf{X}}_h = \mathbf{m}_h \mathbf{V}_h \tag{6.38}$$

where $\mathbf{e}_h$, $\mathbf{E}_h$, $\mathbf{f}_h$, and $\mathbf{F}_h$ are the global force vectors

$$\mathbf{e}_h = \sum_e \mathbf{e}^e \tag{6.39}$$

$$\mathbf{E}_h = \sum_e \mathbf{E}^e \tag{6.40}$$

$$\mathbf{f}_h = \sum_e \mathbf{f}^e \tag{6.41}$$

$$\mathbf{F}_h = \sum_e \mathbf{F}^e \tag{6.42}$$

Equations (6.36), (6.37), and (6.38) are the first sought form of the semidiscrete Euler-Lagrange equations. They are the (semi)discrete counterpart of the continuous Euler-Lagrange equations (5.11), (5.12), (5.13). Notice that the static nodal mechanical and configurational forces $\mathbf{f}_h$ and $\mathbf{F}_h$ will be functions of $(\mathbf{X}_h, \mathbf{x}_h)$ while the dynamic sources will be functions of $\left(\mathbf{X}_h, \mathbf{x}_h, \dot{\mathbf{X}}_h, \dot{\mathbf{x}}_h, \mathbf{V}_h\right)$.

6.1.4.2 Semidiscrete Euler-Lagrange equations, second form

Notice that the Euler-Lagrange equations (6.36), (6.37) involve time derivatives of the mass matrices $(\mathbf{M}_h, \mathbf{m}_h)$ multiplied by the velocity vector $\mathbf{V}_h$. We would like now to rewrite the previous equations in a form that does not involve time differentiation of the mass matrices $(\mathbf{M}_h, \mathbf{m}_h)$ but only time differentiation of the velocity vector $\mathbf{V}_h$. To this end we observe that integrating by parts in time and space appropriately in the variations (6.24) and (6.27) and making use of the identities (5.14) and (5.15), the semidiscrete variations might be rewritten as

$$\begin{aligned}
\langle \delta S_h, \delta x^e_{ai} \rangle &= \int\limits_{t_0}^{t_f} \sum_e \int_{\Omega^e} \left(\delta x^e_{ai} \left(N^e_a B^e_i - \frac{\partial N^e_a}{\partial X_I} P^e_{iI} \right) - \frac{d}{dt} \left(R N^e_a V_{ai} \right) \left(\delta_{ij} \right) N^e_b \delta x^e_{bj} \right) dV dt \\
\langle \delta S_h, \delta X^e_{aI} \rangle &= \int\limits_{t_0}^{t_f} \sum_e \int_{\Omega^e} \left(\delta X^e_{aI} \left(N^e_a B^{inh-static-e}_I - \frac{\partial N^e_a}{\partial X_J} C^{static-e}_{IJ} \right) + \right. \\
& \quad - \frac{d}{dt} \left(R N^e_a V^e_{ai} \right) \left(-F^e_{iJ} \right) N^e_b \delta X^e_{bJ} + \\
& \quad \left. - \delta X^e_{cJ} R N^e_c \frac{\partial \left(V^e_{ai} N^e_a \right)}{\partial X_J} \left(\frac{d}{dt} \left(N^e_b x^e_{bi} \right) - N^e_b V^e_{bi} \right) \right) dV dt \\
\langle \delta S_h, \delta V^e_{ai} \rangle &= \int\limits_{t_0}^{t_f} \sum_e \int_{\Omega^e} R N^e_a \delta V^e_{ai} \delta_{ij} \left(\frac{d}{dt} \left(N^e_b x^e_{bj} \right) - N^e_b V^e_{bj} \right) dV dt
\end{aligned}$$

Making use next of (6.8) and rearranging terms, the semidiscrete variations take the compact form

$$\left\langle \delta S_h, \delta x^e_{bj} \right\rangle = \int_{t_0}^{t_f} \left(\sum_e \delta x^e_{bj} \left(f_{bj} - \dot{V}^e_{ai} m^e_{aibj} - \mu^e_{bjaI} \dot{X}_{aI} \right) \right) dt \tag{6.43}$$

$$\left\langle \delta S_h, \delta X^e_{bJ} \right\rangle = \int_{t_0}^{t_f} \left(\sum_e \int_{\Omega^e} \delta X^e_{bJ} \left(F^e_{bJ} - \dot{V}^e_{ai} M^e_{aibJ} + \left(\dot{x}^e_{ai} - V^e_{ai} \right) \mu^e_{aibJ} \right) \right) dt \tag{6.44}$$

$$\left\langle \delta S_h, \delta V^e_{ai} \right\rangle = \int_{t_0}^{t_f} \left(\sum_e \delta V^e_{ai} \left(m^e_{aibj} \dot{x}^e_{bj} + M^e_{aibJ} \dot{X}^e_{bJ} - m^e_{aibj} V^e_{bj} \right) \right) dt \tag{6.45}$$

where

$$\mu^e_{aibJ} = \int_{\Omega_e} R N^e_a \left(-V^e_{i,J} \right) N^e_b dV$$

is a new mass matrix based on the tensor $V_{i,J}$ (material velocity gradient). The Euler-Lagrange equations therefore become

$$\begin{aligned}
\sum_e \left(\dot{V}^e_{ai} m^e_{aibj} + \mu^e_{bjaI} \dot{X}_{aI} - f_{bj} \right) &= 0 \\
\sum_e \left(\dot{V}^e_{ai} M^e_{aibJ} - \left(\dot{x}^e_{ai} - V^e_{ai} \right) \mu^e_{aibJ} - F^e_{bJ} \right) &= 0 \\
\sum_e \left(m^e_{aibj} \left(\dot{x}^e_{bj} - V^e_{bj} \right) + M^e_{aibJ} \dot{X}^e_{bJ} \right) &= 0
\end{aligned}$$

or assembling the element contributions into global arrays

$$\mathbf{m}^T_h \dot{\mathbf{V}}_h + \boldsymbol{\mu}_h \dot{\mathbf{X}}_h = \mathbf{f}_h \tag{6.46}$$

$$\mathbf{M}^T_h \dot{\mathbf{V}}_h - \boldsymbol{\mu}^T_h \left(\dot{\mathbf{x}}_h - \mathbf{V}_h \right) = \mathbf{F}_h \tag{6.47}$$

$$\mathbf{m}_h \left(\dot{\mathbf{x}}_h - \mathbf{V}_h \right) + \mathbf{M}_h \dot{\mathbf{X}}_h = \mathbf{0} \tag{6.48}$$

where

$$\boldsymbol{\mu}_h = \sum_e \boldsymbol{\mu}^e$$

is the global assembled velocity-gradient–based mass matrix. Equations (6.46), (6.47), (6.48) are the second sought form of the semidiscrete Euler-Lagrange equations and correspond to the (semi)discrete counterpart of the continuous Euler-Lagrange equations written in the form (5.16), (5.17), (5.18). Notice that comparing (6.36), (6.37) with (6.46), (6.47) we have the identities

$$\begin{aligned} \frac{d}{dt}\left(\mathbf{m}_h^T \mathbf{V}_h\right) - \mathbf{e}_h &= \mathbf{m}_h^T \dot{\mathbf{V}}_h + \boldsymbol{\mu}_h \dot{\mathbf{X}}_h \\ \frac{d}{dt}\left(\mathbf{M}_h^T \mathbf{V}_h\right) - \mathbf{E}_h &= \mathbf{M}_h^T \dot{\mathbf{V}}_h - \boldsymbol{\mu}_h^T \left(\dot{\mathbf{x}}_h - \mathbf{V}_h\right) \end{aligned}$$

or equivalently

$$\begin{aligned} \dot{\mathbf{m}}_h^T \mathbf{V}_h - \mathbf{e}_h &= \boldsymbol{\mu}_h \dot{\mathbf{X}}_h \\ \dot{\mathbf{M}}_h^T \mathbf{V}_h - \mathbf{E}_h &= -\boldsymbol{\mu}_h^T \left(\dot{\mathbf{x}}_h - \mathbf{V}_h\right) \end{aligned}$$

that can be derived directly from the definitions of $\mathbf{m}_h$, $\mathbf{M}_h$, $\mathbf{e}_h$, $\mathbf{E}_h$ and $.\boldsymbol{\mu}_h$. Therefore we might avoid the computation (and time discretization) of the time derivative of the mass matrices by evaluating instead the new mass-like matrix $\boldsymbol{\mu}_h$ based on the gradient of the velocity field.

6.1.5 Horizontal-Vertical variations—Tangential-Normal variations

Analogous to what was done in the continuous setting, we now reinterpret the motion in terms of the evolution of the graph of the deformation mapping $(\mathbf{X}, \boldsymbol{\varphi})$ within the space-space bundle $B \times S$. We thus regard nodal coordinates in the reference and deformed configurations $\mathbf{X}_h$ and $\mathbf{x}_h$ as horizontal and vertical components of the generalized dynamical variable $\mathbf{q}_h = (\mathbf{X}_h, \mathbf{x}_h)$ that we now understand as a single variable in the configurational bundle $\mathbb{R}^{dN} \times \mathbb{R}^{dN}$ where d is the spatial dimension and N the total number of nodes. Variations of the semidiscrete action with respect to $\mathbf{X}_h$ and $\mathbf{x}_h$ can be thus interpreted as horizontal and vertical variations and their corresponding Euler-Lagrange equations as horizontal and vertical components of a single equation for the evolution of the dynamical variable $\mathbf{q}_h$.

When comparing this semidiscrete picture against the continuous picture discussed in §3.3.3 we find however a very important difference: The semidiscrete Euler-Lagrange equations (SDEL) corresponding to horizontal variations are not satisfied automatically whenever the semidiscrete Euler-Lagrange equations corresponding to the vertical variations are. Or equivalently, semidiscrete tangential variations do not vanish identically and result in non-trivial tangential SDEL. Horizontal and vertical SDEL or alternatively, tangential and normal SDEL become therefore a non-trivial set of differential equations to solve for the joint unknown $\mathbf{q}_h$.

Figures (6.5) illustrate graphically this fact. Recall that in the continuous setting (see §3.3.7) every horizontal variation can be understood as a vertical variation (figure 3.4). Therefore a stationary point of the action with respect to vertical variations becomes automatically stationary with respect to all horizontal variations. In the discrete setting however horizontal and vertical variations are not equivalent in general and therefore the corresponding Euler-Lagrange equations are independent as a result.

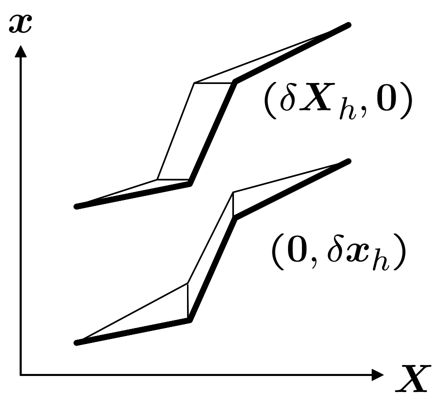

Figure 6.5: Horizontal and vertical variations of the (semi)discretized deformation mapping. Unlike the continuous case, in the discrete case these are not equivalent.

Alternatively we may illustrate the discrepancy by looking at tangential and normal variations as depicted in figure 6.5. We recall that in the continuous setting any perturbation in the tangential direction leaves the configuration unperturbed and, therefore, since the action is a function of the configuration, the tangential Euler-Lagrange equations are trivially satisfied (figure 3.5). In the discrete setting however each discrete configuration does not remain invariant with respect to perturbations in the tangential direction. Therefore the semidiscrete Euler-Lagrange equations corresponding to the tangential direction are not trivially satisfied in general. More precisely, if S is the continuous action and S_h is the semidiscrete action, then we have

$$\langle \delta S, \delta \mathbf{T} \rangle = 0 \qquad \forall \delta \mathbf{T}$$

identically for any tangential variation $\delta \mathbf{T}$, however for its semidiscrete counterpart we obtain

$$\langle \delta S_h, \delta \mathbf{T}_h \rangle \neq 0$$

for arbitrary general variations $\delta \mathbf{T}_h$ in the tangential direction.

In what follows we derive the Euler-Lagrange equations projected into the tangential and normal directions following the procedure outlined for the continuous setting in §3.3.7. To this end we define

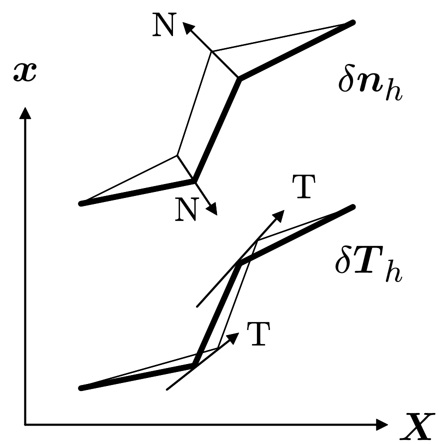

Figure 6.6: Normal and tangential variations of the (semi)discretized deformation mapping. Unlike the continuous case, in the discrete case the mapping does not remain unperturbed under the action of tangential variations.

the following global normal vector $\mathbb{N}_h$ and covector $\mathbb{N}_h^*$

$$\mathbb{N}_h = \begin{pmatrix} \mathbf{M}_h^T \\ \mathbf{m}_h^T \end{pmatrix} \mathbf{m}_h^{-T} \tag{6.49}$$

$$\mathbb{N}_h^* = \mathbf{m}_h^{-1} (\mathbf{M}_h, \mathbf{m}_h) \tag{6.50}$$

and global tangent vector $\mathbb{T}_h$ and covector $\mathbb{T}_h^*$:

$$\mathbb{T}_h = \mathbf{m}_h^{-1} \begin{pmatrix} \mathbf{m}_h \\ -\mathbf{M}_h \end{pmatrix} \tag{6.51}$$

$$\mathbb{T}_h^* = \left(\mathbf{m}_h^T, -\mathbf{M}_h^T\right) \mathbf{m}_h^{-T} \tag{6.52}$$

Notice that the matrices

$$\begin{aligned}
(\mathbf{M}_h, \mathbf{m}_h)_{ab} &= \sum_e (\mathbf{M}^e, \mathbf{m}^e)_{ab} = \sum_e \int_{\Omega^e} R N_a^e N_b^e \, (-\mathbf{F}^e, \mathbf{i}) \, dV \\
\left(\mathbf{m}_h^T, -\mathbf{M}_h^T\right)_{ab} &= \sum_e \left(\mathbf{m}^{eT}, -\mathbf{M}^{eT}\right)_{ab} = \sum_e \int_{\Omega^e} R N_a^e N_b^e \left(\mathbf{I}, \mathbf{F}^{eT}\right) dV \\
\begin{pmatrix} \mathbf{M}_h^T \\ \mathbf{m}_h^T \end{pmatrix}_{ab} &= \sum_e \begin{pmatrix} \mathbf{M}^e \\ \mathbf{m}^e \end{pmatrix}_{ab} = \sum_e \int_{\Omega^e} R N_a^e N_b^e \begin{pmatrix} -\mathbf{F}^{eT} \\ \mathbf{i} \end{pmatrix} dV \\
\begin{pmatrix} \mathbf{m}_h^T \\ -\mathbf{M}_h^T \end{pmatrix}_{ab} &= \sum_e \begin{pmatrix} \mathbf{m}^{eT} \\ -\mathbf{M}^{eT} \end{pmatrix}_{ab} = \sum_e \int_{\Omega^e} R N_a^e N_b^e \begin{pmatrix} \mathbf{I} \\ \mathbf{F}^e \end{pmatrix} dV
\end{aligned}$$

are the assembled weighted averages over element Ω^e of the local normal and tangent vectors and covectors

$$\begin{aligned}
\mathbb{N}^{e*} &= \left(-\mathbf{F}^{e}, \mathbf{i}\right) \\
\mathbb{T}^{e*} &= \left(\mathbf{I}, \mathbf{F}^{eT}\right) \\
\mathbb{N}^{e} &= \begin{pmatrix} -\mathbf{F}^{eT} \\ \mathbf{i} \end{pmatrix} \\
\mathbb{T}^{e} &= \begin{pmatrix} \mathbf{I} \\ \mathbf{F}^{e} \end{pmatrix}
\end{aligned}$$

Notice also that $\mathbb{N}_h$ and $\mathbb{T}_h$ are arrays of dimension $2dN \times dN$ while the dimension of $\mathbb{N}_h^*$ and $\mathbb{T}_h^*$ is $dN \times 2dN$ and that we have the orthogonality properties

$$\begin{aligned}
\mathbb{N}_h^* \cdot \mathbb{T}_h &= \mathbf{m}_h^{-1}\left(\mathbf{M}_h, \mathbf{m}_h\right)\mathbf{m}_h^{-1}\begin{pmatrix} \mathbf{m}_h \\ -\mathbf{M}_h \end{pmatrix} = \mathbf{m}_h^{-1}\left(\mathbf{M}_h - \mathbf{M}_h\right) = \mathbf{0} \\
\mathbb{T}_h^* \cdot \mathbb{N}_h &= \left(\mathbf{m}_h^T, -\mathbf{M}_h^T\right)\mathbf{m}_h^{-T}\begin{pmatrix} \mathbf{M}_h^T \\ \mathbf{m}_h^T \end{pmatrix}\mathbf{m}_h^{-T} = \left(\mathbf{M}_h^T - \mathbf{M}_h^T\right)\mathbf{m}_h^{-T} = \mathbf{0}
\end{aligned}$$

We also define the following differential operators:

$$\begin{aligned}
\begin{pmatrix} \mathcal{F}_{\mathbf{X}}\left(\mathbf{X}_h, \mathbf{x}_h, \mathbf{V}_h\right) \\ \mathcal{F}_{\mathbf{x}}\left(\mathbf{X}_h, \mathbf{x}_h, \mathbf{V}_h\right) \end{pmatrix} &= \frac{d}{dt}\left\{\begin{pmatrix} \mathbf{M}_h^T \\ \mathbf{m}_h^T \end{pmatrix}\mathbf{V}_h\right\} - \begin{pmatrix} \mathbf{E}_h \\ \mathbf{e}_h \end{pmatrix} - \begin{pmatrix} \mathbf{F}_h \\ \mathbf{f}_h \end{pmatrix} \\
&= \begin{pmatrix} \mathbf{M}_h^T \\ \mathbf{m}_h^T \end{pmatrix}\dot{\mathbf{V}}_h + \begin{pmatrix} \boldsymbol{\mu}_h^T\mathbf{m}_h^{-1}\mathbf{M}_h \\ \boldsymbol{\mu}_h \end{pmatrix}\dot{\mathbf{X}}_h - \begin{pmatrix} \mathbf{F}_h \\ \mathbf{f}_h \end{pmatrix}
\end{aligned}$$

that are just the left hand side of the Euler-Lagrange equations ((6.36), (6.37)) and ((6.46), (6.37)) written in a column vector. Using the above definitions, the Euler-Lagrange equations can be rewritten as

$$\begin{aligned}
\begin{pmatrix} \mathcal{F}_{\mathbf{X}}\left(\mathbf{X}_h, \mathbf{x}_h, \mathbf{V}_h\right) \\ \mathcal{F}_{\mathbf{x}}\left(\mathbf{X}_h, \mathbf{x}_h, \mathbf{V}_h\right) \end{pmatrix} &= \frac{d}{dt}\left\{\mathbb{N}_h\mathbf{m}_h\mathbf{V}_h\right\} - \begin{pmatrix} \mathbf{E}_h \\ \mathbf{e}_h \end{pmatrix} - \begin{pmatrix} \mathbf{F}_h \\ \mathbf{f}_h \end{pmatrix} = \\
&= \mathbb{N}_h\mathbf{m}_h\dot{\mathbf{V}}_h + \begin{pmatrix} \boldsymbol{\mu}_h^T\mathbf{m}_h^{-1}\mathbf{M}_h \\ \boldsymbol{\mu}_h \end{pmatrix}\dot{\mathbf{X}}_h - \begin{pmatrix} \mathbf{F}_h \\ \mathbf{f}_h \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \end{pmatrix} \\
\mathbb{N}_h^*\begin{pmatrix} \dot{\mathbf{X}}_h \\ \dot{\mathbf{x}}_h \end{pmatrix} &= \mathbf{V}_h
\end{aligned}$$

Finally, following the same methodology we used in the continuum setting (§3.3.7) we define global tangential and normal variations $\delta\mathbf{n}_h$ and $\delta\mathbf{T}_h$ using the identities

$$\left(\delta\mathbf{X}_h^T, \delta\mathbf{x}_h^T\right) = \delta\mathbf{n}_h^T\mathbb{N}_h^* + \delta\mathbf{T}_h^T\mathbb{T}_h^*$$

The combined horizontal and vertical variations become therefore

$$\begin{aligned}
\langle\delta S_h, \delta\mathbf{X}_h\rangle + \langle\delta S, \delta\mathbf{x}_h\rangle &= \int_{t_0}^{t_f}\left(\delta\mathbf{X}_h^T, \delta\mathbf{x}_h^T\right)\begin{pmatrix}\mathcal{F}_{\mathbf{X}}(\mathbf{X}_h,\mathbf{x}_h,\mathbf{V}_h)\\ \mathcal{F}_{\mathbf{x}}(\mathbf{X}_h,\mathbf{x}_h,\mathbf{V}_h)\end{pmatrix}dt = \\
&= \int_{t_0}^{t_f}\left(\delta\mathbf{n}_h^T\mathbb{N}_h^* + \delta\mathbf{T}_h^T\mathbb{T}_h^*\right)\begin{pmatrix}\mathcal{F}_{\mathbf{X}}(\mathbf{X}_h,\mathbf{x}_h,\mathbf{V}_h)\\ \mathcal{F}_{\mathbf{x}}(\mathbf{X}_h,\mathbf{x}_h,\mathbf{V}_h)\end{pmatrix}dt = \\
&= \langle\delta S_h, \delta\mathbf{T}_h\rangle + \langle\delta S, \delta\mathbf{n}_h\rangle
\end{aligned}$$

with corresponding tangential and normal semidiscrete Euler-Lagrange equations given by

$$\begin{aligned}
\mathcal{F}_{\mathbf{n}}(\mathbf{X}_h,\mathbf{x}_h,\mathbf{V}_h) &= \mathbb{N}_h^*\begin{pmatrix}\mathcal{F}_{\mathbf{X}}(\mathbf{X}_h,\mathbf{x}_h,\mathbf{V}_h)\\ \mathcal{F}_{\mathbf{x}}(\mathbf{X}_h,\mathbf{x}_h,\mathbf{V}_h)\end{pmatrix} = 0\\
\mathcal{F}_{\mathbf{T}}(\mathbf{X}_h,\mathbf{x}_h,\mathbf{V}_h) &= \mathbb{T}_h^*\begin{pmatrix}\mathcal{F}_{\mathbf{X}}(\mathbf{X}_h,\mathbf{x}_h,\mathbf{V}_h)\\ \mathcal{F}_{\mathbf{x}}(\mathbf{X}_h,\mathbf{x}_h,\mathbf{V}_h)\end{pmatrix} = 0
\end{aligned}$$

Using the definitions of the differential operators $\mathcal{F}_{\mathbf{X}}(\mathbf{X}_h,\mathbf{x}_h,\mathbf{V}_h)$ and $\mathcal{F}_{\mathbf{x}}(\mathbf{X}_h,\mathbf{x}_h,\mathbf{V}_h)$ the previous evaluates to

$$\begin{aligned}
\mathcal{F}_{\mathbf{n}}(\mathbf{X}_h,\mathbf{x}_h,\mathbf{V}_h) &= \mathbb{N}_h^*\frac{d}{dt}\{\mathbb{N}_h\mathbf{m}_h\mathbf{V}_h\} - \mathbb{N}_h^*\begin{pmatrix}\mathbf{E}_h\\ \mathbf{e}_h\end{pmatrix} - \mathbb{N}_h^*\begin{pmatrix}\mathbf{F}_h\\ \mathbf{f}_h\end{pmatrix} = \\
&= \left(\mathbb{N}_h^*\cdot\mathbb{N}_h\right)\mathbf{m}_h\dot{\mathbf{V}}_h + \mathbb{N}_h^*\begin{pmatrix}\boldsymbol{\mu}_h^T\mathbf{m}_h^{-1}\mathbf{M}_h\\ \boldsymbol{\mu}_h\end{pmatrix}\dot{\mathbf{X}}_h - \mathbb{N}_h^*\begin{pmatrix}\mathbf{F}_h\\ \mathbf{f}_h\end{pmatrix} = \mathbf{0}
\end{aligned}$$

$$\begin{aligned}
\mathcal{F}_{\mathbf{T}}(\mathbf{X}_h,\mathbf{x}_h,\mathbf{V}_h) &= \mathbb{T}_h^*\frac{d}{dt}\{\mathbb{N}_h\mathbf{m}_h\mathbf{V}_h\} - \mathbb{T}_h^*\begin{pmatrix}\mathbf{E}_h\\ \mathbf{e}_h\end{pmatrix} - \mathbb{T}_h^*\begin{pmatrix}\mathbf{F}_h\\ \mathbf{f}_h\end{pmatrix} = \\
&= \left(\mathbb{T}_h^*\cdot\mathbb{N}_h\right)\mathbf{m}_h\dot{\mathbf{V}}_h + \mathbb{T}_h^*\begin{pmatrix}\boldsymbol{\mu}_h^T\mathbf{m}_h^{-1}\mathbf{M}_h\\ \boldsymbol{\mu}_h\end{pmatrix}\dot{\mathbf{X}}_h - \mathbb{T}_h^*\begin{pmatrix}\mathbf{F}_h\\ \mathbf{f}_h\end{pmatrix} = \\
&= \left(\boldsymbol{\mu}_h^T\mathbf{m}_h^{-1}\mathbf{M}_h - \mathbf{M}_h^T\mathbf{m}_h^{-T}\boldsymbol{\mu}_h\right)\dot{\mathbf{X}}_h - \left(\mathbf{F}_h - \mathbf{M}_h^T\mathbf{m}_h^{-T}\mathbf{f}_h\right) = \mathbf{0}
\end{aligned}$$

We thus arrive at the following important conclusion: as was anticipated, the tangential evolution equations for the dynamical system under consideration are not trivially satisfied. But there is more: This equation *is only first-order in time*; that is to say, it involves only first-order derivatives of the unknown variables $(\mathbf{X}_h, \mathbf{x}_h)$. This is a consequence of the fact that the second-order derivatives enter the equations multiplied by the normal $\mathbb{N}_h$. Therefore, when projecting the equations into the tangential direction, the factor that multiplies the second-order derivatives vanishes. Furthermore, if the matrix $\left(\boldsymbol{\mu}_h^T \mathbf{m}_h^{-1} \mathbf{M}_h\right)$ is symmetric, as happens for example if we use mass lumping, then *also the first-order derivative term vanishes* from the tangential equation and this equation becomes an *algebraic constraint. The dynamical system becomes therefore constrained to evolve within a manifold in the configuration bundle.* This manifold will be given by the global equations

$$\mathbb{T}_h^* \begin{pmatrix} \mathbf{F}_h \\ \mathbf{f}_h \end{pmatrix} = \mathbf{F}_h \left(\mathbf{X}_h, \mathbf{x}_h\right) - \mathbf{M}_h^T \left(\mathbf{X}_h, \mathbf{x}_h\right) \mathbf{m}_h^{-T} \left(\mathbf{X}_h\right) \mathbf{f}_h \left(\mathbf{X}_h, \mathbf{x}_h\right) = \mathbf{0}$$

or more compactly as

$$\mathbb{T}_h^* \cdot \mathbb{F}_h = 0$$

where

$$\mathbb{F}_h = \begin{pmatrix} \mathbf{F}_h \\ \mathbf{f}_h \end{pmatrix}$$

is a global extended vector that combines the static nodal configurational and mechanical forces.

