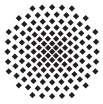


Universität Stuttgart

Institut für
Nichtlineare Mechanik

Master Thesis
Summer Semester

Time Finite Element Methods for Mechanical Systems in Minimal Coordinates

Giuseppe Capobianco

Supervisors: Dr. S. R. Eugster
Prof. Dr. R. I. Leine
Prof. Dr. P. Hora

September 2015

Preface

The present thesis has been carried out at the Institute for Nonlinear Mechanics (INM) of the University of Stuttgart. I had a very good and interesting time here in Stuttgart and I want to thank all the people that made this happen. First of all I want to thank Prof. Dr. Remco Leine for this great opportunity, the interesting discussions and all the support. A special thanks goes to Dr. Simon R. Eugster, who not only was the main supervisor of this thesis, but very much shaped my understanding of mechanics. I appreciated his support, his critical questions and all his time he put into this project. I am very grateful to Prof. Dr. Pavel Hora for allowing me to do my thesis abroad. Many thanks go to all the colleagues at the Institute for Nonlinear Mechanics for their warm welcome in Stuttgart. I am looking forward to my time as doctoral student at the INM. Last but not least I want to thank my friends and especially my family for their support.

Stuttgart, September 2015 *Giuseppe Capobianco*

Abstract

The virtual action as a variational equation is considered to hold as an axiom in mechanics. In this thesis time finite element methods are developed by discretizing the principle of virtual action and related variational principles. Using the Legendre–Fenchel transform, multi-field formulations are induced from the principle of virtual action. For mechanical systems described in minimal coordinates, the infinite dimensional variational formulations are discretized by introducing temporal shape functions. Such a discretization reduces a variational equation to a set of nonlinear equations approximating the dynamical behavior of a mechanical system. For a single-field formulation these nonlinear equations are equivalent to a time stepping algorithm. The various finite element methods are compared with respect to convergence behavior for three different mechanical systems.

Contents

Chapter 1

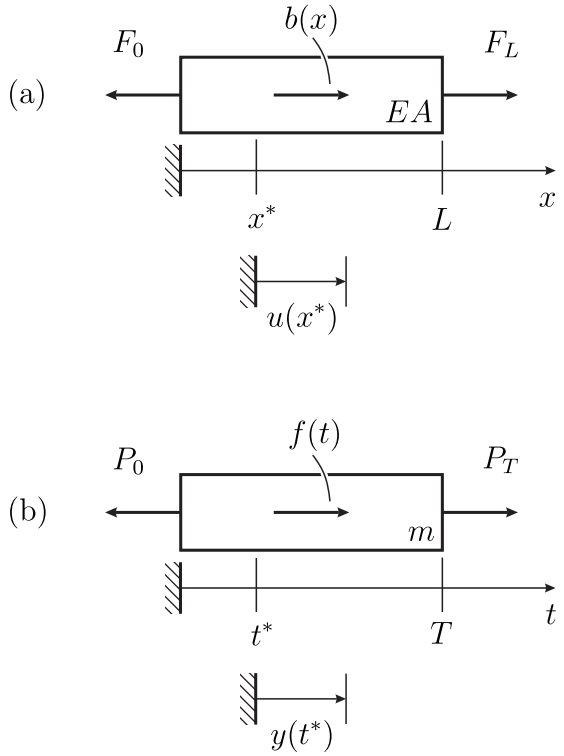
Introduction

This thesis is concerned with the variational formulation of dynamics and its application to time finite element formulations, which are derived by discretizing the principle of virtual action using temporal shape functions.

This capter starts with a motivation for the thesis in Section 1.1. After a literature survey on time finite element methods and variational integrators in Section 1.2, the aim and scope of the thesis is presented in Section 1.3. Lastly an outline of this thesis is given in Section 1.4.

1.1 Motivation

Since the introduction of finite element procedures in the early 1960s and thanks to ongoing research in this field together with the increase of computational power over the years, these methods became indispensable for engineering development. The finite element procedures are employed extensively in the analysis of solids and structures, of heat transfer, and partially even in fluid mechanics. The algorithms used for the nonlinear finite element analysis of solids and structures are known to be very performing in terms of accuracy and robustness. These properties follow inter alia from the fact that the finite element description is derived from a weak variational formulation in the space dimension, e.g. the weak variational form of the principle of virtual work. In this thesis, we state the principle of virtual action as an axiom and use it to derive finite element formulations for dynamical multi body systems. As the principle of virtual action is a weak variational formulation for both, the space and the time dimension, the resulting time finite elements can be expected to have the same qualities as the spatial finite elements. The principle of virtual action can be motivated using the analogy between the static description of a linear elastic one dimensional bar and the motion of a point mass in one dimension. Figure 1.1 (a) shows the static equilibrium condition (seq) and the



$$EAu''(x) = -b(x) \qquad \text{(seq)}$$
$$EAu'(0) = -F_0 \qquad \text{(bc)}$$
$$EAu'(L) = F_L \qquad \text{(bc)}$$

$$m\ddot{y}(t) = f(t) \qquad \text{(eqm)}$$
$$y(0) = y_0 \qquad \text{(ic)}$$
$$\dot{y}(0) = u_0 \qquad \text{(ic)}$$

Figure 1.1: Comparison between the boundary value problem describing the one dimensional static bar (a) and initial value problem describing the motion of a pointmass in one dimension (b).

boundary conditions (bc) for the displacement field $u(x)$ of a statically loaded one-dimensional linear elastic bar of length L. The sole spatial coordinate is x, E is Young's modulus and A is the cross section of the bar. The bar is assumed to be loaded by body forces $b(x)$ and two point forces acting at the boundaries. The latter are denoted with F_0 and F_L. Figure 1.1 (b) illustrates the equation of motion (eqm) and the initial conditions (ic) for the motion $y(t)$ during the time interval $[0, T]$ of a point mass m in one dimension. The point mass is exposed to time dependent forces $f(t)$. By similarity, two point forces, denoted with P_0 and P_T, are introduced to act at the boundaries. As point forces they are impulsive forces, since they act at a single instant of time. The static bar and the motion of the point mass are described both by a second order differential equation with two auxiliary conditions. The big difference between the two descriptions lies in the auxiliary conditions. As the bar has to respect boundary conditions, the dynamics of the point mass has to satisfy the initial conditions. The boundary value problem of Figure 1.1 (a) can be

derived form the the principle of virtual work of a linear elasic bar, which is

$$\delta W = -\int_0^L \{\delta u' \, EAu' - \delta u \, b\} \mathrm{d}x - \delta u(0) \, F_0 + \delta u(L) \, F_L = 0 \quad \forall \delta u \, . \tag{1.1}$$

The principle of virtual action of the form

$$\delta A = -\int_0^T \{\delta \dot{y} \, m\dot{y} + \delta y \, f\} \mathrm{d}t - \delta y(0) \, P_0 + \delta y(T) \, P_T = 0 \quad \forall \delta y \tag{1.2}$$

can therefore be motivated in analogy as a starting point for the derivation of the motion of the point mass. Obviously, the principle of virtual action also induces a boundary value problem. Thus, the conversion of a boundary value problem into an initial value problem must be addressed.

1.2 Literature Survey

The variational view of mechanics, which goes back to Euler, Lagrange and Hamilton, forms the basic of the time finite element methods (TFEM) and the theory of discrete mechanics, from which arises the concept of variational integrators. Although discrete mechanics and TFEM are strongly related, the discretization of time used in both approaches is conceptually different. As TFEM are derived by the discretization of a continuous time variable, discrete mechanics postulates a discrete time. Consequently, the literature survey of this section is therefore devided into the two parts TFEM and discrete mechanics.

Time Finite Element Methods

The idea of discretizing a variational principle using temporal shape functions was introduced by Fried (1969), and Argyris and Scharpf (1969), who discretized the principle of Hamiltion using Hermitian polynomials. Both use a Ritz' method to obtain a set of algebraic equations, describing the dynamic behavior of their system. The set of equations can be considered as a single set of nonlinear equations in several variables. Consequently, we call this approach to be monolithic. The ideas used for time finite element methods are the same as the ideas used for spatial finite element methods. Nevertheless, there is a crucial difference. All the methods used to derive spatial finite element descriptions are developed to solve boundary value problems. In dynamics the solution of an initial value problem is sought and the question of how to impose initial conditions in temporal finite element descriptions becomes important.

The treatment of the initial conditions needs a variational principle with suitable boundary terms. Some effort on adding boundary terms to Hamilton's principle, such that the new variational principle describes an initial value problem was done. An approach with rather little mechanical motivation has been proposed by Wu (1977), and Wu and Simkins (1980). The principle of virtual action and Hamilton's law of varying action, which are more general than Hamilton's principle, have mechanically motivated boundary terms and allow better treatment of the initial conditions. This was recognized by Bailey, who discretized them using global power series as shape functions together with the Galerkin and the Ritz method, cf. Bailey (1975, 1976b, 1980). Many more possibilities for imposing the initial conditions have been discussed. In Simkins (1978) and Agrawal and Saigal (1987) a Lagrangian multiplier approach is used. Baruch and Riff (1982) discuss the modification of the boundary terms of the principle of virtual action in six different ways. Borri (1986) and Izadpanah (1986) point out the importance of using unknown external impulsive forces in the boundary terms. This allows for a natural convergence of the discrete initial velocity to the one of the continuous motion. Early applications of TFEM to simple rigid multi body systems are found in Argyris and Scharpf (1969), Bailey (1976b), and Bailey (1981). More complex applications are found in Hitzl (1980), and Hitzl and Levinson (1980), who compute the planetary motion modeled as a three body problem, and Borri (1986), who analyzes the motion of helicopter rotors using TFEM. The main disadvantage of monolithic TFEM, which are used in all the before mentioned publications, is the computational effort needed to solve one big system of nonlinear algebraic equations. Additionally, stepping schemes, which allow to calculate the state of the system for a subsequent time instants out of the sate of previous time instants, are often preferred. If local shape functions are used in Galerkin or weighted residual methods, the monolithic approach induces an equivalent stepping scheme, which makes the computation of the motion more efficient. This approach is used by Kujawski and Desai (1984) and Adélaïde et al. (2002, 2003), who additionally used some mesh adaption techniques in their TFEM. An alternative approach to arrive at stepping equations is the application of the principle of virtual action on subsequent short time intervals. Imposing the final state of the previous time interval as initial condition of the new one, the dynamics of an interval is obtained. This approach can be found in Borri et al. (1985, 1991, 1992), Aharoni and Bar-Yoseph (1992) and Betsch and Steinmann (2000a,b). Note however that this approach might not be equivalent to a monolithic formulation. The possibility to derive stepping equations from a time finite element formulation rises the possibility to reinterpret known stepping alghorithms. Gillilan and Wilson (1992) derive the central difference method, also known as the Verlet algorithm, discretiz-

ing the principle of Hamilton with linear temporal shape functions. Bottasso (1997) links the Runge–Kutta methods to TFEM. Marsden and West (2001) show that a class of variational integrators derived in the context of discrete mechanics can be derived from Galerkin type TFEM.

Time finite element methods are also used in continuum dynamics, in which both space and time are discretized. First applications can be found in Bailey (1976a), in which the transient behaviour of beams has been analized. Cella et al. (1980) compute a shock wave propagations. Bajer (1986) develops a triangular space-time element for beams. Gellin and Pitarresi (1988), Hughes and Hulbert (1988), Pitarresi and Manolis (1991) and Atilgan et al. (1996) are some further publications that use TFEM in the context of elastodynamics. Finding the motion of a beam, which is loaded with a moving mass can efficiently be solved with TFEM as Bajer and Dyniewicz (2008) showed. A very complete treatment on space-time finite element methods for elastodynamics can be found in Bajer and Dyniewicz (2012). Space-time finite element methods are also applied in fluid dynamics, see Hughes and Hulbert (1988), Hughes et al. (1989) and Shakib and Hughes (1991), to name a few. Note that in general TFEM derived from the the principle of virtual action by applying Galerkin's methods often have higher continuity requirements than TFEM derived by weighted residual methods. This makes the former more popular in rigid multi body dynamics, while in elastodynamics and fluid dynamics time-discontinuous weighted residual approaches are preferred, cf. Bottasso (1997).

Discrete Mechanics and Variational Integrators

The foundations for the development of discrete mechanics were laid in the context of optimal control, where a discrete calculus of variations was introduced. The formulation of a discrete variational problem with discrete Euler equations as necessary and sufficient condition for stationarity is treated in Cadzow (1970). In discrete mechanics, time is modeled as a discrete variable. The possibility of introducing a discrete time in classical mechanics and other branches of physics is discussed in Lee (1983, 1987). Veselov (1988) has developed the theory of discrete mechanics, whose fundamental axiom is the discrete principle of stationary action and the discrete Euler–Lagrange equations, which are the corresponding stationarity conditions. A canonical formulation of the principle of stationary action is first derived in Shibberu (1993). A more recent formulation has been given by Leok and Zhang (2011), which is closer to the view of discrete mechanics. See Marsden et al. (1998) for a detailed discussion of discrete mechanics. As time is treated as a discrete variable, the discrete Euler–Lagrange equations define a stepping scheme, which are called variational integrators (VI). Wendlandt and Marsden (1997), and Marsden and

Wendlandt (1997) derived some VI for conservative mechanical systems and analyze the conservation properties. Some of the well known numerical integration schemes, such as some Newmark β and Runge–Kutta methods, happen to be variational integrators, as is shown by Marsden and West (2001). The concepts of discrete mechanics discussed in Wendlandt and Marsden (1997) have been further developed to arrive at VI with variable time steps, cf. Kane et al. (1999) and to include holonomic and non-holonomic constraints, cf. Cortés and Martínez (2001), Cortés (2002), and Leyendecker et al. (2008). To simulate problems arising in elastodynamics, such as wave propagation, asynchronous VI were developed, which have different time steps for every spatial node, cf. Lew et al. (2003) and Lew (2003). An extension of discrete mechanics to non-smooth phenomena can be found in Fetecau et al. (2003a,b). De León and de Diego (2002) derive VI for non-autonomous conservative systems. As the variational integrators became popular in computer animation, faster update methods for constrained mechanical systems are analyzed in Kharevych et al. (2006), where the update is reformulated as the solution of a minimzation problem. Johnson and Murphey (2009) used tree representations to faster update the states. Lacoursière (2007) developed a VI, which can treat holonomic and non-holonomic bilateral constraints and discusses unilateral constraints with frictional impacts. To simulate flexible multi body systems VI were used by Betsch et al. (2010). An extension of the theory of asynchronous VI to simulate collisions between deformable structures is given by Wolff (2011).
For a more detailed review on discrete mechanics and variational integrators we refer to Lew et al. (2004) or West (2004).

1.3 Aim and Scope

As pointed out in Section 1.1, finite elment methods, especially the spatial discretization using finite elements, are very popular in many fields of engineering. The scope of the present thesis is the temporal discretization with finite elements adapting the well established ideas from spatial finite elments. The aims of this thesis are:

- to derive the most important principles of analytical dynamics for rigid multi body systems in minimal coordinates starting from the principle of virtual action as an axiom.

- to show how the boundary conditions of the equation of motion can be transformed into initial conditions by means of a constitutive force law on the impulsive boundary forces.

- to use the Legendre–Fenchel transform on the kinetic energy to derive multi field formulations of the abovementioned principles of analytical dynamics.

- to discretize the variational principles of analytical dynamics to derive algebraic equations that describe the motion of the multi body system. Both a monolithic and a stepping approach are considered.

- to compare the different approaches using a few examples.

1.4 Outline

In Chapter 2 the thesis begins by stating the principle of virtual action as an axiom to derive the principle of virtual work. By restricting the mechanical system to rigid multi body systems, the equations of motion for this type of systems are derived from the principle of virutal action. Moreover Hamilton's law of varying action and the principle of Hamilton are derived for conservative systems. In Chapter 3 the Legendre–Fenchel transform is introduced and applied to the kinetic energy to derive multi-field formulations of the principle of virtual action and subsequently of Hamiltion's law of varying action and Hamilton's principle. Chapter 4 discusses the derivation of algebraic equations that describe the motion of a rigid multi body system in minimal coordinates by means of a temporal finite element discretization. The discretization is derived for the single- and multi-field formulations of Chapter 2 and Chapter 3. This is done in two different ways, i.e. the monolithic approach and the stepping approach, which give a set of algebraic equation or a stepping scheme. The two approaches are shown to be equivalent under certain conditions. In Chapter 5 the performance of the different approaches is tested. Computations of the harmonic oscillator, the simple pendulum and the two body problem are performed. Finally, in Chapter 6 a conclusion of the thesis is drawn and an outlook on further topics is given.

Chapter 2

Principles in Analytical Dynamics

Starting from the principle of virtual action as an axiom, we, in this chapter, derive some important principles of analytical dynamics. In the first Section 2.1 we introduce the concept of forces in the sense of Eugster (2014) and state the principle of virtual action as an axiom of dynamics. The inertial forces behave according to a linear constitutive law and the principle of virtual work for this case is derived. In Section 2.2 we develop the principle of virtual action for systems with finite degrees of freedom. For this type of systems Hamilton's law of varying action and Hamilton's principle follow from the principle of virtual action, cf. Section 2.3. Finally, the Euler–Lagrange equations of motion are shown to follow from these principles.

2.1 Principle of Virtual Action

Consider a mechanical system $\mathcal{S}$ consisting of material points, e.g. a continuous body or a multi-body system composed of rigid and flexible bodies. It is convenient to chose $\mathcal{S}$ to be the reference configuration of the system, whose material points occupy a subset of the euclidean three-space $\mathbb{E}^3$. The position vectors $\mathbf{X} \in \mathbb{E}^3$ address the material points of $\mathcal{S} \subset \mathbb{E}^3$. The motion of the system during the time interval $\mathcal{I} = [0, T]$

$$\boldsymbol{\xi} \colon \mathcal{S} \times \mathcal{I} \to \mathbb{E}^3, \ (\mathbf{X}, t) \mapsto \mathbf{x} = \boldsymbol{\xi}(\mathbf{X}, t) \tag{2.1}$$

is a parametrization of configurations $\boldsymbol{\xi}(\cdot, t) \colon \mathcal{S} \to \mathbb{E}^3$, which is as smooth as required with respect to time $t \in \mathbb{R}$. A dot $(\dot{\bullet})$ denotes the derivative with respect to time t. The motion induces the velocity field $\dot{\boldsymbol{\xi}}(\mathbf{X}, t)$ and the acceleration field $\ddot{\boldsymbol{\xi}}(\mathbf{X}, t)$, whenever they exist. A variational family of motions

is a differentiable parametrization of motions $\hat{\boldsymbol{\xi}}(\mathbf{X}, t, \varepsilon)$ with respect to a single parameter $\varepsilon \in \mathbb{R}$. The actual motion is embedded in the family $\hat{\boldsymbol{\xi}}$ and is obtained for $\varepsilon = \varepsilon_0$, i.e. $\hat{\boldsymbol{\xi}}(\mathbf{X}, t, \varepsilon_0) = \boldsymbol{\xi}(\mathbf{X}, t)$. The variation of the motion

$$\delta\boldsymbol{\xi}(\mathbf{X}, t) = \frac{\partial \hat{\boldsymbol{\xi}}}{\partial \varepsilon}(\mathbf{X}, t, \varepsilon_0) \tag{2.2}$$

defines the virtual displacement for each material point $\mathbf{X} \in \mathcal{S}$ at each instant of time $t \in \mathcal{I}$. The variational family of velocity fields $\frac{\partial \hat{\boldsymbol{\xi}}}{\partial t}(\mathbf{X}, t, \varepsilon)$ is induced by $\hat{\boldsymbol{\xi}}$ and contains the actual velocity field in the form $\frac{\partial \hat{\boldsymbol{\xi}}}{\partial t}(\mathbf{X}, t, \varepsilon_0) = \dot{\boldsymbol{\xi}}(\mathbf{X}, t)$. Therefore the variation of the velocity field is

$$\delta\dot{\boldsymbol{\xi}}(\mathbf{X}, t) = \frac{\partial}{\partial \varepsilon}\frac{\partial \hat{\boldsymbol{\xi}}}{\partial t}(\mathbf{X}, t, \varepsilon_0) = \frac{\partial}{\partial t}\frac{\partial \hat{\boldsymbol{\xi}}}{\partial \varepsilon}(\mathbf{X}, t, \varepsilon_0) \overset{(2.2)}{=} \frac{\partial(\delta\boldsymbol{\xi})}{\partial t}(\mathbf{X}, t) \ , \tag{2.3}$$

where we applied Schwarz' theorem. Due to the isomorphism between tangent spaces $T_{\mathbf{X}}\mathbb{E}^3$ and the base space $\mathbb{E}^3$, we identify the virtual displacements with elements of the euclidean three-space, i.e. $\delta\boldsymbol{\xi} \in \mathbb{E}^3$. Eugster (2015) introduced the space of forces to be the dual space of the space of virtual displacements. In other words the space of forces is the set of linear, real-valued functionals on the space of virtual displacements. According to this we define the forces acting on the mechanical system $\mathcal{S}$ during the time interval $\mathcal{I}$ to be of the form

$$\int_{\mathcal{I}} \mathrm{d}\mathbf{f} \colon \mathbb{E}^3 \to \mathbb{R}, \ \delta\boldsymbol{\xi} \mapsto \delta A = \int_{\mathcal{I}} \mathrm{d}\mathbf{f}(\delta\boldsymbol{\xi}) \ , \tag{2.4}$$

where the real number δA is called the virtual action of the mechanical system $\mathcal{S}$. As a fundamental principle of mechanics we postulate the principle of virtual action as an axiom.

Axiom 1 (Principle of Virtual Action)**.** *The virtual action of all forces acting on a mechanical system $\mathcal{S}$ vanishes for all virtual displacements, i.e.*

$$\delta A = \int_{\mathcal{I}} \mathrm{d}\mathbf{f}(\delta\boldsymbol{\xi}) = 0 \quad \forall \delta\boldsymbol{\xi} \ . \tag{2.5}$$

The forces acting on a mechanical system are so far a very general construct. In order to get a proper description of the dynamical behavior of a mechanical system we require further specifications of the forces with appropriate force laws. We assume that the virtual action is composed by two parts, the virtual action of dynamical forces δA^{dyn} and the virtual action of spatial forces δA^{spa}, which we express as

$$\delta A = \delta A^{\mathrm{dyn}} + \delta A^{\mathrm{spa}} \ . \tag{2.6}$$

The dynamical forces model the interaction between different time points. In order to respect causality of time, only interactions between neighboring time instants are possible and the virtual action of the dynamical forces is defined as

$$\delta A^{\mathrm{dyn}} = \int_{\mathcal{I}} \int_{\mathcal{S}} \delta\dot{\boldsymbol{\xi}}^{\mathrm{T}} \mathrm{d}\mathbf{P} \mathrm{d}t \; . \tag{2.7}$$

The dynamical forces (2.7) can be interpreted as internal forces in time direction of the extended mechanical system $\mathcal{S} \times \mathcal{I}$. The spatial forces model the internal and external forces of the system $\mathcal{S}$, where internal forces describe the interaction between different spatial points of the system $\mathcal{S}$ and external forces model the interaction of $\mathcal{S}$ with other systems that have no common material point with $\mathcal{S}$. The virtual action of the spatial forces

$$\delta A^{\mathrm{spa}} = \delta A^{\mathrm{int}} + \delta A^{\mathrm{ext}} = -\int_{\mathcal{I}} \int_{\mathcal{S}} \delta\boldsymbol{\xi}^{\mathrm{T}} \mathrm{d}\mathbf{F} \mathrm{d}t - \sum_i \int_{\mathcal{S}} \delta\boldsymbol{\xi}(t_i)^{\mathrm{T}} \mathrm{d}\boldsymbol{\Lambda}_i \tag{2.8}$$

contribute negatively to the total virtual action, where $\mathrm{d}\mathbf{F}$ accounts for forces that act over a certain time interval and $\mathrm{d}\boldsymbol{\Lambda}_i$ account for impulsive forces acting at the time instants t_i. As we restrict us in the following to rigid multi-body systems, the virtual action of stress fields is omitted here. With the virtual action contributions (2.7) and (2.8), the principle of virtual action (2.5) reads as

$$\delta A(\delta\boldsymbol{\xi}) = \int_{\mathcal{I}} \int_{\mathcal{S}} \left\{ \delta\dot{\boldsymbol{\xi}}^{\mathrm{T}} \mathrm{d}\mathbf{P} - \delta\boldsymbol{\xi}^{\mathrm{T}} \mathrm{d}\mathbf{F} \right\} \mathrm{d}t - \sum_i \int_{\mathcal{S}} \delta\boldsymbol{\xi}(t_i)^{\mathrm{T}} \mathrm{d}\boldsymbol{\Lambda}_i = 0 \quad \forall \delta\boldsymbol{\xi} \; . \tag{2.9}$$

In the following the dynamical forces are related to the velocity by the constitutive law

$$\mathrm{d}\mathbf{P} = -\dot{\boldsymbol{\xi}} \mathrm{d}m \; , \tag{2.10}$$

where $\mathrm{d}m$ is the mass distribution of the system $\mathcal{S}$. The constitutive law models the inertia of the system. The corresponding potential to the constitutive law is the kinetic energy

$$T(\dot{\boldsymbol{\xi}}) = \frac{1}{2} \int_{\mathcal{S}} \dot{\boldsymbol{\xi}}^{\mathrm{T}} \dot{\boldsymbol{\xi}} \mathrm{d}m \; , \tag{2.11}$$

which allows us to write

$$\int_{\mathcal{S}} \delta\dot{\boldsymbol{\xi}}^{\mathrm{T}} \mathrm{d}\mathbf{P} \overset{(2.10)}{=} -\int_{\mathcal{S}} \delta\dot{\boldsymbol{\xi}}^{\mathrm{T}} \dot{\boldsymbol{\xi}} \mathrm{d}m = -\delta T(\dot{\boldsymbol{\xi}}) \; . \tag{2.12}$$

For the sake of brevity we restrict the external impulsive forces $\mathrm{d}\boldsymbol{\Lambda}_i$ to act only at the boundaries of the time interval $\mathcal{I}$[1]. Consequently, the principle of

[1] The influence of an impulsive force in the interior of the time interval $\mathcal{I}$ is shown in Section A.3 by means of an example.

virtual action (2.9), together with (2.10), takes the form

$$\delta A = -\int_{\mathcal{I}} \int_{\mathcal{S}} \left\{ \delta\dot{\boldsymbol{\xi}}^{\mathrm{T}} \dot{\boldsymbol{\xi}} \mathrm{d}m + \delta\boldsymbol{\xi}^{\mathrm{T}} \mathrm{d}\mathbf{F} \right\} \mathrm{d}t + \int_{\mathcal{S}} \delta\boldsymbol{\xi}^{\mathrm{T}} \mathrm{d}\boldsymbol{\Lambda} \Big|_{\partial\mathcal{I}} = 0 \quad \forall \delta\boldsymbol{\xi} \,, \tag{2.13}$$

with the notation

$$\int_{\mathcal{S}} \delta\boldsymbol{\xi}^{\mathrm{T}} \mathrm{d}\boldsymbol{\Lambda} \Big|_{\partial\mathcal{I}} = \int_{\mathcal{S}} \delta\boldsymbol{\xi}(T)^{\mathrm{T}} \mathrm{d}\boldsymbol{\Lambda}_T - \int_{\mathcal{S}} \delta\boldsymbol{\xi}(0)^{\mathrm{T}} \mathrm{d}\boldsymbol{\Lambda}_0 \,. \tag{2.14}$$

