Variational Methods for Nonsmooth Mechanics

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Abstract

In this thesis we investigate nonsmooth classical and continuum mechanics and its discretizations by means of variational numerical and geometric methods.

The theory of smooth Lagrangian mechanics is extended to a nonsmooth context appropriate for collisions and it is shown in what sense the system is symplectic and satisfies a Noether-style momentum conservation theorem.

Next, we develop the foundations of a multisymplectic treatment of nonsmooth classical and continuum mechanics. This work may be regarded as a PDE generalization of the previous formulation of a variational approach to collision problems. The multisymplectic formulation includes a wide collection of nonsmooth dynamical models such as rigid-body collisions, material interfaces, elastic collisions, fluid-solid interactions and lays the groundwork for a treatment of shocks.

Discretizations of this nonsmooth mechanics are developed by using the methodology of variational discrete mechanics. This leads to variational integrators which are symplectic-momentum preserving and are consistent with the jump conditions given in the continuous theory. Specific examples of these methods are tested numerically and the longtime stable energy behavior typical of variational methods is demonstrated.

Contents

Chapter 1

Introduction

We shall begin with a survey of some history and literature to put our own work into context. The literature and history is of course quite complex with many points of view, so we focus on selected highlights only.

History and Literature: Theory. The problem of collisions has been extensively treated in the literature since the early days of mechanics. More recently, much work has been done on the rigorous mathematical foundation of impact problems, in particular by generalizing Newton's law to include forces which are measure-valued and hence can include impulses at the point of impact. The contact dynamics is thus governed by a *measure differential inclusion*, a general formulation that can directly incorporate impulsive forces and nonsmooth solutions. In this context, a measure differential inclusion has the form

$$\frac{dv}{dt} \in F(t,x), \ \frac{dx}{dt} = g(t,x,v),$$

where $v(t)$ and $x(t)$ denote the velocity and the position, F is a set-valued function and $v(\cdot)$ is only required to have bounded variation.

The extension of the concept of a differential equation to that of a *differential inclusion* was first considered by Filippov [1964, 1967, 1988]. These works provide a deep study of ordinary differential equations with a discontinuous right-hand side, but the fact that solutions are required to be continuous in the phase space makes the theory inapplicable to collisions. Measure differential inclusions can be found in different contexts in the work of Schatzman [1973, 1978], and the use of this concept to rigid-body dynamics was further developed in the work of Moreau [1986, 1988], where the (unilateral) contact between rigid

bodies received a formulation (called by the author a *sweeping process*) that combines differential inclusions with convex analysis. Since then, an extensive literature has been devoted to the theoretical and numerical study of nonsmooth dynamics within the mathematical framework of measure differential inclusions.

Substantial progress has been made in the last two decades on the existence and uniqueness theory for the generalized solutions of rigid-body dynamics. The first rigorous results in this area were produced by Monteiro Marques [1985] for the case of an inelastic collision with a single convex constraint. Further results generalized the existence theory to more general contacts in Paoli and Schatzman [1993a], to more general (nonconvex, but of class C^1) constraints in Monteiro Marques [1993] or even to a less regular constraint for an arbitrary frictionless impact in Mabrouk [1998]. The recent works of Stewart [1998, 2000] consider the impact dynamics with friction and give a rigorous mathematical solution to the famous problem of Painlevé.

In the same elegant framework of differential inclusions, but oriented towards the control and stability of nonsmooth dynamical systems, we mention the works of Brogliato [1996, 2001] and Brogliato et al. [1997].

History and Literature: Computations. The measure differential inclusion has also been proved to be an excellent mathematical foundation for the study of numerical methods for discontinuous ODEs. It is not our scope to give a complete account of these methods, but we refer the reader to the excellent overviews of numerical methods for differential inclusions by Dontchev and Lempio [1992] and Lempio and Veliov [1998]. In particular, such numerical approaches have been pursued to develop efficient numerical methods for rigid-body dynamics in the sweeping process formalism in Moreau [1986, 1999], Paoli and Schatzman [1999], and Stewart [2000].

Various other numerical methods for rigid-body systems have been studied extensively in the engineering and mathematics literature. We refer to the excellent book of Pfeiffer and Glocker [1996] for a comprehensive account of some of these methods. We particularly remark the approach that reduces the contact to a *complementarity problem*, concept frequently used in constrained optimization, to decide at each step which constraints are active.

However, most existing practical codes are based on smoothing techniques, a class of

methods that use a penalty formulation to regularize the problem. This approach relies on the definition of a proper gap function as a means to detect and penalize the interpenetration; see, for example, Simo et al. [1985], Carpenter et al. [1991], Wriggers and Zavarise [1993], and Taylor and Papadopoulos [1993]. An obvious weakness of the penalty methods is that they cannot handle collisions of irregularly shaped bodies (bodies with corners), where neither normals nor gap functions can be defined. An elegant solution to this problem is offered by the *nonsmooth analysis* approach from Kane et al. [1999b], where new robust contact algorithms are derived using the powerful tools of nonsmooth calculus (see Clarke [1983]).

An important issue in contact dynamics is how to formulate physically correct friction models and an extensive body of literature has addressed this problem. Frictional effects are generally accounted for by introducing a friction law (Coulomb's law is an example) which relates the sliding velocity to the contact forces. An alternative approach uses the *maximum dissipation principle* where the friction force c_f is required to maximize the rate of energy dissipation $-c_f^T v_{rel}$, where v_{rel} is the relative velocity at the contact, out of all possible friction forces allowed by a given contact force c_n. However, the correct modeling of friction still has many open questions which generates controversy in various engineering and mathematical communities. All the various numerical methods for contact that we mentioned above have introduced friction in the dynamics and we refer to Anitescu et al. [1999] and Moreau [1988] for measure differential inclusion methods, and to Jean [1988], Lee and Oden [1993], Peric and Owen [1992], Pires and Oden [1983], White and Oden [1989], Wriggers et al. [1990], Pfeiffer [1999], Armero and Petöcz [1999], for the complementarity and gap function formulation and to Pandolfi et al. [2002] for the nonsmooth analysis approach.