6.1.6 Semidiscrete Euler-Lagrange equations in *Space-Space*

The Euler-Lagrange equations (6.36) and (6.37) (or their equivalents (6.46) and (6.47)) are, respectively, the vertical and horizontal projections of a balance equation for the evolution of the generalized dynamical variable $\mathbf{q}_h = (\mathbf{X}_h, \mathbf{x}_h)$. Being horizontal and vertical components of a higher dimensional combined space (the configuration bundle $\mathbb{R}^{dN} \times \mathbb{R}^{dN}$), it becomes useful (as was done in the continuous setting, see §3.3.8) to restate them as a *joint* system of equations in this combined space, rather than two separate equations in $\mathbb{R}^{dN}$. We will write the joint system for the two alternative expressions, the expression involving time derivatives of the mass matrices (equations (6.36), (6.37), and (6.38)), and the expression involving only the time derivative of the velocity vector $\dot{\mathbf{V}}_h$ and the mass matrix based on velocity gradients $\boldsymbol{\mu}_h$ ((6.46), (6.47), (6.48))

6.1.6.1 Equations in space-space, first form.

Combining horizontal and vertical variations (6.29) and (6.30) we find

$$\begin{aligned}
\langle \delta S_h, \delta X^e_{aI}\rangle + \langle \delta S_h, \delta x^e_{ai}\rangle &= \int_{t_0}^{t_f} \left(\sum_e \left(\delta X^e_{aI}, \delta x^e_{ai}\right) \left(\begin{pmatrix} F^e_{aI} \\ f^e_{ai} \end{pmatrix} + \begin{pmatrix} E^e_{aI} \\ e^e_{ai} \end{pmatrix} \right) \right. \\
&\quad \left. + V^e_{ai} \left(M^e_{aibJ}, m^e_{aibj}\right) \begin{pmatrix} \delta \dot{X}^e_{bJ} \\ \delta \dot{x}^e_{bj} \end{pmatrix} \right) dt \\
\langle \delta S_h, \delta V^e_{ai}\rangle &= \int_{t_0}^{t_f} \sum_e \delta V^e_{ai} \left(\left(M^e_{aibJ}, m^e_{aibj}\right) \begin{pmatrix} \dot{X}^e_{bJ} \\ \dot{x}^e_{bj} \end{pmatrix} - m^e_{aibj} V^e_{bj} \right) dt
\end{aligned}$$

that evaluates to the global form

$$\begin{aligned}
\langle \delta S_h, \delta \mathbf{X}_h\rangle + \langle \delta S, \delta \mathbf{x}_h\rangle &= \int_{t_0}^{t_f} \left(\left(\delta \mathbf{X}^T_h, \boldsymbol{\delta} \mathbf{x}^T_h\right) \left(\begin{pmatrix} \mathbf{E}_h \\ \mathbf{e}_h \end{pmatrix} + \begin{pmatrix} \mathbf{F}_h \\ \mathbf{f}_h \end{pmatrix} \right) \right. \\
&\quad \left. + \mathbf{V}^T_h \left(\mathbf{M}_h, \mathbf{m}_h\right) \begin{pmatrix} \delta \dot{\mathbf{X}}_h \\ \boldsymbol{\delta} \dot{\mathbf{x}}_h \end{pmatrix} \right) dt \\
\langle \delta S_h, \delta \mathbf{V}_h\rangle &= \int_{t_0}^{t_f} \delta \mathbf{V}_h \left(\left(\mathbf{M}_h, \mathbf{m}_h\right) \begin{pmatrix} \dot{\mathbf{X}}_h \\ \dot{\mathbf{x}}_h \end{pmatrix} - \mathbf{m}_h \mathbf{V}_h \right)
\end{aligned}$$

The corresponding Euler-Lagrange equations become

$$\begin{aligned}
\sum_e \left(\frac{d}{dt} \left\{ V_{bj} \begin{pmatrix} M^e_{bjaI} \\ m^e_{bjai} \end{pmatrix} \right\} - \begin{pmatrix} E^e_{aI} \\ e^e_{ai} \end{pmatrix} + \begin{pmatrix} F^e_{aI} \\ F^e_{ai} \end{pmatrix} \right) &= \begin{pmatrix} 0 \\ 0 \end{pmatrix} \\
\sum_e \left(\left(M^e_{aibJ}, m^e_{aibj}\right) \begin{pmatrix} \dot{X}^e_{bJ} \\ \dot{x}^e_{bj} \end{pmatrix} - m^e_{aibj} V^e_{bj} \right) &= 0
\end{aligned}$$

that assembled into global array take the global form

$$\frac{d}{dt} \left\{ \begin{pmatrix} \mathbf{M}^T_h \\ \mathbf{m}^T_h \end{pmatrix} \mathbf{V}_h \right\} = \begin{pmatrix} \mathbf{E}_h \\ \mathbf{e}_h \end{pmatrix} + \begin{pmatrix} \mathbf{F}_h \\ \mathbf{f}_h \end{pmatrix} \tag{6.53}$$

$$\left(\mathbf{M}_h, \mathbf{m}_h\right) \begin{pmatrix} \dot{\mathbf{X}}_h \\ \dot{\mathbf{x}}_h \end{pmatrix} = \mathbf{m}_h \mathbf{V}_h \tag{6.54}$$

Using the definition for the global normal $\mathbb{N}_h$ and conormal $\mathbb{N}_h^*$ (equations (6.49) and (6.50)) the previous might be compactly written as

$$\begin{aligned}\frac{d}{dt}\{\mathbb{N}_h\mathbf{m}_h\mathbf{V}_h\} &= \mathbb{E}_h + \mathbb{F}_h \\ \mathbb{N}_h^*\dot{\mathbf{q}}_h &= \mathbf{V}_h\end{aligned}$$

where $\mathbf{q}_h$ is the combined horizontal/vertical nodal coordinate array

$$\mathbf{q}_h = \begin{pmatrix}\mathbf{X}_h \\ \mathbf{x}_h\end{pmatrix}$$

$\mathbb{E}_h$ and $\mathbb{F}_h$ are the extended dynamic and static forces given by

$$\mathbb{E}_h = \begin{pmatrix}\mathbf{E}_h \\ \mathbf{e}_h\end{pmatrix} \tag{6.55}$$

$$\mathbb{F}_h = \begin{pmatrix}\mathbf{F}_h \\ \mathbf{f}_h\end{pmatrix} \tag{6.56}$$

Combining both, these equations can be rewritten finally in the equivalent form

$$\frac{d}{dt}\left\{\mathbb{M}_h\begin{pmatrix}\dot{\mathbf{X}}_h \\ \dot{\mathbf{x}}_h\end{pmatrix}\right\} = \mathbb{E}_h + \mathbb{F}_h$$

where

$$\begin{aligned}\mathbb{M}_h &= \mathbb{N}_h\mathbf{m}_h\mathbb{N}_h^* = \\ &= \begin{pmatrix}\mathbf{M}_h^T \\ \mathbf{m}_h^T\end{pmatrix}\mathbf{m}_h^{-1}(\mathbf{M}_h, \mathbf{m}_h) = \\ &= \begin{pmatrix}\mathbf{M}_h^T\mathbf{m}_h^{-1}\mathbf{M}_h & \mathbf{M}_h^T \\ \mathbf{M}_h & \mathbf{m}_h^T\end{pmatrix}\end{aligned} \tag{6.57}$$

is the global semidiscrete extended mass matrix, the semidiscrete global analog to the continuous extended mass matrix (3.56).

6.1.6.2 Equations in space-space, second form.

Alternatively, combining horizontal and vertical variations written in the form (6.43) and (6.44) we find

$$
\begin{aligned}
\langle \delta S, \delta X_{bJ}^{e} \rangle + \langle \delta S, \delta x_{bj}^{e} \rangle &= \int_{t_0}^{t_f} \sum_{e} \left(\delta X_{bJ}^{e}, \delta x_{bj}^{e} \right) \left(\left(\begin{array}{c} F_{bJ}^{e} \\ f_{bj} \end{array} \right) - \dot{V}_{ai}^{e} \left(\begin{array}{c} M_{aibJ}^{e} \\ m_{aibj}^{e} \end{array} \right) \right. \\
&\quad \left. - \left(\begin{array}{c} - \left(\dot{x}_{ai}^{e} - V_{ai}^{e} \right) \mu_{aibJ}^{e} \\ \mu_{bjaI}^{e} \dot{X}_{aI} \end{array} \right) \right) dt \\
\langle \delta S_h, \delta V_{ai}^{e} \rangle &= \int_{t_0}^{t_f} \sum_{e} \delta V_{ai}^{e} \left(\left(M_{aibJ}^{e}, m_{aibj}^{e} \right) \left(\begin{array}{c} \dot{X}_{bJ}^{e} \\ \dot{x}_{bj}^{e} \end{array} \right) - m_{aibj}^{e} V_{bj}^{e} \right) dt
\end{aligned}
$$

which in global form evaluates to

$$
\begin{aligned}
\langle \delta S_h, \delta \mathbf{X}_h \rangle + \langle \delta S, \delta \mathbf{x}_h \rangle &= \int_{t_0}^{t_f} \left(\left(\delta \mathbf{X}_h^T, \boldsymbol{\delta} \mathbf{x}_h^T \right) \left(\left(\begin{array}{c} \mathbf{F}_h \\ \mathbf{f}_h \end{array} \right) - \left(\begin{array}{c} \mathbf{M}_h^T \\ \mathbf{m}_h^T \end{array} \right) \mathbf{V}_h \right) \right. \\
&\quad \left. - \left(\begin{array}{c} -\boldsymbol{\mu}_h^T \left(\dot{\mathbf{x}}_h - \mathbf{V}_h \right) \\ \boldsymbol{\mu}_h \dot{\mathbf{X}}_h \end{array} \right) \right) dt \\
\langle \delta S_h, \delta \mathbf{V}_h \rangle &= \int_{t_0}^{t_f} \delta \mathbf{V}_h \left(\left(\mathbf{M}_h, \mathbf{m}_h \right) \left(\begin{array}{c} \dot{\mathbf{X}}_h \\ \dot{\mathbf{x}}_h \end{array} \right) - \mathbf{m}_h \mathbf{V}_h \right)
\end{aligned}
$$

The corresponding local and global Euler-Lagrange equations become respectively

$$
\begin{aligned}
\sum_{e} \left(\left(\begin{array}{c} F_{bJ}^{e} \\ f_{bj} \end{array} \right) - \dot{V}_{ai}^{e} \left(\begin{array}{c} M_{aibJ}^{e} \\ m_{aibj}^{e} \end{array} \right) - \left(\begin{array}{c} - \left(\dot{x}_{ai}^{e} - V_{ai}^{e} \right) \mu_{aibJ}^{e} \\ \mu_{bjaI}^{e} \dot{X}_{aI} \end{array} \right) \right) &= \left(\begin{array}{c} 0 \\ 0 \end{array} \right) \\
\sum_{e} \left(\left(M_{aibJ}^{e}, m_{aibj}^{e} \right) \left(\begin{array}{c} \dot{X}_{bJ}^{e} \\ \dot{x}_{bj}^{e} \end{array} \right) - m_{aibj}^{e} V_{bj}^{e} \right) &= 0
\end{aligned}
$$

and

$$
\begin{aligned}
\left(\begin{array}{c} \mathbf{M}_h^T \\ \mathbf{m}_h^T \end{array} \right) \dot{\mathbf{V}}_h + \left(\begin{array}{c} -\boldsymbol{\mu}_h^T \left(\dot{\mathbf{x}}_h - \mathbf{V}_h \right) \\ \boldsymbol{\mu}_h \dot{\mathbf{X}}_h \end{array} \right) &= \left(\begin{array}{c} \mathbf{F}_h \\ \mathbf{f}_h \end{array} \right) \\
\left(\mathbf{M}_h, \mathbf{m}_h \right) \left(\begin{array}{c} \dot{\mathbf{X}}_h \\ \dot{\mathbf{x}}_h \end{array} \right) - \mathbf{m}_h \mathbf{V}_h &= \mathbf{0}
\end{aligned}
$$

Combining both, we finally obtain

$$\begin{pmatrix} \mathbf{M}_h^T \\ \mathbf{m}_h^T \end{pmatrix} \dot{\mathbf{V}}_h + \begin{pmatrix} \boldsymbol{\mu}_h^T \mathbf{m}_h^{-1} \mathbf{M}_h \\ \boldsymbol{\mu}_h \end{pmatrix} \dot{\mathbf{X}}_h = \begin{pmatrix} \mathbf{F}_h \\ \mathbf{f}_h \end{pmatrix} \tag{6.58}$$

$$(\mathbf{M}_h, \mathbf{m}_h) \begin{pmatrix} \dot{\mathbf{X}}_h \\ \dot{\mathbf{x}}_h - \mathbf{V}_h \end{pmatrix} = \mathbf{0} \tag{6.59}$$

which might be compactly written as

$$\begin{aligned} \mathbb{N}_h \left(\mathbf{m}_h \dot{\mathbf{V}}_h + \boldsymbol{\mu}_h \dot{\mathbf{X}}_h \right) + \begin{pmatrix} (\boldsymbol{\mu}_h^T \mathbf{m}_h^{-1} \mathbf{M}_h - \mathbf{M}_h^T \mathbf{m}_h^{-T} \boldsymbol{\mu}_h) \\ \mathbf{0} \end{pmatrix} \dot{\mathbf{X}}_h &= \mathbb{F}_h \\ \mathbb{N}_h^* \begin{pmatrix} \dot{\mathbf{X}}_h \\ \dot{\mathbf{x}}_h \end{pmatrix} &= \mathbf{V}_h \end{aligned}$$

with $\mathbb{N}_h$ and $\mathbb{N}_h^*$ the normal and conormal defined in (6.49) and (6.50) and $\mathbb{F}_h$ the column vector that group configurational and mechanical nodal forces defined in (6.56).

6.1.7 Comparison with the single-field Hamilton's principle formulation

As was anticipated in the introduction to this section, the use of an independent velocity interpolation (6.6) instead of the consistent velocity interpolation (6.9) is proposed as an approach to overcome severe instability issues inherent to the use of the latter. To understand the difference between both formulations, we derive in this section the Euler-Lagrange equations resulting from the use of the *standard* Lagrangian formulation (the formulation that make use of *consistent* velocities $\mathbf{V}_h \equiv \dot{\boldsymbol{\varphi}}_h$) and compare these equations with those that follow from the *mixed Lagrangian* formulation (using *independent* velocities $\mathbf{V}_h \neq \dot{\boldsymbol{\varphi}}_h$).

Inserting the deformation interpolation (6.10) with deformation gradient given by (6.10) and *consistent* interpolation for the velocities given by (6.9) in the standard (single-field) action (3.4, 3.5) the following semidiscrete action S_h and global and elemental Lagrangians L_h and L^e are obtained:

$$\begin{aligned} S_h (\mathbf{X}_h, \mathbf{x}_h) &= \int_{t_0}^{t_f} L_h \left(\mathbf{X}_h, \mathbf{x}_h, \dot{\mathbf{X}}_h, \dot{\mathbf{x}}_h \right) dt \\ L_h \left(\mathbf{X}_h, \mathbf{x}_h, \dot{\mathbf{X}}_h, \dot{\mathbf{x}}_h \right) &= \sum_e L^e \left(\mathbf{X}^e, \mathbf{x}^e, \dot{\mathbf{X}}^e, \dot{\mathbf{x}}^e \right) \\ L^e \left(\mathbf{X}^e, \mathbf{x}^e, \dot{\mathbf{X}}^e, \dot{\mathbf{x}}^e \right) &= \int_{\Omega^e} \mathcal{L} (\mathbf{X}, t, \boldsymbol{\varphi}_h, \dot{\boldsymbol{\varphi}}_h, \mathbf{F}_h) \, dV \end{aligned}$$

For a Lagrangian density of the form (3.3) the local semidiscrete standard Lagrangian becomes

$$
\begin{aligned}
L^e &= \int_{\Omega_e(t)} \left(\frac{R}{2} \left\| \dot{\boldsymbol{\varphi}}^e \right\|^2 - W\left(X_I, t, \varphi_i^e, F_{iI}^e\right) \right) dV = \\
&= \int_{\Omega_e(t)} \left(\frac{R}{2} \left(N_a^e \left(\dot{x}_{ai}^e - F_{iI}^e \dot{X}_{aI}^e \right) \right)^2 - W\left(N_a^e X_{aI}^e, t, \frac{\partial N_a^e}{\partial X_I} x_{ai}^e \right) \right) dt
\end{aligned}
$$

that can be compactly expressed as

$$
L^e = \frac{1}{2} \left(\dot{\mathbf{X}}^e, \dot{\mathbf{x}}^e \right) \mathbb{M}^e \begin{pmatrix} \dot{\mathbf{X}}^e \\ \dot{\mathbf{x}}^e \end{pmatrix} - I^e
$$

where $\mathbb{M}^e$ is a configuration-dependent mass matrix given by

$$
\begin{aligned}
\mathbb{M}_{aIibJj}^e &= \int_{\Omega_e(t)} R N_a^e N_b^e \begin{pmatrix} -F_{kI}^e \\ \delta_{ki} \end{pmatrix} \left(-F_{kJ}^e, \delta_{kj}\right) dV = \\
&= \int_{\Omega_e(t)} R N_a^e N_b^e \begin{pmatrix} F_{kI}^e F_{kJ}^e & -F_{jI}^e \\ -F_{iJ}^e & \delta_{ij} \end{pmatrix} dV
\end{aligned}
$$

Assembling the elemental contributions into global arrays we obtain the global semidiscrete Lagrangian in the form

$$
L_h\left(\mathbf{x}_h, \mathbf{X}_h, \dot{\mathbf{x}}_h, \dot{\mathbf{X}}_h\right) = \frac{1}{2} \left(\dot{\mathbf{X}}_h, \dot{\mathbf{x}}_h \right) \mathbb{M}_h \begin{pmatrix} \dot{\mathbf{X}}_h \\ \dot{\mathbf{x}}_h \end{pmatrix} - I_h
$$

where

$$
\mathbb{M}_h = \sum_e \mathbb{M}^e
$$

is the assembled global extended mass matrix. We recall that in the mixed Lagrangian formulation the mass matrix was given by

$$
\begin{aligned}
\mathbb{M}_h &= \mathbb{N}_h \mathbf{m}_h \mathbb{N}_h^* = \\
&= \left(\sum_e \int_{\Omega_e(t)} R N_a^e N_b^e \mathbb{N}^e dV \right) \left(\sum_e \int_{\Omega_e(t)} R N_a^e \mathbf{I} N_b^e dV \right)^{-1} \left(\sum_e \int_{\Omega_e(t)} R N_a^e N_b^e \mathbb{N}^{e*} dV \right)
\end{aligned}
$$

while in the standard Lagrangian formulation the mass matrix becomes

$$
\mathbb{M}_h = \sum_e \int_{\Omega_e(t)} \left(R N_a N_b \mathbb{N}^e \mathbb{N}^{e*} \right) dV
$$

Therefore, while in the mixed formulation the extended mass matrix is computed by multiplying the global average of local normals, in the standard Lagrangian formulation the mass matrix is built by averaging the product of local normals. As will be illustrated in the example of the next section, this is indeed an essential difference. In the following table we summarize the main differences between both formulations.

	Standard Formulation	Mixed Formulation
Lagrangian density	$\mathcal{L} = R\frac{\mathbf{V}}{2}^2 - W(\mathbf{X},\boldsymbol{\varphi},\mathbf{F})$	$\mathcal{L}^{mix} = R\frac{\mathbf{V}}{2}^2 - W(\mathbf{X},\boldsymbol{\varphi},\mathbf{F}) + {} + R\mathbf{V}(\dot{\boldsymbol{\varphi}} - \mathbf{V})$
Indep. Variables	$\boldsymbol{\varphi}$	$(\boldsymbol{\varphi}, \mathbf{V})$
Interpolation	$\boldsymbol{\varphi}_h = \sum_a N_a \mathbf{x}_a$ $\dot{\boldsymbol{\varphi}}_h = \sum_a N_a \left(\dot{\mathbf{x}}_a - \mathbf{F}_h \dot{\mathbf{X}}_a\right)$ $\mathbf{F}_h = \sum_a \frac{\partial N_a}{\partial X}\mathbf{x}_a$ $\mathbf{X}_h = \sum_a N_a \mathbf{X}_a$	$\boldsymbol{\varphi}_h =$ same $\mathbf{V}_h = \sum_a N_a V_a$ $\dot{\boldsymbol{\varphi}}_h =$ same $\mathbf{F}_h =$ same $\mathbf{X}_h =$ same
Elemental semidiscr. Lagrangian	$L^e = \frac{1}{2}\left(\dot{\mathbf{X}}^e, \dot{\mathbf{x}}^e\right)\mathbb{M}^e \begin{pmatrix} \dot{\mathbf{X}}^e \\ \dot{\mathbf{x}}^e \end{pmatrix} - I^e$	$L^{mix-e} = \frac{1}{2}\mathbf{V}^{eT}\mathbf{m}^e\mathbf{V}^e - I^e + {} + \mathbf{V}^{eT}\left(\mathbf{m}^e\dot{\mathbf{x}}^e + \mathbf{M}^e\dot{\mathbf{X}}^e - \mathbf{m}^e\mathbf{V}^e\right)$
Elemental mass matrix	$\mathbb{M}^e_{ab} = \int_{\Omega_e} R N^e_a N^e_b \begin{pmatrix} -\mathbf{F}^{eT} \\ \mathbf{i} \end{pmatrix} (-\mathbf{F}^e, \mathbf{i})$	$\begin{pmatrix} \mathbf{M}^{eT}_{ab} \\ \mathbf{m}^{eT}_{ab} \end{pmatrix} = \int_{\Omega_e} R N^e_a N^e_b \begin{pmatrix} -\mathbf{F}^{eT} \\ \mathbf{i} \end{pmatrix}$
Global semidisc. Lagrangian	$L_h = \frac{1}{2}\left(\dot{\mathbf{X}}_h, \dot{\mathbf{x}}_h\right)\mathbb{M}_h \begin{pmatrix} \dot{\mathbf{X}}_h \\ \dot{\mathbf{x}}_h \end{pmatrix} - I_h$	$L^{mix}_h = \frac{1}{2}\mathbf{V}^T_h\mathbf{m}_h\mathbf{V}_h - I_h + \mathbf{V}^T_h\left(\mathbf{m}_h\dot{\mathbf{x}}_h + \mathbf{M}_h\dot{\mathbf{X}}_h - \mathbf{m}_h\mathbf{V}_h\right)$
Global extended mass matrix	$\mathbb{M}_h = \sum_e \mathbb{M}^e$	$\begin{pmatrix} \mathbf{M}^T_h \\ \mathbf{m}^T_h \end{pmatrix} = \sum_e \begin{pmatrix} \mathbf{M}^{eT} \\ \mathbf{m}^{eT} \end{pmatrix}$ $\mathbb{N}_h = \begin{pmatrix} \mathbf{M}^T_h \\ \mathbf{m}^T_h \end{pmatrix} \mathbf{m}^{-T}_h$ $\mathbb{N}^*_h = \mathbf{m}^{-1}_h(\mathbf{M}_h, \mathbf{m}_h)$ $\mathbb{M}_h = \mathbb{N}_h\mathbf{m}_h\mathbb{N}^*_h$
Euler-Lagr. equations	$\frac{d}{dt}(\mathbb{M}_h\dot{\mathbf{q}}_h) = \mathbb{E}_h + \mathbb{F}_h$	$\frac{d}{dt}(\mathbb{N}_h\mathbf{m}_h\mathbf{V}_h) = \mathbb{E}_h + \mathbb{F}_h$ $\mathbb{N}^*_h\dot{\mathbf{q}}_h = \mathbf{V}_h$
Generalized coordinate array	$\mathbf{q}_h = \begin{pmatrix} \mathbf{X}_h \\ \mathbf{x}_h \end{pmatrix}$ $\dot{\mathbf{q}}_h = \begin{pmatrix} \dot{\mathbf{X}}_h \\ \dot{\mathbf{x}}_h \end{pmatrix}$	$\mathbf{q}_h =$ same $\dot{\mathbf{q}}_h =$ same
Forces	$\mathbb{F}_h = \begin{pmatrix} \mathbf{F}_h \\ \mathbf{f}_h \end{pmatrix} = \begin{pmatrix} \frac{\partial}{\partial \mathbf{X}_h} \\ \frac{\partial}{\partial \mathbf{x}_h} \end{pmatrix} I_h$ $\mathbb{E}_h = \begin{pmatrix} \mathbf{E}_h \\ \mathbf{e}_h \end{pmatrix} = \begin{pmatrix} \frac{\partial}{\partial \mathbf{X}_h} \\ \frac{\partial}{\partial \mathbf{x}_h} \end{pmatrix} K_h$ $L_h = K_h - I_h$	$\mathbb{F}_h =$ same $\mathbb{E}_h = \begin{pmatrix} \mathbf{E}_h \\ \mathbf{e}_h \end{pmatrix} = \begin{pmatrix} \frac{\partial}{\partial \mathbf{X}_h} \\ \frac{\partial}{\partial \mathbf{x}_h} \end{pmatrix} K^{mix}_h$ $L^{mix}_h = K^{mix}_h - I_h$

6.1.8 Example: Oscillation of a one-dimensional bar, non-linear material

As an illustrative example we consider a one-dimensional body $B = [0, L]$ fixed on both sides and free of body forces. The body is set to oscillate by applying an initial deformation and releasing it from rest. For simplicity we assume that the body is made of a homogeneous hyperelastic material with total energy density $W(F)$ and that the mass density R is constant.

We will establish the Euler-Lagrange equations for this particular example using the two formulations just outlined: namely, the mixed (two-field) Lagrangian formulation with velocities interpolated independently, and the standard (single-field) Lagrangian formulation with consistent velocity interpolation.