A special choice of virtual displacements allows to deduce the principle of virtual work at each instant of time from the principle of virtual action (2.13). By a telescopic expansion in the virtual action of (2.13) and by applying the fundamental theorem of calculus we obtain

$$\begin{aligned} \delta A = & -\int_{\mathcal{I}} \left\{ \int_{\mathcal{S}} \delta\dot{\boldsymbol{\xi}}^{\mathrm{T}} \dot{\boldsymbol{\xi}} \mathrm{d}m - \frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathcal{S}} \delta\boldsymbol{\xi}^{\mathrm{T}} \dot{\boldsymbol{\xi}} \mathrm{d}m + \int_{\mathcal{S}} \delta\boldsymbol{\xi}^{\mathrm{T}} \mathrm{d}\mathbf{F} \right\} \mathrm{d}t \\ & -\int_{\mathcal{I}} \left\{ \frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathcal{S}} \delta\boldsymbol{\xi}^{\mathrm{T}} \dot{\boldsymbol{\xi}} \mathrm{d}m \right\} \mathrm{d}t + \int_{\mathcal{S}} \delta\boldsymbol{\xi}^{\mathrm{T}} \mathrm{d}\boldsymbol{\Lambda} \Big|_{\partial\mathcal{I}} \\ = & -\int_{\mathcal{I}} \int_{\mathcal{S}} \left\{ \delta\dot{\boldsymbol{\xi}}^{\mathrm{T}} \dot{\boldsymbol{\xi}} \mathrm{d}m - \frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathcal{S}} \delta\boldsymbol{\xi}^{\mathrm{T}} \dot{\boldsymbol{\xi}} \mathrm{d}m + \int_{\mathcal{S}} \delta\boldsymbol{\xi}^{\mathrm{T}} \mathrm{d}\mathbf{F} \right\} \mathrm{d}t \\ & + \int_{\mathcal{S}} \delta\boldsymbol{\xi}^{\mathrm{T}} (\mathrm{d}\boldsymbol{\Lambda} - \dot{\boldsymbol{\xi}} \mathrm{d}m) \Big|_{\partial\mathcal{I}} \,. \end{aligned} \tag{2.15}$$

By the product rule for differentiation (2.15) reads as

$$\delta A = \int_{\mathcal{I}} \int_{\mathcal{S}} \delta\boldsymbol{\xi}^{\mathrm{T}} (\ddot{\boldsymbol{\xi}} \mathrm{d}m - \mathrm{d}\mathbf{F}) \mathrm{d}t + \int_{\mathcal{S}} \delta\boldsymbol{\xi}^{\mathrm{T}} (\mathrm{d}\boldsymbol{\Lambda} - \dot{\boldsymbol{\xi}} \mathrm{d}m) \Big|_{\partial\mathcal{I}} \,, \tag{2.16}$$

which is nothing else but the virtual action of the system after integration by parts. Let $\delta\boldsymbol{\xi}(\mathbf{X}, t)$ be an arbitrary virtual displacement field and let $\delta\boldsymbol{\zeta}(\mathbf{X}, t) = \delta(t - \bar{t}) \delta\boldsymbol{\xi}(\mathbf{X}, \bar{t})$ be a special choice of virtual displacement field, where $\bar{t} \in \mathrm{int}(\mathcal{I})$ is an arbitrary time instant in the interior of the interval $\mathcal{I}$ and $\delta(t - \bar{t})$ is the shifted Dirac distribution. Since the principle of virtual action (2.13) demands (2.16) to vanish for all virtual displacements, it does so also for the special choice $\delta\boldsymbol{\zeta}(\mathbf{X}, t)$. As $\delta(t - \bar{t})$ vanishes on the boundaries of $\mathcal{I}$ for all choices of $\bar{t} \in \mathrm{int}(\mathcal{I})$, the principle of virtual action (2.13) in the form (2.16) induces

$$\delta A = \int_{\mathcal{I}} \int_{\mathcal{S}} \delta(t - \bar{t}) \delta\boldsymbol{\xi}(\mathbf{X}, \bar{t})^{\mathrm{T}} (\ddot{\boldsymbol{\xi}} \mathrm{d}m - \mathrm{d}\mathbf{F}) \mathrm{d}t = 0 \quad \forall \delta\boldsymbol{\xi}(\mathbf{X}, \bar{t}), \ \forall \bar{t} \,. \tag{2.17}$$

Integrating over the time interval $\mathcal{I}$ and labeling $\bar{t}$ by t leads directly to the principle of virtual work.

Principle 1 (Principle of Virtual Work)**.** *The virtual work δW of all forces acting on a mechanical system $\mathcal{S}$ vanishes for all virtuall discplacements $\delta\boldsymbol{\xi}$ and at every instant of time t, i.e.*

$$\delta W = \int_{\mathcal{S}} \delta\boldsymbol{\xi}^{\mathrm{T}}(\ddot{\boldsymbol{\xi}}\mathrm{d}m - \mathrm{d}\mathbf{F}) = 0 \quad \forall\delta\boldsymbol{\xi},\ \forall t\ . \tag{2.18}$$

The virtual work, as defined in (2.18), is the temporal density of the virtual action, as can be seen from (2.16). Furthermore, by comparing the integrand of the time integration in (2.16) to the equivalent integrand in (2.15), the principle of virtual work can be written in the form

$$\delta W = -\int_{\mathcal{S}} \delta\dot{\boldsymbol{\xi}}^{\mathrm{T}}\dot{\boldsymbol{\xi}}\mathrm{d}m + \frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{S}} \delta\boldsymbol{\xi}^{\mathrm{T}}\dot{\boldsymbol{\xi}}\mathrm{d}m - \int_{\mathcal{S}} \delta\boldsymbol{\xi}^{\mathrm{T}}\mathrm{d}\mathbf{F} = 0 \quad \forall\delta\boldsymbol{\xi},\ \forall t\ , \tag{2.19}$$

which, according to Hamel (1967), Heun called Lagrange's central equation.

2.2 Dynamics in Generalized Coordinates

For a finite degree of freedom system the state of the mechanical system at each instant of time t can be completely described by a set of generalized coordinates $\mathbf{q}(t) \in \mathbb{R}^n$. Therefore, we assume the existence of a function $\boldsymbol{\varphi}$, such that

$$\boldsymbol{\xi}(\mathbf{X}, t) = \boldsymbol{\varphi}(\mathbf{X}, \mathbf{q}(t), t)\ . \tag{2.20}$$

Consider the variational family $\hat{\mathbf{q}}(t, \varepsilon)$, which contains the actual motion of the generalized coordinates in the sense that $\hat{\mathbf{q}}(t, \varepsilon_0) = \mathbf{q}(t)$. The variational family is assumed to be differentiable with respect to ε. This allows the definition of the variation of $\mathbf{q}$ as

$$\delta\mathbf{q}(t) = \frac{\partial\hat{\mathbf{q}}}{\partial\varepsilon}(t, \varepsilon_0)\ . \tag{2.21}$$

As $\frac{\partial\hat{\mathbf{q}}}{\partial t}(t, \varepsilon_0) = \dot{\mathbf{q}}(t)$ holds, $\frac{\partial\hat{\mathbf{q}}}{\partial t}(t, \varepsilon)$ is a variational family that contains the generalized velocities $\dot{\mathbf{q}}$. Thus, the variation of the generalized velocities is

$$\delta\dot{\mathbf{q}}(t) = \frac{\partial}{\partial\varepsilon}\frac{\partial\hat{\mathbf{q}}}{\partial t}(t, \varepsilon_0) = \frac{\partial}{\partial t}\frac{\partial\hat{\mathbf{q}}}{\partial\varepsilon}(t, \varepsilon_0) \overset{(2.21)}{=} \frac{\partial(\delta\mathbf{q})}{\partial t}(t)\ , \tag{2.22}$$

where we have used Schwarz' theorem. By means of (2.20), the variational family $\hat{\mathbf{q}}(t, \varepsilon)$ induces a variational family of motions

$$\hat{\boldsymbol{\xi}}(\mathbf{X}, t, \varepsilon) = \boldsymbol{\varphi}(\mathbf{X}, \hat{\mathbf{q}}(t, \varepsilon), t)\ , \tag{2.23}$$

which by the definition (2.2) induces the virtual displacements for each material point $\mathbf{X}$

$$\delta\boldsymbol{\xi}(\mathbf{X}, t) = \frac{\partial\boldsymbol{\varphi}}{\partial\mathbf{q}}(\mathbf{X}, \mathbf{q}(t), t)\ \frac{\partial\hat{\mathbf{q}}}{\partial\varepsilon}(t, \varepsilon_0) \overset{(2.21)}{=} \frac{\partial\boldsymbol{\varphi}}{\partial\mathbf{q}}(\mathbf{X}, \mathbf{q}(t), t)\ \delta\mathbf{q}(t)\ . \tag{2.24}$$

Introducing the Jacobians

$$\mathbf{J}_{\mathbf{X}}(\mathbf{X},\mathbf{q}(t),t)=\frac{\partial\boldsymbol{\varphi}}{\partial\mathbf{q}}(\mathbf{X},\mathbf{q}(t),t)\quad\text{and}\quad\mathbf{J}_t(\mathbf{X},\mathbf{q}(t),t)=\frac{\partial\boldsymbol{\varphi}}{\partial t}(\mathbf{X},\mathbf{q}(t),t)\tag{2.25}$$

we can write the virtual displacements and the velocity field as $\delta\boldsymbol{\xi}=\mathbf{J}_{\mathbf{X}}\delta\mathbf{q}$ and $\dot{\boldsymbol{\xi}}=\mathbf{J}_{\mathbf{X}}\dot{\mathbf{q}}+\mathbf{J}_t$ respectively. The kinetic energy (2.11) therefore yields

$$T(\mathbf{q},\dot{\mathbf{q}},t)=\frac{1}{2}\int_{\mathcal{S}}(\dot{\mathbf{q}}^{\mathrm{T}}\mathbf{J}_{\mathbf{X}}^{\mathrm{T}}+\mathbf{J}_t^{\mathrm{T}})(\mathbf{J}_{\mathbf{X}}\dot{\mathbf{q}}+\mathbf{J}_t)\mathrm{d}m\ .\tag{2.26}$$

For the expression of the kinetic energy (2.11) in terms of generalized coordinates, it is convenient to introduce the integral expressions

$$\begin{aligned}\mathbf{M}(\mathbf{q},t)&=\int_{\mathcal{S}}(\mathbf{J}_{\mathbf{X}})^{\mathrm{T}}\mathbf{J}_{\mathbf{X}}\mathrm{d}m\ ,\\ \mathbf{b}(\mathbf{q},t)^{\mathrm{T}}&=\int_{\mathcal{S}}(\mathbf{J}_t)^{\mathrm{T}}\mathbf{J}_{\mathbf{X}}\mathrm{d}m\ ,\\ \eta(\mathbf{q},t)&=\int_{\mathcal{S}}\frac{1}{2}(\mathbf{J}_t)^{\mathrm{T}}\mathbf{J}_t\mathrm{d}m\ ,\end{aligned}\tag{2.27}$$

where $\mathbf{M}(\mathbf{q},t)$ is the mass matrix. Hence the kinetic energy (2.26) can be expressed as

$$T(\mathbf{q},\dot{\mathbf{q}},t)=\frac{1}{2}\dot{\mathbf{q}}^{\mathrm{T}}\mathbf{M}(\mathbf{q},t)\dot{\mathbf{q}}+\mathbf{b}^{\mathrm{T}}(\mathbf{q},t)\dot{\mathbf{q}}+\eta(\mathbf{q},t)\ .\tag{2.28}$$

Since the mass matrix $\mathbf{M}$ is symmetric and positive definite, the kinetic energy T is convex with respect to the generalized velocities $\dot{\mathbf{q}}$. Note, that the kinetic energy (2.11) for a finite degree of freedom system, with (2.20), actually is $T(\frac{\mathrm{d}\boldsymbol{\varphi}}{\mathrm{d}t}(\mathbf{X},\mathbf{q}(t),t))$, which according to (2.26) can be seen as a function of $\mathbf{q}$, $\dot{\mathbf{q}}$ and t. Hence we write $T(\mathbf{q},\dot{\mathbf{q}},t)$, which introduces an ambiguity in the notion of T. From the context it is always clear what is meant. Using the variation of the kinetic energy (2.12), the induced virtual displacements (2.24) and the principle of virtual action (2.13), the principle of virtual action expressed in generalized coordinates reads as

$$\delta A=-\int_{\mathcal{I}}\left\{\delta T(\mathbf{q},\dot{\mathbf{q}},t)+\delta\mathbf{q}^{\mathrm{T}}\mathbf{f}\right\}\mathrm{d}t+\delta\mathbf{q}^{\mathrm{T}}\mathbf{P}\big|_{\partial\mathcal{I}}=0\quad\forall\delta\mathbf{q}\ ,\tag{2.29}$$

where we have introduced the generalized forces $\mathbf{f}$ and the generalized impulsive forces $\mathbf{P}$ as

$$\mathbf{f}=\int_{\mathcal{S}}(\mathbf{J}_{\mathbf{X}})^{\mathrm{T}}\mathrm{d}\mathbf{F}\quad\text{and}\quad\mathbf{P}=\int_{\mathcal{S}}(\mathbf{J}_{\mathbf{X}})^{\mathrm{T}}\mathrm{d}\boldsymbol{\Lambda}\ .\tag{2.30}$$

Borri (1986) and Izadpanah (1986) point out the importance of modeling the boundary contributions of the virtual action as external forces $\mathbf{P}$, which play a crucial role in the treatment of the initial conditions.[2] The virtual action (2.29) can be split into to the sum of

$$\delta A^{\mathrm{dyn}} = -\int_{\mathcal{I}} \delta T(\mathbf{q}, \dot{\mathbf{q}}, t)\mathrm{d}t \quad \text{and} \quad \delta A^{\mathrm{spa}} = -\int_{\mathcal{I}} \delta \mathbf{q}^{\mathrm{T}} \mathbf{f} \mathrm{d}t + \delta \mathbf{q}^{\mathrm{T}} \mathbf{P}\big|_{\partial \mathcal{I}} \ , \quad (2.31)$$

where the contribution of the dynamical and spatial forces correspond to (2.7) and (2.8). In order to derive a strong variational form of the principle of virtual action, we evaluate the variation

$$\delta T(\mathbf{q}, \dot{\mathbf{q}}, t) = \frac{\partial T}{\partial \dot{\mathbf{q}}} \, \delta \dot{\mathbf{q}} + \frac{\partial T}{\partial \mathbf{q}} \, \delta \mathbf{q} \quad (2.32)$$

of the kinetic energy in (2.29) and by applying integration by parts we obtain the strong variational form of the principle of virtual action

$$\int_{\mathcal{I}} \delta \mathbf{q}^{\mathrm{T}} \left(\frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{\partial T}{\partial \dot{\mathbf{q}}} \right)^{\mathrm{T}} - \left(\frac{\partial T}{\partial \mathbf{q}} \right)^{\mathrm{T}} - \mathbf{f} \right) \mathrm{d}t + \delta \mathbf{q}^{\mathrm{T}} \left(\mathbf{P} - \left(\frac{\partial T}{\partial \dot{\mathbf{q}}} \right)^{\mathrm{T}} \right) \Big|_{\partial \mathcal{I}} = 0 \quad (2.33)$$

for all $\delta \mathbf{q}$. The complete boundary value problem (BVP) with the equations of motion in the interior of $\mathcal{I}$

$$\frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{\partial T}{\partial \dot{\mathbf{q}}} \right)^{\mathrm{T}} - \left(\frac{\partial T}{\partial \mathbf{q}} \right)^{\mathrm{T}} - \mathbf{f} = 0 \quad (2.34)$$

and the boundary conditions on $\partial \mathcal{I}$

$$\begin{aligned} \mathbf{P}_0 &= \left(\frac{\partial T}{\partial \dot{\mathbf{q}}} \right)^{\mathrm{T}} (\mathbf{q}(0), \dot{\mathbf{q}}(0), 0) \ , \\ \mathbf{P}_T &= \left(\frac{\partial T}{\partial \dot{\mathbf{q}}} \right)^{\mathrm{T}} (\mathbf{q}(T), \dot{\mathbf{q}}(T), T) \ , \end{aligned} \quad (2.35)$$

follow by the application of the fundamental lemma of calculus of variations to (2.33). In the description and prediction of the motion of the mechanical system $\mathcal{S}$ one often is confronted with an initial value problem (IVP). An IVP consists in finding the motion $\mathbf{q}(t)$ with known initial configuration $\mathbf{q}(0) = \mathbf{q}_0$ and known initial velocity $\dot{\mathbf{q}}(0) = \mathbf{u}_0$. In order to get an IVP from (2.33) we have to model the impulsive forces $\mathbf{P}_0$ and $\mathbf{P}_T$ according to the following set-valued constitutive laws

$$\begin{aligned} \mathbf{P}_0 &\in \mathbb{R}^n \ s.t. \ \mathbf{q}(0) = \mathbf{q}_0 \ , \\ \mathbf{P}_T &\in \mathbb{R}^n \ s.t. \ \dot{\mathbf{q}}(0) = \mathbf{u}_0 \ . \end{aligned} \quad (2.36)$$

[2] Often the external forces $\mathbf{P}$ are eliminated from (2.29) by (2.35). Further comments on this elimination process can be found in Secion 2.3.

Restricting the strong variational form of the principle of virtual action (2.33) to motions that fullfill the initial conditions this yields

$$\int_{\mathcal{I}} \delta\mathbf{q}^{\mathrm{T}} \left(\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial T}{\partial \dot{\mathbf{q}}}\right)^{\mathrm{T}} - \left(\frac{\partial T}{\partial \mathbf{q}}\right)^{\mathrm{T}} - \mathbf{f} \right) \mathrm{d}t + \delta\mathbf{q}^{\mathrm{T}} \left(\mathbf{P} - \left(\frac{\partial T}{\partial \dot{\mathbf{q}}}\right)^{\mathrm{T}} \right)\Big|_{T} = 0 \quad (2.37)$$

for all $\delta\mathbf{q}$, where $\delta\mathbf{q}(0) = 0$, $\delta\dot{\mathbf{q}}(0) = 0$ and $\mathbf{q}(t)$ fulfills the initial conditions $\mathbf{q}(0) = \mathbf{q}_0$ and $\dot{\mathbf{u}}(0) = \mathbf{u}_0$. The fact that the force $\mathbf{P}_0$ has no contribution to the virtual action of the constrained system shows that $\mathbf{P}_0$ is a perfect bilateral constraint force by means of the principle of d'Alembert–Lagrange. Using the fundamental lemma of the calculus of variations in (2.37) gives the equation of motion (2.34) with $\mathbf{q}(t)$ fulfilling the initial conditions $\mathbf{q}(0) = \mathbf{q}_0$ and $\dot{\mathbf{q}}(0) = \mathbf{u}_0$, which determines the motion $\mathbf{q}(t)$ completely. Additionally we get the boundary condition

$$\mathbf{P}_T - \left(\frac{\partial T}{\partial \dot{\mathbf{q}}}\right)^{\mathrm{T}} (\mathbf{q}(T), \dot{\mathbf{q}}(T), T) = 0 \,, \quad (2.38)$$

which determines the value of the force $\mathbf{P}_T$ necessary to impose the initial condition.

2.3 Hamilton's Law of Varying Action

Consider a finite degree of freedom system $\mathcal{S}$ and assume that all forces can be deduced from a potential $V(\mathbf{q}, t)$, i.e.

$$\mathbf{f} = -\left(\frac{\partial V}{\partial \mathbf{q}}\right)^{\mathrm{T}} \quad \Rightarrow \quad \delta\mathbf{q}^{\mathrm{T}}\mathbf{f} = -\delta\mathbf{q}^{\mathrm{T}}\left(\frac{\partial V}{\partial \mathbf{q}}\right)^{\mathrm{T}} = -\delta V(\mathbf{q}, t) \,. \quad (2.39)$$

The difference between the kinetic energy T and the potential V of a mechanical system is called Lagrangian

$$L(\mathbf{q}, \dot{\mathbf{q}}, t) = T(\mathbf{q}, \dot{\mathbf{q}}, t) - V(\mathbf{q}, t) \,. \quad (2.40)$$

Using (2.39) and (2.40) the principle of virtual action (2.29) takes the form of Hamilton's Law of varying action.

Principle 2 (Hamilton's Law of Varying Action)**.** *A finite degree of freedom system described by the generalized coordinates* $\mathbf{q}(t)$*, which is influenced by potential forces only, has vanishing virtual action for all variations of* $\mathbf{q}(t)$*, i.e*

$$\delta A = -\int_{\mathcal{I}} \delta L(\mathbf{q}, \dot{\mathbf{q}}, t)\mathrm{d}t + \delta\mathbf{q}^{\mathrm{T}}\mathbf{P}\big|_{\partial\mathcal{I}} = 0 \quad \forall\delta\mathbf{q} \,. \quad (2.41)$$

Hamilton (1834) arrived at the formulation

$$\delta A = -\int_{\mathcal{I}} \delta L(\mathbf{q}, \dot{\mathbf{q}}, t)\mathrm{d}t + \delta\mathbf{q}^{\mathrm{T}} \left(\frac{\partial T}{\partial \dot{\mathbf{q}}}\right)^{\mathrm{T}}\Bigg|_{\partial\mathcal{I}} = 0 \quad \forall \delta\mathbf{q} \,, \tag{2.42}$$

which he called the law of varying action. Hamilton's formulation can be derived from (2.41) by inserting in the boundary conditions (2.35). This step, namely inserting strong boundary conditions into a weak formulation, is worrisome, as Papes (2011) showed in an example for a linear elastic bar. Additionally, (2.42) does not represent the whole BVP anymore.

If the positions at the boundaries of the time interval $\mathbf{q}(0)$ and $\mathbf{q}(T)$ are known, then the boundary terms in (2.41) vanish, and (2.41) becomes a stationarity condition, which leads to the principle of Hamilton (1835).

Principle 3 (Principle of Hamilton)**.** *Consider a finite degree of freedom system described by the generalized coordinates $\mathbf{q}(t)$, where the initial and final position are fixed to $\mathbf{q}(0) = \mathbf{q}_0$ and $\mathbf{q}(T) = \mathbf{q}_T$. If all forces acting on the system are potential forces, then the action integral*

$$A = \int_{\mathcal{I}} L(\mathbf{q}, \dot{\mathbf{q}}, t)\mathrm{d}t \tag{2.43}$$

is stationary, where $L = T - V$, cf. (2.40)*.*

A necessary and sufficient condition for the stationarity of the action integral is that its variation vanishes.

$$\begin{aligned} \delta A &= \int_{\mathcal{I}} \left(\delta\dot{\mathbf{q}}^{\mathrm{T}} \left(\frac{\partial L}{\partial \dot{\mathbf{q}}}\right)^{\mathrm{T}} + \delta\mathbf{q}^{\mathrm{T}} \left(\frac{\partial L}{\partial \mathbf{q}}\right)^{\mathrm{T}} \right) \mathrm{d}t \\ &\overset{i.p.}{=} \int_{\mathcal{I}} \delta\mathbf{q}^{\mathrm{T}} \left(-\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{\mathbf{q}}}\right)^{\mathrm{T}} + \left(\frac{\partial L}{\partial \mathbf{q}}\right)^{\mathrm{T}} \right) \mathrm{d}t \\ &= 0 \qquad \forall \delta\mathbf{q} \quad \text{s.t. } \delta\mathbf{q}(0) = \delta\mathbf{q}(T) = 0 \,. \end{aligned} \tag{2.44}$$

The fundamental lemma of calculus of variations leads directly to the Euler–Lagrange equations

$$-\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{\mathbf{q}}}\right)^{\mathrm{T}} + \left(\frac{\partial L}{\partial \mathbf{q}}\right)^{\mathrm{T}} = 0 \,, \tag{2.45}$$

with the boundary conditions $\mathbf{q}(0) = \mathbf{q}_0$ and $\mathbf{q}(T) = \mathbf{q}_T$. The Euler-Lagrange equations are therefore a necessary and sufficient condition for the stationarity of the action integral (2.43). The Euler–Lagrange equations represent the equations of motion (2.34) for systems with potential forces only, and therefore follow also from Hamilton's law of varying action with the same boundary

conditions (2.35) as for systems with non-potential forces. The procedure of transforming the boundary value problem into an initial value problem by means of the constitutive law (2.36) still holds for Hamilton's law of varying action (2.41).

Chapter 3

Multi-field Formulations of Dynamics

In the theory of linear elasticity there are multi-field variational principles, which have become very popular as a starting point for finite element formulations, as phenomena such as locking can be eliminated by this approach, cf. Belytschko et al. (2013). The Hellinger–Reissner principle, proposed by Reissner (1953), is a two-field formulation, whose independent variables are the displacement and stress fields. Hu (1955) and Washizu (1955) introduced independently a three-field formulation with displacement, strain and stress fields as independent quantities. In this chapter we introduce the Legendre–Fenchel transform, which is subsequently used to derive the $(\mathbf{q}, \mathbf{p})$-formulation, the dynamical analogon to the Hellinger–Reissner principle, and the $(\mathbf{q}, \mathbf{u}, \mathbf{p})$-formulation, which is the dynamical analogon to the Hu–Washizu principle. Moreover the Legendre–Fenchel transform is used to derive a generalization of the $(\mathbf{q}, \mathbf{u}, \mathbf{p})$-formulation, which is shown to contain the other formulations. The $(\mathbf{q}, \mathbf{p})$-formulation, which has the generalized positions $\mathbf{q}(t)$ and generalized momenta $\mathbf{p}(t)$ as independent quantities, is called the canonical formulation, cf. Lanczos (1970), and was introduced by Hamilton (1835). In section 3.2 we derive the canonical form of Hamilton's law of varying action and Hamilton's principle, which are often starting point for space-time finite element formulations, cf. e.g. Simkins (1981), Betsch and Steinmann (2000b), and Borri and Bottasso (1993).