In both cases we discretize the body into two finite elements with nodal coordinates of the mid node in both the reference and deformed configuration taken as unknowns:

$$\begin{aligned} x_1 &= x_1(t) \\ X_1 &= X_1(t) \end{aligned}$$

Interpolating deformations and velocities with linear elements we obtain

$$\begin{aligned} \varphi_h(X,t) &= \begin{cases} \frac{X}{X_1(t)} x_1(t) & \text{if } 0 < X < X_1(t) \\ \frac{L-X}{L-X_1(t)} x_1(t) + \frac{X-X_1(t)}{L-X_1(t)} L & \text{if } X_1(t) < X < L \end{cases} \\ V_h(X,t) &= \begin{cases} \frac{X}{X_1(t)} V_1(t) & \text{if } 0 < X < X_1(t) \\ \frac{L-X}{L-X_1(t)} V_1(t) & \text{if } X_1(t) < X < L \end{cases} \end{aligned}$$

where $V_1(t)$ is the coefficient for the interpolation of the velocity also taken as unknown in the mixed Lagrangian formulation. Differentiating with respect to time the deformation mapping $\varphi_h(X,t)$ at constant X, we find

$$\dot{\varphi}_h(X,t) = \begin{cases} \frac{X}{X_1(t)} \left[\dot{x}_1(t) - \left(\frac{x_1(t)}{X_1(t)} \right) \dot{X}_1(t) \right] & \text{if } 0 < X < X_1(t) \\ \frac{L-X}{L-X_1(t)} \left[\dot{x}_1(t) - \left(\frac{L-x_1(t)}{L-X_1(t)} \right) \dot{X}_1(t) \right] & \text{if } X_1(t) < X < L \end{cases}$$

Differentiating next with respect to space X at constant time t we obtain

$$F_h(X,t) = \begin{cases} \frac{x_1(t)}{X_1(t)} & \text{if } 0 < X < X_1(t) \\ \frac{L-x_1(t)}{L-X_1(t)} & \text{if } X_1(t) < X < L \end{cases}$$

6.1.8.1 Mixed Lagrangian formulation

The semidiscrete-mixed action functional and mixed Lagrangian becomes in this case

$$\begin{aligned} S_h\left(X_1\left(t\right), x_1\left(t\right), V_1\left(t\right)\right) &= \int_{t_0}^{t_f} L_h^{mix}\left(x_1\left(t\right), X_1\left(t\right), \dot{x}_1\left(t\right), \dot{X}_1\left(t\right), V_1\left(t\right)\right) dt \\ L_h^{mix}\left(x_1, X_1, \dot{x}_1, \dot{X}_1, V_1\right) &= \int_0^L \left(\frac{1}{2} R V_h^2 - W\left(F_h\right) + R V_h\left(\dot{\varphi}_h - V_h\right)\right) dX = \end{aligned}$$

that making use of the given interpolation and integrating evaluates to

$$L_h^{mix} = \frac{RL}{6} V_1^2 - \left(X_1 W\left(\frac{x_1}{X_1}\right) + \left(L - X_1\right) W\left(\frac{L - x_1}{L - X_1}\right)\right) + \frac{RL}{3} V_1\left(\dot{x}_1 - \dot{X}_1 - V_1\right)$$

Taking variations we obtain

$$\begin{aligned} \left\langle \delta S_h, \delta X_1 \right\rangle &= \int_{t_0}^{t_f} \left(\left(-\frac{RL}{3} V_1\right) \delta \dot{X}_1 - \left(C\left(\frac{x_1}{X_1}\right) - C\left(\frac{L - x_1}{L - x_1}\right)\right) \delta X_1\right) dt \\ \left\langle \delta S_h, \delta x_1 \right\rangle &= \int_{t_0}^{t_f} \left(\left(\frac{RL}{3} V_1\right) \delta \dot{X}_1 - \left(P\left(\frac{x_1}{X_1}\right) - P\left(\frac{L - x_1}{L - x_1}\right)\right) \delta x_1\right) dt \\ \left\langle \delta S_h, \delta V_1 \right\rangle &= \int_{t_0}^{t_f} \left(\frac{RL}{3} \delta V_1\left(\dot{x}_1 - \dot{X}_1 - V_1\right)\right) dt \end{aligned}$$

where

$$\begin{aligned} P\left(F\right) &= \frac{\partial W}{\partial F}\left(F\right) \\ C\left(F\right) &= W\left(F\right) - F \frac{\partial W}{\partial F}\left(F\right) \end{aligned}$$

are, respectively, the first Piolla-Kirchhoff and static Eshelby stress tensors. The corresponding horizontal-vertical Euler-Lagrange equations are

$$\begin{aligned} \frac{RL}{3} \dot{V}_1 &= P\left(\frac{L - x_1}{L - x_1}\right) - P\left(\frac{x_1}{X_1}\right) \\ -\frac{RL}{3} \dot{V}_1 &= C\left(\frac{L - x_1}{L - x_1}\right) - C\left(\frac{x_1}{X_1}\right) \\ V_1 &= \dot{x}_1 - \dot{X}_1 \end{aligned}$$

that can written in matrix form as

$$\begin{aligned} \frac{RL}{3} \begin{pmatrix} -1 \\ 1 \end{pmatrix} \dot{V}_1 &= \begin{pmatrix} C\left(\frac{L - x_1}{L - x_1}\right) - C\left(\frac{x_1}{X_1}\right) \\ P\left(\frac{L - x_1}{L - x_1}\right) - P\left(\frac{x_1}{X_1}\right) \end{pmatrix} \\ V_1 &= \left(-1, 1\right) \begin{pmatrix} \dot{X}_1 \\ \dot{x}_1 \end{pmatrix} \end{aligned}$$

or combining both as

$$\mathbb{M}\begin{pmatrix}\ddot{X}_1\\ \ddot{x}_1\end{pmatrix}=\begin{pmatrix}[C]\\ [P]\end{pmatrix} \tag{6.60}$$

where

$$\begin{aligned}\mathbb{M} &= \begin{pmatrix}-1\\ 1\end{pmatrix}\frac{RL}{3}(-1,1)=\\ &= \frac{RL}{3}\begin{pmatrix}1 & -1\\ -1 & 1\end{pmatrix}\end{aligned}$$

is the extended mass matrix and

$$\begin{pmatrix}[C]\\ [P]\end{pmatrix}=\begin{pmatrix}C\left(\frac{L-x_1}{L-x_1}\right)-C\left(\frac{x_1}{X_1}\right)\\ P\left(\frac{L-x_1}{L-x_1}\right)-P\left(\frac{x_1}{X_1}\right)\end{pmatrix}$$

are the jumps of the Eshelby static and Piolla-kirchhoff stress tensor across the boundary between the two elements. Notice that in this example the extended mass matrix is independent of the configuration (X_1, x_1). In general this is not the case.

The normal and tangential vectors and covectors evaluate in this case simply to

$$\begin{aligned}\mathbb{N} &= \begin{pmatrix}-1\\ 1\end{pmatrix}\\ \mathbb{N}^* &= (-1,1)\\ \mathbb{T} &= \begin{pmatrix}1\\ 1\end{pmatrix}\\ \mathbb{T}^* &= (1,1)\end{aligned}$$

that correspond to a weighted average of the normals and tangents to the graph of φ_h on each element. Tangential and normal Euler-Lagrange equations become therefore

$$\begin{aligned}(-1,1)\left(\frac{RL}{3}\begin{pmatrix}-1\\ 1\end{pmatrix}\dot{V}_1-\begin{pmatrix}[C]\\ [P]\end{pmatrix}\right) &= 0\\ (1,1)\left(\frac{RL}{3}\begin{pmatrix}-1\\ 1\end{pmatrix}\dot{V}_1-\begin{pmatrix}[C]\\ [P]\end{pmatrix}\right) &= 0\end{aligned}$$

that evaluates to

$$\begin{aligned}\frac{2RL}{3}\dot{V}_1 + [C] - [P] &= 0\\ [C] + [P] &= 0\end{aligned}$$

The tangential equation results therefore an algebraic equation and represents a constraint manifold for the evolution of the dynamical variable (X_1, x_1). The constraint equation is thus

$$C\left(\frac{L-x_1}{L-x_1}\right) - C\left(\frac{x_1}{X_1}\right) + P\left(\frac{L-x_1}{L-x_1}\right) - P\left(\frac{x_1}{X_1}\right) = 0$$

Figure (6.7(a)) shows this constraint manifold for the particular case of an incompressible Neo-hookean material, characterized by a strain energy density of the form

$$W(F) = \frac{\mu}{2}\left(F^2 + \frac{2}{F} - 3\right)$$

along with the solution of the above system at different times.

6.1.8.2 Standard Lagrangian formulation

If on the other hand the standard (single-field) Lagrangian formulation is adopted and the velocity is interpolated using $\dot{\varphi}_h$ instead of the independent interpolation $\mathbf{V}_h$ we obtain

$$\begin{aligned}S_h(X_1(t), x_1(t)) &= \int_{t_0}^{t_f} L_h\left(x_1(t), X_1(t), \dot{x}_1(t), \dot{X}_1(t)\right) dt\\ L_h\left(x_1, X_1, \dot{x}_1, \dot{X}_1\right) &= \int_0^L \left(\frac{1}{2}R\dot{\varphi}_h^2 - W(F_h)\right) dX =\end{aligned}$$

that making use of the given interpolation and integrating evaluates to

$$\begin{aligned}L_h\left(x_1, X_1, \dot{x}_1, \dot{X}_1\right) &= \frac{1}{6}R\left(\dot{x}_1 - \frac{x_1}{X_1}\dot{X}_1\right)^2 X_1 + \frac{1}{6}R\left(\dot{x}_1 - \frac{L-x_1}{L-X_1}\dot{X}_1\right)^2 (L-X_1)\\ &\quad - \left(X_1 W\left(\frac{x_1}{X_1}\right) + (L-X_1) W\left(\frac{L-x_1}{L-X_1}\right)\right)\end{aligned}$$

Expanding the square velocity terms, the previous can be written as

$$\begin{aligned}L_h\left(x_1, X_1, \dot{x}_1, \dot{X}_1\right) &= \frac{R}{6}\begin{pmatrix}\dot{X}_1 & \dot{x}_1\end{pmatrix}\begin{pmatrix}\frac{x_1^2}{X_1} + \frac{(L-x_1)^2}{(L-X_1)} & -L\\ -L & L\end{pmatrix}\begin{pmatrix}\dot{X}_1\\ \dot{x}_1\end{pmatrix}\\ &\quad - \left(X_1 W\left(\frac{x_1}{X_1}\right) + (L-X_1) W\left(\frac{L-x_1}{L-X_1}\right)\right)\end{aligned}$$

The variations are

$$\begin{aligned}
\langle \delta S_h, \delta X_1\rangle + \langle \delta S_h, \delta x_1\rangle &= \int_{t_0}^{t_f} \frac{R}{3} \begin{pmatrix} \delta \dot{X}_1 & \delta \dot{x}_1 \end{pmatrix} \begin{pmatrix} \frac{x_1^2}{X_1} + \frac{(L-x_1)^2}{(L-X_1)} & -L \\ -L & L \end{pmatrix} \begin{pmatrix} \dot{X}_1 \\ \dot{x}_1 \end{pmatrix} + \\
&+ \frac{R}{6} \begin{pmatrix} \delta X_1 & \delta x_1 \end{pmatrix} \begin{pmatrix} \left(-\frac{x_1^2}{X_1^2} + \frac{(L-x_1)^2}{(L-X_1)^2}\right) \\ 2\left(\frac{x_1}{X_1} - \frac{L-x_1}{L-X_1}\right) \end{pmatrix} \dot{X}_1^2 + \\
&- \begin{pmatrix} \delta X_1 & \delta x_1 \end{pmatrix} \begin{pmatrix} C\left(\frac{x_1}{X_1}\right) - C\left(\frac{L-x_1}{L-x_1}\right) \\ P\left(\frac{x_1}{X_1}\right) - P\left(\frac{L-x_1}{L-x_1}\right) \end{pmatrix} dt
\end{aligned}$$

and the corresponding Euler-Lagrange equations evaluates to

$$\frac{d}{dt}\left\{\mathbb{M}\begin{pmatrix} \dot{X}_1 \\ \dot{x}_1 \end{pmatrix}\right\} + \frac{R}{6}\begin{pmatrix} -\frac{x_1^2}{X_1^2} + \frac{(L-x_1)^2}{(L-X_1)^2} \\ 2\left(\frac{x_1}{X_1} - \frac{L-x_1}{L-X_1}\right) \end{pmatrix} \dot{X}_1^2 = \begin{pmatrix} [C] \\ [P] \end{pmatrix} \tag{6.61}$$

where

$$\begin{aligned}
\mathbb{M} &= \frac{R}{3}\begin{pmatrix} \frac{x_1^2}{X_1} + \frac{(L-x_1)^2}{L-X_1} & -L \\ -L & L \end{pmatrix} = \\
&= \frac{RL}{3}\begin{pmatrix} 1 + \left(\frac{L}{X_1} + \frac{L}{L-X_1}\right)\left(\frac{x_1 - X_1}{L}\right)^2 & -1 \\ -1 & 1 \end{pmatrix}
\end{aligned}$$

is the extended mass matrix. Notice that when $x_1 = X_1$ the mass matrix becomes identical to the mass matrix obtained with the mixed Lagrangian formulation. The tangential and normal Euler-Lagrange equations become in this case

$$\begin{aligned}
0 &= \frac{d}{dt}\left\{\frac{R}{3}\left(-\frac{x_1^2}{X_1} - \frac{(L-x_1)^2}{(L-X_1)} - L\right)\dot{X}_1 + 2L\dot{x}_1\right\} + \\
&+ \frac{R}{6}\left(2\left(\frac{x_1}{X_1} - \frac{L-x_1}{L-X_1}\right) + \frac{x_1^2}{X_1^2} - \frac{(L-x_1)^2}{(L-X_1)^2}\right)\dot{X}_1^2 + [C] - [P] \\
0 &= \frac{d}{dt}\left\{\frac{R}{3}\left(\frac{x_1^2}{X_1} + \frac{(L-x_1)^2}{(L-X_1)} - L\right)\dot{X}_1\right\} + \\
&\frac{R}{6}\left(2\left(\frac{x_1}{X_1} - \frac{L-x_1}{L-X_1}\right) - \frac{x_1^2}{X_1^2} + \frac{(L-x_1)^2}{(L-X_1)^2}\right)\dot{X}_1^2 - [C] - [P]
\end{aligned}$$

Figure (6.7(b)) shows the solution of the above system for an incompressible Neohookean material. Figure (6.8) shows the phase space for the horizontal motion (X_1, P_1) where

$$P_1 = \frac{\partial L_h^{mix}}{\partial \dot{X}_1} = -\frac{RL}{3}V_1 = \frac{RL}{3}\left(\dot{X}_1 - \dot{x}_1\right)$$

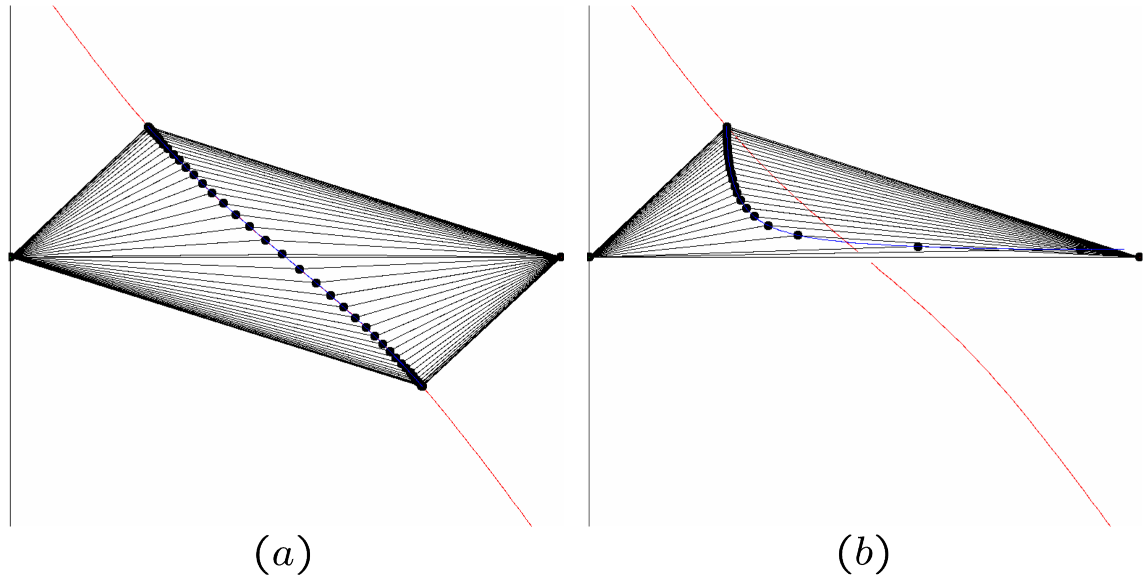

Figure 6.7: Oscillation of a 1D bar discretized with two 1D linear elements. Displacements as a function of position for different times $u(X,t)$. (a) Mixed Lagrangian formulation. (b) Standard Lagrangian formulation

in the case of the mixed Lagrangian formulation and

$$P_1 = \frac{\partial L_h}{\partial \dot{X}_1} = \frac{RL}{3}\left(\dot{X}_1 - \dot{x}_1\right) + \frac{R}{3}\left(\frac{1}{X_1} + \frac{1}{L - X_1}\right)(x_1 - X_1)\,\dot{X}_1$$

in the case of the standard Lagrangian formulation.

6.1.8.3 Comparison between both formulations

Comparing the extended mass matrices of both formulations we find that for the mixed Lagrangian formulation we obtained

$$\mathbb{M}^{mix} = \frac{RL}{3}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$$

whereas for the standard Lagrangian formulation we found

$$\mathbb{M}^{std} = \frac{RL}{3}\begin{pmatrix} 1 + \left(\frac{L}{X_1} + \frac{L}{L-X_1}\right)\left(\frac{x_1 - X_1}{L}\right)^2 & -1 \\ -1 & 1 \end{pmatrix}$$

Subtracting both expressions yields

$$\mathbb{M}^{std} = \mathbb{M}^{mix} + \frac{RL}{3}\begin{pmatrix} \left(\frac{1}{U} + \frac{1}{1-U}\right)u^2 & 0 \\ 0 & 0 \end{pmatrix} \tag{6.62}$$

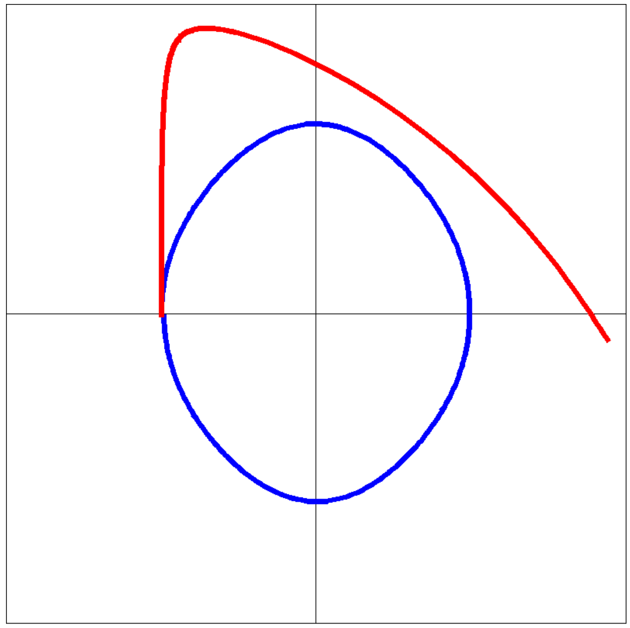

Figure 6.8: Oscillation of 1D bar discretized with two 1D linear elements. Phase space diagram (X_1, P_1) for the mixed Lagrangian formulation (blue) and for the standard Lagrangian formulation (red).

where u and U are the adimensionalized vertical and horizontal displacements of node 1 given by

$$u = \frac{x_1 - X_1}{L} \tag{6.63}$$

$$U = \frac{X_1}{L} \tag{6.64}$$

or more compactly

$$\mathbb{M}^{std} = \mathbb{M}^{mix} + \frac{RL}{3}\begin{pmatrix} A(U)\,u^2 & 0 \\ 0 & 0 \end{pmatrix}$$

where the function $A(U)$ is given by

$$A(U) = \frac{1}{U} + \frac{1}{1-U}$$

Using this notation, the differential equations of motion for the pair (X_1, x_1) (equations (6.60) and (6.61)) might be rewritten as

$$\mathbb{M}^{mix}\begin{pmatrix} \ddot{X}_1 \\ \ddot{x}_1 \end{pmatrix} = \begin{pmatrix} [C] \\ [P] \end{pmatrix}$$

for the mixed Lagrangian formulation, and

$$\frac{d}{dt}\left\{\mathbb{M}^{std}\begin{pmatrix}\dot{X}_1\\ \dot{x}_1\end{pmatrix}\right\}+\frac{R}{6}\begin{pmatrix}-\frac{x_1^2}{X_1^2}+\frac{(L-x_1)^2}{(L-X_1)^2}\\ 2\left(\frac{x_1}{X_1}-\frac{L-x_1}{L-X_1}\right)\end{pmatrix}\dot{X}_1^2=\begin{pmatrix}[C]\\ [P]\end{pmatrix}$$

for the standard Lagrangian formulation. On account of identity (6.62) and definitions (6.63) and (6.64) the previous yields

$$\mathbb{M}^{mix}\begin{pmatrix}\ddot{X}_1\\ \ddot{x}_1\end{pmatrix}+\frac{RL^2}{3}\frac{d}{dt}\begin{pmatrix}A(U)\,u^2\dot{U}\\ 0\end{pmatrix}+\frac{RL^2}{6}\begin{pmatrix}A'(U)\,u^2-2A(U)\,u\\ 2A(U)\,u\end{pmatrix}\dot{U}^2=\begin{pmatrix}[C]\\ [P]\end{pmatrix}$$

where

$$\begin{aligned}A'(U) &= \frac{dA}{dU}=\\ &= -\frac{1}{U^2}+\frac{1}{(1-U)^2}\end{aligned}$$

Assume now that $U=\frac{1}{2}+\varepsilon$ with $\varepsilon\ll 1$, which implies, given definition (6.64), that ε is the offset from a uniform mesh, i.e., if $\varepsilon=0$ then both elements have length $\frac{L}{2}$. Notice that

$$\begin{aligned}A(U) &= A\left(\frac{1}{2}+\varepsilon\right)=4\left(1+4\varepsilon^2+16\varepsilon^4+\cdots\right)\\ A'(U) &= A'\left(\frac{1}{2}+\varepsilon\right)=4\left(8\varepsilon+64\varepsilon^3+\cdots\right)\end{aligned}$$

Inserting the previous expansions into the differential equations we find to leading order in ε

$$\mathbb{M}^{mix}\begin{pmatrix}\ddot{X}_1\\ \ddot{x}_1\end{pmatrix}+\frac{4RL^2}{3}\begin{pmatrix}u^2\ddot{\varepsilon}+2u\dot{u}\dot{\varepsilon}-u\dot{\varepsilon}^2\\ u\dot{\varepsilon}^2\end{pmatrix}=\begin{pmatrix}[C]\\ [P]\end{pmatrix}$$

The differential equation in the tangent direction (which can be obtained by multiplying the horizontal/vertical equations by the tangent vector $\mathbb{T}^*=(1,1)$) evaluates therefore to

$$\frac{4RL^2}{3}\left(u^2\ddot{\varepsilon}+2u\dot{u}\dot{\varepsilon}\right)+[C]+[P]=0$$

which might be contrasted with the tangent differential equation for the mixed Lagrangian formuation

$$[C]+[P]=0$$

We notice that the term $2u\dot{u}$, which operates as a non-linear viscosity coefficient, becomes negative when the bar is returning to its undeformed configuration, i.e., when $u\to 0$. This is the reason why the solution becomes unstable for the standard Lagrangian formulation.

6.1.9 Example: Oscillation of a 1D bar, linear material

As a second illustrative example of the difference between both formulations, we consider again a one-dimensional body $B = [0, L]$ fixed on both sides and free of body forces. The bar is now set to oscillate from an underfomed configuration by applying an initial sinusoidal velocity. We assume a quadratic strain energy function of the form

$$W(F) = \frac{3}{2}\mu (F-1)^2$$

which results in linear stress-strain relation

$$P(F) = 3\mu (F-1)$$

and Eshelby stress

$$\begin{aligned} C(F) &= \left(W(F) - \frac{1}{2}R\dot{\varphi}^2\right) - PF = \\ &= -\frac{3}{2}\mu (F-1)(F+1) - \frac{1}{2}R\dot{\varphi}^2 \end{aligned}$$

The differential equations of motion are in this case

$$\begin{aligned} R\ddot{\varphi} &= \frac{\partial P}{\partial X} = \\ &= \frac{\partial}{\partial X}\left(3\mu \frac{\partial \varphi}{\partial X}\right) \end{aligned}$$

which corresponds to the wave equation. The analytical solution with zero boundary conditions, undeformed initial configuration and sinusoidal initial velocities is

$$\varphi(X,t) = A_k \sin\left(2k\pi \frac{X}{L}\right) \sin\left(2k\pi \frac{ct}{L}\right)$$

with

$$c^2 = \frac{R}{3\mu}$$

Figure (6.9) shows the finite element solution for the displacement field $u(X,t) = \varphi(X,t) - X$ using a different number of elements for both the mixed and standard Lagrangian formulations. It can be noticed that the latter is catastrophically unstable and leads to meaningless solutions.

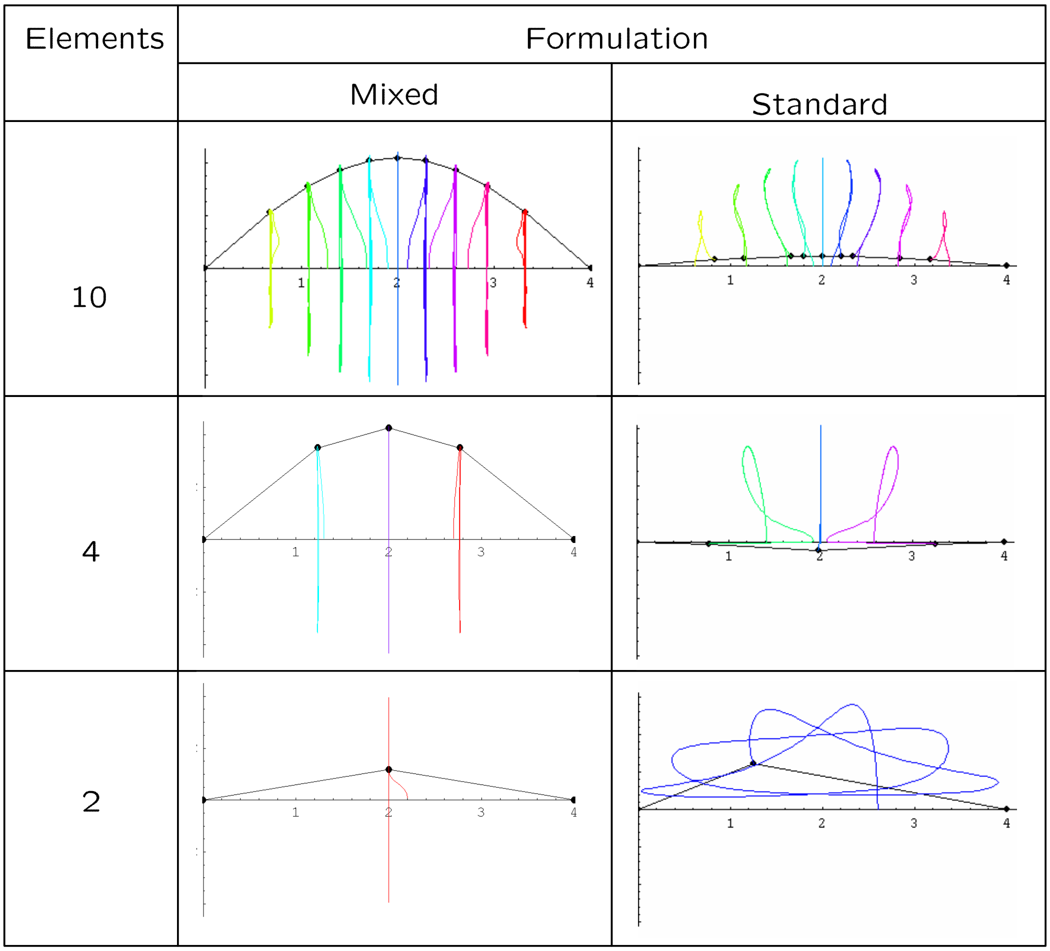

Figure 6.9: Oscillation of a 1D bar discretized with two 1D linear elements. Displacements as a function of position for different times $u(X,t)$ for a linear elastic material. Comparison between the solution for the mixed (left column) and standard (right column) Lagrangian formulations for meshes with a different number of elements

6.1.10 Viscosity and Semidiscrete Mixed Lagrange-d'Alembert principle

The incorporation of viscous effects into the analysis in the context of Lagrange-d'Alembert principle was discussed in sections §3.2, §3.4, and §5.5. We recall that the combined (vertical-horizontal) Lagrange-d'Alembert principle is given by (see §3.4, equations (3.63) or (3.64))

$$\mathbf{0} = \langle \delta S, \delta \boldsymbol{\psi} \rangle + \langle \delta S, \delta \boldsymbol{\phi} \rangle - \int_{t_0}^{t_f} \int_B \mathbf{P}^v \left(\mathbf{F}, \dot{\mathbf{F}} \right) \frac{\partial}{\partial \mathbf{X}} \left(\delta \boldsymbol{\phi} - \mathbf{F} \delta \boldsymbol{\psi} \right) dV\, dt \qquad \forall \left(\delta \boldsymbol{\psi}, \delta \boldsymbol{\phi} \right) \tag{6.65}$$

and that the *mixed* version of this principle (section (5.5), equation (5.19) and (5.20)) is given by

$$\begin{aligned} \mathbf{0} \quad = \quad & \langle \delta S, \delta \boldsymbol{\psi} \rangle + \langle \delta S, \delta \boldsymbol{\phi} \rangle + \langle \delta S, \delta \boldsymbol{\nu} \rangle + \\ & + \int_{t_0}^{t_f} \int_B \left(-\mathbf{P}^v \left(\mathbf{F}, D\mathbf{V} \right) \frac{\partial \delta \boldsymbol{\varphi}}{\partial \mathbf{X}} + \mathbf{R}^v \left(\delta \boldsymbol{\phi} - \mathbf{F} \delta \boldsymbol{\psi} - \delta \boldsymbol{\varphi} \right) \right) dV\, dt \qquad \forall \left(\delta \boldsymbol{\psi}, \delta \boldsymbol{\phi} \right) \end{aligned} \tag{6.66}$$

We noticed also that in the latter there are four unknown fields, namely $(\boldsymbol{\phi}, \boldsymbol{\psi}, \boldsymbol{\nu}, \mathbf{R}^v)$ and four independent variations $(\delta\boldsymbol{\phi}, \delta\boldsymbol{\psi}, \delta\boldsymbol{\nu}, \delta\boldsymbol{\varphi})$. Furthermore, we notice that in the first principle the viscous stress $\mathbf{P}^v$ is weighted with the gradient of

$$\delta\boldsymbol{\phi} - \mathbf{F}\delta\boldsymbol{\psi}$$

while in the second, with the gradient of

$$\delta\boldsymbol{\varphi}$$

As in the case of conservative Lagrangian systems (no viscosity) where the use of independent interpolations for velocities $\mathbf{V}$ and deformations $\boldsymbol{\varphi}$ was required to avoid unstable solutions, we will see in this section that for non-conservative systems (viscous behavior) we might simplify the formulation and reduce notably the computational effort by making use of independent interpolations not only for $\boldsymbol{\varphi}$ and $\mathbf{V}$ but also for the viscous body forces $\mathbf{R}^v$ and for the variations $\delta\boldsymbol{\varphi}$.

To understand this fact (the need for an independent interpolation for $\mathbf{R}^v$ and independent weighting function $\delta\boldsymbol{\varphi}$) consider first that we use the combined horizontal-vertical Lagrange-d'Alembert principle (6.66) with independent interpolations of velocities $\mathbf{V}$ and deformations $\boldsymbol{\varphi}$ but without independent interpolations for $\mathbf{R}^v$, i.e., with $\mathbf{R}^v = \mathrm{DIV}\left(\mathbf{P}^v\right)$ strongly enforced. In this case the mixed Lagrange-d'Alembert principle takes the form

$$\mathbf{0} = \langle \delta S, \delta\boldsymbol{\psi} \rangle + \langle \delta S, \delta\boldsymbol{\phi} \rangle - \int_{t_0}^{t_f} \int_B \mathbf{P}^v\left(\mathbf{F}, D\mathbf{V}\right) \frac{\partial}{\partial \mathbf{X}} \left(\delta\boldsymbol{\phi} - \mathbf{F}\delta\boldsymbol{\psi}\right) dV dt \qquad \forall \left(\delta\boldsymbol{\psi}, \delta\boldsymbol{\phi}\right) \quad (6.67)$$

$$\mathbf{0} = \langle \delta S, \delta\mathbf{V} \rangle \qquad \forall \delta\mathbf{V} \quad (6.68)$$

where the first two terms correspond to the combination of horizontal and vertical variations of the mixed action (equations (5.6) and (5.7)) and the viscous stress $\mathbf{P}^v$ is evaluated on $D\mathbf{V}$ (material velocity gradient) instead of $\dot{\mathbf{F}}$. We would like now to insert the finite element (mixed) interpolation ((6.1), (6.2)) into the previous. To this end we notice that this principle contains a term of the form $\frac{\partial \mathbf{F}}{\partial \mathbf{X}}$ and that if standard finite element shape functions are used, $\mathbf{F}$ will be discontinuous across element boundaries. This implies the presence of delta function contributions to the derivative $\frac{\partial \mathbf{F}_h}{\partial \mathbf{X}}$ of the discretized deformation gradient $\mathbf{F}_h$ will result in delta function contributions. Inserting the (mixed) interpolation (6.1), (6.2) in the mixed Lagrange-d'Alembert principle (6.67, 6.68) we therefore find

$$\begin{aligned}
\mathbf{0} &= \langle \delta S_h, \delta \mathbf{X}_h \rangle + \langle \delta S_h, \delta \mathbf{x}_h \rangle - \int_{t_0}^{t_f} \int_B \mathbf{P}_h^v \frac{\partial}{\partial \mathbf{X}} \left(N_a \left(\delta \mathbf{x}_a - \mathbf{F}_h \delta \mathbf{X}_a \right) \right) dV dt = \\
&= \langle \delta S_h, \delta \mathbf{X}_h \rangle + \langle \delta S_h, \delta \mathbf{x}_h \rangle - \int_{t_0}^{t_f} \left(\sum_e \int_{\Omega^e} \mathbf{P}^{v-e} \frac{\partial}{\partial \mathbf{X}} \left(N_a^e \left(\delta \mathbf{x}_a^e - \mathbf{F}^e \delta \mathbf{X}_a^e \right) \right) dV \right) dt \\
&\quad - \int_{t_0}^{t_f} \left(\sum_f \int_{\Gamma_f} \mathbf{P}^{v-f} N_a^f \delta \mathbf{X}_a^f dS \right) dt \qquad (6.69) \\
\mathbf{0} &= \langle \delta S_h, \delta \mathbf{V}_h \rangle \qquad (6.70)
\end{aligned}$$

where $\mathbf{P}^{v-e}$ is the discretized viscous stress within the element

$$P_{iJ}^{v-e} = P_{iJ}^v \left(\frac{\partial N_a^e}{\partial X_I} x_{ai}^e, \frac{\partial N_a^e}{\partial X_I} V_{ai}^e \right)$$

N_a and N_a^e are, respectively, the global and elemental shape functions, N_a^f is the shape function evaluated on each element face Γ_f, and $\mathbf{P}_b^{v-f}$ are viscous material forces, distributed on every element face Γ_f, conjugate to the (delta-function) singularities occurring as derivatives of the jump discontinuities on $\mathbf{F}_h$ across element boundaries.

Consider as an illustrative example of the jump terms, a one-dimensional domain $[0, L]$ discretized into two linear finite elements $[0, X_1]$ and $[X_1, L]$. In this case both P_h^v and F_h will be piecewise constant and exhibit jump discontinuities at the element boundary X_1, the derivative $\frac{\partial F_h}{\partial X}$ resulting thus in a delta function singularity. Integrating we find

$$\int_0^L P_h^v \frac{\partial F_h}{\partial X} \left(N_a \delta X_a \right) = \frac{(P^v)^+ + (P^v)^-}{2} \left(F^+ - F^- \right) \delta X_1 = F_1^{v-f} \delta X_1$$

where $(P^v)^+$, F^+ and $(P^v)^-$, F^- are, respectively, the viscous stress and deformation gradient in the first and second element and F^{v-f} is the sought viscous material forces distributed over the interelement boundary. Therefore the total configurational (horizontal) viscous force is in this case

$$\begin{aligned}
F_1^v \delta X_1 &= \int_0^L P_h^v \frac{\partial}{\partial X} \left(-F_h N_a \delta X_a \right) = \\
&= \left(F_1^{v-e} + F_1^{v-f} \right) \delta X_1 = \\
&= -\int_0^L P_h^v F_h \left(\frac{\partial N_a}{\partial X} \delta X_a \right) - \int_0^L P_h^v \frac{\partial F_h}{\partial X} \left(N_a \delta X_a \right) = \\
&= \left(-\left(P^{v-} F^- - P^{v+} F^+ \right) - \frac{P^{v+} + P^{v-}}{2} \left(F^+ - F^- \right) \right) \delta X_1
\end{aligned}$$

Using relations (6.29), (6.30), and (6.31), and following the same methodology that led to the semidiscrete Euler-Lagrange equations (6.36), (6.37), and (6.38), the (semi)discretized version of this mixed Lagrange-d'Alembert principle with no independent interpolation for $\mathbf{R}^v$ (the principle defined by equations (6.67) and (6.68)) might be rewritten as

$$\begin{aligned}
\frac{d}{dt}\left(\mathbf{m}_h^T \mathbf{V}_h\right) &= \mathbf{e}_h + \mathbf{f}_h + \mathbf{f}_h^v \\
\frac{d}{dt}\left(\mathbf{M}_h^T \mathbf{V}_h\right) &= \mathbf{E}_h + \mathbf{F}_h + \mathbf{F}_h^v \\
\mathbf{m}_h \dot{\mathbf{x}}_h + \mathbf{M}_h \dot{\mathbf{X}}_h &= \mathbf{m}_h \mathbf{V}_h
\end{aligned}$$

where

$$\mathbf{f}_h^v = \sum_e \mathbf{f}^{v-e} \tag{6.71}$$

$$\mathbf{F}_h^v = \sum_e \mathbf{F}^{v-e} + \sum_f \mathbf{F}^{v-f} \tag{6.72}$$

are the global assembled viscous mechanical (vertical) and configurational (horizontal) nodal forces with elemental forces given by

$$f_{ai}^{v-e} = \int_{\Omega^e} P_{iJ}^{v-e} \frac{\partial N_a^e}{\partial X_J} dV \tag{6.73}$$

$$\begin{aligned}
F_{aI}^{v-e} &= \int_{\Omega^e} P_{iJ}^{v-e} \frac{\partial}{\partial X_J}\left(-F_{iI}^e N_a^e\right) dV = \\
&= \int_{\Omega^e} P_{iJ}^{v-e} \left(-F_{iI}^e \frac{\partial N_a^e}{\partial X_J} - N_a \frac{\partial F_{iI}^e}{\partial X_J}\right) dV
\end{aligned} \tag{6.74}$$

$$F_{aI}^{v-f} = \int_{\Gamma^f} P_I^{v-f} N_a dS \tag{6.75}$$

We thus arrive at a system of equations similar to those obtained for conservative systems but with additional forces $\mathbf{f}_h^v$ and $\mathbf{F}_h^v$ in both the vertical and horizontal equations. Furthermore there are two contributions to the total configurational nodal viscous force $\mathbf{F}_h^v = \mathbf{F}_h^{v-e} + \mathbf{F}_h^{v-f}$, a bulk or elemental term $\mathbf{F}_h^{v-e}$ and a boundary or face term $\mathbf{F}_h^{v-f}$, the latter arising as viscous configurational force conjugate to the delta function singularity terms.

The computation of the boundary term $\mathbf{F}_h^{v-f}$ is cumbersome for two-dimensional and three-dimensional problems and for general grids because to pursue this computation we are required, as definitions (6.72) and (6.75) suggest, to walk and integrate over every element face in the finite element mesh, and this is an expensive and non-standard computation in traditional finite element implementations. As an alternative to avoid this difficult calculation we propose to make use of the mixed Lagrange-d'Alembert principle written in the form of (5.19) and (5.20) with *independent* interpolations for the total bulk viscous force $\mathbf{R}^v$ and *independent* variations $\delta\boldsymbol{\varphi}$ to enforce the identity

$$\mathbf{R}^v = \mathrm{DIV}\left(\mathbf{P}^v\right)$$

Assume therefore the same (independent) interpolations for deformations $\boldsymbol{\varphi}$ and velocities $\mathbf{V}$ used before (equations (6.1) and (6.2)) and, in addition, the following independent interpolation for viscous forces $\mathbf{R}^v$ and variations $\delta\boldsymbol{\varphi}$:

$$\begin{aligned}\mathbf{R}_h^v(\mathbf{X},t) &= \sum_a^N N_a(\mathbf{X},t)\,\mathbf{R}_a^v(t) = \sum_e^E\sum_a^n N_a^e(\mathbf{X},t)\,\mathbf{R}_a^e(t)\\ \boldsymbol{\delta\varphi}_h(\mathbf{X},t) &= \sum_a^N N_a(\mathbf{X},t)\,\boldsymbol{\delta\varphi}_a = \sum_e^E\sum_a^n N_a^e(\mathbf{X},t)\,\boldsymbol{\delta\varphi}_a^e(t)\end{aligned}$$

where N_a (respectively N_a^e) are nodal (respectively elemental) shape functions chosen to be coincident with the shape functions used for to interpolate deformations $\boldsymbol{\varphi}$ and velocities $\mathbf{V}$. Inserting the four independent interpolations into the mixed Lagrange-d'Alembert principle (6.66) we find

$$\begin{aligned}\mathbf{0} &= \langle \delta S_h, \delta\mathbf{X}_h\rangle + \langle \delta S_h, \delta\mathbf{x}_h\rangle + \\ &+\int_{t_0}^{t_f}\int_B -\mathbf{P}_h^v\frac{\partial}{\partial\mathbf{X}}\left(N_a\delta\boldsymbol{\varphi}_a\right) + \left(\mathbf{R}_b^v N_b\right)\left(N_a\left(\delta\mathbf{x}_a - \mathbf{F}_h\delta\mathbf{X}_a - \delta\boldsymbol{\varphi}_a\right)\right)dV\,dt\\ &= \langle \delta S_h, \delta\mathbf{X}_h\rangle + \langle \delta S_h, \delta\mathbf{x}_h\rangle + \\ &+\int_{t_0}^{t_f}\left(\sum_e\int_{\Omega^e} -\mathbf{P}^{v-e}\frac{\partial}{\partial\mathbf{X}}\left(N_a^e\left(\delta\boldsymbol{\varphi}_a^e\right)\right) + \left(\mathbf{R}_b^{v-e}N_b^e\right)\left(N_a^e\left(\delta\mathbf{x}_a^e - \mathbf{F}^e\delta\mathbf{X}_a^e - \delta\boldsymbol{\varphi}_a^e\right)\right)dV\right)dt\\ \mathbf{0} &= \langle \delta S_h, \delta\mathbf{V}_h\rangle\end{aligned}$$

When comparing the previous with (6.69) and (6.70) we can see that we now find a derivative of a *continuous* variation

$$\delta\boldsymbol{\varphi}_h = \sum_a N_a\delta\boldsymbol{\varphi}_a$$

while before we were required to differentiate a *discontinuous* variation

$$\delta\boldsymbol{\varphi}_h = \sum_a N_a\left(\delta\mathbf{x}_a - \mathbf{F}_h\delta\mathbf{X}_a\right)$$

In this way we avoid the computation of the (delta function–related) viscous forces $\mathbf{F}_h^{v-f}$ that arose as a consequence of the discontinuity of $\mathbf{F}_h$. Defining as before the nodal (spatial) viscous force $\mathbf{f}^v$ as

$$\begin{aligned}\mathbf{f}_a^v &= \int_B \mathbf{P}_h^v\frac{\partial N_a}{\partial\mathbf{X}}dV\\ &= \sum_e\int_{\Omega^e}\mathbf{P}^{v-e}\frac{\partial N_a^e}{\partial\mathbf{X}}dV\end{aligned}$$

and the extended mass matrix $(\mathbf{M}_h, \mathbf{m}_h)$ as

$$
\begin{aligned}
(\mathbf{M}_h, \mathbf{m}_h)_{ab} &= \int_B R N_a N_b \left(-\mathbf{F}_h, \mathbf{i}\right) dV = \\
&= \sum_e \int_{\Omega^e} R N_b^e N_a^e \left(-\mathbf{F}^e, \mathbf{i}\right) dV
\end{aligned}
$$

we can rewrite the discretized mixed Lagrange d'Alembert principle as

$$
\begin{aligned}
\mathbf{0} &= \langle \delta S_h, \delta \mathbf{X}_h \rangle + \langle \delta S_h, \delta \mathbf{x}_h \rangle \\
&\quad - \int_{t_0}^{t_f} \left(\delta \boldsymbol{\varphi}_a^T \cdot \mathbf{f}_a^v + (\mathbf{R}_b^v)^T \left((\mathbf{M}_{ba}, \mathbf{m}_{ba}) \cdot \begin{pmatrix} \delta \mathbf{X}_a \\ \delta \mathbf{x}_a \end{pmatrix} - (\mathbf{m}_h)_{ba} \cdot \delta \boldsymbol{\varphi}_a \right) \right) dt \\
\mathbf{0} &= \langle \delta S_h, \delta \mathbf{V}_h \rangle
\end{aligned}
$$

Using relations (6.29), (6.30), and (6.31), and taking into account that the variations $\delta\boldsymbol{\varphi}$ are independent, the following Euler-Lagrange equations are obtained:

$$
\begin{aligned}
\mathbf{0} &= \frac{d}{dt} \left\{ \begin{pmatrix} \mathbf{M}_h^T \\ \mathbf{m}_h^T \end{pmatrix} \mathbf{V}_h \right\} - \begin{pmatrix} \mathbf{E}_h \\ \mathbf{e}_h \end{pmatrix} - \begin{pmatrix} \mathbf{F}_h \\ \mathbf{f}_h \end{pmatrix} + \begin{pmatrix} \mathbf{M}_h^T \\ \mathbf{m}_h^T \end{pmatrix} \mathbf{R}_h^v \\
\mathbf{0} &= \mathbf{f}_h^v + \mathbf{m}_h \mathbf{R}_h^v \\
\mathbf{0} &= (\mathbf{M}_h, \mathbf{m}_h) \begin{pmatrix} \dot{\mathbf{X}}_h \\ \dot{\mathbf{x}}_h \end{pmatrix} - \mathbf{m}_h \mathbf{V}_h
\end{aligned}
$$

Eliminating now the vector $\mathbf{R}^v$ the previous can finally be written as

$$
\begin{aligned}
\frac{d}{dt} \left\{ \begin{pmatrix} \mathbf{M}_h^T \\ \mathbf{m}_h^T \end{pmatrix} \mathbf{V}_h \right\} &= \begin{pmatrix} \mathbf{E}_h \\ \mathbf{e}_h \end{pmatrix} + \begin{pmatrix} \mathbf{F}_h \\ \mathbf{f}_h \end{pmatrix} + \begin{pmatrix} \mathbf{F}_h^v \\ \mathbf{f}_h^v \end{pmatrix} \\
(\mathbf{M}_h, \mathbf{m}_h) \begin{pmatrix} \dot{\mathbf{X}}_h \\ \dot{\mathbf{x}}_h \end{pmatrix} &= \mathbf{m}_h \mathbf{V}_h
\end{aligned}
$$

with

$$
\begin{pmatrix} \mathbf{F}_h^v \\ \mathbf{f}_h^v \end{pmatrix} = \begin{pmatrix} \mathbf{M}_h^T \\ \mathbf{m}_h^T \end{pmatrix} \mathbf{m}_h^{-T} \mathbf{f}_h^v \tag{6.76}
$$

Recalling the definition for the global normal $\mathbb{N}_h$ and conormal $\mathbb{N}_h^*$ (equations (6.49) and (6.50))

$$
\begin{aligned}
\mathbb{N}_h &= \begin{pmatrix} \mathbf{M}_h^T \\ \mathbf{m}_h^T \end{pmatrix} \mathbf{m}_h^{-T} \\
\mathbb{N}_h^* &= \mathbf{m}_h^{-1} (\mathbf{M}_h, \mathbf{m}_h)
\end{aligned}
$$

the (combined horizontal-vertical) Euler-Lagrange equations might be rewritten as

$$\begin{aligned} \frac{d}{dt}\left\{\mathbb{N}_h \mathbf{m}_h \mathbf{V}_h\right\} &= \mathbb{E}_h + \mathbb{F}_h + \mathbb{F}_h^v \\ \mathbb{N}_h^* \dot{\mathbf{q}}_h &= \mathbf{V}_h \end{aligned}$$

where $\mathbf{q}_h$ is the combined (horizontal/vertical) generalized coordinate

$$\mathbf{q}_h = \begin{pmatrix} \mathbf{X}_h \\ \mathbf{x}_h \end{pmatrix}$$

$\mathbb{E}_h$, $\mathbb{F}_h$, and $\mathbb{F}_h^v$ are, respectively, the combined configurational/mechanical (horizontal/vertical) dynamic, static, and viscous forces

$$\begin{aligned} \mathbb{E}_h &= \begin{pmatrix} \mathbf{E}_h \\ \mathbf{e}_h \end{pmatrix} \\ \mathbb{F}_h &= \begin{pmatrix} \mathbf{F}_h \\ \mathbf{f}_h \end{pmatrix} \\ \mathbb{F}_h^v &= \begin{pmatrix} \mathbf{F}_h^v \\ \mathbf{f}_h^v \end{pmatrix} = \mathbb{N}_h \mathbf{f}_h^v \end{aligned}$$

Using continuous variations we therefore obtain the following global configurational (horizontal) viscous force:

$$\mathbf{F}_h^v = \mathbf{M}_h^T \mathbf{m}_h^{-T} \mathbf{f}_h^v \tag{6.77}$$

as opposed to (6.72), (6.74), and (6.75). The semidiscrete Euler-Lagrange equations become modified by a factor of the form

$$\mathbb{N}_h \mathbf{f}_h^v$$

in complete analogy to the continuous case (equation (3.62)) where the continuous horizontal-vertical Euler-lagrange equations result modified by the factor

$$\mathbb{N}\,\mathrm{DIV}\left(\mathbf{P}^v\right)$$

6.1.11 Viscous regularization

We have observed in §6.1.5 that, unlike the continuous case, horizontal and vertical variations are not equivalent in the (semi)discrete setting and therefore horizontal and vertical semidiscrete Euler-Lagrange equations are independent as a result. In some situations, however, the system of equations becomes only *weakly* independent and consequently ill-posed, and a special approach is required to obtain an accurate and stable solution. An example of such a situation is a body undergoing uniform (constant) deformations for every time. In this case the graph of the deformation mapping at every given time is flat both in the continuous and discrete settings and, therefore, horizontal and vertical variations do become equivalent. A possible approach to overcome this difficulty is to influence the horizontal equations of motion with viscous regularizing forces. The semidiscrete system of equations thus becomes

$$\begin{aligned} \frac{d}{dt}\left(\mathbf{m}_h^T \mathbf{V}_h\right) &= \mathbf{e}_h + \mathbf{f}_h + \mathbf{f}_h^v \\ \frac{d}{dt}\left(\mathbf{M}_h^T \mathbf{V}_h\right) &= \mathbf{E}_h + \mathbf{F}_h + \mathbf{F}_h^v + \mathbf{F}_h^{v-reg} \\ \mathbf{m}_h \dot{\mathbf{x}}_h + \mathbf{M}_h \dot{\mathbf{X}}_h &= \mathbf{m}_h \mathbf{V}_h \end{aligned}$$

where $\mathbf{F}_h^{v-reg}$ is the viscous regularization force. We shall assume that this force is composed of two parts, one that penalizes the *total* horizontal nodal velocity $\dot{\mathbf{X}}_h$ and another that accounts for the *relative* horizontal velocity between nodes, namely,

$$\mathbf{F}_h^{v-reg} = \mathbf{F}_h^{v-reg-tot} + \mathbf{F}_h^{v-reg-rel} \tag{6.78}$$

where

$$\begin{aligned} \mathbf{F}_h^{v-reg-tot} &= \mu_1 \dot{\mathbf{X}}_h \\ \mathbf{F}_h^{v-reg-rel} &= \sum_e \mathbf{F}^{v-reg-rel-e} \end{aligned}$$

with

$$\begin{aligned} \mathbf{F}_{aI}^{v-reg-rel-e} &= \int_{\Omega^e} 2\mu_2 \left(\frac{\partial}{\partial X_J} \left(\dot{\psi}_I^e \circ \boldsymbol{\psi}^{-1} \right) \right) \frac{\partial N_a^e}{\partial X_J} dV \\ &= \int_{\Omega^e} 2\mu_2 \dot{\psi}_{I,\alpha} \left(\psi_{\alpha,J}^{-1} \circ \boldsymbol{\psi}^{-1} \right) \frac{\partial N_a^e}{\partial X_J} dV \end{aligned}$$

The relative viscous force is modelled in analogy to the Newtonian viscous force ((3.12), (3.13)) and will be a function of the material gradient of $\mathbf{W} = \dot{\boldsymbol{\psi}}_h \circ \boldsymbol{\psi}_h^{-1}$, the horizontal velocity field.

The modified system of equations may be established finally from the following semidiscrete-mixed Lagrange-d'Alembert principle:

$$\begin{aligned} \langle \delta S_h, \delta \mathbf{X}_h \rangle + \langle \delta S_h, \delta \mathbf{x}_h \rangle - \int_{t_0}^{t_f} (\delta \mathbf{x}_h, \delta \mathbf{X}_h) \begin{pmatrix} \mathbf{F}_h^v + \mathbf{F}_h^{v-reg} \\ \mathbf{f}_h^v \end{pmatrix} dt &= \mathbf{0} \qquad \forall (\delta \mathbf{X}_h, \delta \mathbf{x}_h) && (6.79) \\ \langle \delta S_h, \delta \mathbf{V}_h \rangle &= \mathbf{0} \qquad \forall \delta \mathbf{V}_h && (6.80) \end{aligned}$$

with combined horizontal-vertical semidiscrete Euler-Lagrange equations

$$\frac{d}{dt}\left\{\begin{pmatrix} \mathbf{M}_h^T \\ \mathbf{m}_h^T \end{pmatrix} \mathbf{V}_h\right\} = \begin{pmatrix} \mathbf{E}_h \\ \mathbf{e}_h \end{pmatrix} + \begin{pmatrix} \mathbf{F}_h \\ \mathbf{f}_h \end{pmatrix} + \begin{pmatrix} \mathbf{F}_h^v \\ \mathbf{f}_h^v \end{pmatrix} + \begin{pmatrix} \mathbf{F}_h^{v-reg} \\ \mathbf{0} \end{pmatrix} \tag{6.81}$$

$$(\mathbf{M}_h, \mathbf{m}_h) \begin{pmatrix} \dot{\mathbf{X}}_h \\ \dot{\mathbf{x}}_h \end{pmatrix} = \mathbf{m}_h \mathbf{V}_h \tag{6.82}$$

or alternatively

$$\frac{d}{dt}\{\mathbb{N}_h \mathbf{m}_h \mathbf{V}_h\} = \mathbb{E}_h + \mathbb{F}_h + \mathbb{F}_h^v + \mathbb{F}_h^{v-reg}$$

$$\mathbb{N}_h^* \begin{pmatrix} \dot{\mathbf{X}}_h \\ \dot{\mathbf{x}}_h \end{pmatrix} = \mathbf{V}_h$$

with $\mathbb{N}_h$, $\mathbb{N}_h^*$, $\mathbb{E}_h$, $\mathbb{F}_h$ and $\mathbb{F}_h^v$ defined as before and with

$$\mathbb{F}_h^{v-reg} = \begin{pmatrix} \mathbf{F}_h^{v-reg} \\ \mathbf{0} \end{pmatrix}$$

6.2 Time discretization

In the remainder of this section we turn to the problem of discretizing in *time* the semidiscrete system of differential equations (6.53) and (6.54) and their extension to include viscous effects ((6.81), (6.82)). These equations might be discretized using a direct time-stepping algorithm based on finite difference approximations of the rates in the unknown variables $(\mathbf{X}_h, \mathbf{x}_h, \mathbf{V}_h)$. However widely used direct methods such as those of the Newmark family were not designed for configuration-dependent (and therefore time-dependent) inertia and although they might be generalized to this case, the extension is not unique and relies on ad-hoc considerations. To avoid this difficulty the semidiscrete equations may be alternatively discretized in time by recourse to a *mixed variational integrator* (see Chapter 2, §2.1.4 and §2.1.8) for a review of standard and mixed variational integrators). The use of a semidiscrete finite element interpolation resulted in the formulation of a *semidiscrete* (mixed) action functional S_h and a semidiscrete (mixed) Lagrangian L_h^{mix}. As it was outlined in chapter 2 for the particular case of one-dimensional elasticity (see §2.2.14 and §2.2.15), we will now discretize this semidiscrete action and Lagrangian in time to obtain a *discrete* action sum S_d and *discrete-mixed* Lagrangian L_d^{mix}. We next obtain the *discrete* Euler-Lagrange equations by invoking the stationarity of the discrete action sum with respect to the discrete nodal trajectories. These equations become a discrete version of the semidiscrete Euler-Lagrange equation and define the sought time-stepping algorithm.