3.1 Legendre–Fenchel Transform

Consider a convex function $f\colon \mathbb{R}^n \to \mathbb{R}$, then the convex function $f^*\colon \mathbb{R}^n \to \mathbb{R}$ defined by

$$f^*(\mathbf{z}) = \sup_{\mathbf{x}\in\mathbb{R}^n} \{\mathbf{z}^{\mathrm{T}}\mathbf{x} - f(\mathbf{x})\} \tag{3.1}$$

is said to be conjugate to f. The mapping $f \mapsto f^*$ is called Legendre–Fenchel transform and we say that $\mathbf{x}$ and $\mathbf{z}$ are dual to each other. We assume f to be differentiable, which has the consequence that the biconjugate $f^{**} = (f^*)^*$ is equal to f , i.e. $f^{**} = f$. This allows to represent the function f as

$$f(\mathbf{x}) = \sup_{\mathbf{z}\in\mathbb{R}^n} \{\mathbf{x}^{\mathrm{T}}\mathbf{z} - f^*(\mathbf{z})\} \; . \tag{3.2}$$

Moreover Fenchel's equation

$$\mathbf{x}^{\mathrm{T}}\mathbf{z} = f(\mathbf{x}) + f^*(\mathbf{z}) \quad \Leftrightarrow \quad \mathbf{x}^{\mathrm{T}} = \frac{\partial f^*(\mathbf{z})}{\partial \mathbf{z}} \quad \Leftrightarrow \quad \mathbf{z}^{\mathrm{T}} = \frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} \tag{3.3}$$

holds. For a proof of Fenchel's equation and the property of the biconjugate we refere to Rockafellar and Wets (2009), Chap. 11. Assume that $\mathbf{x}$ depends on a parameter $t \in \mathbb{R}$ then

$$\int f(\mathbf{x})\mathrm{d}t \overset{(3.2)}{=} \int \sup_{\mathbf{z}\in\mathbb{R}^n} \{\mathbf{x}^{\mathrm{T}}\mathbf{z} - f^*(\mathbf{z})\}\mathrm{d}t \tag{3.4}$$

can be expressed as

$$\int f(\mathbf{x})\mathrm{d}t = \int \{\mathbf{x}^{\mathrm{T}}\mathbf{z} - f^*(\mathbf{z})\}\mathrm{d}t \quad \text{iff} \quad \delta\int \{\mathbf{x}^{\mathrm{T}}\mathbf{z} - f^*(\mathbf{z})\}\mathrm{d}t = 0 \;\forall \delta\mathbf{z} \; , \tag{3.5}$$

since the condition $\delta\int\{\mathbf{x}^{\mathrm{T}}\mathbf{z} - f^*(\mathbf{z})\}\mathrm{d}t = 0 \;\forall\delta\mathbf{z}$ in (3.5) corresponds to the stationarity condition of the supremum in (3.4). Alternatively one can look at (3.5) as a consequence of Fenchel's equation (3.3). For the variation of f with respect to $\mathbf{x}$, (3.5) leads to

$$\delta\int f(\mathbf{x})\mathrm{d}t = \delta\int \{\mathbf{x}^{\mathrm{T}}\mathbf{z} - f^*(\mathbf{z})\}\mathrm{d}t \quad \text{iff} \quad \delta\int \{\mathbf{x}^{\mathrm{T}}\mathbf{z} - f^*(\mathbf{z})\}\mathrm{d}t = 0 \;\forall \delta\mathbf{z} \; , \tag{3.6}$$

since $\mathbf{x}$ and $\mathbf{z}$ are independent variables.

Let $a\colon \mathbb{R}^n \to \mathbb{R}$ be the function

$$a(\mathbf{x}) = \frac{1}{2}\mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x} + \mathbf{b}^{\mathrm{T}}\mathbf{x} + c \; , \tag{3.7}$$

where $\mathbf{A} \in \mathbb{R}^{n\times n}$ is symmetric and positive definite, $\mathbf{b} \in \mathbb{R}^n$ and $c \in \mathbb{R}$. According to (3.1) the conjugate $a^*\colon \mathbb{R}^n \to \mathbb{R}$ of a is

$$a^*(\mathbf{z}) = \sup_{\mathbf{x}\in\mathbb{R}^n} \{\mathbf{z}^{\mathrm{T}}\mathbf{x} - \frac{1}{2}\mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x} - \mathbf{b}^{\mathrm{T}}\mathbf{x} - c\} \; . \tag{3.8}$$

Necessary and sufficient condition for the supremum is

$$\mathbf{z} - \mathbf{A}\mathbf{x} - \mathbf{b} = 0 \quad \Leftrightarrow \quad \mathbf{x} = \mathbf{A}^{-1}(\mathbf{z} - \mathbf{b}) \,, \tag{3.9}$$

which can be inserted into (3.8) and yields

$$a^*(\mathbf{z}) = \frac{1}{2}\mathbf{z}^{\mathrm{T}}\mathbf{A}^{-1}\mathbf{z} - \mathbf{b}^{\mathrm{T}}\mathbf{A}^{-1}\mathbf{z} + \frac{1}{2}\mathbf{b}^{\mathrm{T}}\mathbf{A}^{-1}\mathbf{b} - c \,, \tag{3.10}$$

i.e. the Legendre–Fenchel transform of a.

3.2 (q,p)-Formulation

The kinetic energy $T(\mathbf{q}, \dot{\mathbf{q}}, t)$ is differentiable and convex with respect to the generalized velocities $\dot{\mathbf{q}}$, as can be deduced from (2.28). This allows a pointwise Legendre–Fenchel transform of the kinetic energy and defines the conjugate kinetic energy

$$T^*(\mathbf{q}, \mathbf{p}, t) = (T(\mathbf{q}, \cdot, t))^*(\mathbf{p}) \tag{3.11}$$

together with the generalized momentum $\mathbf{p}$, which is the dual variable of the generalized velocities $\dot{\mathbf{q}}$. As seen in (2.28), the kinetic energy has the form of the function a in (3.7), which leads together with (3.10) to the conjugate kinetic energy

$$T^*(\mathbf{q}, \mathbf{p}, t) = \frac{1}{2}\mathbf{p}^{\mathrm{T}}\mathbf{M}^{-1}\mathbf{p} - \mathbf{b}^{\mathrm{T}}\mathbf{M}^{-1}\mathbf{p} + \frac{1}{2}\mathbf{b}^{\mathrm{T}}\mathbf{M}^{-1}\mathbf{b} - \eta(\mathbf{q}, t) \,, \tag{3.12}$$

where the dependency of $\mathbf{M}$ and $\mathbf{b}$ on $(\mathbf{q}, t)$ has been neglected for the sake of brevity. By the use of (3.2), the kinetic energy T can be rewritten as

$$T(\mathbf{q}, \dot{\mathbf{q}}, t) = \sup_{\mathbf{p} \in \mathbb{R}^n} \{\dot{\mathbf{q}}^{\mathrm{T}}\mathbf{p} - T^*(\mathbf{q}, \mathbf{p}, t)\} \,. \tag{3.13}$$

Using (3.6), the virtual action contribution of the dynamical forces (2.31) can be expressed as

$$\delta A^{\mathrm{dyn}} = -\int_{\mathcal{I}} \delta \left\{\dot{\mathbf{q}}^{\mathrm{T}}\mathbf{p} - T^*(\mathbf{q}, \mathbf{p}, t)\right\} \mathrm{d}t \quad \text{with} \quad \delta A^{\mathrm{dyn}} = 0 \ \forall \delta\mathbf{p} \,. \tag{3.14}$$

Since merely the virtual action of the inertial forces δA^{dyn} depends on the generalized momentum $\mathbf{p}$, the stationarity condition in (3.14) can also be stated for the total virtual action of the system, i.e. $\delta A = 0 \ \forall \delta\mathbf{p}$. Using (3.14), the principle of virtual action (2.29) expressed in the two independent variables $\mathbf{q}$ and $\mathbf{p}$ is

$$\delta A = -\int_{\mathcal{I}} \left\{\delta \left(\dot{\mathbf{q}}^{\mathrm{T}}\mathbf{p} - T^*(\mathbf{q}, \mathbf{p}, t)\right) + \delta\mathbf{q}^{\mathrm{T}}\mathbf{f}\right\} \mathrm{d}t + \delta\mathbf{q}^{\mathrm{T}}\mathbf{P}\big|_{\partial\mathcal{I}} = 0 \quad \forall \delta\mathbf{q}, \forall \delta\mathbf{p}. \tag{3.15}$$

Carrying out the variation of the conjugate kinetic energy and using integration by parts the strong variational form of the principle of virtual action

$$\begin{aligned}\delta A = \int_{\mathcal{I}} \left\{ \delta \mathbf{q}^{\mathrm{T}} \left(\dot{\mathbf{p}} - \mathbf{f} + \left(\frac{\partial T^*}{\partial \mathbf{q}} \right)^{\mathrm{T}} \right) - \delta \mathbf{p}^{\mathrm{T}} \left(\dot{\mathbf{q}} - \left(\frac{\partial T^*}{\partial \mathbf{p}} \right)^{\mathrm{T}} \right) \right\} \mathrm{d}t \\ + \delta \mathbf{q}^{\mathrm{T}} (\mathbf{P} - \mathbf{p}) \big|_{\partial \mathbf{I}} = 0 \quad \forall \delta \mathbf{q},\ \forall \delta \mathbf{p}\end{aligned} \tag{3.16}$$

is attained. By the fundamental lemma of calculus of variations, the terms in the round brackets have to vanish pointwise, which leads to the equations of motion

$$\dot{\mathbf{p}} + \left(\frac{\partial T^*}{\partial \mathbf{q}} \right)^{\mathrm{T}} = \mathbf{f} \quad \text{and} \quad \dot{\mathbf{q}} = \left(\frac{\partial T^*}{\partial \mathbf{p}} \right)^{\mathrm{T}}, \tag{3.17}$$

together with the boundary conditions $\mathbf{p}(0) = \mathbf{P}_0$ and $\mathbf{p}(T) = \mathbf{P}_T$. Sometimes it is useful to use Fenchel's equation (3.3) to transform the equations of motion (3.17) to

$$\dot{\mathbf{p}} + \left(\frac{\partial T^*}{\partial \mathbf{q}} \right)^{\mathrm{T}} = \mathbf{f} \quad \text{and} \quad \mathbf{p} = \left(\frac{\partial T}{\partial \dot{\mathbf{q}}} \right)^{\mathrm{T}}. \tag{3.18}$$

The two-field formulation of dynamics in terms of generalized coordinates $\mathbf{q}(t)$ and generalized momenta $\mathbf{p}(t)$ for mechanical systems with potential forces only, has been introduced by Hamilton (1835), where he used a function H, which we hence call Hamiltonian of the system. Often the $(\mathbf{q}, \mathbf{p})$-formulation is called the canonical formulation or canonical formalism, cf. Lanczos (1970). The Hamiltonian of the system

$$H(\mathbf{q}, \mathbf{p}, t) = (L(\mathbf{q}, \cdot, t))^*(\mathbf{p}) \overset{(2.40)}{=} T^*(\mathbf{q}, \mathbf{p}, t) + V(\mathbf{q}, t) \tag{3.19}$$

is the conjugate of the Lagrangian with respect to its dependency on the generalized velocities, where $V(\mathbf{q}, t)$ denotes the potential of the forces. Rewriting the virtual action of the non-impulsive forces of (3.15) for a conservative system as

$$\begin{aligned}\delta A &= -\int_{\mathcal{I}} \left\{ \delta(\dot{\mathbf{q}}^{\mathrm{T}} \mathbf{p} - T^*(\mathbf{q}, \mathbf{p}, t)) + \delta V(\mathbf{q}, t) \right\} \mathrm{d}t \\ &= -\int_{\mathcal{I}} \left\{ \delta(\dot{\mathbf{q}}^{\mathrm{T}} \mathbf{p}) - \delta(T^*(\mathbf{q}, \mathbf{p}, t) + V(\mathbf{q}, t)) \right\} \mathrm{d}t \\ &\overset{(3.19)}{=} -\int_{\mathcal{I}} \left\{ \delta(\dot{\mathbf{q}}^{\mathrm{T}} \mathbf{p}) - \delta H(\mathbf{q}, \mathbf{p}, t) \right\} \mathrm{d}t \\ &= -\delta \int_{\mathcal{I}} \left\{ \dot{\mathbf{q}}^{\mathrm{T}} \mathbf{p} - H(\mathbf{q}, \mathbf{p}, t) \right\} \mathrm{d}t\end{aligned} \tag{3.20}$$

leads to the canonical formulation of Hamilton's law of varying action (2.41)

$$\delta A = -\delta \int_{\mathcal{I}} \left\{ \dot{\mathbf{q}}^{\mathrm{T}} \mathbf{p} - H(\mathbf{q}, \mathbf{p}, t) \right\} \mathrm{d}t + \delta \mathbf{q}^{\mathrm{T}} \mathbf{P} \big|_{\partial \mathcal{I}} = 0 \quad \forall \delta \mathbf{q},\ \forall \delta \mathbf{p}\,. \tag{3.21}$$

Hamilton's law of varying action in canonical coordinates is the dynamic analogon to the principle of Hellinger–Reissner, cf. Reissner (1953), which corresponds to a two-field formulation in linear elasticity, i.e. a formulation in displacement and stress field. If the generalized positions are known on the boundaries of the time interval, i.e. $\mathbf{q}(0) = \mathbf{q}_0$ and $\mathbf{q}(T) = \mathbf{q}_T$ for known values $\mathbf{q}_0$ and $\mathbf{q}_T$, then Hamilton's law of varying action reduces to Hamilton's principle (2.43) in canonical coordinates, which demands the canonical action integral

$$A = \int_{\mathcal{I}} \left\{ \dot{\mathbf{q}}^{\mathrm{T}} \mathbf{p} - H(\mathbf{q}, \mathbf{p}, t) \right\} \mathrm{d}t \tag{3.22}$$

to be stationary. By means of the fundamental lemma of calculus of variation both Hamilton's law of varying action and Hamilton's principle lead to the canonical equations of motion

$$\dot{\mathbf{p}} = -\left(\frac{\partial H}{\partial \mathbf{q}} \right)^{\mathrm{T}} \quad \text{and} \quad \dot{\mathbf{q}} = \left(\frac{\partial H}{\partial \mathbf{p}} \right)^{\mathrm{T}} , \tag{3.23}$$

with the boundary conditions $\mathbf{p}(0) = \mathbf{P}_0$ and $\mathbf{p}(T) = \mathbf{P}_T$ for the law of varying action, and $\mathbf{q}(0) = \mathbf{q}_0$ and $\mathbf{q}(T) = \mathbf{q}_T$ for Hamilton's principle.

3.3 (q,u,p)-Formulation

The generalized velocity $\mathbf{u}$ is introduced as an independent variable in a similar way as we have introduced the generalized momentum $\mathbf{p}$ before. By definition (3.1) the conjugate kinetic energy defined in (3.11) is

$$T^*(\mathbf{q}, \mathbf{p}, t) = \sup_{\mathbf{u} \in \mathbb{R}^n} \left\{ \mathbf{u}^{\mathrm{T}} \mathbf{p} - T(\mathbf{q}, \mathbf{u}, t) \right\} . \tag{3.24}$$

We therefore can write the virtual action contribution of the dynamical forces (3.14) as

$$\begin{aligned} \delta A^{\mathrm{dyn}} &= -\int_{\mathcal{I}} \delta \left\{ \dot{\mathbf{q}}^{\mathrm{T}} \mathbf{p} - \left(\mathbf{u}^{\mathrm{T}} \mathbf{p} - T(\mathbf{q}, \mathbf{u}, t) \right) \right\} \mathrm{d}t \\ \text{s.t.} \qquad & \delta A^{\mathrm{dyn}} = 0 \ \forall \delta \mathbf{p}, \forall \delta \mathbf{u} , \end{aligned} \tag{3.25}$$

where we made use of (3.6). Considering this representation of the virtual action contribution of the dynamical forces, the principle of virtual action (3.15) can be written as

$$\delta A = -\int_{\mathcal{I}} \left\{ \delta \left(T(\mathbf{q}, \mathbf{u}, t) + \mathbf{p}^{\mathrm{T}} (\dot{\mathbf{q}} - \mathbf{u}) \right) + \delta \mathbf{q}^{\mathrm{T}} \mathbf{f} \right\} \mathrm{d}t + \delta \mathbf{q}^{\mathrm{T}} \mathbf{P} \big|_{\partial \mathcal{I}} = 0 \tag{3.26}$$

for all variations $\delta\mathbf{q}$, $\delta\mathbf{u}$ and $\delta\mathbf{p}$. Using integration by parts in (3.26) the strong variational form

$$\delta A = \int_{\mathcal{I}} \left\{ \delta\mathbf{q}^{\mathrm{T}} \left(\dot{\mathbf{p}} - \mathbf{f} + \left(\frac{\partial T}{\partial \mathbf{q}} \right)^{\mathrm{T}} \right) + \delta\mathbf{p}^{\mathrm{T}} \left(\dot{\mathbf{q}} - \mathbf{u} \right) + \delta\mathbf{u}^{\mathrm{T}} \left(\left(\frac{\partial T}{\partial \mathbf{u}} \right)^{\mathrm{T}} - \mathbf{p} \right) \right\} \mathrm{d}t + \delta\mathbf{q}^{\mathrm{T}} (\mathbf{P} - \mathbf{p}) \big|_{\partial\mathcal{I}} = 0 \quad \forall \delta\mathbf{q},\ \forall \delta\mathbf{p},\ \forall \delta\mathbf{u} \tag{3.27}$$

follows directly. Except the boundary terms Borri et al. (1992) use a variational three-field formulation, which corresponds to the strong variational form of the principle of virtual action (3.27). As the dynamic analogon of the Hu–Washizu principle, cf. Hu (1955) and Washizu (1955), Borri et al. (1992) call (3.27) the Hu–Washizu form. The Hu–Washizu principle is a three-field formulation in linear elasticity with the displacements, strains and stresses as independent fields. For systems, in which all forces are potential forces with potential $V(\mathbf{q}, t)$ the principle of virtual action (3.26) translates to

$$\delta A = -\int_{\mathcal{I}} \delta \big\{ L(\mathbf{q}, \mathbf{u}, t) + \mathbf{p}^{\mathrm{T}} (\dot{\mathbf{q}} - \mathbf{u}) \big\} \, \mathrm{d}t + \delta\mathbf{q}^{\mathrm{T}} \mathbf{P} \big|_{\partial\mathcal{I}} = 0 \quad \forall \delta\mathbf{q}, \forall \delta\mathbf{p}, \forall \delta\mathbf{u} \,, \tag{3.28}$$

which is the three field formulation of Hamilton's law of varying action (2.41). If furthermore the initial and final positions are known, i.e. $\mathbf{q}(0) = \mathbf{q}_0$ and $\mathbf{q}(T) = \mathbf{q}_T$, then the three field form of the principle of Hamilton (2.43) follows, as the action integral

$$A = -\int_{\mathcal{I}} \big\{ L(\mathbf{q}, \mathbf{u}, t) + \mathbf{p}^{\mathrm{T}} (\dot{\mathbf{q}} - \mathbf{u}) \big\} \, \mathrm{d}t \tag{3.29}$$

is stationary due to (3.28) with vanishing boundary terms. Using the fundamental lemma of calculus of variation for the strong variational form (3.27), the equations of motion

$$\dot{\mathbf{p}} + \left(\frac{\partial T}{\partial \mathbf{q}} \right)^{\mathrm{T}} = \mathbf{f} \,, \quad \mathbf{p} = \left(\frac{\partial T}{\partial \mathbf{u}} \right)^{\mathrm{T}} \quad \text{and} \quad \mathbf{u} = \dot{\mathbf{q}} \tag{3.30}$$

with boundary conditions $\mathbf{p}(0) = \mathbf{P}_0$ and $\mathbf{p}(T) = \mathbf{P}_T$ are attained, as the terms in the round brackets in (3.27) have to vanish pointwise.

3.4 Generalized (q,u,p)-Formulation

By introducing two parameters $\alpha \in [0, 1]$ and $\beta \in [0, 1]$ a generalization of the $(\mathbf{q}, \mathbf{u}, \mathbf{p})$-formulation of the principle of virtual action can be derived. For any value of $\alpha \in [0, 1]$ the dynamical part of the virtual action (2.31) can be written as the convex combination

$$\delta A^{\mathrm{dyn}} = (1 - \alpha) \delta A^{\mathrm{dyn}} + \alpha \, \delta A^{\mathrm{dyn}} \,. \tag{3.31}$$

Representing the second term as in (3.14) and using (2.31), (3.31) reads

$$\delta A^{\mathrm{dyn}} = -\int_{\mathcal{I}} \left\{ (1-\alpha)\delta T(\mathbf{q},\dot{\mathbf{q}},t) + \alpha\, \delta \left(\dot{\mathbf{q}}^{\mathrm{T}}\mathbf{p} - T^*(\mathbf{q},\mathbf{p},t) \right) \right\} \mathrm{d}t \;, \tag{3.32}$$

where $\delta A^{\mathrm{dyn}} = 0 \;\forall \delta\mathbf{p}$. Using the definition of the conjugate kinetic energy (3.24) write the conjugate energy as the convex combination

$$\begin{aligned} T^*(\mathbf{q},\mathbf{p},t) &= (1-\beta)T^*(\mathbf{q},\mathbf{p},t) + \beta T^*(\mathbf{q},\mathbf{p},t) \\ &\overset{(3.24)}{=} (1-\beta)T^*(\mathbf{q},\mathbf{p},t) + \beta \sup_{\mathbf{u}\in\mathbb{R}^n} \{\mathbf{u}^{\mathrm{T}}\mathbf{p} - T(\mathbf{q},\mathbf{u},t)\} \end{aligned} \tag{3.33}$$

for any value of $\beta \in [0,1]$. Inserting (3.33) into (3.32) and using (3.6) the virtual action contribution of the dynamical forces is

$$\delta A^{\mathrm{dyn}} = -\int_{\mathcal{I}} \left\{ (1-\alpha)\delta T(\dot{\mathbf{q}}) + \alpha\delta(\dot{\mathbf{q}}^{\mathrm{T}}\mathbf{p} - (1-\beta)T^*(\mathbf{p}) - \beta(\mathbf{u}^{\mathrm{T}}\mathbf{p} - T(\mathbf{u}))) \right\} \mathrm{d}t, \tag{3.34}$$

where $\delta A^{\mathrm{dyn}} = 0 \;\forall \delta\mathbf{p},\; \forall \delta\mathbf{u}$ and the dependences on $\mathbf{q}$ and t have been suppressed for the sake of brevity. By (3.34) the principle of virtual action takes the form

$$\begin{aligned} \delta A = -\int_{\mathcal{I}} \Bigg\{ & \delta\mathbf{q}^{\mathrm{T}} \left((1-\alpha)\left(\frac{\partial T}{\partial \mathbf{q}}\right)^{\mathrm{T}} - \alpha(1-\beta)\left(\frac{\partial T^*}{\partial \mathbf{q}}\right)^{\mathrm{T}} + \alpha\beta\left(\frac{\partial T}{\partial \mathbf{q}}\right)^{\mathrm{T}} + \mathbf{f} \right) \\ & + \delta\dot{\mathbf{q}}^{\mathrm{T}} \left((1-\alpha)\left(\frac{\partial T}{\partial \dot{\mathbf{q}}}\right)^{\mathrm{T}} + \alpha\mathbf{p} \right) + \alpha\, \delta\mathbf{p}^{\mathrm{T}} \left(\dot{\mathbf{q}} - (1-\beta)\left(\frac{\partial T^*}{\partial \mathbf{p}}\right)^{\mathrm{T}} - \beta\mathbf{u} \right) \\ & + \alpha\beta\, \delta\mathbf{u}^{\mathrm{T}} \left(\left(\frac{\partial T}{\partial \mathbf{u}}\right)^{\mathrm{T}} - \mathbf{p} \right) \Bigg\} \mathrm{d}t + \delta\mathbf{q}^{\mathrm{T}}\mathbf{P}\big|_0^{\mathrm{T}} = 0 \quad \forall\delta\mathbf{q}, \forall\delta\mathbf{p}, \forall\delta\mathbf{u} \;, \end{aligned} \tag{3.35}$$

as the condition $\delta A^{\mathrm{dyn}} = 0 \;\forall \delta\mathbf{p},\; \forall \delta\mathbf{u}$ is equivalent to $\delta A = 0 \;\forall \delta\mathbf{p},\; \forall \delta\mathbf{u}$. As the Fenchel equation (3.3) holds for the kinetic energy, we have

$$T(\mathbf{q},\dot{\mathbf{q}},t) = \mathbf{p}^{\mathrm{T}}\dot{\mathbf{q}} - T^*(\mathbf{q},\mathbf{p},t) \quad \Rightarrow \quad \frac{\partial T}{\partial \mathbf{q}} = -\frac{\partial T^*}{\partial \mathbf{q}} \;, \tag{3.36}$$

which allows to rewrite the integrand in the first row in (3.35) as

$$\delta\mathbf{q}^{\mathrm{T}} \left((1-\alpha)\left(\frac{\partial T}{\partial \mathbf{q}}\right)^{\mathrm{T}} - \alpha(1-\beta)\left(\frac{\partial T^*}{\partial \mathbf{q}}\right)^{\mathrm{T}} + \alpha\beta\left(\frac{\partial T}{\partial \mathbf{q}}\right)^{\mathrm{T}} \right) = \delta\mathbf{q}^{\mathrm{T}} \left(\frac{\partial T}{\partial \mathbf{q}}\right)^{\mathrm{T}} . \tag{3.37}$$

Using (3.37) in the principle of virtual action (3.35) and applying integration by parts, the equations of motion

$$\begin{aligned} 0 &= (1-\alpha)\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial T}{\partial \dot{\mathbf{q}}}\right)^{\mathrm{T}} + \alpha\dot{\mathbf{p}} - \left(\frac{\partial T}{\partial \mathbf{q}}\right)^{\mathrm{T}} - \mathbf{f} \ , \\ 0 &= \alpha\dot{\mathbf{q}} - \alpha\left((1-\beta)\left(\frac{\partial T^*}{\partial \mathbf{p}}\right)^{\mathrm{T}} + \beta\mathbf{u}\right) \ , \\ 0 &= \alpha\beta\left(\left(\frac{\partial T}{\partial \mathbf{u}}\right)^{\mathrm{T}} - \mathbf{p}\right) \ , \end{aligned} \tag{3.38}$$

with the boundary condtitions

$$(1-\alpha)\left(\frac{\partial T}{\partial \dot{\mathbf{q}}}\right)^{\mathrm{T}}(\mathbf{q}(t), \dot{\mathbf{q}}(t), t) + \alpha\mathbf{p}(t) = \mathbf{P}_t \quad \text{for} \quad t \in \{0, T\} \tag{3.39}$$

follow by means of the fundamental lemma of calculus of variations. Note that the generalized $(\mathbf{q}, \mathbf{u}, \mathbf{p})$-formulation of the principle of virtual action (3.35) contains the formulations encountered so far. The choice $\alpha = \beta = 0$ leads to the formulation in (2.29), where the only unknown is the generalized position $\mathbf{q}$. By choosing $\alpha = 1$ and $\beta = 0$ we get the $(\mathbf{q}, \mathbf{p})$-formulation in (3.15) and for $\alpha = \beta = 1$ the $(\mathbf{q}, \mathbf{u}, \mathbf{p})$-formulation in (3.26). We introduce the notion of pure multi-field formulations for the $(\mathbf{q}, \mathbf{p})$, and $(\mathbf{q}, \mathbf{u}, \mathbf{p})$-formulation and mixed multi-field formulations all other formulations, which arise from other values of α and β.

Chapter 4

Time Finite Elements

In this chapter we discretize the principle of virtual action with respect to time, in order to obtain a finite element formulation, which results in a system of algebraic equations describing the motion of the mechanical system $\mathcal{S}$. In Section 4.1 we derive a set of nonlinear algebraic equations by subdividing the time interval into a sequence of time intervals, i.e. elements, and by restricting the continuous motion within an element to a motion that can be described by finite degrees of freedom only. This procedure is similar to the procedure in a spatial finite element discretization, cf. Belytschko et al. (2013). As the solution of such a set of nonlinear algebraic equations fully describes the motion of the system, we call this method the *monolithic approach* for the single-field approach it is shown in Section 4.2, that the solution of the nonlinear algebraic equations of the monolithic approach can be solved by sequentially solve a smaller set of equations, which is given by the motion within a single time element. As we solve element by element, stepping forward in time, we call this procedure the *stepping approach*. Within this section, we derive three different formulations of equivalent stepping approaches and show that these are the same as the variational integrators that can be derived using concepts of discrete mechanics, cf. Marsden and Wendlandt (1997), Kane (1999), and West (2004).