6.2.1 Discrete mixed Lagrangian and Discrete mixed Hamilton's principle

We recall from §6.1.3 that the semidiscrete-mixed action and semidiscrete-mixed Lagrangian are given by

$$S_h(\mathbf{X}_h,\mathbf{x}_h,\mathbf{V}_h)=\int_{t_0}^{t_f} L_h^{mix}\left(\mathbf{X}_h(t),\mathbf{x}_h(t),\dot{\mathbf{X}}_h(t),\dot{\mathbf{x}}_h(t),\mathbf{V}_h(t)\right)dt$$

and

$$\begin{aligned}L_h^{mix}\left(\mathbf{X}_h,\mathbf{x}_h,\dot{\mathbf{X}}_h,\dot{\mathbf{x}}_h,\mathbf{V}_h\right) &= \frac{1}{2}\mathbf{V}_h^T\mathbf{m}_h\mathbf{V}_h - I_h(\mathbf{X}_h,\mathbf{x}_h)+\\ &\quad +\mathbf{V}_h^T\left((\mathbf{M}_h,\mathbf{m}_h)\begin{pmatrix}\dot{\mathbf{X}}_h\\ \dot{\mathbf{x}}_h\end{pmatrix}-\mathbf{m}_h\mathbf{V}_h\right)\\ &= \frac{1}{2}\mathbf{V}_h^T\mathbf{m}_h\mathbf{V}_h - I_h(\mathbf{X}_h,\mathbf{x}_h)+\\ &\quad +\mathbf{V}_h^T\mathbf{m}_h\left(\mathbb{N}_h^*\begin{pmatrix}\dot{\mathbf{X}}_h\\ \dot{\mathbf{x}}_h\end{pmatrix}-\mathbf{V}_h\right)\end{aligned}$$

with semidiscrete Euler-Lagrange equations

$$\begin{aligned}\frac{d}{dt}\left(\mathbf{M}_h^T\mathbf{V}_h\right) &= \mathbf{E}_h\left(\mathbf{X}_h,\mathbf{x}_h,\dot{\mathbf{X}}_h,\dot{\mathbf{x}}_h,\mathbf{V}_h\right)+\mathbf{F}_h(\mathbf{X}_h,\mathbf{x}_h)\\ \frac{d}{dt}\left(\mathbf{m}_h^T\mathbf{V}_h\right) &= \mathbf{e}_h\left(\mathbf{X}_h,\mathbf{x}_h,\dot{\mathbf{X}}_h,\dot{\mathbf{x}}_h,\mathbf{V}_h\right)+\mathbf{f}_h(\mathbf{X}_h,\mathbf{x}_h)\\ \mathbf{m}_h\dot{\mathbf{x}}_h+\mathbf{M}_h\dot{\mathbf{X}}_h &= \mathbf{m}_h\mathbf{V}_h\end{aligned}$$

where the mass matrices $\mathbf{M}_h(\mathbf{X}_h,\mathbf{x}_h)$ and $\mathbf{m}_h(\mathbf{X}_h)$ are given by (6.17), (6.18), (6.20) and (6.21); I_h is the total potential energy defined in (6.19) and (6.22); the forces $(\mathbf{F}_h,\mathbf{f}_h)$ and $(\mathbf{E}_h,\mathbf{e}_h)$ are the static and dynamic internal forces given in compact notation by

$$\begin{pmatrix}\mathbf{F}_h\\ \mathbf{f}_h\end{pmatrix}=-\begin{pmatrix}\frac{\partial}{\partial\mathbf{X}_h}\\ \frac{\partial}{\partial x_h}\end{pmatrix}I_h$$

$$\begin{pmatrix}\mathbf{E}_h\\ \mathbf{e}_h\end{pmatrix}=\begin{pmatrix}\frac{\partial}{\partial\mathbf{X}_h}\\ \frac{\partial}{\partial x_h}\end{pmatrix}\left(\frac{1}{2}\mathbf{V}_h^T\mathbf{m}_h\mathbf{V}_h+\mathbf{V}_h^T\left((\mathbf{M}_h,\mathbf{m}_h)\begin{pmatrix}\dot{\mathbf{X}}_h\\ \dot{\mathbf{x}}_h\end{pmatrix}-\mathbf{m}_h\mathbf{V}_h\right)\right)$$

(see equations (6.32), (6.33), (6.34), (6.35), (6.41), (6.42), (6.39), (6.40)) and $\mathbb{N}_h^*$ is the global (co)normal defined as

$$\mathbb{N}_h^*=\mathbf{m}_h^{-1}(\mathbf{M}_h,\mathbf{m}_h)$$

(see equation (6.50)).

In order to obtain a fully discrete system of equations, the time variable needs to be discretized.

To this end we begin by collecting all dynamical variables into the generalized coordinate array

$$\mathbf{q}_h = (\mathbf{X}_h, \mathbf{x}_h)$$

whereupon the semidiscrete-mixed action and Lagrangian adopt the simplified form

$$S_h(\mathbf{q}_h, \mathbf{V}_h) = \int_{t_0}^{t_f} L_h^{mix}(\mathbf{q}_h(t), \dot{\mathbf{q}}_h(t), \mathbf{V}_h(t))\, dt$$

$$L_h^{mix}(\mathbf{q}_h, \dot{\mathbf{q}}_h, \mathbf{V}_h) = \frac{1}{2}\mathbf{V}_h^T \mathbf{m}_h(\mathbf{q}_h)\mathbf{V}_h - I_h(\mathbf{q}_h) + \mathbf{V}_h^T \mathbf{m}_h(\mathbf{q}_h)(\mathbb{N}_h^*(\mathbf{q}_h)\dot{\mathbf{q}}_h - \mathbf{V}_h)$$

and the Euler-Lagrange equations reduce to

$$\begin{aligned} \frac{d}{dt}\left(D_2 L_h^{mix}(\mathbf{q}_h, \dot{\mathbf{q}}_h, \mathbf{V}_h)\right) &= D_1 L_h^{mix}(\mathbf{q}_h, \dot{\mathbf{q}}_h, \mathbf{V}_h) \\ 0 &= D_3 L_h^{mix}(\mathbf{q}_h, \dot{\mathbf{q}}_h, \mathbf{V}_h) \end{aligned}$$

where we are using the classical notation $D_i L$ to denote the partial derivative with respect to variables in the ith slot of the dependent variable list of L. We thus arrive at a dynamical system of the class studied in Chapter 2, (see §2.1).

We next partition the time interval $[t_0, t_f]$ into discrete times $\left(t^0 = t_0, \cdots, t^k, \cdots, t^K = t_f\right)$ where K is the number of time subintervals and where we are using a supraindex to denote time step. As suggested by the analysis performed in the second chapter, we proceed by interpolating the trajectories $\mathbf{q}_h(t)$ and velocities $\mathbf{V}_h(t)$, respectively, with piecewise linear functions of time and piecewise constant functions, namely,

$$\begin{aligned} \mathbf{q}_h(t) &= \mathbf{q}_h^k \left(\frac{t^{k+1} - t}{t^{k+1} - t^k}\right) + \mathbf{q}_h^{k+1}\left(\frac{t - t^k}{t^{k+1} - t^k}\right) \qquad \forall t \in \left[t^k, t^{k+1}\right] \\ \mathbf{V}_h(t) &= \mathbf{V}_h^{k+\beta} \qquad \forall t \in \left[t^k, t^{k+1}\right] \end{aligned}$$

where $\mathbf{V}_h^{k+\beta}$ is constant in the interval $\left(t^k, t^{k+1}\right)$. We recall from our discussion in chapter 2 (section (2.1.10)) that an arbitrary choice of interpolation spaces might lead to the presence of *arbitrary global modes in time* and that to avoid these modes a careful selection of interpolation spaces is required.

This results in the discrete-mixed action sum

$$S_d\left(\cdots, \mathbf{q}_h^k, \cdots, \mathbf{V}_h^{k+\beta}, \cdots, t^k, \cdots\right) = \sum_{k=0}^{K} L_d^{mix}\left(\mathbf{q}_h^k, \mathbf{q}_h^{k+1}, \mathbf{V}_h^{k+\beta}, t^k, t^{k+1}\right) \tag{6.83}$$

where

$$L_d^{mix}\left(\mathbf{q}_h^k,\mathbf{q}_h^{k+1},\mathbf{V}_h^{k+\beta},t^k,t^{k+1}\right)=\int_{t^k}^{t^{k+1}} L_h^{mix}\left(\mathbf{q}_h^k\left(\tfrac{t^{k+1}-t}{t^{k+1}-t^k}\right)+\mathbf{q}_h^{k+1}\left(\tfrac{t-t^k}{t^{k+1}-t^k}\right),\tfrac{\mathbf{q}_h^{k+1}-\mathbf{q}_h^k}{t^{k+1}-t^k},\mathbf{V}_h^{k+\beta}\right)dt \tag{6.84}$$

is the discrete-mixed Lagrangian. Different alternative variational integrators follow now from the selection of an appropriate quadrature rule to approximate the previous integral. We will use in particular a selective quadrature rule that combines midpoint integration (one single quadrature point at $t^{k+\beta}$) for the kinetic energy term and Lagrange multiplier term, combined with a trapezoidal rule (two quadrature points sampled at $t^{k+\alpha}=(1-\alpha)\,t^k+(\alpha)\,t^{k+1}$ and $t^{k+1-\alpha}=(\alpha)\,t^k+(1-\alpha)\,t^{k+1}$) for the potential energy term I_h (see §2.1.11), equations (2.20), (2.21), (2.22)). The discrete mixed Lagrangian thus obtained is

$$\begin{aligned}L_d^{mix}\left(\mathbf{q}_h^k,\mathbf{q}_h^{k+1},\mathbf{V}_h^{k+\beta},t^k,t^{k+1}\right) &= \left(t^{k+1}-t^k\right)\left(\frac{1}{2}\mathbf{V}_h^{(k+\beta)T}\mathbf{m}_h^{k+\beta}\mathbf{V}_h^{k+\beta}-\frac{1}{2}\left(I_h^{k+\alpha}+I_h^{k+1-\alpha}\right)\right)+\\ &+\left(t^{k+1}-t^k\right)\left(\mathbf{V}_h^{(k+\beta)T}\mathbf{m}_h^{k+\beta}\left(\mathbb{N}_h^{*(k+\beta)}\frac{\mathbf{q}_h^{k+1}-\mathbf{q}_h^k}{t^{k+1}-t^k}-\mathbf{V}_h^{k+\beta}\right)\right)\end{aligned}$$

where

$$\begin{aligned}I_h^{k+\alpha} &= I_h\left(\mathbf{q}_h^{k+\alpha}\right)\\ I_h^{k+1-\alpha} &= I_h\left(\mathbf{q}_h^{k+1-\alpha}\right)\\ \mathbf{m}_h^{k+\beta} &= \mathbf{m}_h\left(\mathbf{q}_h^{k+\beta}\right)\\ \mathbb{N}_h^{*(k+\beta)} &= \mathbb{N}_h^*\left(\mathbf{q}_h^{k+\beta}\right)=\mathbf{m}_h^{-1}\left(\mathbf{M}_h,\mathbf{m}_h\right)\big|_{\mathbf{q}_h^{k+\beta}}\end{aligned}$$

with

$$\begin{aligned}\mathbf{q}_h^{k+\beta} &= (1-\beta)\,\mathbf{q}_h^k+(\beta)\,\mathbf{q}_h^{k+1}\\ \mathbf{V}_h^{k+\beta} &= (1-\beta)\,\mathbf{V}_h^k+(\beta)\,\mathbf{V}_h^{k+1}\\ \mathbf{q}_h^{k+\alpha} &= (1-\alpha)\,\mathbf{q}_h^k+(\alpha)\,\mathbf{q}_h^{k+1}\\ \mathbf{q}_h^{k+1-\alpha} &= (\alpha)\,\mathbf{q}_h^k+(1-a)\,\mathbf{q}_h^{k+1}\end{aligned}$$

and $\alpha,\beta\in[0,1]$ are integration parameters. In terms of the individual dynamic variables $(\mathbf{X}_h,\mathbf{x}_h)$

the discrete-mixed Lagrangian reads

$$L_d^{mix}\left(\mathbf{X}_h^k, \mathbf{x}_h^k, \mathbf{X}_h^{k+1}, \mathbf{x}_h^{k+1}, \mathbf{V}_h^{k+\beta}, t^k, t^{k+1}\right) =$$
$$= \left(t^{k+1}-t^k\right)\left(\frac{1}{2}\mathbf{V}_h^{(k+\beta)T}\mathbf{m}_h^{k+\beta}\mathbf{V}_h^{n+\beta} - \frac{1}{2}\left(I_h^{k+\alpha}+I_h^{k+1-\alpha}\right)\right) +$$
$$+\left(t^{k+1}-t^k\right)\mathbf{V}_h^{(k+\beta)T}\left(\left(\mathbf{M}_h^{k+\beta}, \mathbf{m}_h^{k+\beta}\right)\left(\begin{array}{c}\frac{\mathbf{X}_h^{k+1}-\mathbf{X}_h^k}{t^{k+1}-t^k}\\ \frac{\mathbf{x}_h^{k+1}-\mathbf{x}_h^k}{t^{k+1}-t^k}\end{array}\right) - \mathbf{m}_h^{k+\beta}\mathbf{V}_h^{k+\beta}\right) \tag{6.85}$$

The discrete action sum expands in this case to the form

$$S_d\left(\cdots, \mathbf{X}_h^k, \cdots, \mathbf{x}_h^k, \cdots, \mathbf{V}_h^{k+\beta}, \cdots, t^k, \cdots\right) = \sum_{k=0}^{K} L_d^{mix}\left(\mathbf{X}_h^k, \mathbf{x}_h^k, \mathbf{X}_h^{k+1}, \mathbf{x}_h^{k+1}, \mathbf{V}_h^{k+\beta}, t^k, t^{k+1}\right) \tag{6.86}$$

Discrete trajectories are next obtained by invoking the stationarity of the discrete-mixed action sum S_d with respect to variations of all of its argument. The resulting variational principle will be referred to as the "mixed" discrete Hamilton's principle:

$$\begin{aligned}\frac{\partial S_d}{\partial \mathbf{X}_h^k} &= \mathbf{0}\\ \frac{\partial S_d}{\partial \mathbf{x}_h^k} &= \mathbf{0}\\ \frac{\partial S_d}{\partial \mathbf{V}_h^{k+\beta}} &= \mathbf{0}\end{aligned}$$

It bears emphasis that only one single velocity sample $V^{k+\beta}$ per time interval $[t_k, t_{k+1}]$ is taken.

6.2.2 Discrete Euler-Lagrange equations

We next turn to the derivation of the discrete Euler-Lagrange equations. Differentiating the discrete-mixed action sum S_d (6.83) with discrete-mixed Lagrangian (6.84), the following *discrete-mixed Euler-Lagrange* equations are obtained (see equations (2.21), (2.22))

$$\begin{aligned}D_1 L_d^{mix}\left(\mathbf{q}_h^k, \mathbf{q}_h^{k+1}, \mathbf{V}_h^{k+\beta}, t^k, t^{k+1}\right) + D_2 L_d^{mix}\left(\mathbf{q}_h^{k-1}, \mathbf{q}_h^k, \mathbf{V}_h^{k-1+\beta}, t^{k-1}, t^k\right) &= \mathbf{0}\\ D_3 L_d^{mix}\left(\mathbf{q}_h^k, \mathbf{q}_h^{k+1}, \mathbf{V}_h^{k+\beta}, t^k, t^{k+1}\right) &= \mathbf{0}\end{aligned}$$

that evaluate to

$$\begin{pmatrix} \mathbf{M}_h^{(k+\beta)T} \\ \mathbf{m}_h^{(k+\beta)T} \end{pmatrix} \mathbf{V}_h^{k+\beta} - \begin{pmatrix} \mathbf{M}_h^{(k-1+\beta)T} \\ \mathbf{m}_h^{(k-1+\beta)T} \end{pmatrix} \mathbf{V}_h^{k-1+\beta} = (1-\beta)\left(t^{k+1}-t^k\right) \begin{pmatrix} \mathbf{E}_h^{k+\beta} \\ \mathbf{e}_h^{k+\beta} \end{pmatrix}$$
$$+ (\beta)\left(t^k - t^{k-1}\right) \begin{pmatrix} \mathbf{E}_h^{k-1+\beta} \\ \mathbf{e}_h^{k-1+\beta} \end{pmatrix}$$
$$+ \frac{t^{k+1}-t^k}{2} \begin{pmatrix} (1-\alpha)\,\mathbf{F}_h^{k+\alpha} + (\alpha)\,\mathbf{F}_h^{k+1-\alpha} \\ (1-\alpha)\,\mathbf{f}_h^{k+\alpha} + (\alpha)\,\mathbf{f}_h^{k+1-\alpha} \end{pmatrix}$$
$$+ \frac{t^k-t^{k-1}}{2} \begin{pmatrix} (\alpha)\,\mathbf{F}_h^{k-1+\alpha} + (1-\alpha)\,\mathbf{F}_h^{k-\alpha} \\ (\alpha)\,\mathbf{f}_h^{k-1+\alpha} + (1-\alpha)\,\mathbf{f}_h^{k-\alpha} \end{pmatrix}$$

$$\mathbf{0} = \left(\mathbf{M}_h^{n+\beta}, \mathbf{m}_h^{n+\beta}\right) \begin{pmatrix} \frac{\mathbf{X}_h^{n+1}-\mathbf{X}_h^{n+1}}{\Delta t} \\ \frac{\mathbf{x}_h^{n+1}-\mathbf{x}_h^{n+1}}{\Delta t} \end{pmatrix} - \mathbf{m}_h^{n+\beta}\mathbf{V}_h^{n+\beta}$$

where

$$\begin{aligned} \mathbf{E}_h^{k+\beta} &= \mathbf{E}_h\left(\mathbf{X}_h^{k+\beta}, \mathbf{x}_h^{k+\beta}, \frac{\mathbf{X}_h^{n+1}-\mathbf{X}_h^{n+1}}{\Delta t}, \frac{\mathbf{x}_h^{n+1}-\mathbf{x}_h^{n+1}}{\Delta t}, \mathbf{V}_h^{k+\beta}\right) \\ \mathbf{e}_h^{k+\beta} &= \mathbf{e}_h\left(\mathbf{X}_h^{k+\beta}, \mathbf{x}_h^{k+\beta}, \frac{\mathbf{X}_h^{n+1}-\mathbf{X}_h^{n+1}}{\Delta t}, \frac{\mathbf{x}_h^{n+1}-\mathbf{x}_h^{n+1}}{\Delta t}, \mathbf{V}_h^{k+\beta}\right) \end{aligned}$$

and

$$\begin{pmatrix} \mathbf{F}_h^{k+\alpha} \\ \mathbf{f}_h^{k+\alpha} \end{pmatrix} = \begin{pmatrix} \mathbf{F}_h\left(\mathbf{q}_h^{k+\alpha}\right) \\ \mathbf{f}_h\left(\mathbf{q}_h^{k+\alpha}\right) \end{pmatrix}$$

$$\begin{pmatrix} \mathbf{F}_h^{k+1-\alpha} \\ \mathbf{f}_h^{k+1-\alpha} \end{pmatrix} = \begin{pmatrix} \mathbf{F}_h\left(\mathbf{q}_h^{k+1-\alpha}\right) \\ \mathbf{f}_h\left(\mathbf{q}_h^{k+1-\alpha}\right) \end{pmatrix}$$

and with $\mathbf{E}_h, \mathbf{e}_h, \mathbf{F}_h, \mathbf{f}_h$ defined in (6.34), (6.35), (6.32), (6.33), (6.39), (6.40), (6.41), and (6.42).

For implementation purposes it result more convenient to rewrite the discrete Euler-Lagrange equations in the so-called "position-momentum" form. To this end we define the discrete momentum $\boldsymbol{\pi}_h^k$ at time k to be

$$\boldsymbol{\pi}_h^k = D_2 L_d^{mix}\left(\mathbf{q}_h^{k-1}, \mathbf{q}_h^k, \mathbf{V}_h^{k-1+\beta}, t^k, t^{k+1}\right) = -D_1 L_d^{mix}\left(\mathbf{q}_h^k, \mathbf{q}_h^{k+1}, \mathbf{V}_h^{k+\beta}, t^k, t^{k+1}\right) \tag{6.87}$$

whereupon the discrete-mixed Euler-Lagrange equations take the form

$$\begin{aligned} \boldsymbol{\pi}_h^k &= -D_1 L_d^{mix}\left(\mathbf{q}_h^k, \mathbf{q}_h^{k+1}, \mathbf{V}_h^{k+\beta}, t^k, t^{k+1}\right) \\ \boldsymbol{\pi}_h^{k+1} &= D_2 L_d^{mix}\left(\mathbf{q}_h^k, \mathbf{q}_h^{k+1}, \mathbf{V}_h^{k+\beta}, t^k, t^{k+1}\right) \\ \mathbf{0} &= D_3 L_d^{mix}\left(\mathbf{q}_h^k, \mathbf{q}_h^{k+1}, \mathbf{V}_h^{k+\beta}, t^k, t^{k+1}\right) \end{aligned}$$

Using the given form of L_d^{mix} the previous evaluates to

$$\begin{aligned}
\begin{pmatrix} \mathbf{P}_h^k \\ \mathbf{p}_h^k \end{pmatrix} &= \begin{pmatrix} \mathbf{M}_h^{(k+\beta)T} \\ \mathbf{m}_h^{(k+\beta)T} \end{pmatrix} \mathbf{V}_h^{k+\beta} - (1-\beta)\left(t^{k+1}-t^k\right) \begin{pmatrix} \mathbf{E}_h^{k+\beta} \\ \mathbf{e}_h^{k+\beta} \end{pmatrix} \\
&\quad - \frac{t^{k+1}-t^k}{2} \begin{pmatrix} (1-\alpha)\,\mathbf{F}_h^{k+\alpha} + (\alpha)\,\mathbf{F}_h^{k+1-\alpha} \\ (1-\alpha)\,\mathbf{f}_h^{k+\alpha} + (\alpha)\,\mathbf{f}_h^{k+1-\alpha} \end{pmatrix} \\
\begin{pmatrix} \mathbf{P}_h^{k+1} \\ \mathbf{p}_h^{k+1} \end{pmatrix} &= \begin{pmatrix} \mathbf{M}_h^{(k+\beta)T} \\ \mathbf{m}_h^{(k+\beta)T} \end{pmatrix} \mathbf{V}_h^{k+\beta} + (\beta)\left(t^{k+1}-t^k\right) \begin{pmatrix} \mathbf{E}_h^{k+\beta} \\ \mathbf{e}_h^{k+\beta} \end{pmatrix} \\
&\quad + \frac{t^{k+1}-t^k}{2} \begin{pmatrix} (1-\alpha)\,\mathbf{F}_h^{k+\alpha} + (\alpha)\,\mathbf{F}_h^{k+1-\alpha} \\ (1-\alpha)\,\mathbf{f}_h^{k+\alpha} + (\alpha)\,\mathbf{f}_h^{k+1-\alpha} \end{pmatrix}
\end{aligned}$$

$$\mathbf{0} = \left(\mathbf{M}_h^{n+\beta}, \mathbf{m}_h^{n+\beta}\right) \begin{pmatrix} \frac{\mathbf{X}_h^{n+1}-\mathbf{X}_h^{n+1}}{\Delta t} \\ \frac{\mathbf{x}_h^{n+1}-\mathbf{x}_h^{n+1}}{\Delta t} \end{pmatrix} - \mathbf{m}_h^{n+\beta}\mathbf{V}_h^{n+\beta}$$

where

$$\boldsymbol{\pi}_h = \begin{pmatrix} \mathbf{P}_h \\ \mathbf{p}_h \end{pmatrix} \tag{6.88}$$

is an array that collects horizontal and vertical discrete momentum $\mathbf{P}_h$ and $\mathbf{p}_h$. Given $\left(\mathbf{q}_h^k, \boldsymbol{\pi}_h^k\right)$ the first and third equations represent an implicitly system to solve for the unknowns $\left(\mathbf{q}_h^{k+1}, \mathbf{V}_h^{k+\beta}\right)$. Using this result we then obtain $\boldsymbol{\pi}^{k+1}$ by evaluating the second equation.

6.2.3 Comparison with Lagrangian system with constant inertia

It becomes useful at this point to compare the obtained discrete Euler-Lagrange equations with those corresponding to a Lagrangian system with constant inertia. In this case the discrete-mixed Lagrangian reduces to

$$\begin{aligned}
L_d^{mix}\left(\mathbf{q}_h^k, \mathbf{q}_h^{k+1}, \mathbf{V}_h^{k+\beta}, t^k, t^{k+1}\right) &= \left(t^{k+1}-t^k\right)\left(\frac{1}{2}\mathbf{V}_h^{(k+\beta)T}\mathbf{m}_h\mathbf{V}_h^{k+\beta} - \frac{1}{2}\left(I_h^{k+\alpha} + I_h^{k+1-\alpha}\right)\right) + \\
&\quad + \left(t^{k+1}-t^k\right)\left(\mathbf{V}_h^{(k+\beta)T}\mathbf{m}_h\left(\mathbb{N}_h^*\frac{\mathbf{q}^{k+1}-\mathbf{q}^k}{t^{k+1}-t^k} - \mathbf{V}_h^{k+\beta}\right)\right)
\end{aligned}$$

with corresponding discrete-mixed Euler-Lagrange equations given by

$$\begin{aligned}
\mathbb{N}_h\mathbf{m}_h^T\left(\mathbf{V}_h^{k+\beta} - \mathbf{V}_h^{k-1+\beta}\right) &= -\frac{t^{k+1}-t^k}{2}\left((1-\alpha)\frac{\partial I_h^{k+\alpha}}{\partial \mathbf{q}_h} + (\alpha)\frac{\partial I_h^{k+1-\alpha}}{\partial \mathbf{q}_h}\right) \\
&\quad - \frac{t^k-t^{k-1}}{2}\left((1-\alpha)\frac{\partial I_h^{k-1+\alpha}}{\partial \mathbf{q}_h} + (\alpha)\frac{\partial I_h^{k-\alpha}}{\partial \mathbf{q}_h}\right) \\
\mathbf{0} &= \mathbb{N}_h^*\frac{\mathbf{q}^{k+1}-\mathbf{q}^k}{t^{k+1}-t^k} - \mathbf{V}_h^{k+\beta}
\end{aligned}$$

Eliminating velocities from the second equation we obtain

$$\mathbb{M}_h \left(\frac{\mathbf{q}^{k+1} - \mathbf{q}^k}{t^{k+1} - t^k} - \frac{\mathbf{q}^k - \mathbf{q}^{k-1}}{t^k - t^{k-1}} \right) = -\frac{t^{k+1} - t^k}{2} \left((1-\alpha) \frac{\partial I_h^{k+\alpha}}{\partial \mathbf{q}_h} + (\alpha) \frac{\partial I_h^{k+1-\alpha}}{\partial \mathbf{q}_h} \right) - \frac{t^k - t^{k-1}}{2} \left((1-\alpha) \frac{\partial I_h^{k-1+\alpha}}{\partial \mathbf{q}_h} + (\alpha) \frac{\partial I_h^{k-\alpha}}{\partial \mathbf{q}_h} \right)$$

where

$$\mathbb{M}_h = \mathbb{N}_h \mathbf{m}_h^T \mathbb{N}_h^*$$

is the mass matrix. These equations correspond to the Euler-Lagrange equations of the standard single-field discrete Lagrangian

$$L_d \left(\mathbf{q}_h^k, \mathbf{q}_h^{k+1}, t^k, t^{k+1} \right) = \left(t^{k+1} - t^k \right) \left(\frac{1}{2} \left(\frac{\mathbf{q}^{k+1} - \mathbf{q}^k}{t^{k+1} - t^k} \right)^T \mathbb{M}_h \left(\frac{\mathbf{q}^{k+1} - \mathbf{q}^k}{t^{k+1} - t^k} \right) - \frac{1}{2} \left(I_h^{k+\alpha} + I_h^{k+1-\alpha} \right) \right)$$

As was shown in [20], for the particular case of affine forces, i.e., when the forces have the property

$$\frac{\partial I_h^{k+\alpha}}{\partial \mathbf{q}_h} = (1-\alpha) \frac{\partial I_h^k}{\partial \mathbf{q}_h} + (\alpha) \frac{\partial I_h^{k+1}}{\partial \mathbf{q}_h}$$

this integrator is equivalent to the implicit Newmark integrator with $\gamma = \frac{1}{2}$ and $\beta = \alpha (1 - \alpha)$. The proposed variational integrator is its generalization for configuration-dependent inertia.

6.2.4 Discrete-mixed Lagrange-d'Alembert principle

In this subsection we extend the discrete-mixed Hamilton's principle developed in the previous section to systems with viscous effects. This is accomplished by discretizing in time the semidiscrete Lagrange-d'Alembert principle ((6.79), (6.80)). We recall that this variational principle can be written as

$$\begin{aligned} \langle \delta S_h, \delta \mathbf{X}_h \rangle + \langle \delta S_h, \delta \mathbf{x}_h \rangle - \int_{t_0}^{t_f} (\delta \mathbf{X}_h, \delta \mathbf{x}_h) \begin{pmatrix} \mathbf{F}_h^v + \mathbf{F}_h^{v-reg} \\ \mathbf{f}_h^v \end{pmatrix} dt &= \mathbf{0} \qquad \forall (\delta \mathbf{X}_h, \delta \mathbf{x}_h) \\ \langle \delta S_h, \delta \mathbf{V}_h \rangle &= \mathbf{0} \qquad \forall \delta \mathbf{V}_h \end{aligned}$$

with mechanical (vertical) viscous forces $\mathbf{f}_h^v$ given in (6.71) and (6.73), configurational (horizontal) forces computed from (6.77), and horizontal regularization forces defined in (6.78). We notice also that these viscous forces depend on the dynamical variables in the form

$$\begin{aligned}\mathbf{f}_h^v &= \mathbf{f}_h^v\left(\mathbf{X}_h, \mathbf{x}_h, \mathbf{V}_h\right)\\ \mathbf{F}_h^v &= \mathbf{F}_h^v\left(\mathbf{X}_h, \mathbf{x}_h, \mathbf{V}_h\right)\\ \mathbf{F}_h^{v-reg} &= \mathbf{F}_h^{v-reg}\left(\mathbf{X}_h, \dot{\mathbf{X}}_h\right)\end{aligned}$$

The above principle may be compactly expressed as

$$\langle \delta S_h, \delta \mathbf{q}_h \rangle + \int_{t_0}^{t_f} \delta \mathbf{q}_h^T \cdot \mathbb{F}^v\left(\mathbf{q}_h, \dot{\mathbf{q}}_h, \mathbf{V}_h\right) dt = 0$$

where $\mathbf{q}_h = \{\mathbf{X}_h, \mathbf{x}_h\}$ and

$$\mathbb{F}^v\left(\mathbf{q}_h, \dot{\mathbf{q}}_h \mathbf{V}_h\right) = \begin{pmatrix} \mathbf{F}_h^v + \mathbf{F}_h^{v-reg} \\ \mathbf{f}_h^v \end{pmatrix}$$

are arrays that collects respectively the viscous physical and regularization forces.

Following the ideas presented in [20] we may discretize in time the semidiscrete Lagrange-d'Alembert principle in the form

$$0 = \left\langle \delta S_d, \delta \mathbf{q}_h^k \right\rangle + \sum_{k=0}^{K} \left(\delta \mathbf{q}_h^k\right)^T \cdot \mathbb{F}^{v-}\left(\mathbf{q}_h^k, \mathbf{q}_h^{k+1}, \mathbf{V}_h^{k+\beta}, t^k, t^{k+1}\right) + \left(\delta \mathbf{q}_h^{k+1}\right)^T \cdot \mathbb{F}^{v+}\left(\mathbf{q}_h^k, \mathbf{q}_h^{k+1}, \mathbf{V}_h^{k+\beta}, t^k, t^{k+1}\right)$$

where $\mathbb{F}^{v-}$ and $\mathbb{F}^{v+}$ are the left and right discrete viscous forces that should satisfy the identity

$$\begin{aligned}\int_{t^k}^{t^{k+1}} \delta \mathbf{q}_h^T \cdot \mathbb{F}^v\left(\mathbf{q}_h(t), \mathbf{V}_h(t)\right) dt &= \left(\delta \mathbf{q}_h^k\right)^T \cdot \mathbb{F}^{v-}\left(\mathbf{q}_h^k, \mathbf{q}_h^{k+1}, \mathbf{V}_h^{k+\beta}, t^k, t^{k+1}\right)\\ &\quad + \left(\delta \mathbf{q}_h^{k+1}\right)^T \cdot \mathbb{F}^{v+}\left(\mathbf{q}_h^k, \mathbf{q}_h^{k+1}, \mathbf{V}_h^{k+\beta}, t^k, t^{k+1}\right)\end{aligned}$$

and where only one velocity sample for the whole time interval $[t_k, t_{k+1}]$ is used. For simplicity this velocity is taken to coincide with that used for the kinetic energy term, namely $\mathbf{V}_h^{n+\beta}$. The corresponding discrete Euler-Lagrange equations follow as

$$\begin{aligned}\mathbf{0} &= D_1 L_d^{mix}\left(\mathbf{q}_h^k, \mathbf{q}_h^{k+1}, \mathbf{V}_h^{k+\beta}, t^k, t^{k+1}\right) + D_2 L_d^{mix}\left(\mathbf{q}_h^{k-1}, \mathbf{q}_h^k, \mathbf{V}_h^{k-1+\beta}, t^{k-1}, t^k\right) + \\ &\quad + \mathbb{F}^{v-}\left(\mathbf{q}_h^k, \mathbf{q}_h^{k+1}, \mathbf{V}_h^{k+\beta}, t^k, t^{k+1}\right) + \mathbb{F}^{v+1}\left(\mathbf{q}_h^{k-1}, \mathbf{q}_h^k, \mathbf{V}_h^{k-1+\beta}, t^{k-1}, t^k\right)\\ \mathbf{0} &= D_3 L_d^{mix}\left(\mathbf{q}_h^k, \mathbf{q}_h^{k+1}, \mathbf{V}_h^{k+\beta}, t^k, t^{k+1}\right)\end{aligned}$$

The left and right physical and regularization viscous forces may be chosen to be simply

$$\begin{aligned}
\mathbb{F}^{v-}\left(\mathbf{q}_h^k, \mathbf{q}_h^{k+1}, \mathbf{V}_h^k, \mathbf{V}_h^{k+1}, t^k, t^{k+1}\right) &= (1-\gamma)\left(t^{k+1}-t^k\right)\mathbb{F}^v\left(\mathbf{q}_h^{k+\beta}, \frac{\mathbf{q}_h^{k+1}-\mathbf{q}_h^k}{t^{k+1}-t^k}, \mathbf{V}_h^{k+\beta}\right) \\
\mathbb{F}^{v+}\left(\mathbf{q}_h^k, \mathbf{q}_h^{k+1}, \mathbf{V}_h^k, \mathbf{V}_h^{k+1}, t^k, t^{k+1}\right) &= (\gamma)\left(t^{k+1}-t^k\right)\mathbb{F}^v\left(\mathbf{q}_h^{k+\beta}, \frac{\mathbf{q}_h^{k+1}-\mathbf{q}_h^k}{t^{k+1}-t^k}, \mathbf{V}_h^{k+\beta}\right)
\end{aligned}$$

where $\gamma \in [0,1]$ is a new integration parameter.

In terms of the individual dynamic variables $(\mathbf{X}_h, \mathbf{x}_h, \mathbf{V}_h)$ the discrete-mixed Euler-Lagrange equations evaluates to

$$\begin{aligned}
\begin{pmatrix} \mathbf{M}_h^{(k+\beta)T} \\ \mathbf{m}_h^{(k+\beta)T} \end{pmatrix}\mathbf{V}_h^{k+\beta} - \begin{pmatrix} \mathbf{M}_h^{(k-1+\beta)T} \\ \mathbf{m}_h^{(k-1+\beta)T} \end{pmatrix}\mathbf{V}_h^{k-1+\beta} &= \frac{t^{k+1}-t^k}{2}\begin{pmatrix} (1-\alpha)\,\mathbf{F}_h^{k+\alpha} + (\alpha)\,\mathbf{F}_h^{k+1-\alpha} \\ (1-\alpha)\,\mathbf{f}_h^{k+\alpha} + (\alpha)\,\mathbf{f}_h^{k+1-\alpha} \end{pmatrix} \\
&+ \frac{t^k-t^{k-1}}{2}\begin{pmatrix} (\alpha)\,\mathbf{F}_h^{k-1+\alpha} + (1-\alpha)\,\mathbf{F}_h^{k-\alpha} \\ (\alpha)\,\mathbf{f}_h^{k-1+\alpha} + (1-\alpha)\,\mathbf{f}_h^{k-\alpha} \end{pmatrix} \\
&+ (1-\beta)\left(t^{k+1}-t^k\right)\begin{pmatrix} \mathbf{E}_h^{k+\beta} \\ \mathbf{e}_h^{k+\beta} \end{pmatrix} \\
&+ (\beta)\left(t^k-t^{k-1}\right)\begin{pmatrix} \mathbf{E}_h^{k-1+\beta} \\ \mathbf{e}_h^{k-1+\beta} \end{pmatrix} \\
&+ (1-\gamma)\left(t^{k+1}-t^k\right)\begin{pmatrix} \left(\mathbf{F}_h^v\right)^{k+\beta} + \left(\mathbf{F}_h^{v-reg}\right)^{k+\beta} \\ \left(\mathbf{f}_h^v\right)^{k+\beta} \end{pmatrix} + \\
&+ (\gamma)\left(t^k-t^{k-1}\right)\begin{pmatrix} \left(\mathbf{F}_h^v\right)^{k-1+\beta} + \left(\mathbf{F}_h^{v-reg}\right)^{k-1+\beta} \\ \left(\mathbf{f}_h^v\right)^{k-1+\beta} \end{pmatrix}
\end{aligned}$$

$$\mathbf{0} = \left(\mathbf{M}_h^{n+\beta}, \mathbf{m}_h^{n+\beta}\right)\begin{pmatrix} \frac{\mathbf{X}_h^{n+1}-\mathbf{X}_h^{n+1}}{\Delta t} \\ \frac{\mathbf{x}_h^{n+1}-\mathbf{x}_h^{n+1}}{\Delta t} \end{pmatrix} - \mathbf{m}_h^{n+\beta}\mathbf{V}_h^{n+\beta}$$

where

$$\begin{aligned}
\left(\mathbf{f}_h^v\right)^{k+\beta} &= \mathbf{f}_h^v\left(\mathbf{X}_h^{k+\beta}, \mathbf{x}_h^{k+\beta}, \mathbf{V}_h^{k+\beta}\right) \\
\left(\mathbf{F}_h^v\right)^{k+\beta} &= \mathbf{F}_h^v\left(\mathbf{X}_h^{k+\beta}, \mathbf{x}_h^{k+\beta}, \mathbf{V}_h^{k+\beta}\right) \\
\left(\mathbf{F}_h^{v-reg}\right)^{k+\beta} &= \mathbf{F}_h^{v-reg}\left(\mathbf{X}_h^{k+\beta}, \frac{\mathbf{X}_h^{k+1}-\mathbf{X}_h^k}{t^{k+1}-t^k}\right)
\end{aligned}$$

Using the discrete momentum definitions (6.87) and (6.88), the previous may be rewritten in the position-momentum form:

$$\begin{pmatrix} \mathbf{P}_h^k \\ \mathbf{p}_h^k \end{pmatrix} = \begin{pmatrix} \mathbf{M}_h^{(k+\beta)T} \\ \mathbf{m}_h^{(k+\beta)T} \end{pmatrix} \mathbf{V}_h^{k+\beta} - \frac{t^{k+1}-t^k}{2} \begin{pmatrix} (1-\alpha)\,\mathbf{F}_h^{k+\alpha} + (\alpha)\,\mathbf{F}_h^{k+1-\alpha} \\ (1-\alpha)\,\mathbf{f}_h^{k+\alpha} + (\alpha)\,\mathbf{f}_h^{k+1-\alpha} \end{pmatrix} + \\ - (1-\beta)\left(t^{k+1}-t^k\right) \begin{pmatrix} \mathbf{E}_h^{k+\beta} \\ \mathbf{e}_h^{k+\beta} \end{pmatrix} + \\ - (1-\gamma)\left(t^{k+1}-t^k\right) \begin{pmatrix} \left(\mathbf{F}_h^v\right)^{k+\beta} \\ \left(\mathbf{f}_h^v\right)^{k+\beta} \end{pmatrix} + \\ - (1-\delta)\left(t^{k+1}-t^k\right) \begin{pmatrix} \left(\mathbf{F}_h^{v-reg}\right)^{k+\beta} \\ \mathbf{0} \end{pmatrix} \tag{6.89}$$

$$\begin{pmatrix} \mathbf{P}_h^{k+1} \\ \mathbf{p}_h^{k+1} \end{pmatrix} = \begin{pmatrix} \mathbf{M}_h^{(k+\beta)T} \\ \mathbf{m}_h^{(k+\beta)T} \end{pmatrix} \mathbf{V}_h^{k+\beta} + \frac{t^{k+1}-t^k}{2} \begin{pmatrix} (1-\alpha)\,\mathbf{F}_h^{k+\alpha} + (\alpha)\,\mathbf{F}_h^{k+1-\alpha} \\ (1-\alpha)\,\mathbf{f}_h^{k+\alpha} + (\alpha)\,\mathbf{f}_h^{k+1-\alpha} \end{pmatrix} + \\ + (\beta)\left(t^{k+1}-t^k\right) \begin{pmatrix} \mathbf{E}_h^{k+\beta} \\ \mathbf{e}_h^{k+\beta} \end{pmatrix} \\ + (\gamma)\left(t^{k+1}-t^k\right) \begin{pmatrix} \left(\mathbf{F}_h^v\right)^{k+\beta} \\ \left(\mathbf{f}_h^v\right)^{k+\beta} \end{pmatrix} \\ + (\delta)\left(t^{k+1}-t^k\right) \begin{pmatrix} \left(\mathbf{F}_h^{v-reg}\right)^{k+\beta} \\ 0 \end{pmatrix} \tag{6.90}$$

$$\mathbf{0} = \left(\mathbf{M}_h^{n+\beta}, \mathbf{m}_h^{n+\beta}\right) \begin{pmatrix} \frac{\mathbf{X}_h^{n+1}-\mathbf{X}_h^{n+1}}{\Delta t} \\ \frac{\mathbf{x}_h^{n+1}-\mathbf{x}_h^{n+1}}{\Delta t} \end{pmatrix} - \mathbf{m}_h^{n+\beta}\mathbf{V}_h^{n+\beta} \tag{6.91}$$

where we are using a different integration parameters $\delta \in [0,1]$ in the viscous regularizing force. Given $\left(\mathbf{X}_h^k, \mathbf{x}_h^k, \mathbf{P}_h^k, \mathbf{p}_h^k\right)$ the first of the above equations (equation (6.89)) is a non-linear system to solve for $\left(\mathbf{X}_h^{k+1}, \mathbf{x}_h^{k+1}\right)$ with $\mathbf{V}_h^{k+\beta}$ given by the third equation (equation (6.91)). Once the first equation is solved, the second (equation (6.90)) yields the identity for the update of the momentum $\left(\mathbf{P}_h^{k+1}, \mathbf{p}_h^{k+1}\right)$.

Chapter 7

Numerical tests

In this section we present a collection of tests and examples designed to assess the performance of the method developed in the following. The first example is designed to measure the accuracy of the method and concern the propagation of compressive waves along a shock tube for which the exact analytical solution can be obtained in closed form. The solutions of both the one-dimensional and three-dimensional wave propagation problems are presented as well as a three-dimensional example where the wave propagates and expands along a tube with a non-uniform cross-section. The second example relates to the natural oscillation of a one-dimensional bar and illustrates how the node motion in the combined horizontal-vertical plane result constrained to oscillate within a manifold as predicted by the theory. The third example involves a block of non-linear elastic material subjected to the application of a moving point load, and the last example concerns the propagation of a crack along a preexisting crack path.

7.1 Shock propagation example

The first test involves the propagation of a plane wave travelling down a highly compressive material and has been used as a benchmark example to assess the convergence and accuracy of other mesh adaption strategies (c.f. [55]).

7.1.1 Analytical solution

Assume a solid body undergoing planar deformations in the direction of the X_1 axis. Then the motion may be fully described by a deformation mapping of the form $\boldsymbol{\varphi}\left(X_1, X_2, X_3, t\right) = \left(\varphi_1\left(X_1, t\right), X_2, X_3\right)$.

The corresponding deformation gradient will be

$$\mathbf{F} = \begin{pmatrix} \varphi_{1,1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

with rate of deformation

$$\mathbf{d} = \dot{\mathbf{F}}\mathbf{F}^{-1} = \begin{pmatrix} \frac{\dot{\varphi}_{1,1}}{\varphi_{1,1}} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

We assume that there are no body forces and that the material is homogeneous. Therefore the total energy density is dependent only on $\mathbf{F}$, i.e.,

$$W = W(\mathbf{F}) = W\left(\varphi_{1,1}\right)$$

The action will be given by

$$S(\varphi_1) = \int_{t_0}^{t_f} \int_{-\infty}^{\infty} \left(\frac{R}{2}\dot{\varphi}_1^2 - W\left(\varphi_{1,1}\right) \right) dX\, dt$$

where we assume that the body extends unbounded in the X_1 direction. The equations of balance of mechanical and configurational force balance (3.14) and (3.58) reduce in this case to

$$R\ddot{\varphi}_1 = P^e_{11,1} + P^v_{11,1} \tag{7.1}$$

$$R\left(-\varphi_{1,1}\right)\ddot{\varphi}_1 = C_{11,1} + \left(-\varphi_{1,1}\right) P^v_{11,1} \tag{7.2}$$

where P^e_{11} and C_{11} are, respectively, the equilibrium part of the first Piolla-Kirchhoff stress and the dynamic Eshelby stress given by

$$\begin{aligned} P^e_{11} &= \frac{\partial W}{\partial \varphi_{1,1}} \\ C_{11} &= \left(W - \frac{R}{2}\dot{\varphi}_1^2 \right) - \varphi_{1,1}\frac{\partial W}{\partial \varphi_{1,1}} \end{aligned}$$

and P^v_{11} is the viscous Newtonian stress given by (3.12) and (3.13), which in this one-dimensional case simplifies to

$$P^v_{11} = \frac{4}{3}\mu\frac{\dot{\varphi}_{1,1}}{\varphi_{1,1}}$$

Inserting the previous into (7.1) and (7.2) leads to the governing equations

$$\begin{aligned} R\ddot{\varphi}_1 &= \left(\frac{\partial W}{\partial \varphi_{1,1}} + \frac{4}{3}\mu \frac{\dot{\varphi}_{1,1}}{\varphi_{1,1}}\right)_{,1} \\ \frac{d}{dt}\left(R\left(-\varphi_{1,1}\right)\dot{\varphi}_1\right) &= \left(\left(W - \frac{R}{2}\dot{\varphi}_1^w\right) - \varphi_{1,1}\frac{\partial W}{\partial \varphi_{1,1}}\right)_{,1} + \left(-\varphi_{1,1}\right)\left(\frac{4}{3}\mu \frac{\dot{\varphi}_{1,1}}{\varphi_{1,1}}\right)_{,1} \end{aligned}$$

For a certain simple class of constitutive relations $W(F)$, the solution of the previous can be carried out analytically. A particular example is the constitutive equation

$$W(J) = \frac{K}{4}\left(J^2 - 1 - 2\log(J)\right)$$

where $J = \det(\mathbf{F})$. In this case the analytical solution is given by

$$\frac{\varphi_1(X_1, t) - X_1}{l} = f\left(\frac{X_1 - ct}{l}\right)$$

where

$$\begin{aligned} f(\eta) &= \left(\frac{J^+ + J^-}{2} - 1\right)\eta + \left(J^+ - J^-\right)\log\left(\frac{1}{2}\cosh\left(\frac{\eta}{2}\right)\right) && (7.3) \\ c^2 &= \frac{K}{2R}\left(1 + \frac{1}{J^-J^+}\right) && (7.4) \\ l &= \frac{8\mu c}{3K}\frac{J^-J^+}{J^+ - J^-} && (7.5) \end{aligned}$$

and J^+ and J^- are given boundary conditions

$$J^{\pm} = \lim_{X_1 \to \pm\infty} \varphi_{1,1}(X_1, t)$$

The velocity field is given by

$$\dot{\varphi}_1 = -cf'\left(\frac{X_1 - ct}{l}\right)$$

where

$$f'(\eta) = \left(\frac{J^+ + J^-}{2} - 1\right) + \frac{J^+ - J^-}{2}\tanh\left(\frac{\eta}{2}\right)$$

The analytical solution for the displacement $u_1 = \varphi_1 - X_1$, velocity $\dot{\varphi}_1$, deformation gradient $\varphi_{1,1}$ and acceleration fields $\ddot{\varphi}_1$ is shown in figure 7.1 for the following parameters

R	1
K	1
μ	0.025
J^-	1
J^+	0.1

The analytic computed value for the shock velocity is in this case

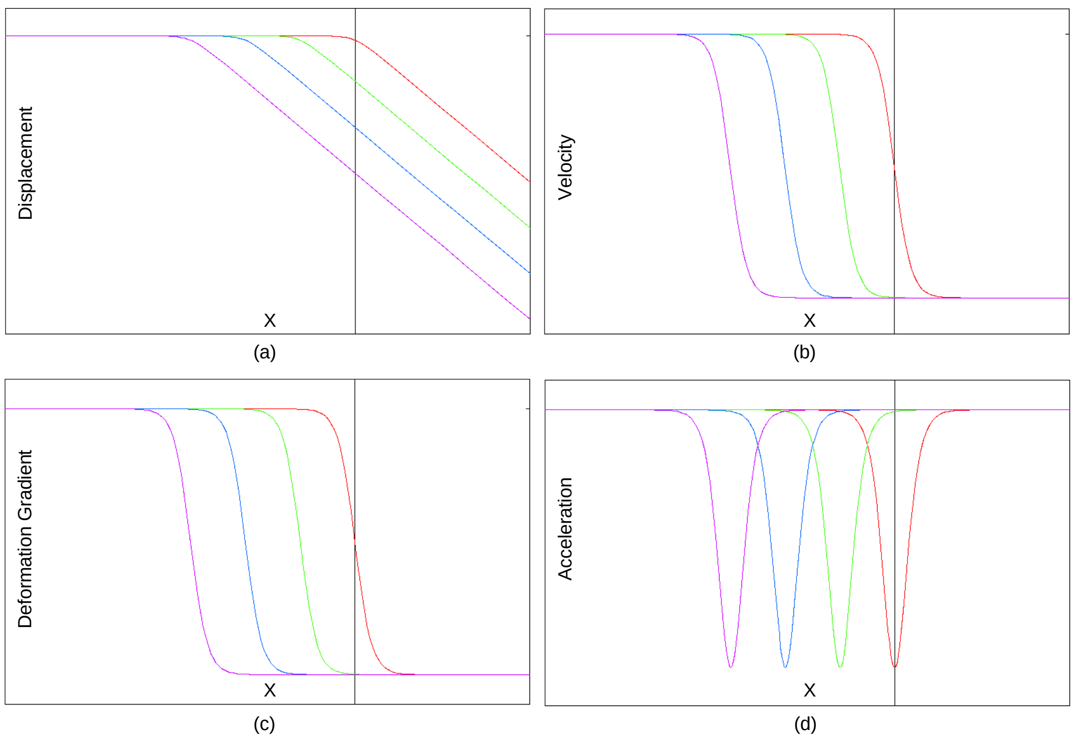

Figure 7.1: Propagation of a planar isothermal compression shock. Time evolution of (a) displacement, (b) velocity, (c) deformation gradient, and (d) acceleration fields. Analytical solution.

$$c = \sqrt{5.5} \simeq 2.3452$$

and the corresponding computed shock thickness is

$$l = 1.737\,2 \times 10^{-2}$$

The problem is solved both using a one-dimensional and a three-dimensional model. The domain of analysis is discretized using linear elements in one dimensions and four-noded linear tetrahedral elements in three dimensions. The governing equations are discretized in time using the mixed variational integrator described in §6.2.1 and §6.2.2, (see equations (6.89), (6.90) and (6.91)) with integration parameters $\alpha = \frac{1}{2}$, $\beta = \frac{1}{2}$, $\gamma = \frac{1}{2}$, $\delta = 0$. The non-linear system of equations (6.89) for the update of referencial and spatial nodal coordinates is solved using the Polak-Ribiere variant of the non-linear conjugate-gradient method. A stable time step was estimated as

$$\Delta t \leq \frac{h_{\min}}{c}$$

where $h_{\min}$ is the measure of the element size and c is the shock velocity given by (7.4). The parameters listed in table 1 are used in the calculations. The length of the domain of analysis is $L = 70l$ where l is the length of the shock, computed from (7.4).