4.1 Monolithic Approach

In this section we first derive the temporal finite element discretization of the principle of virtual action (2.29) in Section 4.1.1 and then the temporal finite element discretization of the multi-field formulations of Chapter 3 in Section 4.1.2.

4.1.1 Discretization of the Single-field Formulation

Let $(t_1, \dots, t_{n_N})$ be the n_N temporal nodes, which subdivide the time interval $\mathcal{I} = [0, T]$ into n_{el} elements $\Omega^e = [t_e, t_{e+1}]$ indexed by $(\bullet)^e$, where $e = 1, \dots, n_{el}$. The time interval $\Delta t^e = t_{e+1} - t_e$ denotes the temporal length of the element e. With the indicator function $\chi_{\Omega^e}(t)$, which is 1 for $t \in \Omega^e$ and zero elsewhere, we can define the motion within an element to be $\mathbf{q}^e(t) = \chi_{\Omega^e}(t)\mathbf{q}(t)$. This allows us to write the virtual action (2.29) of the system as the sum of the virtual actions of each element, i.e.

$$\delta A = -\sum_{e=1}^{n_{el}} \int_{\Omega^e} \left\{ \delta T(\mathbf{q}^e, \dot{\mathbf{q}}^e, t) + \delta \mathbf{q}^{e\mathrm{T}} \mathbf{f} \right\} \mathrm{d}t + \delta \mathbf{q}^{\mathrm{T}} \mathbf{P} \Big|_0^{\mathrm{T}} = 0 \quad \forall \delta \mathbf{q} \, . \tag{4.1}$$

For every element e let $\boldsymbol{\phi}^e$ be the shape function of the element, which constrains the motion of the element to

$$\mathbf{q}^e(t) = \boldsymbol{\phi}^e(s^e(t), \mathbf{z}^e) \quad \text{with} \quad s^e(t) = \frac{t - t_e}{\Delta t^e} \, , \tag{4.2}$$

where we have introduced the element coordinate $s^e \in [0, 1]$ for $t \in \Omega^e$ and the N_e element coordinates $\mathbf{z}^e = (z_1^e, \dots, z_{N_e}^e)^{\mathrm{T}}$, which are the degrees of freedom of the element e. Assume that the actual element coordinates $\mathbf{z}^e$ are embedded into a variational family $\hat{\mathbf{z}}^e(\varepsilon)$ with $\hat{\mathbf{z}}^e(\varepsilon_0) = \mathbf{z}^e$ for some ε_0. The variation of the element coordinate

$$\delta \mathbf{z}^e = \frac{\partial \hat{\mathbf{z}}^e}{\partial \varepsilon}(\varepsilon_0) \tag{4.3}$$

induces a variation of the motion

$$\delta \mathbf{q}^e(t) = \frac{\partial \boldsymbol{\phi}^e}{\partial \mathbf{z}^e}(s^e(t), \mathbf{z}^e) \delta \mathbf{z}^e = \mathbf{N}^e(s^e(t), \mathbf{z}^e) \delta \mathbf{z}^e \, , \tag{4.4}$$

where we have introduced the function $\mathbf{N}^e(s^e(t), \mathbf{z}^e) = \frac{\partial \boldsymbol{\phi}^e}{\partial \mathbf{z}^e}(s^e(t), \mathbf{z}^e)$. The variation (4.4) is by construction admissible with respect to the constraints (4.2). The notation $\dot{\mathbf{N}}^e(s^e(t), \mathbf{z}^e) = \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{N}^e(s^e(t), \mathbf{z}^e) = \frac{\partial \mathbf{N}^e}{\partial s^e}(s^e(t), \mathbf{z}^e)\dot{s}^e$ allows to write the variation of the velocity field as

$$\delta \dot{\mathbf{q}}^e(t) = \dot{\mathbf{N}}^e(s^e(t), \mathbf{z}^e) \delta \mathbf{z}^e \, . \tag{4.5}$$

We constrain the motion in (4.1) to the special form (4.2) by means of ideal constraint forces, which by the principle of d'Alembert–Lagrange have no contribution to the virtual action in unconstrained direction. Therefore, the principle of virtual action (4.1) for admissible virtual displacements (4.4) is

$$\begin{aligned} &-\sum_{e=1}^{n_{el}} \int_{\Omega^e} \left\{ \delta T(\boldsymbol{\phi}^e(s^e(t), \mathbf{z}^e), \dot{\boldsymbol{\phi}}^e(s^e(t), \mathbf{z}^e), t) + \delta \mathbf{z}^{e\mathrm{T}} \mathbf{N}^e(s^e(t), \mathbf{z}^e)^{\mathrm{T}} \mathbf{f} \right\} \mathrm{d}t \\ &+ \delta \mathbf{z}^{n_{el}\mathrm{T}} \mathbf{N}^{n_{el}}(s^{n_{el}}(T), \mathbf{z}^{n_{el}})^{\mathrm{T}} \mathbf{P}_T - \delta \mathbf{z}^{1\mathrm{T}} \mathbf{N}^1(s^1(0), \mathbf{z}^1)^{\mathrm{T}} \mathbf{P}_0 = 0 \quad \forall \delta \mathbf{z}^e \, . \end{aligned} \tag{4.6}$$

The virtual action contribution of the dynamic forces of an element e is

$$\delta A^{\mathrm{dyn},e} = -\delta \mathbf{z}^{e\mathrm{T}} \int_{\Omega^e} \left\{ \mathbf{N}^{e\mathrm{T}} \left(\frac{\partial T}{\partial \mathbf{q}} \right)^{\mathrm{T}} + \dot{\mathbf{N}}^{e\mathrm{T}} \left(\frac{\partial T}{\partial \dot{\mathbf{q}}} \right)^{\mathrm{T}} \right\} \mathrm{d}t \ , \tag{4.7}$$

where we have used (2.32) for the variation of the kinetic energy and for the sake of brevity the functional dependecies are suppressed. For a more compact formulation, we define the discrete dynamic forces of the element e

$$\tilde{\mathbf{f}}^{\mathrm{dyn},e}(\mathbf{z}^e) = \int_{\Omega^e} \left\{ \mathbf{N}^{e\mathrm{T}} \left(\frac{\partial T}{\partial \mathbf{q}} \right)^{\mathrm{T}} (\boldsymbol{\phi}^e, \dot{\boldsymbol{\phi}}^e, t) + \dot{\mathbf{N}}^{e\mathrm{T}} \left(\frac{\partial T}{\partial \dot{\mathbf{q}}} \right)^{\mathrm{T}} (\boldsymbol{\phi}^e, \dot{\boldsymbol{\phi}}^e, t) \right\} \mathrm{d}t \ , \tag{4.8}$$

the discrete spatial forces acting on the element e as

$$\tilde{\mathbf{f}}^{\mathrm{spa},e}(\mathbf{z}^e) = \int_{\Omega^e} \mathbf{N}^e(s^e(t), \mathbf{z}^e)^{\mathrm{T}} \mathbf{f} \left(\boldsymbol{\phi}^e(s^e(t), \mathbf{z}^e), \dot{\boldsymbol{\phi}}^e(s^e(t), \mathbf{z}^e), t \right) \mathrm{d}t \ , \tag{4.9}$$

and the discrete impulsive forces as

$$\tilde{\mathbf{P}}_0^1 = \mathbf{N}^1(s^1(0), \mathbf{z}^1)^{\mathrm{T}} \mathbf{P}_0 \quad \text{and} \quad \tilde{\mathbf{P}}_T^{n_{el}} = \mathbf{N}^{n_{el}}(s^{n_{el}}(T), \mathbf{z}^{n_{el}})^{\mathrm{T}} \mathbf{P}_T \ . \tag{4.10}$$

Using the definitions (4.8), (4.9) and (4.10) the principle of virtual action (4.6) can be written as

$$\delta A = -\sum_{e=1}^{n_{el}} \delta \mathbf{z}^{e\mathrm{T}} \left(\tilde{\mathbf{f}}^{\mathrm{dyn},e}(\mathbf{z}^e) + \tilde{\mathbf{f}}^{\mathrm{spa},e}(\mathbf{z}^e) \right) + \delta \mathbf{z}^{n_{el}\ \mathrm{T}} \tilde{\mathbf{P}}_T^{n_{el}} - \delta \mathbf{z}^{1\ \mathrm{T}} \tilde{\mathbf{P}}_0^1 = 0 \tag{4.11}$$

for all $\delta \mathbf{z}^e$. For a discrete global formulation, we define $\mathbf{z} = (\mathbf{z}^{1\mathrm{T}}, \ldots, \mathbf{z}^{n_{el}\mathrm{T}})^{\mathrm{T}}$ to be the vector of global coordinates and $\mathbf{C}^e$ to be the connectivity matrix of the element, which extracts the element coordinates out of the global coordinates, i.e. $\mathbf{z}^e = \mathbf{C}^e \mathbf{z}$. Since the connectivity matrix is constant, the variation $\delta \mathbf{z}^e = \mathbf{C}^e \delta \mathbf{z}$ of the element coordinates are induced by the the variation of the global coordinates $\delta \mathbf{z}$. This allows to rewrite (4.11) in the global form

$$\delta \mathbf{z}^T \left\{ \sum_{e=1}^{n_{el}} -\mathbf{C}^{e\mathrm{T}} \left(\tilde{\mathbf{f}}^{\mathrm{dyn},e}(\mathbf{C}^e \mathbf{z}) + \tilde{\mathbf{f}}^{\mathrm{spa},e}(\mathbf{C}^e \mathbf{z}) \right) + \mathbf{C}^{n_{el}\mathrm{T}} \tilde{\mathbf{P}}_T^{n_{el}} - \mathbf{C}^{1\mathrm{T}} \tilde{\mathbf{P}}_0^1 \right\} = 0 \tag{4.12}$$

for all $\delta \mathbf{z}$. By the fundamental lemma of calculus of variations the term in the curly brackets in (4.12) has to vanish, which leads to the system of equations

$$-\tilde{\mathbf{f}}^{\mathrm{dyn}}(\mathbf{z}) - \tilde{\mathbf{f}}^{\mathrm{spa}}(\mathbf{z}) + \tilde{\mathbf{P}}_T - \tilde{\mathbf{P}}_0 = 0 \ , \tag{4.13}$$

where we have introduced the global vector of dynamical and spatial forces

$$\tilde{\mathbf{f}}^{\mathrm{dyn}}(\mathbf{z}) = \sum_{e=1}^{n_{el}} \mathbf{C}^{e\mathrm{T}} \tilde{\mathbf{f}}^{\mathrm{dyn},e}(\mathbf{C}^e \mathbf{z}) \ , \quad \tilde{\mathbf{f}}^{\mathrm{spa}}(\mathbf{z}) = \sum_{e=1}^{n_{el}} \mathbf{C}^{e\mathrm{T}} \tilde{\mathbf{f}}^{\mathrm{spa},e}(\mathbf{C}^e \mathbf{z}) \ , \tag{4.14}$$

and the global impulsive forces

$$\tilde{\mathbf{P}}_0 = \mathbf{C}^{1\mathrm{T}}\tilde{\mathbf{P}}_0^1 \,, \quad \tilde{\mathbf{P}}_T = \mathbf{C}^{n_{el}\mathrm{T}}\tilde{\mathbf{P}}_T^{n_{el}} \,. \tag{4.15}$$

Equation (4.13) is a system of $ndof = n_{el}N_e$ non-linear algebraic equations, which follows from the principle of virtual action through discretization and describes the motion of the mechanical system. For given external impulsive forces $\mathbf{P}$ the solution $\mathbf{z} \in \mathbb{R}^{ndof}$ of the nonlinear equation (4.13) can for example be found by using the Newton–Raphson method. The global discrete coordinates $\mathbf{z}$ can be used to construct the discretized motion of the system

$$\mathbf{q}(t) = \sum_{e=1}^{n_{el}} \chi_{\Omega^e}(t)\boldsymbol{\phi}^e(s^e(t), \mathbf{C}^e\mathbf{z}) \,. \tag{4.16}$$

As introduced in (2.36), the impulsive forces $\mathbf{P}_0$ and $\mathbf{P}_T$ are chosen such that the initial conditions $\mathbf{q}(0) = \mathbf{q}_0$ and $\dot{\mathbf{q}}(0) = \mathbf{u}_0$ are satisfied. By (4.2), the initial conditions can be expressed as a function of the discrete coordinates, i.e.

$$\begin{aligned} \boldsymbol{\phi}^1(s^1(0), \mathbf{z}^1) &= \boldsymbol{\phi}^1(0, \mathbf{C}^1\mathbf{z}) = \mathbf{q}_0 \,, \\ \dot{\boldsymbol{\phi}}^1(s^1(0), \mathbf{z}^1) &= \dot{\boldsymbol{\phi}}^1(0, \mathbf{C}^1\mathbf{z}) = \mathbf{u}_0 \,. \end{aligned} \tag{4.17}$$

Thus, the impulsive forces in (4.13) can be treated as unknown variables and the initial conditions can be added to the system of equation (4.13), such that the resulting system of equations

$$\begin{pmatrix} -\tilde{\mathbf{f}}^{\mathrm{dyn}}(\mathbf{z}) - \tilde{\mathbf{f}}^{\mathrm{spa}}(\mathbf{z}) + \tilde{\mathbf{P}}_T - \tilde{\mathbf{P}}_0 \\ \boldsymbol{\phi}^1(0, \mathbf{C}^1\mathbf{z}) - \mathbf{q}_0 \\ \dot{\boldsymbol{\phi}}^1(0, \mathbf{C}^1\mathbf{z}) - \dot{\mathbf{q}}_0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \tag{4.18}$$

fully describes the initial value problem, where the motion of the system is restricted to the form (4.16) with initial conditions (4.17). For the numerical treatment of (4.18) it might be convenient to approximate the time integrations used to calculate the spatial and dynamical forces in (4.8) and (4.9) by some quadrature rule. Imposing the initial velocity in the form $\dot{\boldsymbol{\phi}}^1(0, \mathbf{z}^1) = \mathbf{u}_0$ introduced in (4.17) is often a bad choice, albeit this condition forces the initial velocity of the first element to be the same as the initial velocity of the analytical solution, it also influences the shape of the first element all over the time interval Ω^1, which is due to the finite degree of freedom of the element. This can lead to a first element, which fulfills the initial condition exactly, but due to the abovementioned effect approximates the analytical solution badly[1]. To eliminate the distance effects of the initial condition for the velocity, the

[1] This effect is shown in Section A.1 by means of an example

initial conditions $\mathbf{q}(0) = \mathbf{q}_0$ and $\dot{\mathbf{q}}(0) = \mathbf{u}_0$ are used to determine the impulsive force $\mathbf{P}_0$ by means of the boundary condition (2.35). Replacing the initial condition for the velocity in (4.17) with the boundary condition for $\mathbf{P}_0$ in (4.18) leads to the system of equations

$$\begin{pmatrix} -\tilde{\mathbf{f}}^{\mathrm{dyn}}(\mathbf{z}) - \tilde{\mathbf{f}}^{\mathrm{spa}}(\mathbf{z}) + \tilde{\mathbf{P}}_T - \mathbf{C}^{1\mathrm{T}}\mathbf{N}^1(0, \mathbf{C}^1\mathbf{z})^{\mathrm{T}} \left(\frac{\partial T}{\partial \dot{\mathbf{q}}}\right)^{\mathrm{T}} (\mathbf{q}_0, \dot{\mathbf{q}}_0, 0) \\ \boldsymbol{\phi}^1(0, \mathbf{C}^1\mathbf{z}) - \mathbf{q}_0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \tag{4.19}$$

which fully describes the motion of the system restricted to the form (4.16). This procedure is also used in Borri (1986) and Izadpanah (1986), who point out that it should be preferred to other treatments of the boundary conditions, as this procedure leads to a natural convergence of the discrete motion towards the analytical one.

Box 1 gives a summary of the monolithic single-field approach in form of a flowchart.

Box 1 Monolithic Single-field Approach Flowchart

1. Devide time interval $\mathcal{I}$ into disjoint elements Ω^e such that $\mathcal{I} = \bigcup_{e=1}^{n_{el}} \Omega^e$.
2. Choose shape functions $\boldsymbol{\phi}^e(s^e, \mathbf{z}^e)$.
3. Calculate $\tilde{\mathbf{f}}^{\mathrm{dyn},e}(\mathbf{z})$, $\tilde{\mathbf{f}}^{\mathrm{spa},e}(\mathbf{z})$, $\mathbf{P}_T^{n_{el}}$ and $\mathbf{P}_0^1$ from (4.8–4.10), where the time integration might be approximated using a quadrature rule.
4. Assemble the global forces $\tilde{\mathbf{f}}^{\mathrm{dyn}}(\mathbf{z})$, $\tilde{\mathbf{f}}^{\mathrm{spa}}(\mathbf{z})$, $\mathbf{P}_T$ and $\mathbf{P}_0$ using (4.14) and (4.15).
5. Choose how to treat the initial conditions and solve (4.18) or (4.19) for the discrete global solution $\mathbf{z}$. E.g. use the Newton–Raphson method.
6. Construct discretized solution by means of (4.16).

4.1.2 Discretization of the Multi-field Formulations

Let $(t_1, \ldots, t_{n_N})$ be the n_N temporal nodes, which subdivide the time interval $\mathcal{I} = [0, T]$ into n_{el} elements $\Omega^e = [t_e, t_{e+1}]$. With the indicator function $\chi_{\Omega^e}(t)$, we define the fields within an element to be $\mathbf{q}^e(t) = \chi_{\Omega^e}(t)\mathbf{q}(t)$, $\mathbf{u}^e(t) = \chi_{\Omega^e}(t)\mathbf{u}(t)$ and $\mathbf{p}^e(t) = \chi_{\Omega^e}(t)\mathbf{p}(t)$, respectively. This allows us to

write the virtual action (3.35) of the system as the sum of the virtual actions of the elements, i.e.

$$\begin{aligned}\delta A = &-\sum_{e=1}^{n_{el}} \int_{\Omega^e} \Bigg\{ \delta\mathbf{q}^{e\mathrm{T}} \left((1-\alpha)\left(\frac{\partial T}{\partial \mathbf{q}}\right)^{\mathrm{T}} - \alpha(1-\beta)\left(\frac{\partial T^*}{\partial \mathbf{q}}\right)^{\mathrm{T}} + \alpha\beta\left(\frac{\partial T}{\partial \mathbf{q}}\right)^{\mathrm{T}} + \mathbf{f} \right) \\ &+ \delta\dot{\mathbf{q}}^{e\mathrm{T}} \left((1-\alpha)\left(\frac{\partial T}{\partial \dot{\mathbf{q}}}\right)^{\mathrm{T}} + \alpha\mathbf{p}^e \right) + \alpha\ \delta\mathbf{p}^{e\mathrm{T}} \left(\dot{\mathbf{q}}^e - (1-\beta)\left(\frac{\partial T^*}{\partial \mathbf{p}}\right)^{\mathrm{T}} - \beta\mathbf{u}^e \right) \\ &+ \alpha\beta\ \delta\mathbf{u}^{e\mathrm{T}} \left(\left(\frac{\partial T}{\partial \mathbf{u}}\right)^{\mathrm{T}} - \mathbf{p}^e \right) \Bigg\} \,\mathrm{d}t + \delta\mathbf{q}^{\mathrm{T}}\mathbf{P}\big|_0^{\mathrm{T}} = 0 \quad \forall\delta\mathbf{q}, \forall\delta\mathbf{p}, \forall\delta\mathbf{u}\ , \end{aligned} \tag{4.20}$$

where the kinetic energy terms are evaluated at $(\mathbf{q}^e, \dot{\mathbf{q}}^e, t)$, $(\mathbf{q}^e, \mathbf{u}^e, t)$ and $(\mathbf{q}^e, \mathbf{p}^e, t)$, respectively. For every element e let the field be given by a respective shape function, which constrains the motion of the element to

$$\begin{aligned} \mathbf{q}^e(t) &= \boldsymbol{\phi}^e_{\mathbf{q}}(s^e(t), \mathbf{z}^e_{\mathbf{q}})\ , \\ \mathbf{u}^e(t) &= \boldsymbol{\phi}^e_{\mathbf{u}}(s^e(t), \mathbf{z}^e_{\mathbf{u}})\ , \\ \mathbf{p}^e(t) &= \boldsymbol{\phi}^e_{\mathbf{p}}(s^e(t), \mathbf{z}^e_{\mathbf{p}})\ . \end{aligned} \tag{4.21}$$

Assume that the actual element coordinates $\mathbf{z}^e_\bullet$ are embedded into a variational family $\hat{\mathbf{z}}^e_\bullet(\varepsilon)$ with $\hat{\mathbf{z}}^e_\bullet(\varepsilon_0) = \mathbf{z}^e_\bullet$ for some ε_0, where we have introduced the notation $(\bullet)$ as a placeholder for $\mathbf{q}$, $\mathbf{u}$ and $\mathbf{p}$. The variation of the element coordinate

$$\delta\mathbf{z}^e_\bullet = \frac{\partial \hat{\mathbf{z}}^e_\bullet}{\partial\varepsilon}(\varepsilon_0) \tag{4.22}$$

induces the variation of the corresponding fields

$$\begin{aligned} \delta\mathbf{q}^e(t) &= \mathbf{N}^e_{\mathbf{q}}\delta\mathbf{z}^e_{\mathbf{q}}\ , \\ \delta\mathbf{u}^e(t) &= \mathbf{N}^e_{\mathbf{u}}\delta\mathbf{z}^e_{\mathbf{u}}\ , \\ \delta\mathbf{p}^e(t) &= \mathbf{N}^e_{\mathbf{p}}\delta\mathbf{z}^e_{\mathbf{p}}\ , \end{aligned} \tag{4.23}$$

where we have introduced the function $\mathbf{N}^e_\bullet(s^e(t), \mathbf{z}^e_\bullet) = \frac{\partial \boldsymbol{\phi}^e_\bullet}{\partial \mathbf{z}^e_\bullet}(s^e(t), \mathbf{z}^e_\bullet)$. Introducing $\dot{\mathbf{N}}^e_{\mathbf{q}}(s^e(t), \mathbf{z}^e_{\mathbf{q}}) = \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{N}^e_{\mathbf{q}}(s^e(t), \mathbf{z}^e_{\mathbf{q}}) = \frac{\partial \mathbf{N}^e_{\mathbf{q}}}{\partial s^e}(s^e(t), \mathbf{z}^e_{\mathbf{q}})\dot{s}^e$ the variation of the velocity field is

$$\delta\dot{\mathbf{q}}^e(t) = \dot{\mathbf{N}}^e_{\mathbf{q}}(s^e(t), \mathbf{z}^e_{\mathbf{q}})\delta\mathbf{z}^e_{\mathbf{q}}\ . \tag{4.24}$$

Using (4.21) and (4.23) together with the connectivity matrices, which extract the element coordinates out of the global coordinates in the form $\mathbf{z}^e_\bullet = \mathbf{C}^e_\bullet\mathbf{z}_\bullet$,

the principle of virtual action (4.20) for with (4.21) admissible variations is

$$
\begin{aligned}
&\delta\mathbf{z_q}^{\mathrm{T}} \left\{ \sum_{e=1}^{n_{el}} (\mathbf{C}_\mathbf{q}^e)^{\mathrm{T}} \int_{\Omega^e} \left[-(\mathbf{N}_\mathbf{q}^e)^{\mathrm{T}} \left((1-\alpha) \left(\frac{\partial T}{\partial \mathbf{q}} \right)^{\mathrm{T}} - \alpha(1-\beta) \left(\frac{\partial T^*}{\partial \mathbf{q}} \right)^{\mathrm{T}} \right.\right.\right. \\
&\left.\left.\left. + \ \alpha\beta \left(\frac{\partial T}{\partial \mathbf{q}} \right)^{\mathrm{T}} + \mathbf{f} \right) - (\dot{\mathbf{N}}_\mathbf{q}^e)^{\mathrm{T}} \left((1-\alpha) \left(\frac{\partial T}{\partial \dot{\mathbf{q}}} \right)^{\mathrm{T}} + \alpha \boldsymbol{\phi}_\mathbf{p}^e \right) \right] \mathrm{d}t + (\mathbf{C}_\mathbf{q}^e)^{\mathrm{T}} \mathbf{P} \big|_0^{\mathrm{T}} \right\} \\
&+ \delta\mathbf{z_p}^{\mathrm{T}} \left\{ \sum_{e=1}^{n_{el}} (\mathbf{C}_\mathbf{p}^e)^{\mathrm{T}} \int_{\Omega^e} \left[-(\mathbf{N}_\mathbf{p}^e)^{\mathrm{T}} \left(\alpha \dot{\boldsymbol{\phi}}_\mathbf{q}^e - \alpha(1-\beta) \left(\frac{\partial T^*}{\partial \mathbf{p}} \right)^{\mathrm{T}} - \alpha\beta \boldsymbol{\phi}_\mathbf{u}^e \right) \right] \mathrm{d}t \right\} \\
&+ \delta\mathbf{z_u}^{\mathrm{T}} \left\{ \sum_{e=1}^{n_{el}} (\mathbf{C}_\mathbf{u}^e)^{\mathrm{T}} \int_{\Omega^e} \left[-(\mathbf{N}_\mathbf{u}^e)^{\mathrm{T}} \left(\alpha\beta \left(\frac{\partial T}{\partial \mathbf{u}} \right)^{\mathrm{T}} - \alpha\beta \boldsymbol{\phi}_\mathbf{p}^e \right) \right] \mathrm{d}t \right\} = 0
\end{aligned}
\tag{4.25}
$$

for all variations $\delta\mathbf{z_q}$, $\delta\mathbf{z_u}$ and $\delta\mathbf{z_p}$. As the terms in curly brackets of (4.25) have to vanish by the fundamental lemma of calculus of variations, together with the treatment of the initial condition as in (4.18) or (4.19) leads to the set of nonlinear algebraic equations

$$
\begin{aligned}
0 &= \sum_{e=1}^{n_{el}} (\mathbf{C}_\mathbf{q}^e)^{\mathrm{T}} \int_{\Omega^e} \left[-(\mathbf{N}_\mathbf{q}^e)^{\mathrm{T}} \left((1-\alpha) \left(\frac{\partial T}{\partial \mathbf{q}} \right)^{\mathrm{T}} - \alpha(1-\beta) \left(\frac{\partial T^*}{\partial \mathbf{q}} \right)^{\mathrm{T}} \right.\right. \\
&\quad \left.\left. + \ \alpha\beta \left(\frac{\partial T}{\partial \mathbf{q}} \right)^{\mathrm{T}} + \mathbf{f} \right) - (\dot{\mathbf{N}}_\mathbf{q}^e)^{\mathrm{T}} \left((1-\alpha) \left(\frac{\partial T}{\partial \dot{\mathbf{q}}} \right)^{\mathrm{T}} + \alpha \boldsymbol{\phi}_\mathbf{p}^e \right) \right] \mathrm{d}t + (\mathbf{C}_\mathbf{q}^e)^{\mathrm{T}} \mathbf{P} \big|_0^{\mathrm{T}} \\
0 &= \sum_{e=1}^{n_{el}} (\mathbf{C}_\mathbf{p}^e)^{\mathrm{T}} \int_{\Omega^e} \left[-(\mathbf{N}_\mathbf{p}^e)^{\mathrm{T}} \left(\alpha \dot{\boldsymbol{\phi}}_\mathbf{q}^e - \alpha(1-\beta) \left(\frac{\partial T^*}{\partial \mathbf{p}} \right)^{\mathrm{T}} - \alpha\beta \boldsymbol{\phi}_\mathbf{u}^e \right) \right] \mathrm{d}t \\
0 &= \sum_{e=1}^{n_{el}} (\mathbf{C}_\mathbf{u}^e)^{\mathrm{T}} \int_{\Omega^e} \left[-(\mathbf{N}_\mathbf{u}^e)^{\mathrm{T}} \left(\alpha\beta \left(\frac{\partial T}{\partial \mathbf{u}} \right)^{\mathrm{T}} - \alpha\beta \boldsymbol{\phi}_\mathbf{p}^e \right) \right] \mathrm{d}t \\
0 &= \boldsymbol{\phi}_\mathbf{q}^1(0, \mathbf{C}_\mathbf{q}^1 \mathbf{z_q}) - \mathbf{q}_0 \ ,
\end{aligned}
\tag{4.26}
$$

where the initial condition for the velocity can be one of the following

$$
\begin{aligned}
\dot{\boldsymbol{\phi}}_\mathbf{q}^1(0, \mathbf{C}_\mathbf{q}^1 \mathbf{z_q}) &= \dot{\mathbf{q}}_0 \ , \\
\boldsymbol{\phi}_\mathbf{u}^1(0, \mathbf{C}_\mathbf{u}^1 \mathbf{z_u}) &= \dot{\mathbf{q}}_0 \ , \\
\boldsymbol{\phi}_\mathbf{p}^1(0, \mathbf{C}_\mathbf{p}^1 \mathbf{z_p}) &= \left(\frac{\partial T}{\partial \dot{\mathbf{q}}} \right)^{\mathrm{T}} (\mathbf{q}_0, \dot{\mathbf{q}}_0, 0) \ .
\end{aligned}
\tag{4.27}
$$