Figure (7.2) shows the convergence curves. The accuracy of the solution is measured using the $L_2\left(B \times [t_0, t_f]\right)$ norm of the difference between the analytic and finite element solutions of deformations and velocity fields, namely,

$$\begin{aligned} \|\boldsymbol{\varphi} - \boldsymbol{\varphi}_h\|_{L_2(B\times[t_0,t_f])} &= \int_{t_0}^{t_f} \int_B \|\boldsymbol{\varphi} - \boldsymbol{\varphi}_h\|^2 \, dV \, dt \\ \|\mathbf{V} - \mathbf{V}_h\|_{L_2(B\times[t_0,t_f])} &= \int_{t_0}^{t_f} \int_B \|\mathbf{V} - \mathbf{V}_h\|^2 \, dV \, dt \end{aligned}$$

These errors are plotted against the number of degrees of freedom in a log-log axes. Figure (7.3) and

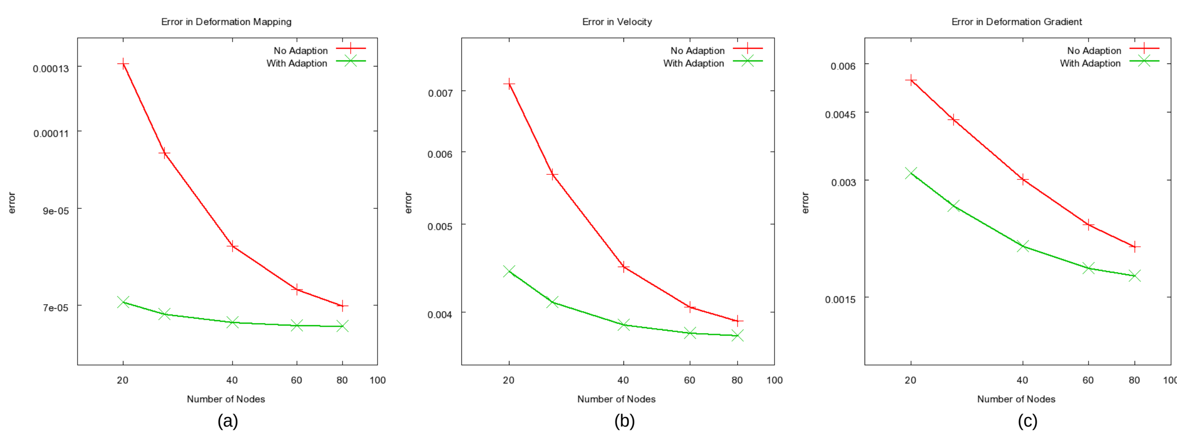

Figure 7.2: Convergence plot for isothermal compressive shock example. (a) Displacement field. (b) Velocity field. (c) Deformation gradient.

(7.4) show the time evolution of the deformation mapping and material velocity fields along with the node trajectory. Figure (7.5) displays the time evolution of nodes in the reference configuration.

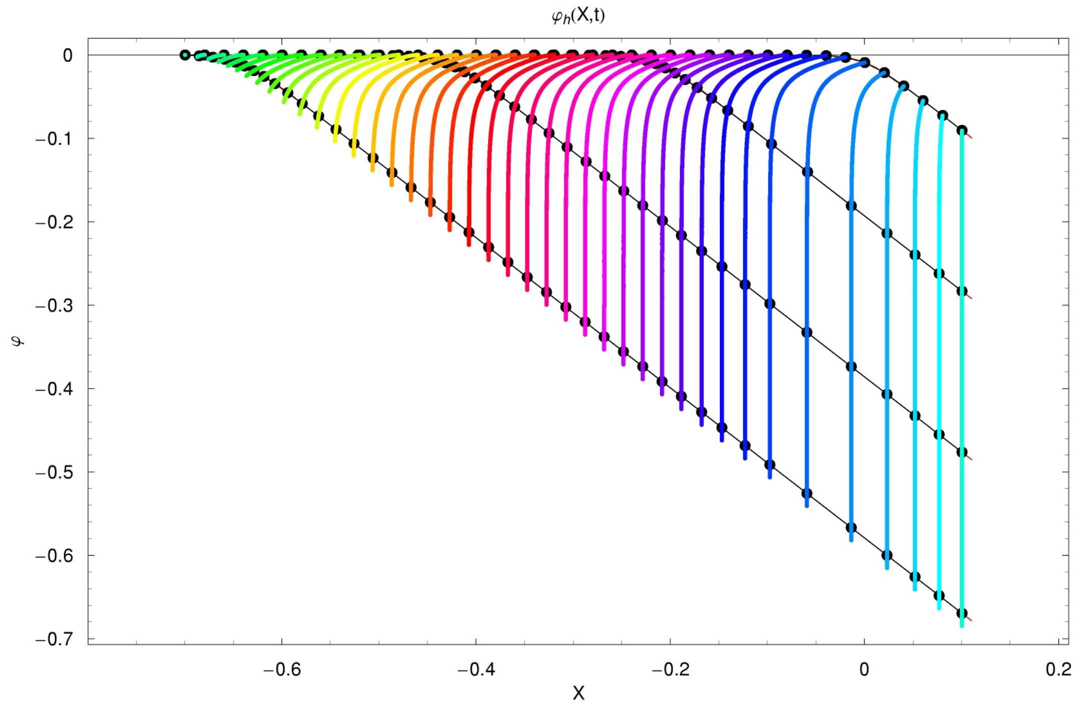

Figure 7.3: Time evolution of displacements profile. Node trajectories and analytical solution are also displayed. The shock advances from right to left in the figure.

Figures (7.6), (7.7), and (7.8) show a sequence of snapshots of the adapted mesh during the three-dimensional simulation both in the reference and deformed configurations. It can be observed that the nodes cluster in the neighborhood of the shock front and follow the shock as it propagates along the domain.

For the three dimensional model we used a mesh composed of 11520 elements and 3270 nodes. Figure (7.9) shows the profile and contour plot of the axial velocity over a plane that contains the cylinder axis and for three different times during the simulation.

As a complementary demonstrative example we modeled also the propagation of a plane wave down a highly compressive cylinder that exhibits a sudden expansion in the cross-section. The material and material parameters are identical to those used in the example of the previous section. Figure (7.10) shows a sequence of snapshots of the evolution of the adapted mesh in the reference configuration at different times. The ability of the mesh to cluster in the neighborhood of the shock as it travels down the tube and expands is remarkable.

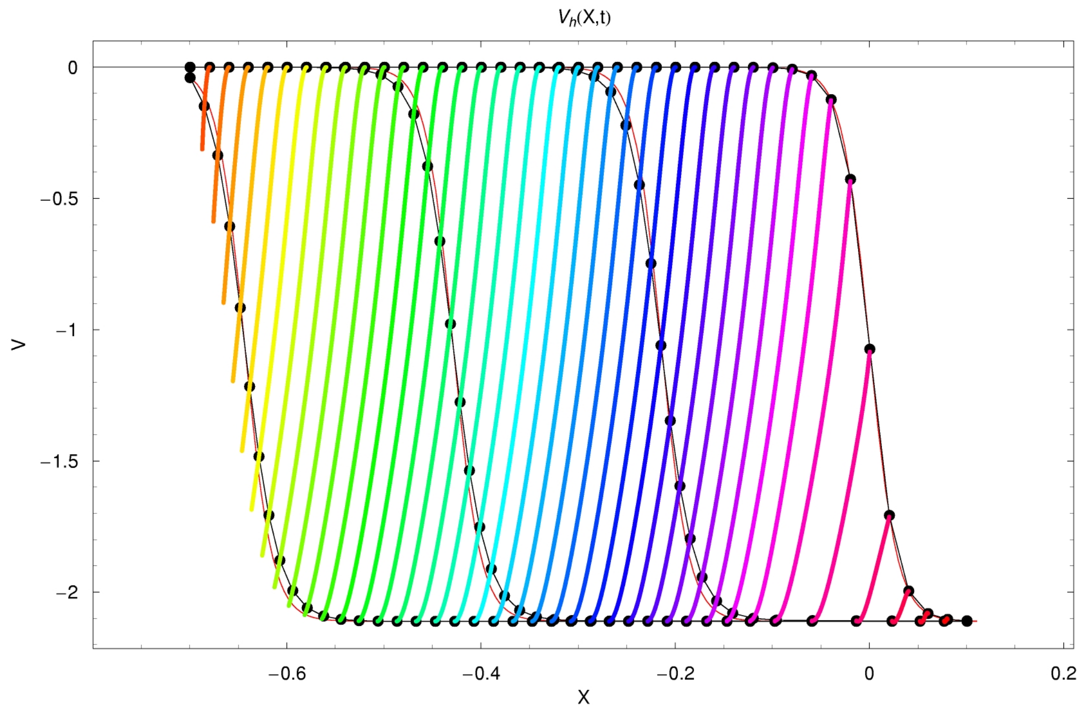

Figure 7.4: Time evolution of velocity profiles. Node trajectories and analytical solution are also displayed.

7.2 Wave propagation example

The second test involves the natural oscillation of an incompressible body that is released from rest from a distorted configuration. We first assume that the body is stretched in one direction, the X_1 axes, and contracts symmetrically in the other two directions due to the incompressibility constraint. The motion is thus assumed to be of the form

$$\boldsymbol{\varphi}\left(X_1, X_2, X_3, t\right) = \left(\varphi_1\left(X_1, t\right), \varphi_2\left(X_1, X_2, t\right), \varphi_3\left(X_1, X_3, t\right)\right)$$

whereupon the deformation gradient reduces to

$$\mathbf{F} = \begin{pmatrix} \varphi_{1,1} & 0 & 0 \\ \varphi_{21} & \varphi_{2,2} & 0 \\ \varphi_{3,1} & 0 & \varphi_{3,3} \end{pmatrix}$$

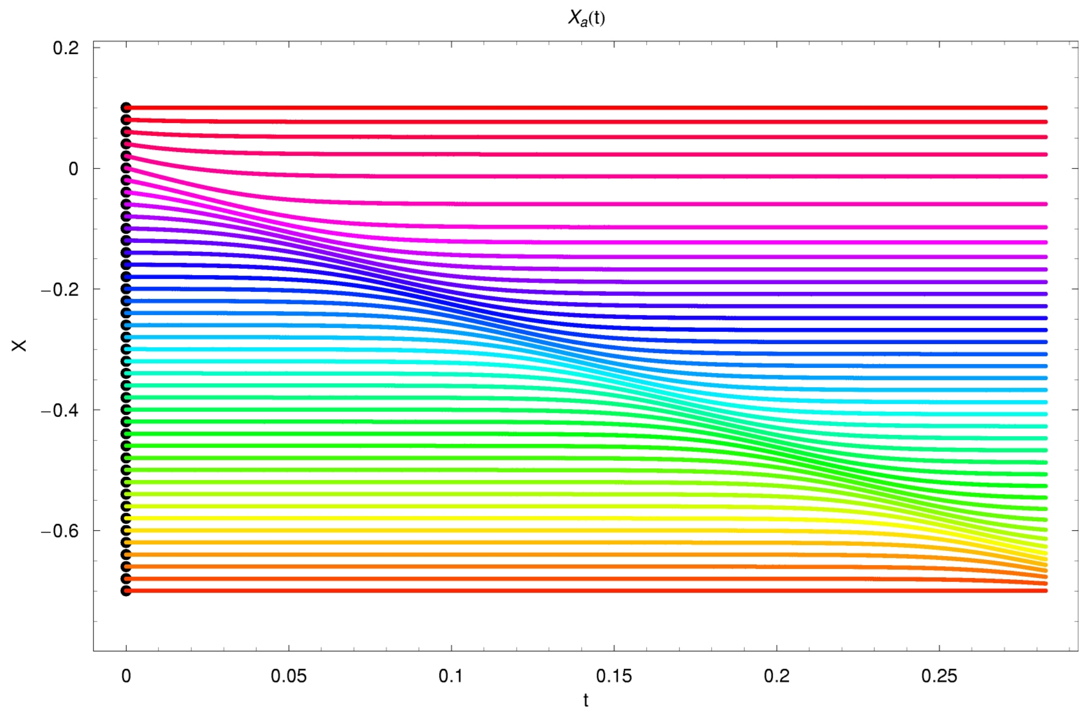

Figure 7.5: Time evolution of nodes in the reference configuration. The shock propagates from top to bottom in the figure. As time progresses the nodes cluster in the neighborhood of the shock front.

Enforcing the incompressibility constraint $J = \det(\mathbf{F}) = 1$ and symmetry condition $F_{22} = F_{33}$ we find

$$\varphi_{2,2} = \varphi_{3,3} = \frac{1}{\sqrt{\varphi_{1,1}}}$$

We will assume that the body is free of body forces and made of a homogeneous (incompressible) Neohookean material with no viscous behavior, characterized by a strain energy density of the form

$$W(\mathbf{F}) = \frac{K}{2}\left(\mathrm{tr}\left(\mathbf{F}^T\mathbf{F}\right) - 3\right)$$

For the particular class of deformations here considered the strain energy density reduces to

$$W(F_{11}) = \frac{K}{2}\left(F_{11}^2 + \frac{2}{F_{11}} - 3\right)$$

The action functional per unit of area is given by

$$S(\varphi_1) = \int_{t_0}^{t_f} \int_0^L \left(\frac{R}{2}\dot{\varphi}_1^2 - W\left(\varphi_{1,1}\right)\right) dX_1 dt$$

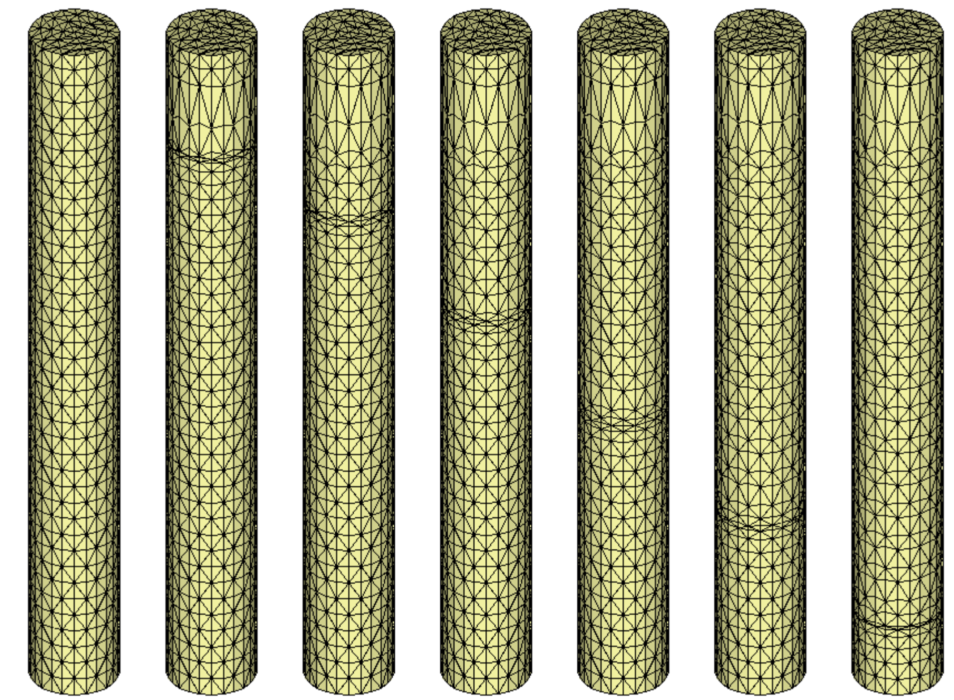

Figure 7.6: Propagation of a compression wave down a cylinder. Adapted 3D meshes at different times. Reference configuration.

where we assume that the reference configuration of the body is $B = [0, L]$. The equations of balance of mechanical force balance (3.14) and (7.2) in the direction of stretch reduce in this case to

$$\begin{aligned} R\ddot{\varphi}_1 &= P_{11,1} \\ \frac{d}{dt}\left(R\left(-\varphi_{1,1}\right)\dot{\varphi}_1\right) &= C_{11,1} \end{aligned}$$

where P_{11} and C_{11} are, respectively, the first Piolla-Kirchhoff stress tensor and Eshelby stress tensor given by

$$\begin{aligned} P_{11} &= \frac{\partial W}{\partial F_{11}} = \\ &= K\left(F_{11} - \frac{1}{F_{11}^2}\right) \\ C_{11} &= \left(\left(W - \frac{R}{2}\dot{\varphi}_1^2\right) - F_{11}\frac{\partial W}{\partial F_{11}}\right) = \\ &= \frac{K}{2}\left(-F_{11}^2 + \frac{4}{F_{11}} - 3\right) - \frac{R}{2}\dot{\varphi}_1^2 \end{aligned}$$

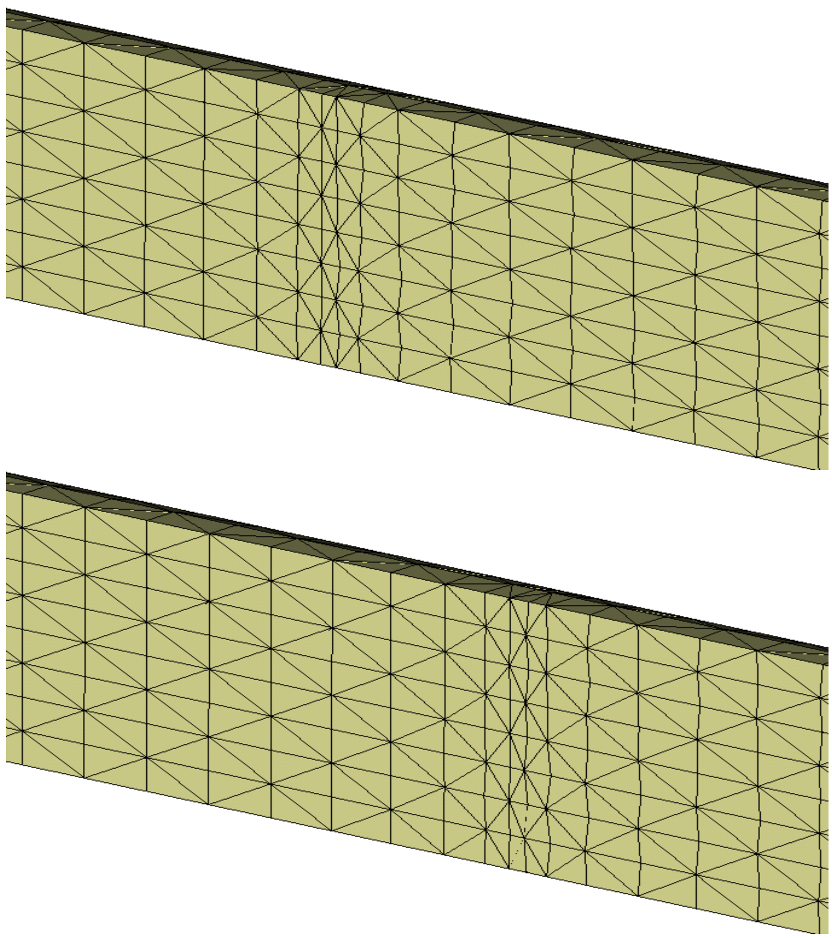

Figure 7.7: Propagation of a compression wave down a cylinder. Detail of the adapted 3D meshes at different times. Reference configuration.

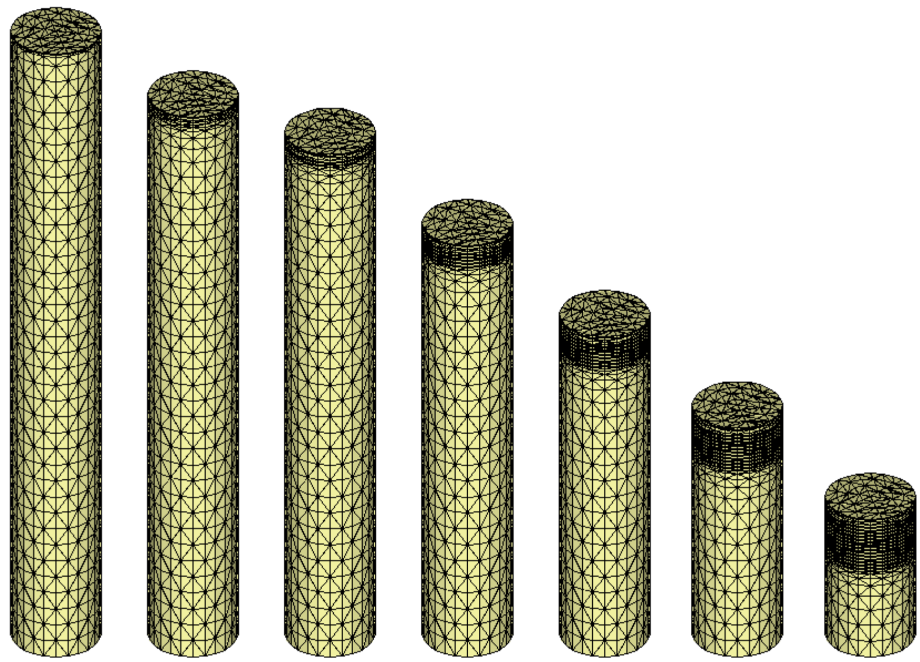

Figure 7.8: Propagation of a compression wave down a cylinder. Adapted 3D meshes at different times. Deformed configuration.

For small deformations $F_{11} \simeq 1$ the strain energy density might be approximated with the first term of its Taylor series expansion

$$W\left(F_{11}\right) \simeq \frac{3}{2} K \left(F_{11} - 1\right)^2$$

whereupon the Piolla-Kirchhoff stress and Eshelby stress reduce to

$$\begin{aligned} P_{11} &= 3K\left(F_{11} - 1\right) \\ C_{11} &= -\frac{3}{2} K \left(F_{11} - 1\right)\left(F_{11} + 1\right) - \frac{R}{2} \dot{\varphi}_1^2 \end{aligned}$$

The equation of balance of mechanical forces becomes in this case

$$R \ddot{\varphi}_1 = 3K \varphi_{,11}$$

which corresponds to the wave equation. The solution with zero boundary conditions and zero initial velocities $\dot{\varphi}_1\left(X, 0\right) = 0$ is

$$\varphi_1\left(X, t\right) = A_k \sin\left(2k\pi \frac{X}{L}\right) \cos\left(2k\pi \frac{ct}{L}\right)$$

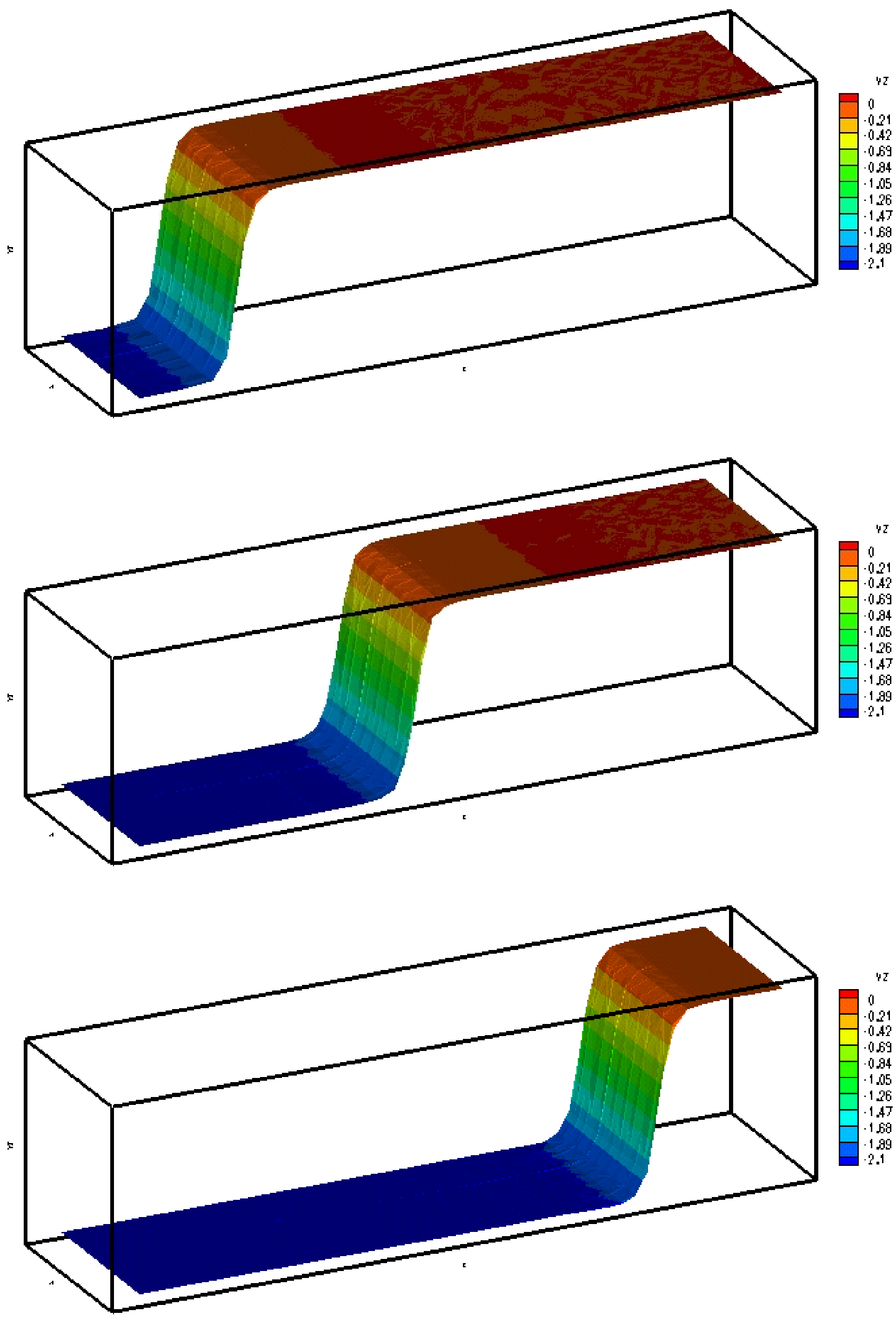

Figure 7.9: Profile and contour plot of axial velocity at different times of the simulation on a plane that contains the axis of the cylinder.