The set of equations (4.26) together with an initial condition from (4.27) can be solved for $\mathbf{z_q}$, $\mathbf{z_u}$, $\mathbf{z_p}$, $\mathbf{P}_0$ and $\mathbf{P}_T$. These discrete solutions define the continuous

motion of the mechanical system by means of

$$\begin{aligned}
\mathbf{q}(t) &= \sum_{e=1}^{n_{el}} \chi_{\Omega^e}(t) \boldsymbol{\phi}_{\mathbf{q}}^e(s^e(t), \mathbf{C}^e \mathbf{z}_{\mathbf{q}}) \ , \\
\mathbf{u}(t) &= \sum_{e=1}^{n_{el}} \chi_{\Omega^e}(t) \boldsymbol{\phi}_{\mathbf{u}}^e(s^e(t), \mathbf{C}^e \mathbf{z}_{\mathbf{u}}) \ , \\
\mathbf{p}(t) &= \sum_{e=1}^{n_{el}} \chi_{\Omega^e}(t) \boldsymbol{\phi}_{\mathbf{p}}^e(s^e(t), \mathbf{C}^e \mathbf{z}_{\mathbf{p}}) \ .
\end{aligned} \tag{4.28}$$

Equation (4.26) represent the finite element discretization of the generalized $(\mathbf{q}, \mathbf{u}, \mathbf{p})$-formulation of Section 3.4. As mentioned, the corresponding choice of the parameters α and β allows to derive the $(\mathbf{q}, \mathbf{u}, \mathbf{p})$-formulation, the $(\mathbf{q}, \mathbf{p})$-formulation and even the $\mathbf{q}$-formulation. Therefore, by choosing $\alpha = \beta = 0$ the finite element discretization of the $\mathbf{q}$-formulation (4.18) or (4.19) are attained. The finite element discretization of the $(\mathbf{q}, \mathbf{p})$-formulation is given by the choice $\alpha = 1$ and $\beta = 0$, and $\alpha = \beta = 1$ leads to the discretization of the $(\mathbf{q}, \mathbf{u}, \mathbf{p})$-formulation. Box 2 gives a flowchart for the monolithic multi-field approach.

Box 2 Monolithic Multi-field Approach Flowchart

1. Devide time interval $\mathcal{I}$ into disjoint elements Ω^e such that $\mathcal{I} = \bigcup_{e=1}^{n_{el}} \Omega^e$.
2. Choose shape functions $\boldsymbol{\phi}_{\mathbf{q}}^e$, $\boldsymbol{\phi}_{\mathbf{u}}^e$ and $\boldsymbol{\phi}_{\mathbf{p}}^e$.
3. Assemble the system of equations (4.26) with an initial condition from (4.27), where the time integration might be approximated by some quadrature rule.
4. Solve the system of equations from 3. using for example the Newton–Raphson method.
5. Construct continuous solution by means of (4.28).

4.2 Stepping Approach

Let the n_N temporal nodes $(t_1, \ldots, t_{n_N})$ subdivide the time interval $\mathcal{I} = [0, T]$ into the n_{el} elements $\Omega^e = [t_e, t_{e+1}]$. The virtual action of the mechanical system can be written as the sum of the virtual actions of the elements as in

(4.1). For an arbitrary element k the virtual action of (4.1) can be rearranged to

$$\begin{aligned}\delta A &= -\int_{\Omega^k} \left\{\delta T(\mathbf{q},\dot{\mathbf{q}},t) + \delta\mathbf{q}^{\mathrm{T}}\mathbf{f}\right\} \mathrm{d}t - \sum_{\substack{e=1\\e\neq k}}^{n_{el}} \int_{\Omega^e} \left\{\delta T(\mathbf{q},\dot{\mathbf{q}},t) + \delta\mathbf{q}^{\mathrm{T}}\mathbf{f}\right\} \mathrm{d}t + \delta\mathbf{q}^{\mathrm{T}}\mathbf{P}\big|_{\partial\mathcal{I}} \\ &= -\int_{\Omega^k} \left\{\delta T(\mathbf{q},\dot{\mathbf{q}},t) + \delta\mathbf{q}^{\mathrm{T}}\mathbf{f}\right\} \mathrm{d}t - \int_{\mathcal{I}\backslash\Omega^k} \left\{\delta T(\mathbf{q},\dot{\mathbf{q}},t) + \delta\mathbf{q}^{\mathrm{T}}\mathbf{f}\right\} \mathrm{d}t + \delta\mathbf{q}^{\mathrm{T}}\mathbf{P}\big|_{\partial\mathcal{I}} \,. \end{aligned} \tag{4.29}$$

Using integration by parts for the complement $\mathcal{I}\backslash\Omega^k$ leads to

$$\begin{aligned}\delta A = -\int_{\Omega^k} \left\{\delta T(\mathbf{q},\dot{\mathbf{q}},t) + \delta\mathbf{q}^{\mathrm{T}}\mathbf{f}\right\} \mathrm{d}t + \int_{\mathcal{I}\backslash\Omega^k} \delta\mathbf{q}^{\mathrm{T}} \left(\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial T}{\partial\dot{\mathbf{q}}}\right)^{\mathrm{T}} - \left(\frac{\partial T}{\partial\mathbf{q}}\right)^{\mathrm{T}} - \mathbf{f}\right) \mathrm{d}t \\ + \delta\mathbf{q}^{\mathrm{T}}\mathbf{P}\big|_{\partial\mathcal{I}} - \delta\mathbf{q}^{\mathrm{T}}\left(\frac{\partial T}{\partial\dot{\mathbf{q}}}\right)^{\mathrm{T}}\Bigg|_{\partial(\mathcal{I}\backslash\Omega^k)} \,. \end{aligned} \tag{4.30}$$

The principle of virtual action (4.1) demands $\delta A = 0$ fpr all $\delta\mathbf{q}$. Hence, the virtual action has to vanish also for the special choice $\delta\mathbf{q}(t) = \delta\mathbf{q}^k(t)$, where $\delta\mathbf{q}^k(t)$ is arbitrary for $t \in \Omega^k$ and $\delta\mathbf{q}(t) = 0$ on $\mathcal{I}\backslash\Omega^k$. Using $\mathbf{q}^k(t) = \chi_{\Omega^k}(t)\mathbf{q}(t)$ together with (4.30), the principle of virtual action for the k^{th} element is

$$\delta A^k = -\int_{\Omega^k} \left\{\delta T(\mathbf{q}^k,\dot{\mathbf{q}}^k,t) + \delta{\mathbf{q}^k}^{\mathrm{T}}\mathbf{f}\right\} \mathrm{d}t - \delta\mathbf{q}(t_k)^{\mathrm{T}}\mathbf{P}_k + \delta\mathbf{q}(t_{k+1})^{\mathrm{T}}\mathbf{P}_{k+1} \,, \tag{4.31}$$

where the external impulsive forces with respect to the element are

$$\mathbf{P}_k = \begin{cases} \mathbf{P}_0 & \text{for} \quad k = 1 \\ \left(\frac{\partial T}{\partial\dot{\mathbf{q}}}\right)^{\mathrm{T}}\Big|_{t=t_k} & \text{for} \quad k = 2,\ldots,n_{el} \\ \mathbf{P}_T & \text{for} \quad k = n_{el}+1 \end{cases} \,. \tag{4.32}$$

As for the monolithic approach, the shape function $\boldsymbol{\phi}^k(s^k(t),\mathbf{z}^k)$ with $\mathbf{z}^k \in \mathbb{R}^{N_k}$ constrains the motion as in (4.2). Assume that the shape function fulfills

$$\boldsymbol{\phi}^k(0,\mathbf{z}^k) = \mathbf{z}_1^k \quad \text{and} \quad \boldsymbol{\phi}^k(1,\mathbf{z}^k) = \mathbf{z}_{N_k}^k \,, \tag{4.33}$$

then

$$\mathbf{q}(t_k) = \mathbf{z}_1^k \quad \text{and} \quad \mathbf{q}(t_{k+1}) = \mathbf{z}_{N_k}^k \tag{4.34}$$

holds. Condition (4.33) is fulfilled by most of the common choices of shape functions, such as Lagrange polynomials, Bézier curves, B-splines and NURBS,

cf. Hartmann and Katz (2013) and Hughes et al. (2005). Restricting the principle of virtual action of the k^{th} element (4.31) to admissible virtual displacements $\delta\mathbf{q}^k = \mathbf{N}^k \delta\mathbf{z}^k$ with $\mathbf{N}^k = \frac{\partial \boldsymbol{\phi}^k}{\partial \mathbf{z}^k}$ gives

$$\delta A^k = -\int_{\Omega^k} \left\{ \delta T(\boldsymbol{\phi}^k, \dot{\boldsymbol{\phi}}^k, t) + \delta\mathbf{z}^{k\mathrm{T}} \mathbf{N}^{k\mathrm{T}} \mathbf{f} \right\} \mathrm{d}t - \delta\mathbf{z}^{k\mathrm{T}} \mathbf{e}^1 \mathbf{P}_k + \delta\mathbf{z}^{k\mathrm{T}} \mathbf{e}^{N_k} \mathbf{P}_{k+1} = 0 \tag{4.35}$$

for all variations $\delta\mathbf{z}^k$, where by (4.33) $\mathbf{N}^{k\mathrm{T}}$ for the boundary terms is given by the $\mathbf{e}^1$ and $\mathbf{e}^N$, which are the first and N^{th} canonical basis vector of $\mathbb{R}^N$. Carrying out the variation of the kinetic energy and by the fundamental lemma of calculus of variations we obtain the nonlinear system of equations

$$-\int_{\Omega^k} \left\{ \dot{\mathbf{N}}^{k\mathrm{T}} \left(\frac{\partial T}{\partial \dot{\mathbf{q}}} \right)^{\mathrm{T}} + \mathbf{N}^{k\mathrm{T}} \left(\frac{\partial T}{\partial \mathbf{q}} \right)^{\mathrm{T}} + \mathbf{N}^{k\mathrm{T}} \mathbf{f} \right\} \mathrm{d}t - \mathbf{e}^1 \mathbf{P}_k + \mathbf{e}^{N_k} \mathbf{P}_{k+1} = 0 \ . \tag{4.36}$$

For given initial conditions $\mathbf{z}_1^k = \mathbf{q}(t_k)$ and $\mathbf{P}_k$ of the k^{th} element, (4.36) can be solved for $\mathbf{z}^k$ and $\mathbf{P}_{k+1}$, which fully determines the motion within the element by means of $\mathbf{q}^k(t) = \boldsymbol{\phi}^k(s^k(t), \mathbf{z}^k)$. By (4.34) we have

$$\mathbf{q}(t_{k+1}) = \mathbf{z}_{N_k}^k = \mathbf{z}_1^{k+1} \quad \text{for} \quad k \notin \{1, n_{el}\} \ . \tag{4.37}$$

Knowing the motion of the k^{th} element in terms of $\mathbf{z}^k$ and $\mathbf{P}_{k+1}$, (4.37) implies the initial conditions $\mathbf{z}_1^{k+1} = \mathbf{q}(t_{k+1}) = \mathbf{z}_{N_k}^k$ and the impulsive force $\mathbf{P}_{k+1}$ for the element $k+1$. This allows to find the global motion, i.e. the motion of the system during the time interval $\mathcal{I}$, by sequentially finding the motion within the elements. The initial conditions for the first element are the same as for the global motion, i.e. $\mathbf{z}_1^1 = \mathbf{q}(0) = \mathbf{q}_0$ for the initial position, and $\dot{\boldsymbol{\phi}}^1(0, \mathbf{z}^1) = \dot{\mathbf{q}}_0$ or $\mathbf{P}_1 = \left(\frac{\partial T}{\partial \dot{\mathbf{q}}} \right)^{\mathrm{T}} (\mathbf{q}_0, \dot{\mathbf{q}}_0, 0)$ for the initial velocity. Imposing the initial impulsive force $\mathbf{P}_1$ is the more natural choice, as the initial condition for all other elements than the first is given by an initial impulsive force. For the numerical treatment of (4.36), the time integration might be approximated by a quadrature rule and solutions are found by means of the Newton–Raphson method. Box 3 shows the resulting stepping scheme, where for the sake of brevity the shape function are chosen to be the same for each element, i.e. $\boldsymbol{\phi}^k = \boldsymbol{\phi}$ for all k, and the initial condition is treated in the sense of (4.19). Let the external forces of the system be given by $\mathbf{f} = \mathbf{f}^{\mathrm{p}} + \mathbf{f}^{\mathrm{np}}$, with $\mathbf{f}^{\mathrm{p}}$ being potential forces deduced from a potential $V(\mathbf{q}, t)$ and $\mathbf{f}^{\mathrm{np}}$ being non-potential forces. Using (2.39) the principle of virtual action of the k^{th} element (4.35) takes the from

$$\delta A^k = -\int_{\Omega^k} \left\{ \delta L(\boldsymbol{\phi}^k, \dot{\boldsymbol{\phi}}^k, t) + \delta\mathbf{z}^{k\mathrm{T}} \mathbf{N}^{k\mathrm{T}} \mathbf{f}^{\mathrm{np}} \right\} \mathrm{d}t - \delta\mathbf{z}^{k\mathrm{T}} \mathbf{e}^1 \mathbf{P}_k + \delta\mathbf{z}^{k\mathrm{T}} \mathbf{e}^{N_k} \mathbf{P}_{k+1} = 0 \ , \tag{4.38}$$

Box 3 Stepping Scheme

1. Divide the time interval $\mathcal{I}$ into disjoint elements Ω^k, such that $\mathcal{I} = \bigcup_{k=1}^{n_{el}} \Omega^k$.

2. Choose the shape function $\boldsymbol{\phi}$ for every element and compute

$$\mathbf{I}(\mathbf{z}^k) = -\int_{\Omega^k} \left\{ \dot{\mathbf{N}}^{\mathrm{T}} \left(\frac{\partial T}{\partial \dot{\mathbf{q}}} \right)^{\mathrm{T}} + \mathbf{N}^{\mathrm{T}} \left(\frac{\partial T}{\partial \mathbf{q}} \right)^{\mathrm{T}} + \mathbf{N}^{\mathrm{T}} \mathbf{f} \right\} \mathrm{d}t$$

   exactly or by applying a quadrature rule.

3. Find the motion of the first element ($k = 1$) by solving

$$\mathbf{I}(\mathbf{z}^1) - \mathbf{e}^1 \left(\frac{\partial T}{\partial \dot{\mathbf{q}}} \right)^{\mathrm{T}} (\mathbf{q}_0, \dot{\mathbf{q}}_0, 0) + \mathbf{e}^N \mathbf{P}_2 \overset{(4.36)}{=} 0$$

   with $\mathbf{z}_1^1 = \mathbf{q}_0$ for $\mathbf{z}^1$ and $\mathbf{P}_2$, using e.g. the Newton–Raphson method.

4. For each $k > 1$ solve

$$\mathbf{I}(\mathbf{z}^k) - \mathbf{e}^1 \mathbf{P}_k + \mathbf{e}^N \mathbf{P}_{k+1} \overset{(4.36)}{=} 0$$

   with $\mathbf{z}_1^k = \mathbf{z}_N^{k-1}$ for $\mathbf{z}^k$ and $\mathbf{P}_{k+1}$, using e.g. the Newton–Raphson method. Use $\mathbf{P}_k$ and $\mathbf{z}_N^{k-1}$ from the solution of the previous element.

5. Construct continuous solution by means of (4.28).

for all variations $\delta \mathbf{z}^k$, where $L = T - V$. Introducing the discrete Lagrangian

$$L_d^k(\mathbf{z}^k) := \int_{\Omega^k} L(\boldsymbol{\phi}^k, \dot{\boldsymbol{\phi}}^k, t) \mathrm{d}t \tag{4.39}$$

and the discrete non-potential forces

$$\tilde{\mathbf{f}}^{\mathrm{np},k}(\mathbf{z}^k) := \int_{\Omega^k} \mathbf{N}^{k\mathrm{T}} \mathbf{f}^{\mathrm{np}} \mathrm{d}t \ , \tag{4.40}$$

the principle of virtual action (4.38) can be rewritten as

$$-\delta L_d^k(\mathbf{z}^k) - \delta \mathbf{z}^{k\mathrm{T}} \tilde{\mathbf{f}}^{\mathrm{np},k}(\mathbf{z}^k) - \delta \mathbf{z}^{k\mathrm{T}} \mathbf{e}^1 \mathbf{P}_k + \delta \mathbf{z}^{k\mathrm{T}} \mathbf{e}^{N_k} \mathbf{P}_{k+1} = 0 \quad \forall \delta \mathbf{z}^k \ . \tag{4.41}$$

For a numerical treatment of (4.41) the time integration in the definition of the discrete Lagrangian (4.39) and the discrete non-potential forces (4.40) has to

be approximated by means of a quadrature rule. Using the notation $\mathrm{D}_i := \frac{\partial}{\partial \mathbf{z}_i^k}$ and reformulating (4.41) to

$$\begin{aligned} -\delta A^k = {} & \delta \mathbf{z}_1^{k\,\mathrm{T}} \left(\mathrm{D}_1 L_d^k(\mathbf{z}^k) + \tilde{\mathbf{f}}_1^{\mathrm{np},k}(\mathbf{z}^k) + \mathbf{P}_k \right) \\ & + \sum_{i=2}^{N_k-1} \delta \mathbf{z}_i^{k\,\mathrm{T}} \left(\mathrm{D}_i L_d^k(\mathbf{z}^k) + \tilde{\mathbf{f}}_i^{\mathrm{np},k}(\mathbf{z}^k) \right) \\ & + \delta \mathbf{z}_{N_k}^{k\,\mathrm{T}} \left(\mathrm{D}_N L_d^k(\mathbf{z}^k) + \tilde{\mathbf{f}}_{N_k}^{\mathrm{np},k}(\mathbf{z}^k) - \mathbf{P}_{k+1} \right) = 0 \quad \forall \delta \mathbf{z}^k \,, \end{aligned} \tag{4.42}$$

this leads to the system of equations

$$\begin{aligned} & \mathrm{D}_1 L_d^k(\mathbf{z}^k) + \tilde{\mathbf{f}}_1^{\mathrm{np},k}(\mathbf{z}^k) + \mathbf{P}_k = 0 \\ & \mathrm{D}_i L_d^k(\mathbf{z}^k) + \tilde{\mathbf{f}}_i^{\mathrm{np},k}(\mathbf{z}^k) = 0 \quad \text{for } i = 2, \ldots, N_k - 1 \\ & \mathrm{D}_N L_d^k(\mathbf{z}^k) + \tilde{\mathbf{f}}_{N_k}^{\mathrm{np},k}(\mathbf{z}^k) - \mathbf{P}_{k+1} = 0 \end{aligned} \tag{4.43}$$

as a consequence of the fundamental lemma of calculus of variations. The system of equations (4.43) is equivalent to the system of equations (4.36), as merely a new notation has been introduced. Therefore, (4.43) defines the same stepping scheme as (4.36). Box 4 shows the stepping scheme of Box 3 reformulated in terms of the discrete Lagrangian as defined by (4.43), where again the shape functions are chosen to be the same for each element, i.e. $\boldsymbol{\phi}^k = \boldsymbol{\phi}$ for all k, and the initial condition is treated in the sense of (4.19). Since for each element k, except the first, the initial impulsive force $\mathbf{P}_k$ stems from the solution of the previous element $k-1$, the last row of(4.43)

$$\mathbf{P}_k = \mathrm{D}_N L_d^{k-1}(\mathbf{z}^{k-1}) + \tilde{\mathbf{f}}_N^{\mathrm{np},k-1}(\mathbf{z}^{k-1}) \,, \tag{4.44}$$

and the impulsive force $\mathbf{P}_k$ can be eliminated in the stepping scheme for $k \neq 1$ and (4.43) is reformulated to

$$\begin{aligned} & \mathrm{D}_1 L_d^k(\mathbf{z}^k) + \mathrm{D}_{N_k} L_d^{k-1}(\mathbf{z}^{k-1}) + \tilde{\mathbf{f}}_{N_k}^{\mathrm{np},k-1}(\mathbf{z}^{k-1}) + \tilde{\mathbf{f}}_1^{\mathrm{np},k}(\mathbf{z}^k) = 0 \\ & \mathrm{D}_i L_d^k(\mathbf{z}^k) + \tilde{\mathbf{f}}_i^{\mathrm{np},k}(\mathbf{z}^k) = 0 \quad \text{for } i = 2, \ldots, N_k - 1 \,. \end{aligned} \tag{4.45}$$

For given $\mathbf{z}^{k-1}$, the system of equations (4.45) can be solved for $\mathbf{z}^k$ and gives the motion within the k^{th} element. (4.45) is called the extended set of discrete Euler–Lagrange equations, cf. West (2004) Sec. 3.5. Note that Marsden and West (2001) derived the extended set of discrete Euler–Lagrange equations using concepts of discrete mechanics and they assumed the discrete Lagrangian to be the same for every element. Box 5 represents a reformulation of the stepping scheme of Box 4 by means of (4.45). For linear elements, the element

coordinates are $\mathbf{z}^k = (\mathbf{q}(t_k), \mathbf{q}(t_{k+1}))^{\mathrm{T}}$. Introducing the notation $\mathbf{q}^k = \mathbf{q}(t_k)$, for linear elements (4.45) reduces to the discrete Euler–Lagrange equations

$$\mathrm{D}_1 L_d(\mathbf{q}^k, \mathbf{q}^{k+1}) + \mathrm{D}_2 L_d(\mathbf{q}^{k-1}, \mathbf{q}^k) + \tilde{\mathbf{f}}_2^{\mathrm{np},k-1}(\mathbf{q}^{k-1}, \mathbf{q}^k) + \tilde{\mathbf{f}}_1^{\mathrm{np},k}(\mathbf{q}^k, \mathbf{q}^{k+1}) = 0 \; . \tag{4.46}$$

Marsden and West (2001) derived (4.46) using the viewpoint of discrete mechanics. For linear elements (4.43) yields

$$\begin{aligned} \mathbf{P}_k &= -\mathrm{D}_1 L_d(\mathbf{q}^k, \mathbf{q}^{k+1}) - \tilde{\mathbf{f}}_1^{\mathrm{np},k}(\mathbf{q}^k, \mathbf{q}^{k+1}) \\ \mathbf{P}_{k+1} &= \mathrm{D}_2 L_d(\mathbf{q}^k, \mathbf{q}^{k+1}) + \tilde{\mathbf{f}}_2^{\mathrm{np},k}(\mathbf{q}^k, \mathbf{q}^{k+1}) \; , \end{aligned} \tag{4.47}$$

which are the equations derived in Marsden and West (2001) p. 424 by means of a discrete Legendre transformation.

To show that the solution found by the stepping approach is equivalent to the solution found by the monolithic approach, the virtual action of the system is written as the sum of the virtual actions of the elements. As the principle of virtual action (4.31) holds, the global virtual action

$$\begin{aligned} \delta A &= \sum_{k=1}^{n_{el}} \delta A^k \\ &\overset{(4.31)}{=} -\sum_{k=1}^{n_{el}} \int_{\Omega^k} \Big\{ \delta T(\boldsymbol{\phi}^k, \dot{\boldsymbol{\phi}}^k, t) + \delta \mathbf{z}^{k\mathrm{T}} \mathbf{N}^{k\mathrm{T}} \mathbf{f} \Big\} \, \mathrm{d}t \\ &\quad - \delta \mathbf{z}^{k\mathrm{T}} \mathbf{e}^1 \mathbf{P}_k + \delta \mathbf{z}^{k\mathrm{T}} \mathbf{e}^N \mathbf{P}_{k+1} \end{aligned} \tag{4.48}$$

vanishes for all variations of $\mathbf{z}^k$ and every k. Using (4.37), which implies $\delta \mathbf{z}_N^k = \delta \mathbf{z}_1^{k+1}$ for $k \notin \{1, n_{el}\}$, after rearranging (4.48) to

$$\begin{aligned} \delta A = &-\sum_{k=1}^{n_{el}} \int_{\Omega^k} \Big\{ \delta T(\boldsymbol{\phi}^k, \dot{\boldsymbol{\phi}}^k, t) + \delta \mathbf{z}^{k\mathrm{T}} \mathbf{N}^{k\mathrm{T}} \mathbf{f} \Big\} \, \mathrm{d}t - \delta \mathbf{z}^{1\mathrm{T}} \mathbf{e}^1 \mathbf{P}_1 + \delta \mathbf{z}^{n_{el}\mathrm{T}} \mathbf{e}^{N_k} \mathbf{P}_{n_{el}+1} \\ &+ \sum_{k=2}^{n_{el}-1} (\delta \mathbf{z}_{N_k}^{k\;\mathrm{T}} - \delta \mathbf{z}_1^{k+1\mathrm{T}}) \mathbf{P}_k = 0 \quad \forall \delta \mathbf{z}^k \end{aligned} \tag{4.49}$$

yields the principle of virtual action

$$\begin{aligned} \delta A = &-\sum_{k=1}^{n_{el}} \int_{\Omega^k} \Big\{ \delta T(\boldsymbol{\phi}^k, \dot{\boldsymbol{\phi}}^k, t) + \delta \mathbf{z}^{k\mathrm{T}} \mathbf{N}^{k\mathrm{T}} \mathbf{f} \Big\} \, \mathrm{d}t \\ &- \delta \mathbf{z}^{1\mathrm{T}} \mathbf{e}^1 \mathbf{P}_1 + \delta \mathbf{z}^{n_{el}\mathrm{T}} \mathbf{e}^{N_k} \mathbf{P}_{n_{el}+1} = 0 \quad \forall \delta \mathbf{z}^k \; . \end{aligned} \tag{4.50}$$

By (4.32) and (4.33), which gives $\mathbf{N}^1(0, \mathbf{z}^1) = \mathbf{e}^1$ and $\mathbf{N}^{n_{el}}(0, \mathbf{z}^{n_{el}}) = \mathbf{e}^{N_k}$, (4.50) is the same as (4.6), which is used to derive the monolithic apporach. As the

stepping approach and the monolithic approach both fulfill the same form of the principle of virtual action, the motions found by the two approaches are the same if the same shape functions, the same temporal nodes are used, and the initial conditions are treated in the same way.

Box 4 Stepping Scheme

1. Divide the time interval $\mathcal{I}$ into disjoint elements Ω^k, such that $\mathcal{I} = \bigcup_{k=1}^{n_{el}} \Omega^k$.

2. Choose a shape function $\boldsymbol{\phi}$ for each element and compute

$$L_d(\mathbf{z}^k) = \int_{\Omega^k} L(\boldsymbol{\phi}, \dot{\boldsymbol{\phi}}, t)\mathrm{d}t, \quad \text{and} \quad \tilde{\mathbf{f}}^{\mathrm{np},k}(\mathbf{z}^k) = \int_{\Omega^k} \mathbf{N}^{\mathrm{T}}\mathbf{f}^{\mathrm{np}}\mathrm{d}t$$

   exactly or by applying a quadrature rule.

3. Find the motion of the first element ($k = 1$) solving

$$\begin{aligned}
&\mathrm{D}_1 L_d(\mathbf{z}^1) + \tilde{\mathbf{f}}_1^{\mathrm{np},1}(\mathbf{z}^1) + \left(\frac{\partial T}{\partial \dot{\mathbf{q}}}\right)^{\mathrm{T}}(\mathbf{q}_0, \dot{\mathbf{q}}_0, 0) = 0 \\
&\mathrm{D}_i L_d(\mathbf{z}^1) + \tilde{\mathbf{f}}_i^{\mathrm{np},1}(\mathbf{z}^1) = 0 \quad \text{for } i = 2, \ldots, N_k - 1 \\
&\mathrm{D}_N L_d^k(\mathbf{z}^1) + \tilde{\mathbf{f}}_N^{\mathrm{np},1}(\mathbf{z}^1) - \mathbf{P}_2 = 0
\end{aligned}$$

   with $\mathbf{z}_1^1 = \mathbf{q}_0$ for $\mathbf{z}^1$ and $\mathbf{P}_2$, using e.g. the Newton–Raphson method.

4. For each $k > 1$ solve

$$\begin{aligned}
&\mathrm{D}_1 L_d(\mathbf{z}^k) + \tilde{\mathbf{f}}_1^{\mathrm{np},k}(\mathbf{z}^k) + \mathbf{P}_k = 0 \\
&\mathrm{D}_i L_d(\mathbf{z}^k) + \tilde{\mathbf{f}}_i^{\mathrm{np},k}(\mathbf{z}^k) = 0 \quad \text{for } i = 2, \ldots, N_k - 1 \\
&\mathrm{D}_N L_d(\mathbf{z}^k) + \tilde{\mathbf{f}}_{N_k}^{\mathrm{np},k}(\mathbf{z}^k) - \mathbf{P}_{k+1} = 0
\end{aligned}$$

   with $\mathbf{z}_1^k = \mathbf{z}_N^{k-1}$ for $\mathbf{z}^k$ and $\mathbf{P}_{k+1}$, using e.g. the Newton–Raphson method. Use $\mathbf{P}_k$ and $\mathbf{z}_N^{k-1}$ from the solution of the previous element.

5. Construct continuous solution by means of (4.28).

Box 5 Stepping Scheme

1. Divide the time interval $\mathcal{I}$ into disjoint elements Ω^k such that $\mathcal{I} = \bigcup_{k=1}^{n_{el}} \Omega^k$.

2. Choose a shape function $\boldsymbol{\phi}$ for each element and compute

$$L_d(\mathbf{z}^k) = \int_{\Omega^k} L(\boldsymbol{\phi}, \dot{\boldsymbol{\phi}}, t)\mathrm{d}t, \quad \text{and} \quad \tilde{\mathbf{f}}^{\mathrm{np},k}(\mathbf{z}^k) = \int_{\Omega^k} \mathbf{N}^{\mathrm{T}}\mathbf{f}^{\mathrm{np}}\mathrm{d}t$$

   exactly or by using a quadrature rule.

3. Find the motion of the first element ($k = 1$) by solving

$$\begin{aligned}
&\mathrm{D}_1 L_d(\mathbf{z}^1) + \tilde{\mathbf{f}}_1^{\mathrm{np},1}(\mathbf{z}^1) + \left(\frac{\partial T}{\partial \dot{\mathbf{q}}}\right)^{\mathrm{T}}(\mathbf{q}_0, \dot{\mathbf{q}}_0, 0) = 0 \\
&\mathrm{D}_i L_d(\mathbf{z}^1) + \tilde{\mathbf{f}}_i^{\mathrm{np},1}(\mathbf{z}^1) = 0 \quad \text{for } i = 2, \ldots, N_k - 1 \\
&\mathrm{D}_N L_d(\mathbf{z}^1) + \tilde{\mathbf{f}}_N^{\mathrm{np},1}(\mathbf{z}^1) - \mathbf{P}_2 = 0
\end{aligned}$$

   with $\mathbf{z}_1^1 = \mathbf{q}_0$ for $\mathbf{z}^1$ and $\mathbf{P}_2$, using e.g. the Newton–Raphson method.

4. For each $k > 1$ solve

$$\begin{aligned}
&\mathrm{D}_1 L_d(\mathbf{z}^k) + \mathrm{D}_N L_d(\mathbf{z}^{k-1}) + \tilde{\mathbf{f}}_N^{\mathrm{np},k-1}(\mathbf{z}^{k-1}) + \tilde{\mathbf{f}}_1^{\mathrm{np},k}(\mathbf{z}^k) = 0 \\
&\mathrm{D}_i L_d(\mathbf{z}^k) + \tilde{\mathbf{f}}_i^{\mathrm{np},k}(\mathbf{z}^k) = 0 \quad \text{for } i = 2, \ldots, N - 1 \,.
\end{aligned}$$

   for $\mathbf{z}^k$ and $\mathbf{P}_{k+1}$, using e.g. the Newton–Raphson method. Use $\mathbf{P}_k$ and $\mathbf{z}^{k-1}$ from the solution of the previous element.

5. Construct continuous solution by means of (4.28).

Chapter 5

Examples

In this chapter the finite element formulations of Chapter 4 are applied to find the motions of the harmonic oscillator, the pendulum and the two body problem. All fields are discretized using linear Lagrange polynomials. Additionally, the single-field formulation is discretized by quadratic Lagrange polynomials. All these formulations are compared in terms of convergence to the analytical, or to a very accurate numerical solution. Furthermore, the energy conservation property of the numerical schemes are analyzed.

Preliminaries

The linear element described by the element coordinate $\mathbf{z}^e = (\mathbf{z}_1^e, \mathbf{z}_2^e)^{\mathrm{T}}$ is defined by the shape function

$$\boldsymbol{\phi}(s, \mathbf{z}^e) = (1-s)\mathbf{z}_1^e + s\mathbf{z}_2^e \, . \tag{5.1}$$

The quadratic element described by the element coordinate $\mathbf{z}^e = (\mathbf{z}_1^e, \mathbf{z}_2^e, \mathbf{z}_3^e)^{\mathrm{T}}$ is defined by the shape function

$$\boldsymbol{\phi}(s, \mathbf{z}^e) = (2s-1)(s-1)\mathbf{z}_1^e - 4(s^2-s)\mathbf{z}_2^e + (2s-1)s\mathbf{z}_3^e \, . \tag{5.2}$$

To study the convergence behavior of the finite element solution (4.16) defined by the global vector of element coordinates $\mathbf{z}$ towards a reference solution $\mathbf{q}^{\mathrm{ref}}(t)$ of the mechanical system, we introduce the error function

$$e = \frac{1}{T}\int_{\mathcal{I}} \left(\mathbf{q}^{\mathrm{ref}}(t) - \sum_{e=1}^{n_{el}} \chi_{\Omega^e}(t)\boldsymbol{\phi}^e(s^e(t), \mathbf{C}^e\mathbf{z}) \right)^2 \mathrm{d}t \, . \tag{5.3}$$

The error function e measures the mean quadratic error between the finite element solution and the reference solution. Furthermore the relative energy error

$$e_E = \frac{E_{\mathrm{disc}} - E_{\mathrm{ref}}}{E_{\mathrm{ref}}} \tag{5.4}$$

of the discrete finite element solution with respect to the reference solution is defined, where $E = T+V$ is the total energy consisting of kinetic and potential energy T and V, respectively.

5.1 Harmonic Oscillator

Consider the mechanical system consisting of a mass m, which is connected to the inertial origin with a spring of stiffness c. The displacement of the mass is measured by the coordinate $q\colon \mathbb{R} \to \mathbb{R}$ which is a function of time. The mass-spring system is depicted in Figure 5.1. The kinetic and potential energy

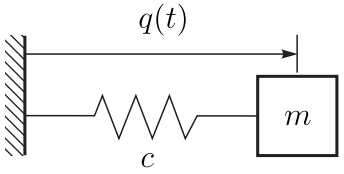


Figure 5.1: Sketch of the harmonic oscillator modeled as mass-spring system with mass m and stiffness c.

of the system are given by

$$T(\dot{q}) = \frac{1}{2} m \dot{q}^2 \quad \text{and} \quad V(q) = \frac{1}{2} c q^2 \,. \tag{5.5}$$

Using the energy representations (5.5) in Hamilton's law of varying action (2.41) yields

$$\delta A = -\int_{\mathcal{I}} \{\delta\dot{q}(t)\, m\dot{q}(t) - \delta q(t)\, cq(t)\} \mathrm{d}t + \delta q(t)\, P|_{\partial\mathcal{I}} = 0 \quad \forall\, \delta q(t) \,, \tag{5.6}$$

which describes the motion of the mass-spring system during the time interval $\mathcal{I}$, where the external impulsive forces are given by the constitutive equations (2.36). The Euler–Lagrange equations (2.45) lead to the initial value problem given by

$$m\ddot{q}(t) + cq(t) = 0 \quad \text{s.t.} \quad q(0) = q_0, \quad \dot{q}(0) = u_0 \,, \tag{5.7}$$

where the values of q_0 and u_0 are given initial conditions. The analytical solution

$$q^{\mathrm{ref}}(t) = q_0 \cos(\sqrt{c/m}\, t) + \frac{u_0}{\sqrt{c/m}} \sin(\sqrt{c/m}\, t) \tag{5.8}$$

of (5.7) is used as the reference solution for this example. Assume that the time interval $\mathcal{I}$ is discretized using a uniform grid of nodes $(t_1, \ldots, t_{n_N}) = (0, \Delta t, 2\Delta t, \ldots, T)$, with $\Delta t = T/(n_N - 1)$ for a chosen number of nodes n_N.

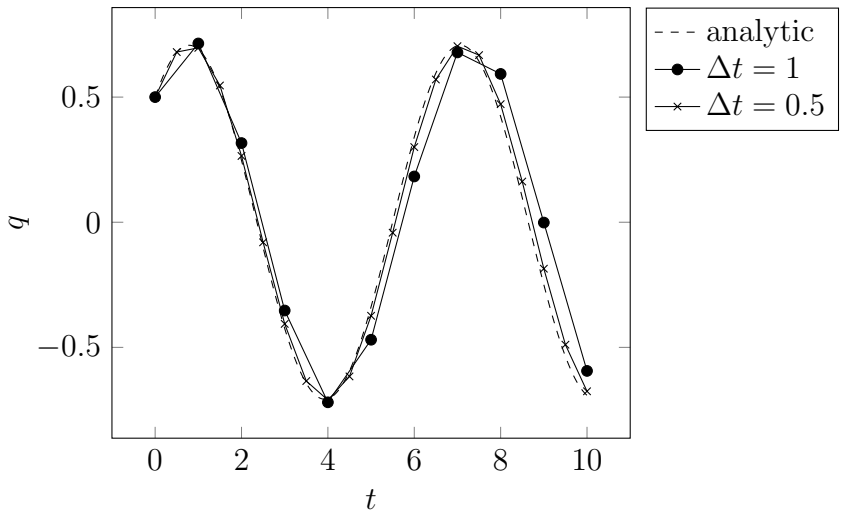


Figure 5.2: Motion of the harmonic oscillator defined by $m = 1$ and $c = 1$ with initial conditions $q(0) = 0.5$ and $\dot{q}(0) = 0.5$ during the time interval $\mathcal{I} = [0, 10]$. Analytical solution (5.8) and single-field finite element solution using linear elements with temporal length $\Delta t = 1$ and $\Delta t = 0.5$.

Figure 5.2 shows two discretized trajectories of the mass-spring system calculated using the single-field formulation described by (4.19) with linear shape functions. It can be seen, that the analytical solution (5.8) is better approximated by the discrete solution with more elements. This can be quantified by means of the error defined in (5.3), which measures the mean quadratic error between the finite element solution and the analytical solution of the harmonic oscillator. Figure 5.3 shows the convergence behavior of the single- and multi-field formulations with linear elements, which can be seen to be quadratic. Moreover, the convergence behavior of the single-field formulation with quadratic elements is shown to be cubic.

For this example, all pure multi-field formulations have the same convergence behavior and for each number of elements chosen, lead to solutions with the smallest error compared to the other formulations with linear elements. Further investigations have shown that the order of the error e of the mixed multi-field formulations seem to depend only on the value of the parameter α and not on β. As shown in Figure 5.3 the formulation with $\alpha = 0.5$ leads to smaller errors than the single-field formulation. Using the pure multi-field formulations the error can be reduced by one order of magnitude with respect to the single-field formulation. The single-field formulation with quadratic elements performs best, as the error compared to the other formulations is between one and two orders of magnitude smaller.

Figure 5.4 shows the temporal evolution of the energy error (5.4), which

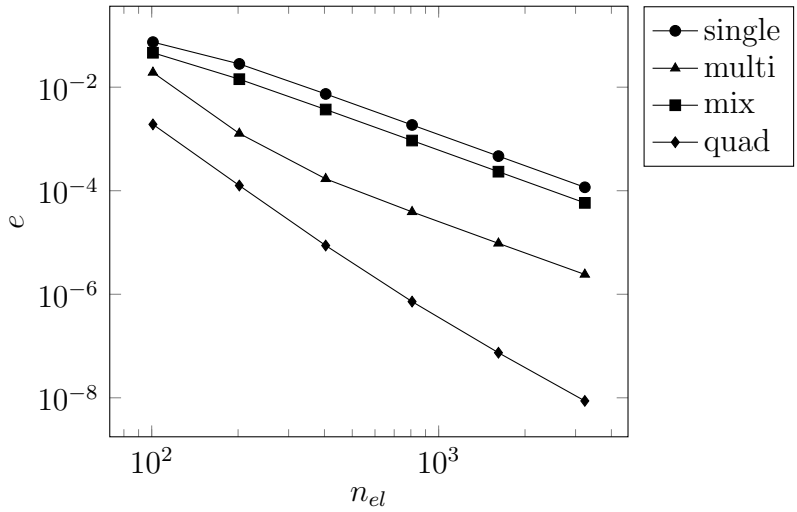


Figure 5.3: Convergence towards analytcal solution of the harmonic oscillator defined by $m = 1$ and $c = 1$ with initial conditions $q(0) = 0.5$ and $\dot{q}(0) = 0.5$ during the time interval $\mathcal{I} = [0, 100]$. Linear elements used for single-field (single), pure multi-field formulation (multi), mixed multi-field (mix) with $\alpha = 0.5$. The single-field formulation with quadratic elements (quad) has slope below -3 in the double logarithmic scale, while the others have a slope of approximately -2.

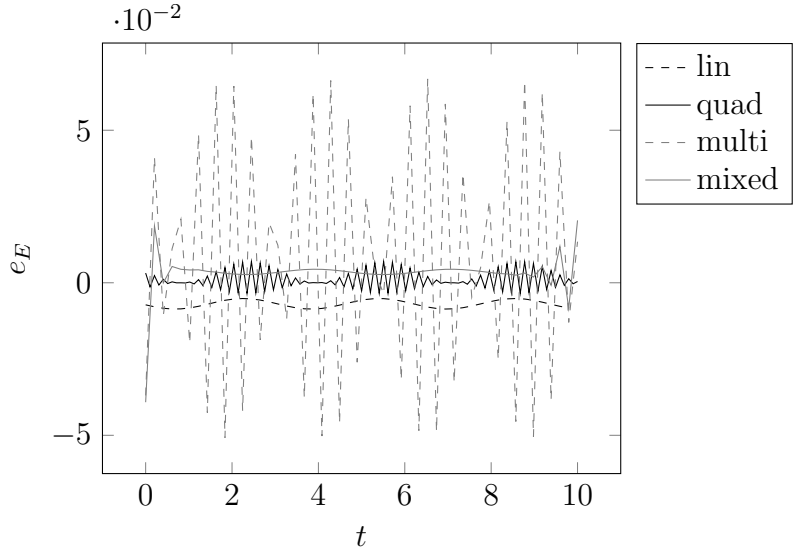


Figure 5.4: Energy error (5.4) of the harmonic oscillator defined by $m = 1$ and $c = 1$ with initial conditions $q(0) = 0.5$ and $\dot{q}(0) = 0.5$ during the time interval $\mathcal{I} = [0, 10]$. Linear elements used for single-field (single), pure multi-field formulation (multi), mixed multi-field (mix) with $\alpha = 0.5$ and quadratic elements (quad) for single-field formulation. All formulations have been computed with $\Delta t = 0.2$.

oscillates around a constant error level. The energy error is bounded for all formulations. Further investigations have shown that the energy error remains bounded even for much longer time intervals $\mathcal{I}$ and that these bounds converge to zero if the number of elements are increased. The best energy performance is achieved by the single-field formulation with the quadratic element, as it oscillates around the smallest error level with very small amplitudes. The mixed multi-field formulation performs very well too, but exhibits error peaks near the boundaries of $\mathcal{I}$.

Concluding from the convergence behavior and the energy considerations, the single-field formulation with quadratic elements is the numerical approach with the best performance. Note that the time integration in the principle of virtual action (5.6), after discretization, can be computed exactly. Therefore the performances seen for this example are due to the choice of the shape function only and are not biased by the choice of some quadrature rule for the time integration.

5.2 Simple Pendulum

The simple pendulum consists of a mass m, which is attached to a mass-less rigid bar of length l and is pivoted on an inertial point. The only degree of freedom of this planar mechanical system is described by the time dependent generalized coordinate $q(t) \in \mathbb{R}$. A sketch of the pendulum is given in Figure 5.5. The kinetic and potential energy of the pendulum are given by

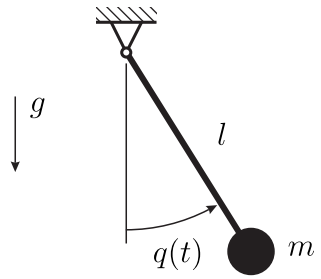


Figure 5.5: Sketch of a pendulum with length l and mass m.

$$T(\dot{q}) = \frac{1}{2} m l^2 \dot{q}^2 \quad \text{and} \quad V(q) = -mgl \cos q(t) \,, \tag{5.9}$$

where the potential energy models the influence of gravitation on the pendulum. Using (5.9) the principle of virtual action for the pendulum is

$$\delta A = -\int_{\mathcal{I}} \{\delta\dot{q}(t)\, ml^2 \dot{q}(t) - \delta q(t)\, mgl \sin q(t)\} \mathrm{d}t + \delta q(t)\, P|_{\partial\mathcal{I}} = 0 \quad \forall\, \delta q \tag{5.10}$$

by Hamilton's law of varying action (2.41). The equation of motion (2.45) takes the form of the initial value problem

$$ml^2 \ddot{q}(t) + mgl \sin q(t) = 0 \quad \text{s.t.} \quad q(0) = q_0, \quad \dot{q}(0) = u_0 \tag{5.11}$$

and follow from (5.10) by means of the fundamental lemma of calculus of variations applied after integration by parts. As the differential equation (5.11) has no analytical solution, a very accurate numerical solution of (5.11), computed by the `ode45` solver of MATLAB, is used as the reference motion $q^{\mathrm{ref}}(t)$.

Figure 5.6 shows a trajectory of the pendulum calculated by a single-field finite element approach, where the elements are chosen to be linear and the time integral in (4.36) is approximated by the trapezoidal rule. Linear elements together with the trapezoidal rule lead to an explicit stepping scheme, the Verlet algorithm[1], which is computationally very cheap. If quadratic elements are

[1] cf. Appendix A.5.

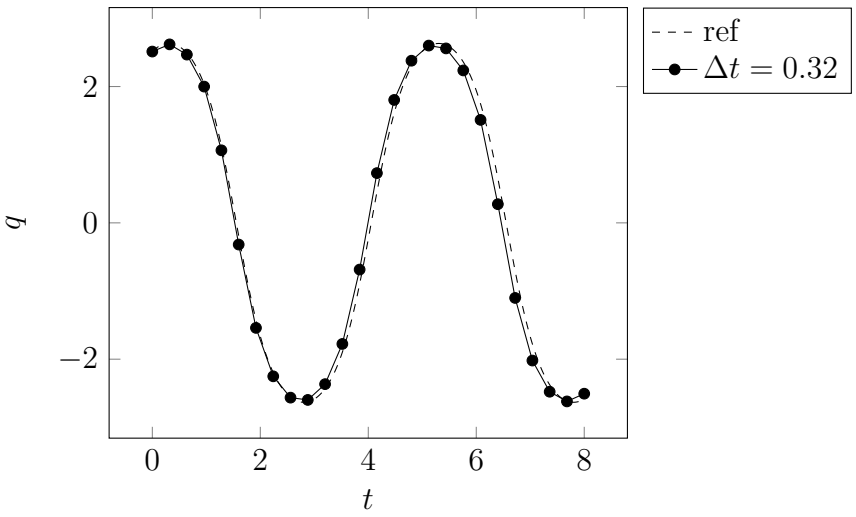


Figure 5.6: Motion of the pendulum characterized by $m = 1$ and $l = 2$ with initial conditions $q(0) = \frac{4\pi}{5}$ and $\dot{q}(0) = 0.8$ during the time interval $\mathcal{I} = [0, 8]$. Reference solution and single-field finite element solution with linear elements whose temporal length is $\Delta t = 0.32$. The virtual action of the gravitational force is integrated using the trapezoidal rule.

used instead of linear ones, the stepping scheme becomes implicit and therefore more costly. Nevertheless, it has the advantage that the discrete velocities are continuous in time, whereas the linear elements give piecewise constant velocities, as shown in Figure 5.7. The velocity field given by the multi-field formulations with linear elements have the same properties as the ones of the single-field formulation with quadratic elements, but as the multi-field formulations are monolithic approaches, they are computationally very expensive. For long time intervals $\mathcal{I}$ and high number of elements, the set of implicit nonlinear equations associated with the multi-field formulations gets very large. In addition to that, the matrices which arise, when the set of equations is solved using the Newton-Raphson method, are often badly conditionned and the Newton-Raphson method does not converge. The matrices of the mixed multi-field approach show a better condition number as the ones of the pure multi-field formulation, this is due to the parameters α and β, which can be used to influence the condition number of the matrices. When a high number of elements is chosen, the Netwton–Raphson method used to solve the pure multi-field formulation does not converge for this example. Thus, Figure 5.8 shows only the convergence behavior of the discrete finite element solutions towards the reference solution for the single-field formulation with linear and quadratic elements, and for a mixed multi-field formulation. The convergence of all approaches is quadratic and the error of the single-field formulation with quadratic elements is about half order of magnitude smaller compared to the

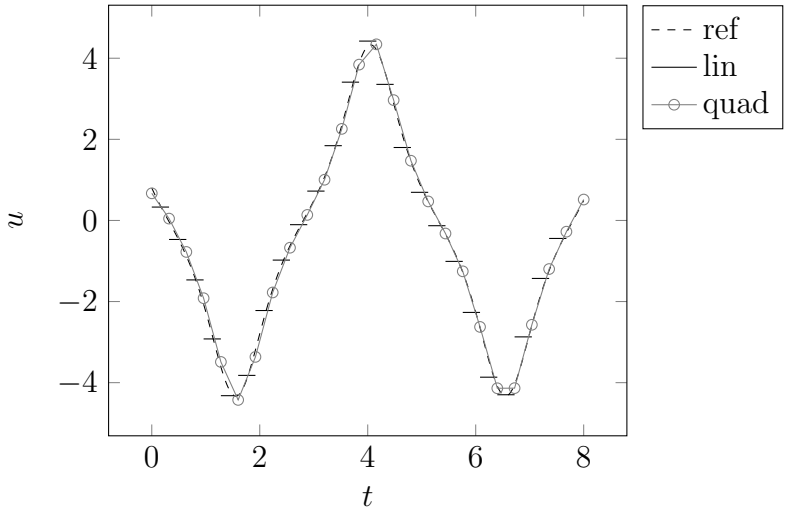


Figure 5.7: Velocity field of the pendulum characterized by $m = 1$ and $l = 2$ with initial conditions $q(0) = \frac{4\pi}{5}$ and $\dot{q}(0) = 0.8$ during the time interval $\mathcal{I} = [0, 8]$. Reference solution (ref) and single-field finite element solution with linear (lin) and quadratic (quad) elements, whose temporal length is $\Delta t = 0.32$. The virtual action of the gravitational force is integrated using the trapezoidal rule.