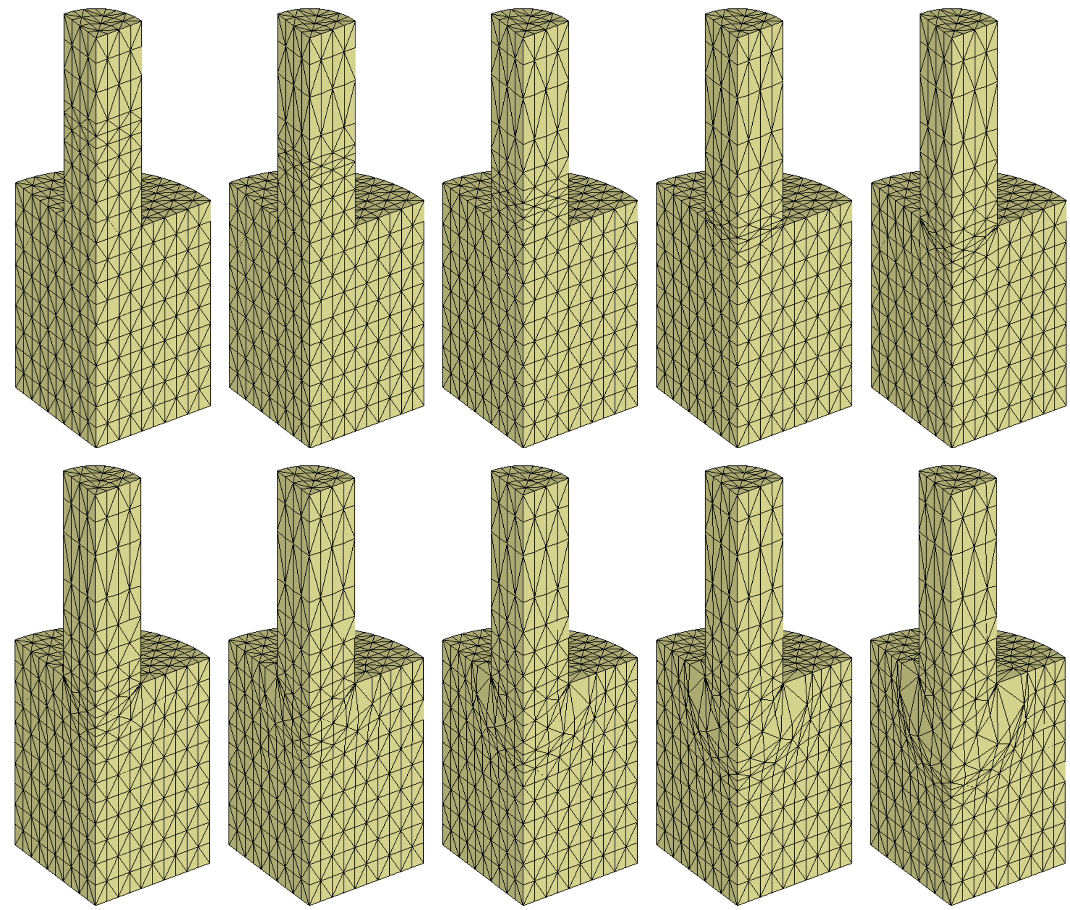

Figure 7.10: Propagation of a plane wave down a cylinder with a sudden expansion. Snapshots of the instantanous mesh (in the reference configuration) at different time steps.

with

$$c^2 = \frac{R}{3K}$$

Figure (7.11) shows the evolution for displacements and adaptive mesh the bar is released from rest $(\dot{\varphi}(X,0) = 0)$ from an initial position that is the superposition of the two first modes of oscillation

$$\varphi(X,0) = A_1 \sin\left(2\pi\frac{X}{L}\right)\cos\left(2\pi\frac{ct}{L}\right) + A_2 \sin\left(4\pi\frac{X}{L}\right)\cos\left(4\pi\frac{ct}{L}\right)$$

with

$$\begin{aligned} A_1 &= 1 \\ A_2 &= 0.2 \end{aligned}$$

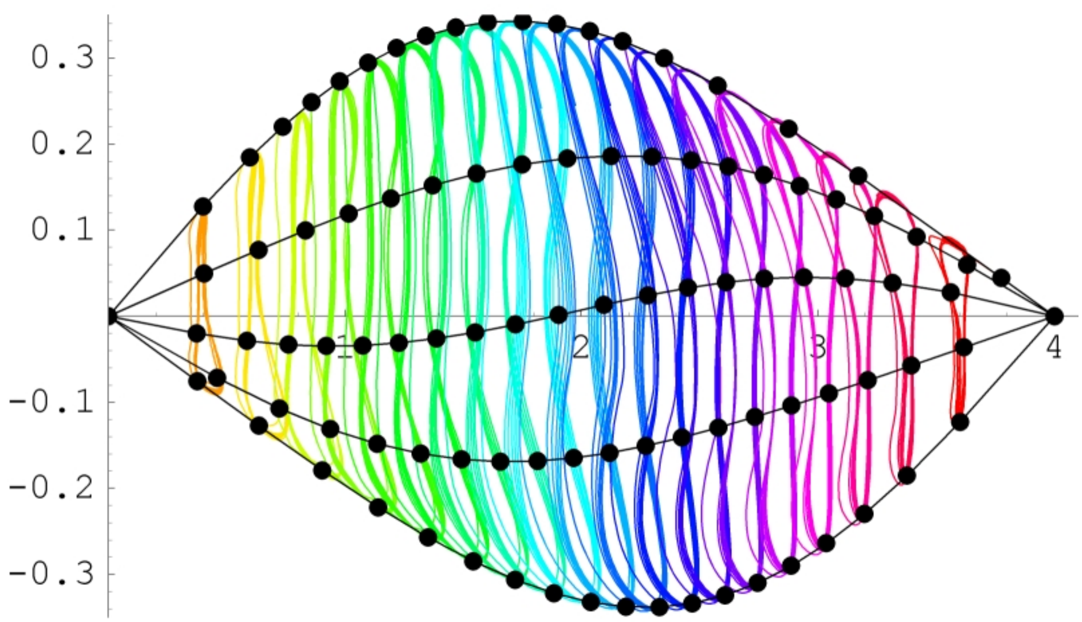

Figure 7.11: Displacement evolution and mesh evolution for the bar oscillation problem.

7.3 Neohookean block under a moving point load

The method has been applied to the case of a three-dimensional Neohookean block subjected to the action of a moving point load. The block dimensions are $1 \times 1 \times 0.5$ and zero normal displacement boundary conditions are enforced on the base and on the face closest to the initial point of application of the load. Only half of the block is simulated due to the symmetry of the loads and geometry. The material chosen is Neohookean extended to the compressible level, which is described by a strain energy density given by

$$W(\mathbf{X},\mathbf{F}) = \frac{\lambda_0(\mathbf{X})}{2}\log(\det(\mathbf{F}))^2 - \mu_0(\mathbf{X})\log(\det(\mathbf{F})) + \frac{\mu_{0(\mathbf{X})}}{2}\operatorname{tr}\left(\mathbf{F}^T\mathbf{F}\right)$$

where λ_0 and μ_0 are to the Lame constants. The material constants used are young modulus $E_0 = 3E10^6$, Poisson constant $\nu_0 = 0.3$, which results in Lame constants

$$\begin{aligned}\lambda_0 &= \frac{E_0\nu_0}{(1+\nu_0)(1-2\nu_0)} = 1.73E\hat{}6 \\ \mu_0 &= \frac{E_0}{2(1+\nu_0)} = 1.15E\hat{}6\end{aligned}$$

The mass density per unit of underformed volume is $R = 100$. The load moves at 1/10 of the characteristic shear wave speed of the material. The mesh consists of 2160 tetrahedral linear finite elements and 637 nodes. To maintain the geometry during the computation the node motion within the reference configuration is restricted in the normal direction to each face. Figure (7.12) show snapshots of the adapted mesh at different times of the simulation. Figure (7.13) shows the deformed configuration and adapted mesh along with a contour plot of the vertical displacement. As a result of mesh adaption and due to the fact that dynamic forces are small compared to the static contact forces, the nodes tend to concentrate in the neighborhood of the point of application of the load. Due to the effect of viscous regularizing forces and due to the fact that configurational forces are small away from the loading area, no rearrangement of nodes takes place in the wake of the moving load.

7.4 Crack propagation example

An application area where variational adaptivity might be particularly advantageous is dynamic fracture mechanics. An alternative for the accurate tracking of dynamically growing cracks is the use of cohesive elements and cohesive laws (see for example [52]). Cohesive elements are surface elements that are inserted within bulk interelement faces and govern their separation and consequent generation of new surfaces and crack growth according to a cohesive law. A immediate limitation of this approach is that crack paths are restricted to the bulk element boundaries. The combination of cohesive finite elements with variational adaptivity would be an approach to overcome this limitation and improve dynamic crack path predictability since both crack evolution and node rearrangement would be driven by the same forces, i.e., dynamic configurational forces.

The potential use of this approach is investigated by modeling an externally driven mode I growing crack in a square slab of Neohookean material as depicted in figure 7.14. Due to the symmetry of the geometry and loading, only the upper half of the body is simulated. To avoid changes in geometry, the motion of nodes in the reference configuration is constrained to remain within the faces. The material properties are Young modulus $E = 1.0E^6$, Poisson ratio $\nu = 0.3$, and mass density per unit of undeformed volume $R = 2300$. The mesh consists of 720 linear tetrahedral finite elements and 273 nodes. Vertical displacement-boundary conditions corresponding to the linear elastic K_1 field were applied with $K_1 = 1.E^5$. The K field is given by

$$\begin{aligned} u_1(x_1, x_2) &= \frac{K_1}{2\mu_0}\sqrt{\frac{r}{2\pi}} \cos\left(\frac{\theta}{2}\right)(K_1 - \cos(\theta)) \\ u_2(x_1, x_2) &= \frac{K_1}{2\mu_0}\sqrt{\frac{(x_1 - a)^2 + x_2^2}{2\pi}} \sin\left(\frac{\theta}{2}\right)(K_1 - \cos(\theta)) \end{aligned}$$

where

$$\begin{aligned} r &= (x_1 - a)^2 + x_2^2 \\ \theta &= \tan^{-1}(y, x - a) \end{aligned}$$

The crack is advanced by assuming a constant crack tip velocity of $\dot{a} = \frac{1}{10}c_s$ where c_s is the characteristic shear wave speed of the material. The node closest to the instantaneous theoretical placement of the crack tip $a(t) = a_0 + \dot{a}t$ is kept fixed and only released after the assumed crack tip position $a(t)$ reaches the subsequent node in the direction of crack advance. Figure (7.15) shows the adapted mesh within the reference configuration for different times of the simulation. Figure (7.16) shows the adaptive mesh in the deformed configuration along with contour plots of vertical displacements. The ability of the method to cluster nodes in the neighborhood of the crack tip while simultaneously following dynamic waves emanating from the advancing crack is noteworthy.

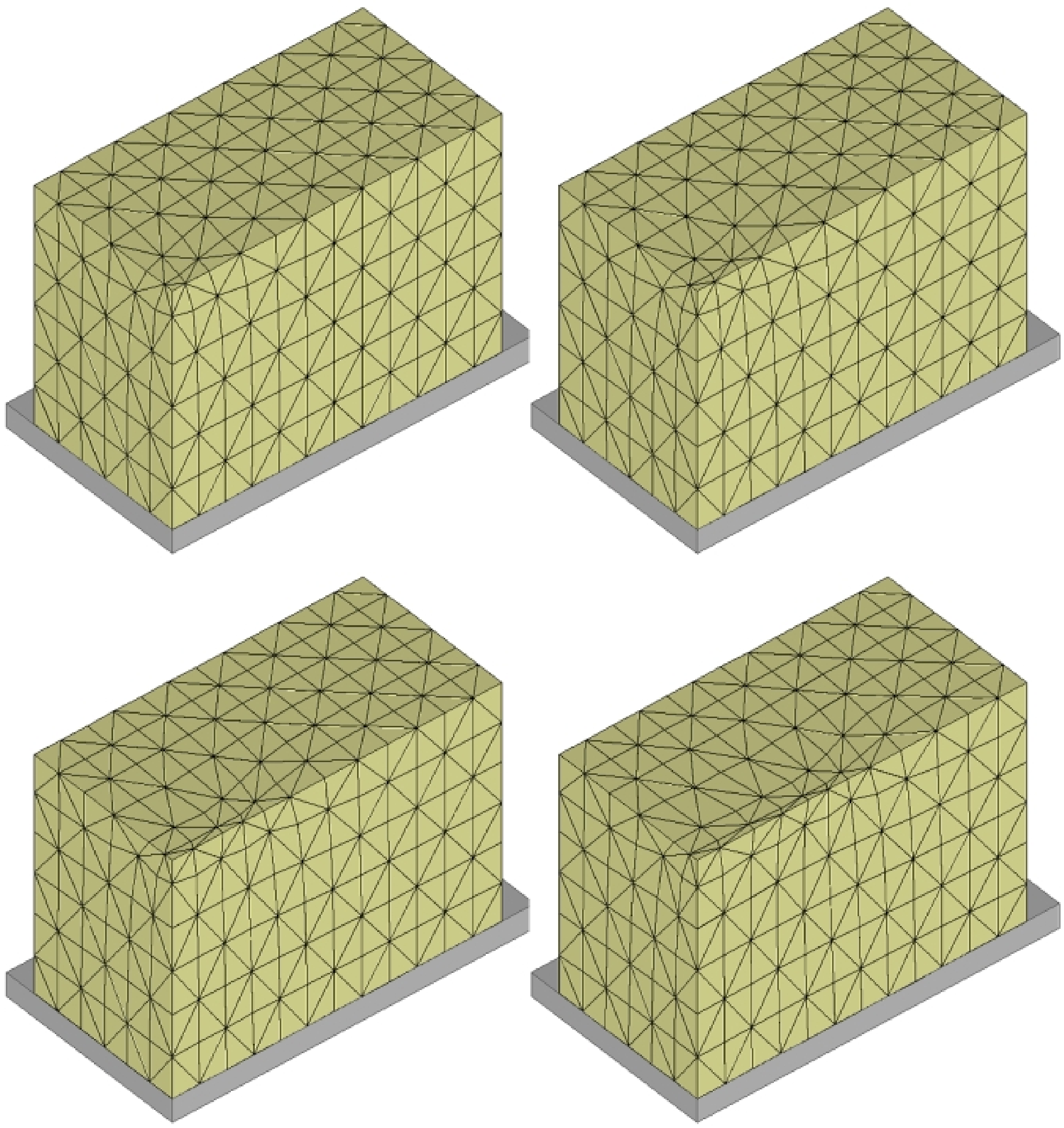

Figure 7.12: Neohookean block subjected to a moving point load. Reference configuration and adapted mesh at different times of the simulation.

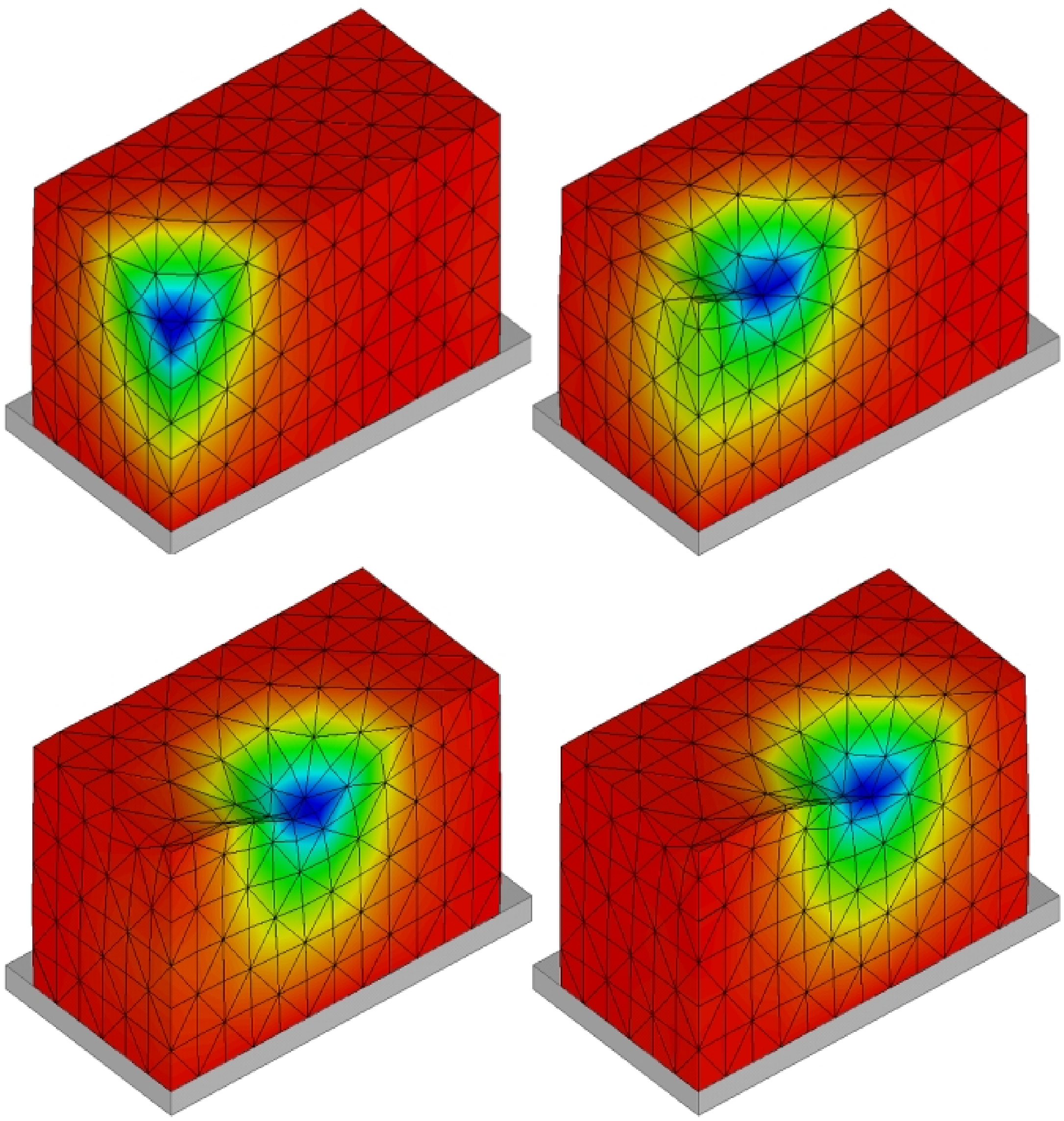

Figure 7.13: Neohookean block subjected to a moving point load. Adapted mesh in the deformed at different times of the simulation and countour plot of vertical displacements.

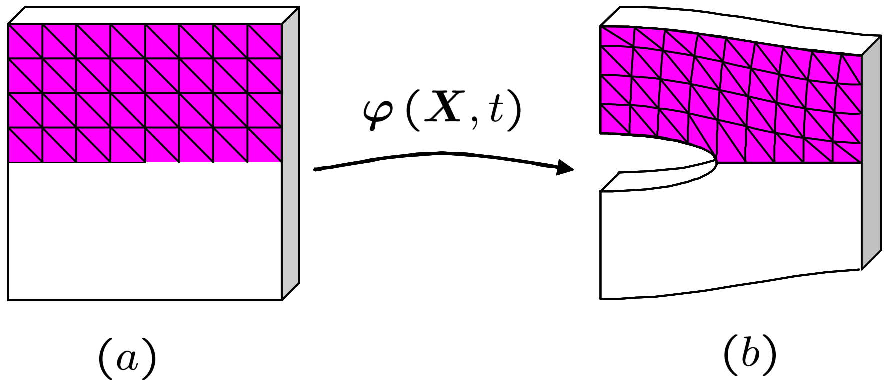

Figure 7.14: Dynamic propagation of a crack along a slab of Neohookean material. (a) Reference configuration. (b) Deformed configuration at time t.

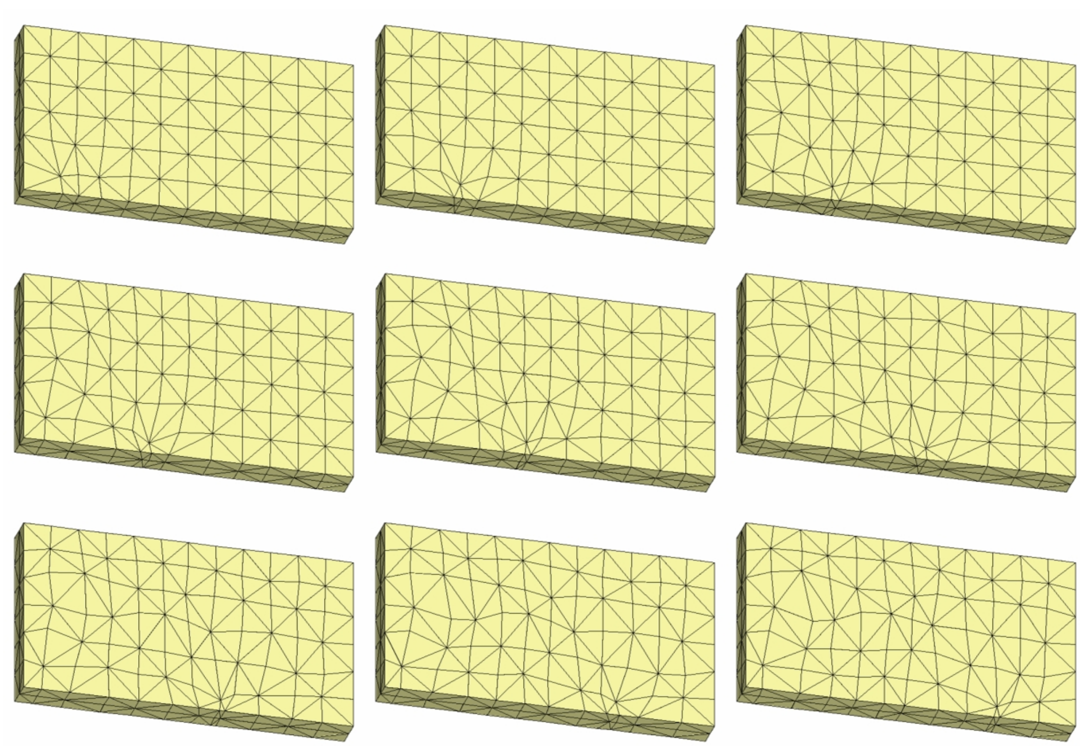

Figure 7.15: Propagation of a crack along a slab of Neohookean material. Adapted mesh in the reference configuration at different time steps of the simulation.

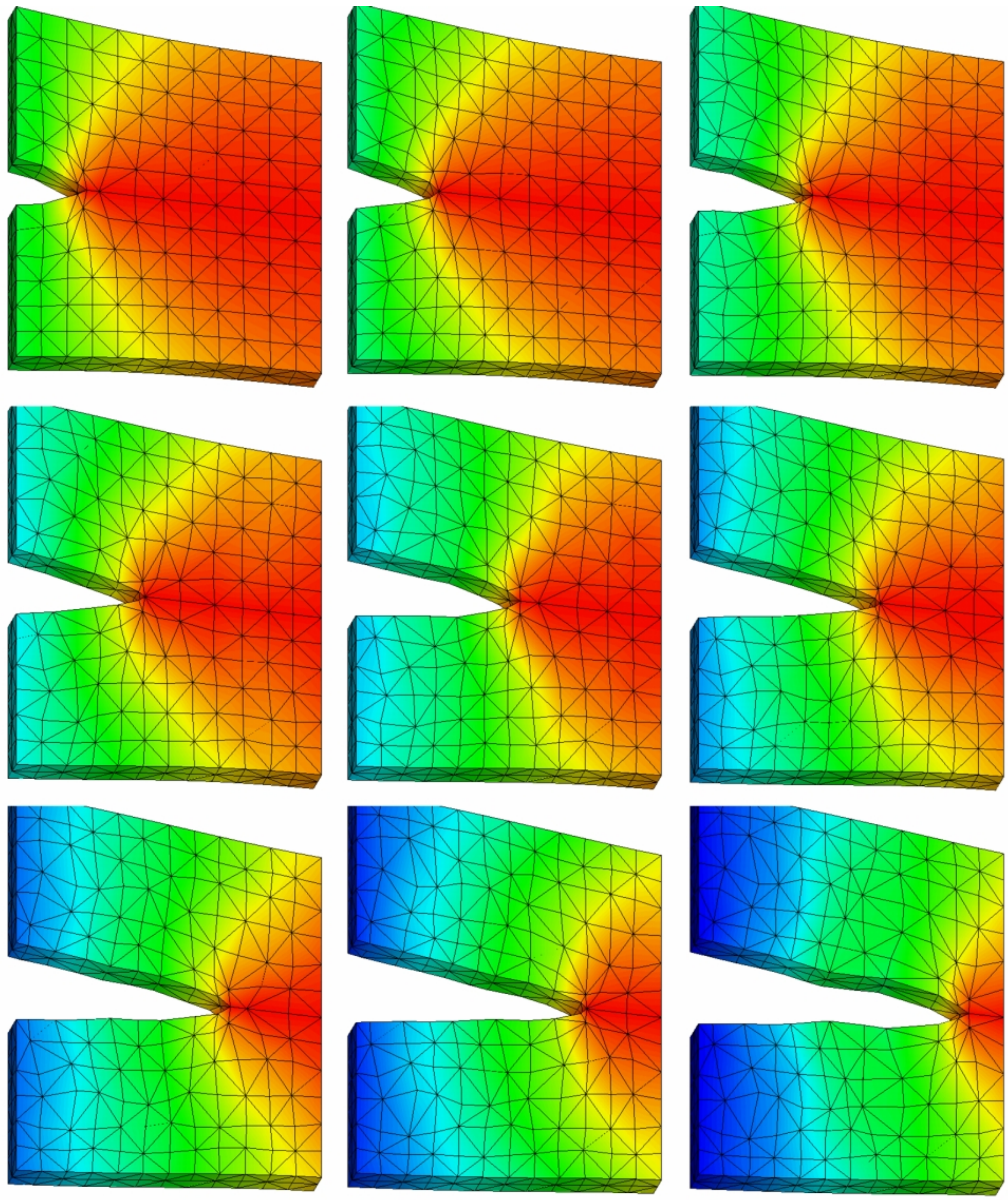

Figure 7.16: Crack propagation along a Neohookean body. The nodes cluster following the crack tip. Countour plots indicate vertical displacements.

Chapter 8

Conclusions and future directions

We have developed in this thesis a variational finite element mesh adaption framework for solid dynamic applications and its conceptual links with the theory of dynamic configurational forces. A mixed, multifield version of Hamilton's principle and a mixed extended version of Lagrange-d'Alembert principle are proposed as underlying variational principles for the formulation. Generalizations of these principles to account for dissipative behavior are conceptualized and and extended class of variational integrators for the integration in time of the resulting differential equations is formulated.

The basic ingredients of this framework are, in addition to the use of the *mixed* form of Hamilton's and Lagrange d'Alembert principles, (i) the use of uncoupled space and time discretizations, (ii) the use of independent space interpolations for velocities and deformations (iii) the application of these interpolations over a continuously varying adaptive mesh, (iv) the application of mixed variational integrators with independent time interpolations for velocities and nodal parameters. The result is a robust adaptive finite element formulation for dynamic applications that satisfies the balance of mechanical forces (or balance of spatial momentum) and the balance of dynamic configurational forces (or balance of material momentum), and, as a result of its variational nature, exhibits excelent long term energy stability behavior.

A *space-space configurational bundle* perspective, complementary to the space-time-based bundle framework developed in the context of multisimplectic continuum mechanics and variational integrators, is proposed as a theoretical base for the formulation. After careful examination of the variational adaption concept as it applies to time adaption for both finite degree-of-freedom dynamical systems and solid dynamics (space-time) problems it was concluded that attempting simultaneous space and time variational adaptivity was too costly. Variational space adaptivity was then pursued, which led to abandoning the space-time framework and implementations based on space-time finite elements and to adopting a staggered approach with an initial semidiscretization in space followed by a discretization in time. Since time is kept continuous during the first stage of the computation, and since time adaption is no longer pursued, it was found that the space-space framework became more useful to analyze the underlying structure of the method.

It was then found that the use of Hamilton's principle led to unstable and meaningless solutions. After careful examination and testing it was concluded that these instabilities were caused by inaccuracy of the velocity approximation whose interpolation was derived, or *consistent*, with the interpolation for deformations. An *independent* interpolation for the velocity was then proposed and a variational framework that allowed for the use of incompatible velocity interpolations was required. This led to the development of the mixed multifield version of Hamilton's and related principles and stable solutions were obtained. To our knowledge, this is the first successful application of this multifield principle whose theoretical conceptualization can be traced back to a century ago.

In attempting to use the variational mesh adaptivity framework in problems involving shocks a generalization to account for viscosity was required. An extended version of the Lagrange-d'Alembert principle was thus developed. This principle acts as a variational restatement both of the equations of motion and the equations of configurational force balance in the presence of viscosity. It was then observed that the application of this principle required the computation of interelement viscous boundary sources, which proved to be prohibitive for three-dimensional tetrahedral meshes. A mixed version of the extended Lagrange-d'Alembert principle was then developed as an approach to avoid the computation of interelement boundary forces and successfully tested in a shock propagation example. A finite element implementation was developed and exercised in several one and three dimensional problems and tests designed to assess convergence, robustness, and scope of the method.

A generalization of all these principles to account for thermal and inelastic processes was then conceptualized. This extension is accomplished by making use of thermal displacements as opposed to temperature as independent thermal variables. An additive decomposition for the heat flux into conservative or dissipationless and non-conservative or dissipative parts was proposed. This decomposition parallels the well-established additive decomposition of mechanical stresses into elastic (conservative) and viscous (nonconservative) factors and facilitates the full identification of different components in the mechanical and thermal balance equations. Then this parallelism was exploited to establish a thermomechanical analog of the mixed Hamilton's principle and extended, mixed Lagrange-d'Alembert principles developed for isothermal elastic materials with viscosity.

Many possible directions might be taken in the future to further the scope of application of this methodology. Immediate steps would be the extension of the methodology to h-adaptivity (work in progress), a direction that has already been explored within the context of static applications in [49], the application to fully coupled thermomechanical problems, the combination with cohesive elements or the coupling with asynchronous variational integrators or discontinuous Galerkin approximations. From the numerical analysis point of view more optimized solvers for the resulting non-linear and ill-posed system of equations and parallel implementations might be devised.

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