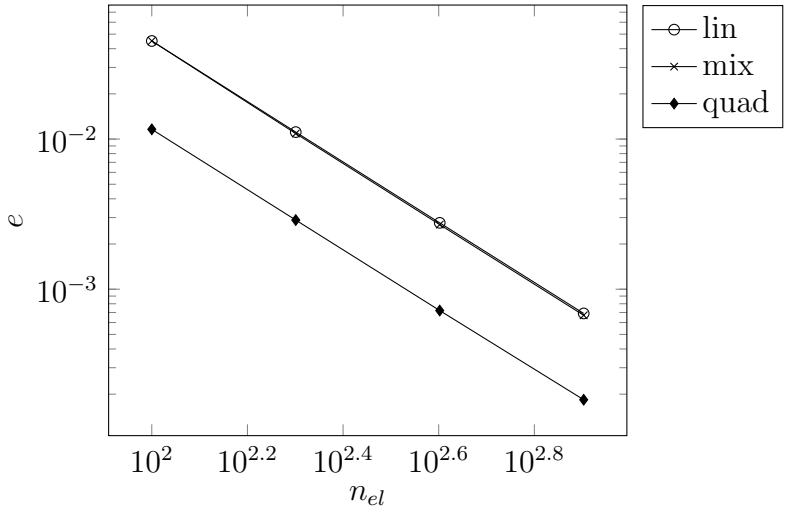


Figure 5.8: Convergence towards reference solution of the simple pendulum defined by $m = 2$ and $l = 1.5$ with initial conditions $q(0) = \frac{3\pi}{5}$ and $\dot{q}(0) = 0.2$ during the time interval $\mathcal{I} = [0, 20]$. Single-field formulation with linear (lin) and quadratic (quad) elements, and mixed multi-field formulation (mix) with $\alpha = 0.5$.

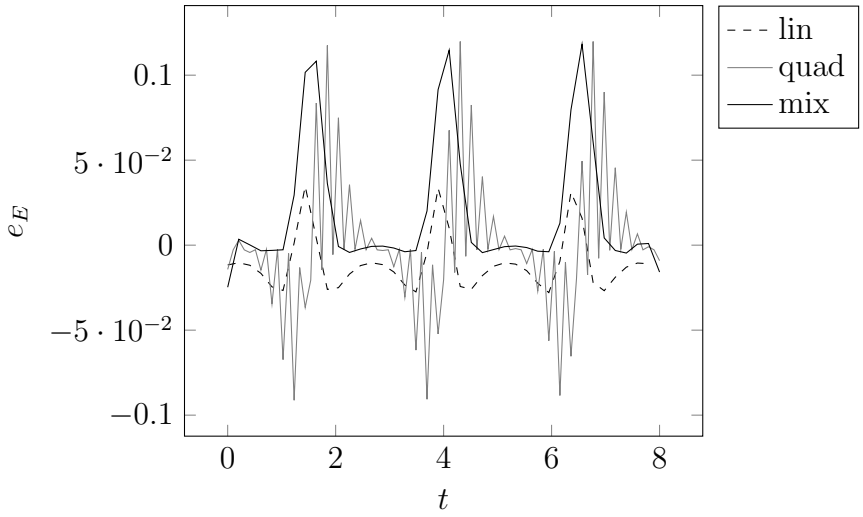


Figure 5.9: Motion of the harmonic oscillator defined by $m = 1$ and $c = 1$ with initial conditions $q(0) = 0.5$ and $\dot{q}(0) = 0.5$ during the time interval $\mathcal{I} = [0, 10]$. Analytical solution and single-field finite element solution with linear elements whose temporal length is $\Delta t = 1$ and $\Delta t = 0.5$, respectively.

formulations with linear elements.

Figure 5.9 shows the temporal evolution of the energy error (5.4) of the different finite element approaches. The energy error is seen to be bounded and oscillates around constant error levels. Further investigations have shown that the error bounds converge to zero, if the number of elements is increased.

The single-field approach with quadratic elements is the preferable approach to find the discrete trajectory of the simple pendulum, as it shows the smallest errors with respect to the reference solution and is computationally cheap compared to the multi-field formulations. As it can be formulated as a stepping equation, the performance does not depend on the length of the time interval $\mathcal{I}$ chosen, but it depends only on the length of the single element. Hence, long term simulations can be performed, which is not possible with the monolithic approaches because of the bad convergence of the Newton–Raphson method described above.

5.3 Two-Body Problem

Let a body of mass M be attached to the origin of the inertial $\mathbf{e}_x^I$-$\mathbf{e}_y^I$-frame, cf. Figure 5.10. The position of the body with mass m, which moves under the influence of the gravitational field of M, is addressed by the coordinate vector $\mathbf{q} = (x, y)^{\mathrm{T}}$ in the $\mathbf{e}_x^I$-$\mathbf{e}_y^I$-frame. The kinetic energy and the potential energy,

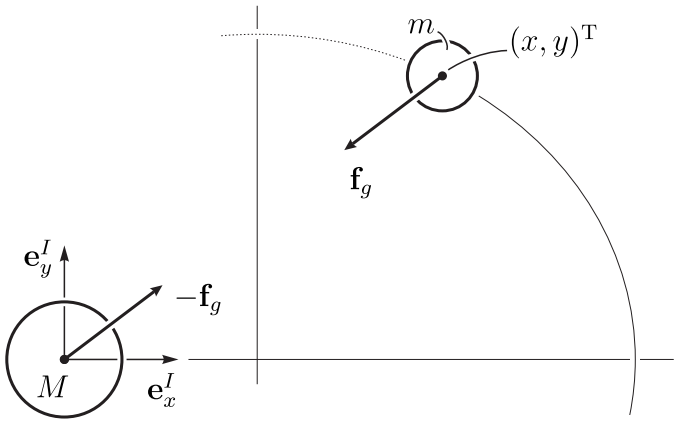


Figure 5.10: Sketch of two-body problem. Body with mass m orbiting around body with mass M under the influence of the gravitational force $\mathbf{f}_g$.

which models gravity, are given by

$$T(\dot{\mathbf{q}}) = \frac{1}{2} m\, \dot{\mathbf{q}}^{\mathrm{T}} \dot{\mathbf{q}} \quad \text{and} \quad V(\mathbf{q}) = -\frac{GMm}{\sqrt{\mathbf{q}^{\mathrm{T}}\mathbf{q}}}\,, \tag{5.12}$$

where G denotes the gravitational constant. The gravitational force acting on m is

$$\mathbf{f}_g = -\left(\frac{\partial V}{\partial \mathbf{q}}\right)^{\mathrm{T}} = -\frac{GMm}{(\mathbf{q}^{\mathrm{T}}\mathbf{q})^{3/2}}\,\mathbf{q}\,, \tag{5.13}$$

which inserted in the principle of virtual action (2.29) yields

$$\delta A = -\int_{\mathcal{I}} \{\delta\dot{\mathbf{q}}^{\mathrm{T}}\, m\dot{\mathbf{q}} - \delta\mathbf{q}^{\mathrm{T}}\, \frac{GMm}{(\mathbf{q}^{\mathrm{T}}\mathbf{q})^{3/2}}\,\mathbf{q}\}\mathrm{d}t + \delta\mathbf{q}^{\mathrm{T}}\,\mathbf{P}\big|_{\partial\mathcal{I}} = 0 \quad \forall\,\delta\mathbf{q}\,. \tag{5.14}$$

The equations of motion (2.34) together with the constitutive law for the boundary impulsive forces (2.36) define the initial value problem

$$m\ddot{\mathbf{q}} = -\frac{GMm}{(\mathbf{q}^{\mathrm{T}}\mathbf{q})^{3/2}}\,\mathbf{q} \quad \text{s.t.} \quad \mathbf{q}(0) = \mathbf{q}_0, \quad \dot{\mathbf{q}}(0) = \mathbf{u}_0\,, \tag{5.15}$$

where $\mathbf{q}_0$ and $\mathbf{u}_0$ are given initial conditions. As the initial value problem (5.15) has no analytical solution, a very accurate numerical solution of (5.15),

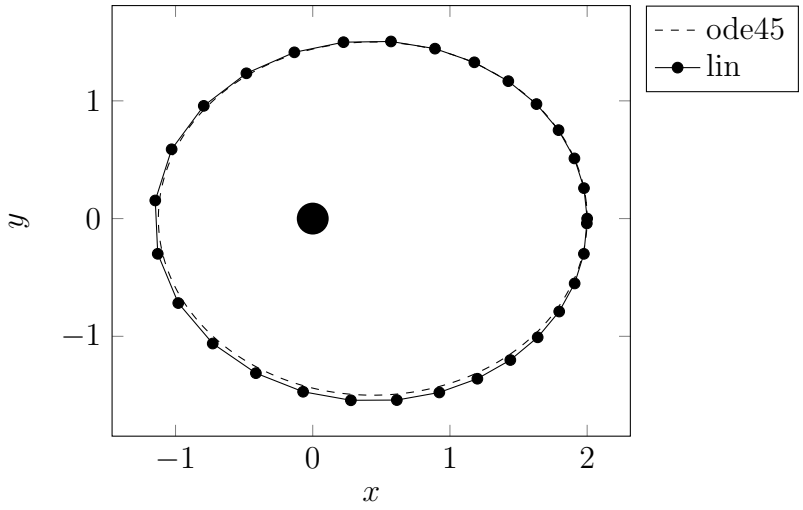


Figure 5.11: Trajectory of the two-body problem defined by $m = 1$ and $GM = 1$, with initial conditions $\mathbf{q}(0) = (2, 0)^{\mathrm{T}}$ and $\dot{\mathbf{q}}(0) = (0, 0.6)^{\mathrm{T}}$. Reference solution (ref) and single-field finite element solution (lin) with linear elements.

computed by the `ode45` solver of MATLAB, is used as the reference motion $\mathbf{q}^{\mathrm{ref}}(t)$.

Figure 5.11 shows a trajectory of the two body problem calculated with the single-field finite element approach with linear elements. The time integration in (4.36) is approximated by means of the trapezoidal rule.

Figure 5.12 shows the convergence of the single-field finite element solutions with linear and quadratic elements and the mixed multi-field finite element solution of (5.14) towards the very accurate reference solution $\mathbf{q}^{\mathrm{ref}}(t)$. For both, the linear and the quadratic shape functions, the convergence is quadratic. The finite element solution with quadratic shape functions shows an error, which is one order of magnitude smaller than the one for the linear element. That means, it needs approximately four times more linear elements to get the same accuracy as achieved with the quadratic element. The mixed multi-field formulation shows the largest error and is computationally very costly, as it has to be solved monolithically. Furthermore the convergence of the Newton–Raphson method used to solve the associated nonlinear set of equations is very poor. For the pure multi-field approaches this convergence is even worse and did not converge at all for this example, which is why no convergence plot is given in Figure 5.12. If the chosen time interval is longer than $\mathcal{I} = [0, 10]$, which corresponds roughly to one period of the body of mass m around the one of mass M, the mixed multi-field finite element approach does not converge either. Hence, the energy error plotted in Figure 5.13 is only shown for the single-field formulations, as these are the sole that allow a long-term simulation.

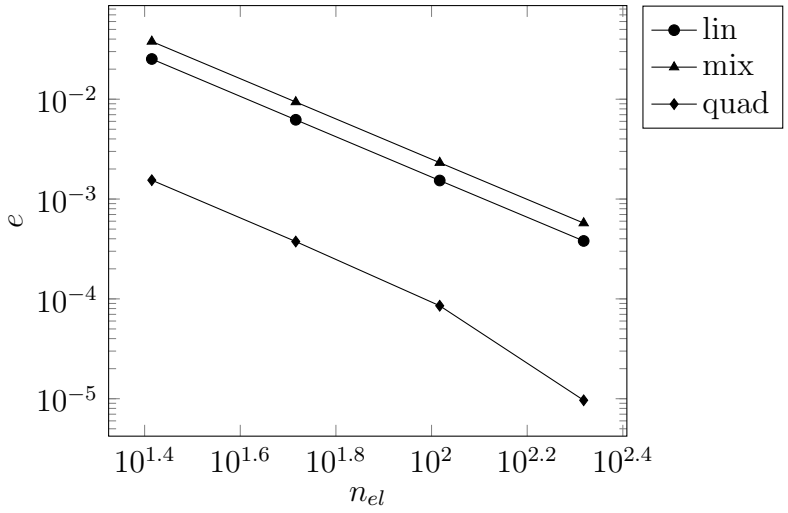


Figure 5.12: Convergence plot of the two-body problem defined by $m = 1$ and $GM = 1$, with initial conditions $\mathbf{q}(0) = (2, 0)^{\mathrm{T}}$ and $\dot{\mathbf{q}}(0) = (0, 0.6)^{\mathrm{T}}$. Single-field finite element approach with linear (lin) and quadratic (quad) elements, with integration time $T = 50$.

This is due to the fact that the single-field formulation can be reformulated to a stepping scheme. Figure 5.13 shows that the energy error is bounded, and of the same order for both, the linear and quadratic element. Further investigations have shown that the boundaries converge to zero energy error, if the number of elements is increased. In other words, the energy error decreases with decreasing time step Δt.

As for the other examples, the single-field finite element approach with quadratic elements is the preferable approach, as it is the most accurate and is computationally cheap due to the possibility to implement it as a stepping scheme. Moreover it is seen that the monolithic multi-field approaches, which seem to have no equivalent stepping scheme, are computationally very expensive and are not suitable for long-term simulations. Note however that multi-field stepping schemes exist, cf. Borri et al. (1992) and Betsch and Steinmann (2000a). Nevertheless, it is not clear yet if they can be deduced from the principle of virtual action (5.14) in the sense of a finite element method.

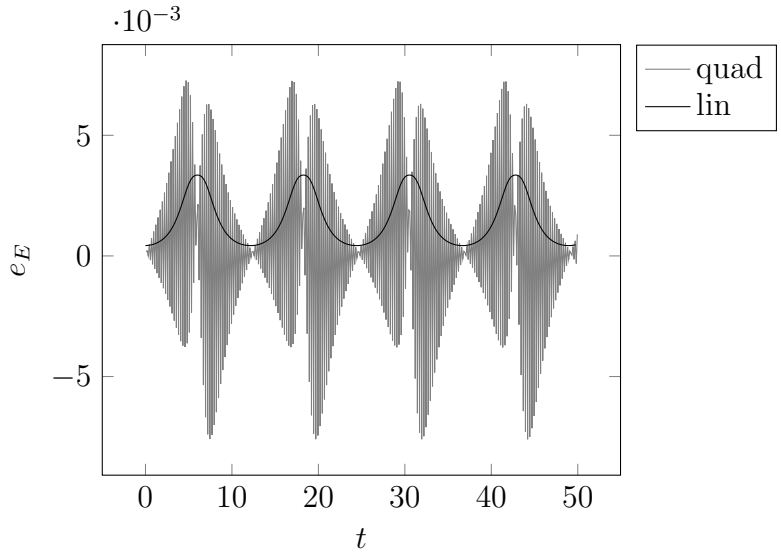


Figure 5.13: Convergence plot of the two-body problem defined by $m = 1$ and $GM = 1$, with initial conditions $\mathbf{q}(0) = (2, 0)^{\mathrm{T}}$ and $\dot{\mathbf{q}}(0) = (0, 0.6)^{\mathrm{T}}$. Single-field finite element approach with linear (lin) and quadratic (quad) elements, with integration time $T = 50$.

Chapter 6

Conclusions and Outlook

In this thesis a systematic approach is presented, which allows to derive different numerical schemes for the computation of the motion of mechanical systems in minimal coordinates. Starting from the principle of virtual action as an axiom of mechanics, single- and multi-field formulations of the principle of virtual action have been derived by imposing perfect motion constraints and using the Legendre–Fenchel transform. These formulations have been discretized using temporal finite elements. The choice of the shape function used for the time finite element discretization, together with the choice of the formulation of the principle of virtual action, results in different numerical schemes. Monolithic numerical schemes have been derived for all formulations. For the single-field formulation it is shown that there is an equivalent stepping scheme.

The main achievement of this thesis can be summarized as follows:

- The dynamical forces have been interpreted as internal forces in time direction. Relating them to the velocity by means of a linear constitutive law, leads to a version of the principle of virtual action, which can be used to derive the principle of virtual work and Lagrange's central equation.

- For finite degree of freedom systems, a formulation of the principle of virtual action has been derived, which depends on the generalized coordinates only. Moreover, Hamilton's law of varying action and the principle of Hamilton have been shown to be special cases of the principle of virtual action.

- Using the Legendre–Fenchel transform, multi-field formulations of the principle of virtual action for finite degree of freedom systems have been derived. Namely, the canonical formulation, whose independent fields are the generalized position and the generalized momentum, and the three-field formulations.

- Finite elements in time have been used to discretize the different formulations of the principle of virtual action. The performance of the resulting monolithic finite element formulations has been tested on three simple mechanical systems. It is shown that the monolithic approaches are computationally very expensive and lead to algorithms with poor convergence.

- It is shown that the monolithic single-field formulation is equivalent to a stepping scheme. The stepping schemes are found to be very performing in terms of numerical stability and computational cost. Moreover, as for all the finite element discretizations of the principle of virtual action, they have good numerical conservation properties.

- The equivalence of the stepping schemes derived by the finite element approach and the stepping schemes derived in the sense of discrete mechanics is shown.

The above insights make the time finite element methods very promising for the application in industrial design and development, but for a good applicability further research is required. The following open questions and tasks are identified:

- The theory has to be extended to describe mechanical systems with perfect holonomic and non-holonomic constraints.

- To describe frictional impacts, it has to be analyzed, how unilateral constraints with set-valued constitutive force laws can be treated using the principle of virtual action. Moreover, the finite element discretization of the principle of virtual action, and especially the set-valued force laws have to be addressed.

- The interaction of differential geometry, measure theory and functional analysis in all derivations presented in this thesis has to be analyzed. For the restriction of the virtual action to the virtual action of one element, integration by parts and the choice of a discontinuous virtual displacement field is required. It is not completely clear, what happens at the boundary of the element and where the boundary conditions arise from.

- It has to be understood, how the point wise Legendre–Fenchel transform, used for the derivation of the multi-field formulations, interacts with the motion constraints, which are used to arrive at finite element formulations by the choice of shape functions. Apparently it is not possible

to find stepping schemes, which are equivalent to the monolithic multi-field approach. This might be proven or disproved, if this interaction is understood.

- From a numerical point of view the performance of time finite element methods should be compared to the common integrators, the efficient implementation should be addressed and the conservation properties of the numerical schemes should be proven.

Appendix A

Miscellaneous

In this chapter we address some miscellaneous topics. In Section A.1, an example is used to visualize the claim of Chapter 4, which says that the velocity initial condition should be imposed by means of the initial impulsive force as this is the most natural way to do it. In Section A.2 the influence of the quadrature rule chosen to approximate the time integration in the finite element formulations is shown by an example. The possiblity to derive time finite element methods for the description of frictional impacts is discussed briefly in Section A.3. A reinterpretation of the generalized momentum together with an alternative derivation of the multi-field formulations is discussed in Section A.4. In Section A.5, the Verlet algorithm is derived using the time finite element stepping approach of Section 4.2.

A.1 On the Initial Condition

At the end of Section 4.1 two ways of treating the initial conditions are introduced, i.e. demanding the first element to have the same initial velocity as the analytical solution as in (4.18) or imposing the initial condition by the use of the initial impulsive force as in (4.19). From the treatment of the finite element discretization through a stepping approach, imposing the initial condition using the initial impulsive force appears to be the more natural choice, cf. end of Section 4.2. Figure A.1 shows two discretized motions of the mass-spring system described in Section 5.1, which are compared with the analytical solution of the harmonic oscillator. The discretized motion, where the initial condition is treated as in (4.18) has the same initial velocity as the analytical solution, therefore the first element is tangent to the analytical solution. As the discrete motion is piecewise linear, the discrete motion, which fulfills the initial condition on the velocity exactly, overshoots and therefore approximates the exact solution poorly. The exact motion is better approximated by the second dis-

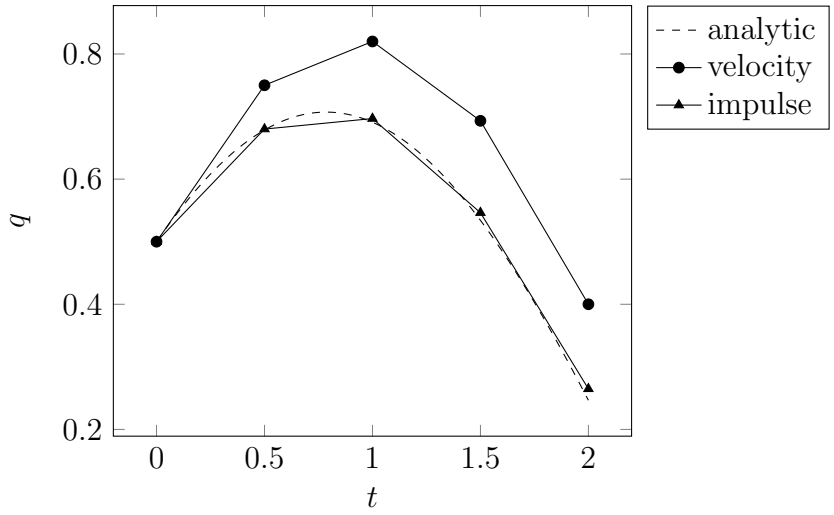


Figure A.1: Motion of the harmonic oscillator defined by $m = 1$ and $c = 1$ with initial conditions $q(0) = 0.5$ and $\dot{q}(0) = 0.5$ during the time interval $\mathcal{I} = [0, 2]$. Analytical solution (analytic), discrete solution with exact initial velocity (velocity) as in (4.18) and discrete solution with given initial impulsive force (impulse) as in (4.19). Both discretizations use $\Delta t = 0.5$.

crete motion, where the initial conditions are imposed by an initial impulsive force. This confirms that imposing the initial condition in such a way is the better and more natural choice. Note however that by augmenting the number of elements, both discrete motions converge to the exact motion.

A.2 On the Time Integration

In all the examples of Chapter 5 the time integrals are approximated by the trapezoidal rule. In this section we show for the simple pendulum of Section (5.2) that the choice of different quadrature rules has an impact on the error (5.3). Therefore take the principle of virtual action for the k^{th} element (4.35) and use linear shape functions (5.1). The variation of the kinetic energy in (4.35) is integrated exactly and by the fundamental lemma of calculus of variations leads to the stepping scheme defined by the equation

$$\frac{m}{\Delta t}\begin{pmatrix}-1 & 1\\ -1 & 1\end{pmatrix} + \Delta t \int_0^1 \begin{pmatrix}1-s\\ s\end{pmatrix} mgl \sin((1-s)z_1^k + sz_2^k) + \begin{pmatrix}-P_k\\ P_{k+1}\end{pmatrix} = 0\ , \quad \text{(A.1)}$$

which corresponds to (4.36). The integral of the external forces is approximated by the quadrature rule defined in Box 6. Figure A.2 shows the convergence of the finite element solution found by the stepping scheme (A.1) towards a very accurate reference solution of the simple pendulum in terms of

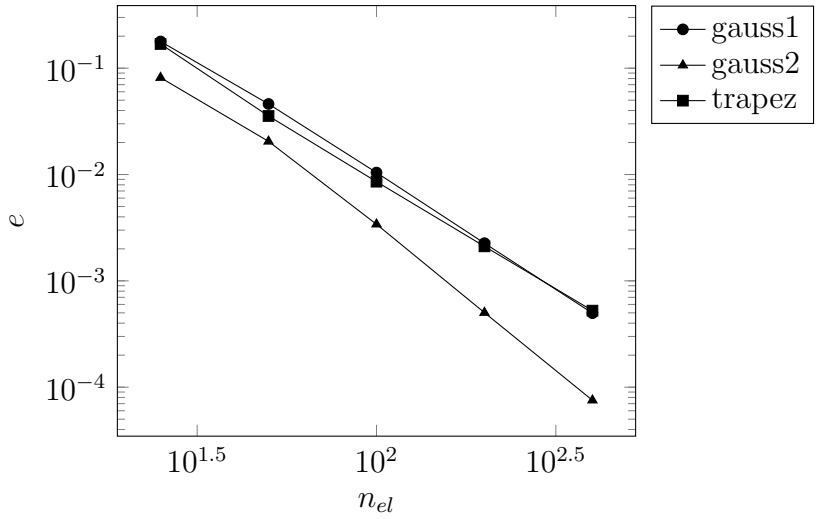


Figure A.2: Convergence towards reference solution of the simple pendulum defined by $m = 2$ and $l = 1.5$ with initial conditions $q(0) = \frac{2\pi}{5}$ and $\dot{q}(0) = 0.2$ during the time interval $\mathcal{I} = [0, 10]$. Single-field formulation with linear elements. The external forces are integrated using a one point gaussian (gauss1), two point gaussian (gauss2) and the trapezoidal (trapez) quadrature rule.

the error (5.3). Figure A.2 shows that the convergence is quadratic and that the two point gaussian quadrature rule leads to the most accurate solutions. This is not surprising, as the two point gaussian quadrature rule is the one that approximates the integral of the external forces best. Note however that for linear elements, the trapezoidal rule leads to an explicit stepping scheme, which is called the Verlet algorithm, cf. Section A.5. The other quadrature rules do not lead to explicit stepping schemes.

Box 6 Quadrature Rules

The integral of a function $\mathbf{g}(s)$ over the interval $[0, 1]$ can be approximated by a quadrature rule of the form

$$\int_0^1 \mathbf{g}(s)\,\mathrm{d}t \approx \sum_{i=1}^{n} w_i \mathbf{g}(s_i)\ . \tag{A.2}$$

There are different possibilities to choose the weights w_i, the number of quadrature points n and the quadrature points s_i.

	n	w_1	s_1	w_2	s_2
gaussian	1	1	1/2	-	-
gaussian	2	1/2	$(1-\sqrt{1/3})/2$	1/2	$(1+\sqrt{1/3})/2$
trapezoidal	2	1/2	0	1/2	1

A.3 On Impulsive Forces

In this section we show that the presence of an impulsive force $\overline{\mathbf{P}}$ acting on a mechanical system at a time instant $\bar{t} \in \mathrm{int}(\mathcal{I})$ of the considered time interval $\mathcal{I} = [0, T]$ results in an impact equation or equivalently in a jump condition for the velocities at $t = \bar{t}$.

The virtual action contribution $\delta\mathbf{q}(\bar{t})^{\mathrm{T}}\overline{\mathbf{P}}$ of the impulsive force is added to the principle of virtual action (2.29), which gives

$$\delta A = -\int_{\mathcal{I}} \left\{\delta T(\mathbf{q}, \dot{\mathbf{q}}, t) + \delta\mathbf{q}^{\mathrm{T}}\mathbf{f}\right\} \mathrm{d}t + \delta\mathbf{q}(\bar{t})^{\mathrm{T}}\overline{\mathbf{P}} + \delta\mathbf{q}^{\mathrm{T}}\mathbf{P}\big|_{\partial\mathcal{I}} = 0 \quad \forall\delta\mathbf{q}\,. \tag{A.3}$$

Applying integration by parts to (A.3) leads to the strong variational formulation of the principle of virtual action

$$\begin{aligned} \delta A = \int_{\mathcal{I}\setminus\{\bar{t}\}} \delta\mathbf{q}^{\mathrm{T}} \left(\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial T}{\partial\dot{\mathbf{q}}}\right)^{\mathrm{T}} - \left(\frac{\partial T}{\partial\mathbf{q}}\right)^{\mathrm{T}} - \mathbf{f}\right) \mathrm{d}t \\ + \delta\mathbf{q}(\bar{t})^{\mathrm{T}} \left(\overline{\mathbf{P}} + \left(\frac{\partial T^-}{\partial\dot{\mathbf{q}}}\right)^{\mathrm{T}} - \left(\frac{\partial T^+}{\partial\dot{\mathbf{q}}}\right)^{\mathrm{T}}\right)\Big|_{\partial\mathcal{I}} \\ + \delta\mathbf{q}^{\mathrm{T}} \left(\mathbf{P} - \left(\frac{\partial T}{\partial\dot{\mathbf{q}}}\right)^{\mathrm{T}}\right)\Big|_{\partial\mathcal{I}} = 0 \quad \forall\delta\mathbf{q}\,, \end{aligned} \tag{A.4}$$

where we have introduced the notation

$$\begin{aligned} \left(\frac{\partial T^-}{\partial\dot{\mathbf{q}}}\right)^{\mathrm{T}} &:= \lim_{t\uparrow\bar{t}} \left(\frac{\partial T}{\partial\dot{\mathbf{q}}}\right)^{\mathrm{T}} (\mathbf{q}(t), \dot{\mathbf{q}}(t), t) \\ \left(\frac{\partial T^+}{\partial\dot{\mathbf{q}}}\right)^{\mathrm{T}} &:= \lim_{t\downarrow\bar{t}} \left(\frac{\partial T}{\partial\dot{\mathbf{q}}}\right)^{\mathrm{T}} (\mathbf{q}(t), \dot{\mathbf{q}}(t), t) \end{aligned} \tag{A.5}$$

and have assumed that $\mathbf{q}(t)$ is continuous in $t = \bar{t}$. By the fundamental lemma of calculus of variations, the terms in brackets of (A.4) vanish pointwise. Therefore the equation of motion

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial T}{\partial\dot{\mathbf{q}}}\right)^{\mathrm{T}} - \left(\frac{\partial T}{\partial\mathbf{q}}\right)^{\mathrm{T}} = \mathbf{f} \tag{A.6}$$

holds for all time instants $t \in \mathcal{I}\setminus\{\bar{t}\}$, in which no impulsive force acts. For the time instant $t = \bar{t}$, in which the impulsive force acts, the equation of motion (A.6) is replaced by the impact equation

$$\left(\frac{\partial T^+}{\partial\dot{\mathbf{q}}}\right)^{\mathrm{T}} - \left(\frac{\partial T^-}{\partial\dot{\mathbf{q}}}\right)^{\mathrm{T}} = \overline{\mathbf{P}}\,. \tag{A.7}$$

The boundary terms give the boundary conditions

$$\begin{aligned} \left(\frac{\partial T}{\partial \dot{\mathbf{q}}}\right)^{\mathrm{T}} (\mathbf{q}(0), \dot{\mathbf{q}}(0), 0) &= \mathbf{P}_0 \\ \left(\frac{\partial T}{\partial \dot{\mathbf{q}}}\right)^{\mathrm{T}} (\mathbf{q}(T), \dot{\mathbf{q}}(T), T) &= \mathbf{P}_T \ , \end{aligned} \tag{A.8}$$

which are the same as (2.35). The equation of motion (A.6) and the impact equation (A.8) are used together with a contact model and impact constitutive equations to model frictional impacts between rigid bodies, cf. Glocker (2006). Using a finite element discretization in the sense of Chapter 4, numerical schemes for the simulation of rigid multi body systems with frictional impacts can be derived from (A.3).

A.4 Multi-field Formulations Revisited

Instead of using the Legendre–Fenchel transform to derive the $(\mathbf{q}, \mathbf{u}, \mathbf{p})$- and canonical formulation of the principle of virtual action, as described in Chapter 3, they can be derived using a Lagrangian multiplier approach. In this framework the generalized velocity $\dot{\mathbf{q}}$ in the kinetic energy of the principle of virtual action (2.29) is replaced by the independent generalized velocity $\mathbf{u}$ and the equality $\mathbf{u} = \dot{\mathbf{q}}$ is enforced by the Lagrangian multiplier $\mathbf{p}$, which is the generalized momentum. This procedure yields the $(\mathbf{q}, \mathbf{u}, \mathbf{p})$-formulation of the principle of virtual action (3.26), which is restated here

$$\delta A = -\int_{\mathcal{I}} \left\{ \delta \left(T(\mathbf{q}, \mathbf{u}, t) + \mathbf{p}^{\mathrm{T}} (\dot{\mathbf{q}} - \mathbf{u}) \right) + \delta \mathbf{q}^{\mathrm{T}} \mathbf{f} \right\} \mathrm{d}t + \delta \mathbf{q}^{\mathrm{T}} \mathbf{P} \big|_{\partial \mathcal{I}} = 0 \ . \tag{A.9}$$

To arrive at the canonical formulation the dependence of (A.9) on $\mathbf{u}$ has to be eliminated. Looking at the strong variational form (3.27) of the $(\mathbf{q}, \mathbf{u}, \mathbf{p})$-formulation of the principle of virtual action, it is clear that the generalized velocity $\mathbf{u}$ can be eliminated by the choice

$$\mathbf{u} = \overline{\mathbf{u}}(\mathbf{q}, \mathbf{p}, t) \quad \text{s.t.} \quad \mathbf{p} = \left(\frac{\partial T}{\partial \mathbf{u}}\right)^{\mathrm{T}} (\mathbf{q}, \overline{\mathbf{u}}, t) \ . \tag{A.10}$$

Due to convexity of the kinetic energy (2.28) it is always possible to express $\overline{\mathbf{u}}$ in dependence of $(\mathbf{q}, \mathbf{p}, t)$ explicitly. Using the definition of the conjugate kinetic energy in the form

$$T^*(\mathbf{q}, \mathbf{p}, t) = \mathbf{p}^{\mathrm{T}} \overline{\mathbf{u}} - T(\mathbf{q}, \overline{\mathbf{u}}, t) \quad \text{s.t.} \quad \mathbf{p} = \left(\frac{\partial T}{\partial \mathbf{u}}\right)^{\mathrm{T}} (\mathbf{q}, \overline{\mathbf{u}}, t) \ , \tag{A.11}$$

which is equivalent to the definition given in (3.11), and eliminating $\mathbf{u}$ from (A.9) by means of (A.10) gives the canonical formulation of the principle of virtual action

$$\delta A = -\int_{\mathcal{I}} \left\{ \delta \left(\dot{\mathbf{q}}^{\mathrm{T}} \mathbf{p} - T^*(\mathbf{q}, \mathbf{p}, t) \right) + \delta \mathbf{q}^{\mathrm{T}} \mathbf{f} \right\} \mathrm{d}t + \delta \mathbf{q}^{\mathrm{T}} \mathbf{P} \big|_{\partial \mathcal{I}} = 0 \; \forall \delta \mathbf{q}, \forall \delta \mathbf{p} \,. \quad \text{(A.12)}$$

This derivation allows to interpret the generalized momentum as constraint force which enforces the velocity constraint $\mathbf{u} = \dot{\mathbf{q}}$, but this interpretation is not very satisfying as in the canonical formalism $\mathbf{p}$ appears but $\mathbf{u}$ does not. This indicates that the role of $\mathbf{p}$ is still not clear. Moreover, this derivation, proposed by Lanczos (1970), does not allow the derivation of the generalized $(\mathbf{q}, \mathbf{u}, \mathbf{p})$-formulation presented in Section 3.4.

A.5 The Verlet Algorithm

Let the motion of the mechanical system $\mathcal{S}$ be described by the generalized coordinates $\mathbf{q}(t)$ and a constant mass matrix $\mathbf{M}$. Then by (2.28) the kinetic energy of the system is

$$T(\dot{\mathbf{q}}) = \frac{1}{2} \mathbf{q}^{\mathrm{T}} \mathbf{M} \mathbf{q} \,. \quad \text{(A.13)}$$

The motion of the system $\mathcal{S}$ during the time interval $\mathcal{I} = [0, T]$ is described by the principle of virtual action

$$\delta A = -\int_{\mathcal{I}} \left\{ \delta \dot{\mathbf{q}}^{\mathrm{T}} \mathbf{M} \dot{\mathbf{q}} + \delta \mathbf{q}^{\mathrm{T}} \mathbf{f}(\mathbf{q}(t)) \right\} \mathrm{d}t + \delta \mathbf{q}^{\mathrm{T}} \mathbf{P} \big|_{\partial \mathcal{I}} = 0 \quad \forall \delta \mathbf{q} \,. \quad \text{(A.14)}$$

Introducing the n_N temporal nodes $(t_1, \ldots, t_{n_N})$ that subdivide the time interval $\mathcal{I} = [0, T]$ into the n_{el} elements $\Omega^e = [t_e, t_{e+1}]$, as done in Section 4.2 the principle of virtual action for the k^{th} element (4.31) is

$$-\int_{\Omega^k} \left\{ \delta \dot{\mathbf{q}}^{k\mathrm{T}} \mathbf{M} \dot{\mathbf{q}}^k + \delta \mathbf{q}^{k\mathrm{T}} \mathbf{f}(\mathbf{q}^k(t)) \right\} \mathrm{d}t - \delta \mathbf{q}(t_k)^{\mathrm{T}} \mathbf{P}_k + \delta \mathbf{q}(t_{k+1})^{\mathrm{T}} \mathbf{P}_{k+1} = 0 \quad \text{(A.15)}$$

for all $\delta \mathbf{q}^k$.Restricting the motion $\mathbf{q}^k(t)$ of the element to the motion described by the linear polynomial

$$\mathbf{q}^k(t) = (1 - s(t)) \mathbf{z}^k + s(t) \mathbf{z}^{k+1}) \,, \quad \text{(A.16)}$$

where the element coordinate $s(t)$ is defined as in (4.2), and the notation $\mathbf{z}^k = \mathbf{q}(t_k)$ has been introduced. The motion of the k^{th} element, which is

restricted to the linear polynomial (A.16) is described by the principle of virtual action (4.35), i.e.

$$\begin{aligned}\delta A^k = &-\int_{\Omega^k} \frac{1}{\Delta t^2}(-\delta\mathbf{z}^{k\mathrm{T}} + \delta\mathbf{z}^{k+1\mathrm{T}})\mathbf{M}(-\mathbf{z}^k + \mathbf{z}^{k+1})\mathrm{d}t \\ &-\int_{\Omega^k}((1-s(t))\delta\mathbf{z}^{k\mathrm{T}} + s(t)\delta\mathbf{z}^{k+1\mathrm{T}}))\mathbf{f}((1-s(t))\mathbf{z}^k + s(t)\mathbf{z}^{k+1}))\mathrm{d}t \\ &- \delta\mathbf{z}^{k\mathrm{T}}\mathbf{P}_k + \delta\mathbf{z}^{k+1\mathrm{T}}\mathbf{P}_{k+1}\ . \end{aligned} \tag{A.17}$$

Approximating the time integration in (A.17) by the trapezoidal rule (A.2) together with the fundamental lemma of calculus of variations leads to the stepping equations

$$\begin{aligned}&\frac{1}{\Delta t}\mathbf{M}(\mathbf{z}^k - \mathbf{z}^{k+1}) + \frac{1}{2}\Delta t\ \mathbf{f}(\mathbf{z}^k) + \mathbf{P}_k = 0 \\ &\frac{1}{\Delta t}\mathbf{M}(-\mathbf{z}^k + \mathbf{z}^{k+1}) + \frac{1}{2}\Delta t\ \mathbf{f}(\mathbf{z}^{k+1}) - \mathbf{P}_{k+1} = 0\ .\end{aligned} \tag{A.18}$$

which correspond to the stepping equations (4.43). For $k > 1$ the impulsive force $\mathbf{P}_k$ can be expressed in terms of the motion of the previous element, which by the second equation of (A.18) is

$$\mathbf{P}_k = \frac{1}{\Delta t}\mathbf{M}(-\mathbf{z}^{k-1} + \mathbf{z}^k) + \frac{1}{2}\Delta t\ \mathbf{f}(\mathbf{z}^k) \tag{A.19}$$

and can be inserted into the first equation of (A.18) yielding

$$\frac{1}{\Delta t}\mathbf{M}(-\mathbf{z}^{k+1} + 2\mathbf{z}^k - \mathbf{z}^{k-1}) + \Delta t\ \mathbf{f}(\mathbf{z}^k) = 0\ , \tag{A.20}$$

the discrete Euler–Lagrange equations (4.46). Rearranging (A.20) leads to the stepping equation

$$\mathbf{z}^{k+1} = 2\mathbf{z}^k - \mathbf{z}^{k-1} + \Delta t^2\ \mathbf{M}^{-1}\mathbf{f}(\mathbf{z}^k)\ , \tag{A.21}$$

which is often called the Verlet algorithm, cf. Verlet (1967). This stepping scheme corresponds to the Newmark β-method with the parameter choice $\beta = 0$ and $\gamma = 1/2$. Note that the Verlet algorithm is explicit because the trapezoidal rule was chosen for the time integration in (A.18). Equation (A.20) can be derived by approximating the time derivative of the equation of motion (2.34) of the system $\mathcal{S}$, which is

$$\mathbf{M}\ddot{\mathbf{q}}(t) = \mathbf{f}(\mathbf{q}(t))\ , \tag{A.22}$$

by means of a central difference as

$$\mathbf{M}\frac{1}{\Delta t^2}\left(\mathbf{q}(t_{k+1}) - 2\mathbf{q}(t_k) + \mathbf{q}(t_{k-1})\right) = \mathbf{f}(\mathbf{q}(t_k)) \tag{A.23}$$

at $t = t_k$, which is equivalent to (A.20). The derivation of the Verlet algorithm using the central difference does not show the variational nature of the algorithm. Therefore, all the convenient properties of the algorithm, such as the discrete energy conservation, have to be shown separately. In the framework of variational integrators, the conservation properties can be shown generally, cf. Marsden and West (2001). For further reading on the central difference method and the Newmark β-method we refer to Belytschko et al. (2013) Chap. 6.

Bibliography

H. Adélaïde, C. Bohatier, and F. Jourdan. New Results on Mesh Adaptation in Space-Time Finite Element Method. In *ASME 2002 Engineering Technology Conference on Energy*, pages 963–972. American Society of Mechanical Engineers, 2002.

L. Adélaïde, F. Jourdan, and C. Bohatier. Méthodes des éléments finis espace-temps et remaillage. *Revue Européenne des Eléments*, 12(4):427–458, 2003.

O. Agrawal and S. Saigal. A novel, computationally efficient, approach for Hamilton's law of varying action. *International journal of mechanical sciences*, 29(4):285–292, 1987.

D. Aharoni and P. Bar-Yoseph. Mixed finite element formulations in the time domain for solution of dynamic problems. *Computational mechanics*, 9(5): 359–374, 1992.

J. Argyris and D. Scharpf. Finite elements in time and space. *Nuclear Engineering and Design*, 10(4):456–464, 1969.

A. Atilgan, D. Hodges, M. Özbek, and W. Zhou. Space-time mixed finite elements for rods. *Journal of sound and vibration*, 192(3):731–739, 1996.

C. Bailey. Hamilton, Ritz, and elastodynamics. *Journal of Applied Mechanics*, 43(4):684–688, 1976a.

C. Bailey. The Galerkin formulation and the Hamilton-Ritz formulation: a comparison. *Acta Mechanica*, 36(1-2):63–70, 1980.

C. Bailey. Application of Hamilton's law to forced, damped, stationary systems. *Journal of Sound and Vibration*, 75(1):117–126, 1981.

C. D. Bailey. Application of Hamilton's law of varying action. *AIAA Journal*, 13(9):1154–1157, 1975.

C. D. Bailey. The method of Ritz applied to the equation of Hamilton. *Computer Methods in Applied Mechanics and Engineering*, 7(2):235–247, 1976b.

C. I. Bajer. Triangular and tetrahedral space-time finite elements in vibration analysis. *International journal for numerical methods in engineering*, 23(11): 2031–2048, 1986.

C. I. Bajer and B. Dyniewicz. Space-time approach to numerical analysis of a string with a moving mass. *International journal for numerical methods in engineering*, 76(10):1528–1543, 2008.

C. I. Bajer and B. Dyniewicz. Space-time finite element method. In *Numerical Analysis of Vibrations of Structures under Moving Inertial Load*, pages 123–180. Springer, 2012.

M. Baruch and R. Riff. Hamilton's principle, Hamilton's law-6 to the n power correct formulations. *AIAA Journal*, 20(5):687–692, 1982.

T. Belytschko, W. K. Liu, B. Moran, and K. Elkhodary. *Nonlinear finite elements for continua and structures*. John Wiley & Sons, 2013.

P. Betsch and P. Steinmann. Conservation properties of a time FE method. Part I: time-stepping schemes for N-body problems. *International Journal for Numerical Methods in Engineering*, 49(5):599–638, 2000a.

P. Betsch and P. Steinmann. Inherently energy conserving time finite elements for classical mechanics. *Journal of Computational Physics*, 160(1):88–116, 2000b.

P. Betsch, C. Hesch, N. Sänger, and S. Uhlar. Variational integrators and energy-momentum schemes for flexible multibody dynamics. *Journal of Computational and Nonlinear Dynamics*, 5(3):031001, 2010.

M. Borri. Helicopter rotor dynamics by finite element time approximation. *Computers & mathematics with applications*, 12(1):149–160, 1986.

M. Borri and C. Bottasso. A general framework for interpreting time finite element formulations. *Computational Mechanics*, 13(3):133–142, 1993.

M. Borri, G. Ghiringhelli, M. Lanz, P. Mantegazza, and T. Merlini. Dynamic response of mechanical systems by a weak Hamiltonian formulation. *Computers & Structures*, 20(1):495–508, 1985.

M. Borri, F. Mello, and S. Atluri. Primal and mixed forms of Hamiltons's principle for constrained rigid body systems: numerical studies. *Computational Mechanics*, 7(3):205–220, 1991.

M. Borri, C. Bottasso, and P. Mantegazza. Basic features of the time finite element approach for dynamics. *Meccanica*, 27(2):119–130, 1992.

C. L. Bottasso. A new look at finite elements in time: a variational interpretation of Runge-Kutta methods. *Applied Numerical Mathematics*, 25(4): 355–368, 1997.

J. A. Cadzow. Discrete calculus of variations. *International Journal of Control*, 11(3):393–407, 1970.

A. Cella, M. Lucchesi, and G. Pasquinelli. Space–time elements for the shock wave propagation problem. *International Journal for Numerical Methods in Engineering*, 15(10):1475–1488, 1980.

J. Cortés. Energy conserving nonholonomic integrators. *arXiv preprint math/0209314*, 2002.

J. Cortés and S. Martínez. Non-holonomic integrators. *Nonlinearity*, 14(5): 1365, 2001.

M. De León and D. M. de Diego. Variational integrators and time-dependent Lagrangian systems. *Reports on Mathematical Physics*, 49(2):183–192, 2002.

S. R. Eugster. *On the Foundations of Continuum Mechanics and its Application to Beam Theories*. PhD thesis, ETH Zurich, 2014.

S. R. Eugster. *Geometric Continuum Mechanics and Induced Beam Theories*. Springer, 2015.

R. Fetecau, J. E. Marsden, and M. West. Variational multisymplectic formulations of nonsmooth continuum mechanics. In *Perspectives and Problems in Nolinear Science*, pages 229–261. Springer, 2003a.

R. C. Fetecau, J. E. Marsden, M. Ortiz, and M. West. Nonsmooth Lagrangian mechanics and variational collision integrators. *SIAM Journal on Applied Dynamical Systems*, 2(3):381–416, 2003b.

I. Fried. Finite-element analysis of time-dependent phenomena. *AIAA Journal*, 7(6):1170–1173, 1969.

S. Gellin and J. M. Pitarresi. Nonlinear analysis using temporal finite elements. *Engineering analysis*, 5(3):126–132, 1988.

R. E. Gillilan and K. R. Wilson. Shadowing, rare events, and rubber bands. A variational Verlet algorithm for molecular dynamics. *The Journal of chemical physics*, 97(3):1757–1772, 1992.

C. Glocker. *An introduction to impacts*. Springer, 2006.

G. Hamel. *Theoretische Mechanik: Eine einheitliche Einführung in die gesamte Mechanik*. Springer, 1967.

W. R. Hamilton. On a general method in dynamics; by which the study of the motions of all free systems of attracting or repelling points is reduced to the search and differentiation of one central relation, or characteristic function. *Philosophical transactions of the Royal Society of London*, 124: 247–308, 1834.

W. R. Hamilton. Second essay on a general method in dynamics. *Philosophical Transactions of the Royal Society of London*, 125:95–144, 1835.

F. Hartmann and C. Katz. *Structural analysis with finite elements*. Springer Science & Business Media, 2013.

D. L. Hitzl. Implementing Hamilton's law of varying action with shifted Legendre polynomials. *Journal of Computational Physics*, 38(2):185–211, 1980.

D. L. Hitzl and D. A. Levinson. Application of Hamilton's law of varying action to the restricted three-body problem. *Celestial mechanics*, 22(3):255–266, 1980.

H.-C. Hu. On some variational principles in the theory of elasticity and the theory of plasticity. *Scientia Sinica*, 4(1):33–54, 1955.

T. J. Hughes and G. M. Hulbert. Space-time finite element methods for elastodynamics: formulations and error estimates. *Computer methods in applied mechanics and engineering*, 66(3):339–363, 1988.

T. J. Hughes, L. P. Franca, and G. M. Hulbert. A new finite element formulation for computational fluid dynamics: VIII. The Galerkin/least-squares method for advective-diffusive equations. *Computer Methods in Applied Mechanics and Engineering*, 73(2):173–189, 1989.

T. J. Hughes, J. A. Cottrell, and Y. Bazilevs. Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement. *Computer methods in applied mechanics and engineering*, 194(39):4135–4195, 2005.

A. P. Izadpanah. *p-version finite elements for the space-time domain with application to Floquet theory*. PhD thesis, Georgia Institute of Technology, 1986.

E. R. Johnson and T. D. Murphey. Scalable variational integrators for constrained mechanical systems in generalized coordinates. *Robotics, IEEE Transactions on*, 25(6):1249–1261, 2009.

C. Kane. *Variational integrators and the Newmark algorithm for conservative and dissipative mechanical systems*. PhD thesis, caltech, 1999.

C. Kane, J. E. Marsden, and M. Ortiz. Symplectic-energy-momentum preserving variational integrators. *Journal of mathematical physics*, 40(7):3353–3371, 1999.

L. Kharevych, W. Yang, Y. Tong, E. Kanso, J. E. Marsden, P. Schröder, and M. Desbrun. Geometric, variational integrators for computer animation. In *Proceedings of the 2006 ACM SIGGRAPH/Eurographics symposium on Computer animation*, pages 43–51. Eurographics Association, 2006.

J. Kujawski and C. S. Desai. Generalized time finite element algorithm for nonlinear dynamic problems. *Engineering Computations*, 1(3):247–251, 1984.

C. Lacoursière. *Ghosts and machines: regularized variational methods for interactive simulations of multibodies with dry frictional contacts*. PhD thesis, Umeå University, 2007.

C. Lanczos. *The variational principles of mechanics*, volume 4. Courier Corporation, 1970.

T. Lee. Difference equations and conservation laws. *Journal of Statistical Physics*, 46(5):843–860, 1987.

T.-D. Lee. Can time be a discrete dynamical variable? *Physics Letters B*, 122 (3):217–220, 1983.

M. Leok and J. Zhang. Discrete Hamiltonian variational integrators. *IMA Journal of Numerical Analysis*, page drq027, 2011.

A. Lew. *Variational time integrators in computational solid mechanics*. PhD thesis, California Institute of Technology, 2003.

A. Lew, J. E. Marsden, M. Ortiz, and M. West. Asynchronous variational integrators. *Archive for Rational Mechanics and Analysis*, 167(2):85–146, 2003.

A. Lew, J. E. Marsden, M. Ortiz, and M. West. An overview of variational integrators. In *Finite Element Methods: 1970's and Beyond*. International Center for Numerical Methods in Engineering (CIMNE), 2004.

S. Leyendecker, J. E. Marsden, and M. Ortiz. Variational integrators for constrained dynamical systems. *ZAMM-Journal of Applied Mathematics and Mechanics/Zeitschrift für Angewandte Mathematik und Mechanik*, 88 (9):677–708, 2008.

J. Marsden and J. Wendlandt. Mechanical Systems with Symmetry, Variational Principles, and Integration Algorithms. In M. Alber, B. Hu, and J. Rosenthal, editors, *Current and Future Directions in Applied Mathematics*, pages 219–261. Birkhäuser Boston, 1997. ISBN 978-1-4612-7380-6.

J. E. Marsden and M. West. Discrete mechanics and variational integrators. *Acta Numerica 2001*, 10:357–514, 2001.

J. E. Marsden, G. W. Patrick, and S. Shkoller. Multisymplectic geometry, variational integrators, and nonlinear PDEs. *Communications in Mathematical Physics*, 199(2):351–395, 1998.

O. Papes. *Nonlinear continuum mechanics in modern engineering applications*. PhD thesis, Diss., Eidgenössische Technische Hochschule ETH Zürich, 2011.

J. Pitarresi and G. Manolis. The temporal finite element method in structural dynamics. *Computers & structures*, 41(4):647–655, 1991.

E. Reissner. On a variational theorem for finite elastic deformations. *Journal of Mathematics and Physics*, 32:129–135, 1953.

R. T. Rockafellar and R. J.-B. Wets. *Variational analysis*, volume 317. Springer Science & Business Media, 2009.

F. Shakib and T. J. Hughes. A new finite element formulation for computational fluid dynamics: IX. Fourier analysis of space-time Galerkin/least-squares algorithms. *Computer Methods in Applied Mechanics and Engineering*, 87(1):35–58, 1991.

Y. Shibberu. Time-discretization of Hamiltonian dynamical systems. Technical report, Rose-Hulman Institute of Technology, 1993.

T. Simkins. Unconstrained variational statements for initial and boundary-value problems. *AIAA Journal*, 16(6):559–563, 1978.

T. Simkins. Finite elements for initial value problems in dynamics. *AIAA Journal*, 19(10):1357–1362, 1981.

L. Verlet. Computer "experiments" on classical fluids. I. Thermodynamical properties of Lennard-Jones molecules. *Physical review*, 159(1):98, 1967.

A. P. Veselov. Integrable discrete-time systems and difference operators. *Functional Analysis and its Applications*, 22(2):83–93, 1988.

K. Washizu. On the variational principles of elasticity and plasticity. Technical report, DTIC Document, 1955.

J. M. Wendlandt and J. E. Marsden. Mechanical integrators derived from a discrete variational principle. *Physica D: Nonlinear Phenomena*, 106(3): 223–246, 1997.

M. West. *Variational integrators*. PhD thesis, California Institute of Technology, 2004.

D. I. S. Wolff. *Asynchronous variational integration of structural collision dynamics*. PhD thesis, Technische Universität Wien, 2011.

J. Wu. Solutions to initial value problems by use of finite elements - unconstrained variational formulationsb. *Journal of Sound and Vibration*, 53(3): 341–356, 1977.

J. Wu and T. Simkins. A numerical comparison between two unconstrained variational formulations. *Journal of Sound and Vibration*, 72(4):491–505, 1980.

Eigenständigkeitserklärung

Ich erkläre mit meiner Unterschrift, die Prüfungsordnung meines Studiengangs zur Kenntnis genommen, die vorliegende Arbeit selbständig verfasst und die im betroffenen Fachgebiet üblichen Zitiervorschriften eingehalten zu haben. Weiter versichere ich, dass das elektronische Exemplar mit den eingereichten gedruckten Exemplaren übereinstimmt.

Prüfungsordnungen:
`www.uni-stuttgart.de/studieren/studium/admin/po/`

Ort, Datum Unterschrift