Variational Methodology. Our approach, in contrast, is based on a variational methodology that goes back to Young [1969], which allows the direct handling of the nonsmooth nature of contact problems. We also use a variational approach to develop numerical integrators for nonsmooth rigid-body dynamics. The procedure is based on a discrete Lagrangian principle and automatically generates a symplectic-momentum preserving integrator. Near impact, we introduce a collision point and a collision time and solve for them using a variational method.

Variational integrators are known to have remarkable near energy preserving properties and we will recover this excellent energy behavior even in the nonsmooth case. We want to emphasize that the variational point of view is not confined to conservative systems, but also applies to forced and dissipative systems as demonstrated in Kane et al. [2000]. In future works we will investigate how forces and friction can be added to our collision algorithm and also how to incorporate other dissipative effects (inelastic collisions).

Issues Addressed in This Thesis. We first show that by introducing a space of configuration trajectories extended by introducing curve parameterizations as variables, that the traditional approach to the calculus of variations can be applied. Moreover, the formulation in the extended setting enables us to address and give a rigorous interpretations to the sense in which the flow map of a mechanical system subjected to dissipationless impact dynamics is symplectic. The nonautonomous variational approach also leads to Weierstrass-Erdmann type conditions for impact, in terms of energy and momentum conservation at the contact point (see Hestenes [1966] and Young [1969]).

A part of this thesis develops the foundations of a multisymplectic treatment of nonsmooth classical and continuum mechanics. The formulation includes a wide collection of nonsmooth dynamical models: rigid-body collisions, material interfaces, elastic collisions, shocks and fluid-solid interactions. From a computational viewpoint, the multisymplectic-momentum integrators for variational PDE's, as formulated in Marsden et al. [1998], have already proved of value in discrete mechanics, particularly in the development of multisymplectic spatially and temporally adaptive algorithms (asynchronous variational integrators). From this perspective, the formalism developed in this work sets the stage for the development of variational multisymplectic algorithms in the nonsmooth context.

The variational approach to nonsmooth multisymplectic field theory gives the existence of the fundamental geometric structures as well as the jump in the Cartan form (the multisymplectic analogue of the Lagrangian $1-$form from particle mechanics). We reconsider the need for both *vertical* and *horizontal* variations in the nonsmooth case and give an alternative motivation for such a generalization. Moreover, we show how to apply the formalism to various multisymplectic models of continuum mechanics such as free surfaces in fluids, fluid-solid interactions, elastic collisions and also lay the groundwork for a treatment of shocks.

On the discrete side, the variational formalism leads to symplectic-momentum preserving integrators that are consistent with the jump conditions and the continuous theory.

The theory of geometric integration (see, for example, Sanz-Serna and Calvo [1994] and Hairer and Wanner [1996]) is typically concerned with smooth Hamiltonian or Lagrangian systems posed on smooth spaces. These techniques do not immediately apply to nonsmooth settings, and naive applications can result in extremely bad behavior, as demonstrated in Stewart [2000].

Our methods answer an important question posed by Stewart [2000], *how can geometric integrators be formulated and implemented for collision problems?* In fact, the algorithms developed in this work show how a symplectic method can be constructed for nonsmooth systems so that it retains the good behavior normally associated with symplectic methods.

Some existing work has been done on extensions of geometric integration to collision problems. In particular, Barth et al. [1999] have constructed time-symmetric methods for contact and Houndonougbo et al. [2000] (see also Houndonougbo and Laird [2002]) have developed methods for impacts of hard spheres. To date there have been no symplectic methods for collisions presented, in part due to difficulties with understanding symplecticity in a nonsmooth setting. However, the variational formulation of continuous time nonsmooth systems that we develop here is a key which allows us to understand the geometric structure of the problem, both before and after discretization. Our methods can be considered extensions of the large body of work on geometric integration of ODEs (see, for example, Hairer et al. [1993], Hairer and Wanner [1996], Iserles et al. [2000], Leimkuhler and Reich [2001], as well as Marsden and West [2001]).

We caution that the algorithm presented here is implicit and very expensive, and thus may not be appropriate for use with large collision systems. Nonetheless, it is the first geometric integrator for collision problems, and thus serves as a basis for the construction of more efficient methods in the future. In fact, the methods of this work have already led to the development of more computationally feasible collision integrators (see Cirak and West [2003]).

We also discuss how nonsmooth analysis techniques (Kane et al. [1999b]) can be incorporated into the variational procedure such that the integrator can cope with nonsmooth contact geometries (such as corner to corner collisions). As we mentioned before, this is the case which most existing algorithms cannot handle (the standard penalty methods simply

fail since no proper gap function can be defined for such geometries).

Summary of main results:

- rigorous understanding and proofs of the symplectic structure for collisions
- extension of the variational multisymplectic formalism to include various nonsmooth problems in continuum mechanics
- setting the stage for the development of multisymplectic discretizations for fluid-solid interactions, material interfaces, elastic collisions and shocks
- extension of the variational integration methods to include collisions
- the usual properties of variational integrators such as symplecticy, energy conservation were shown either numerically or analytically to hold in the case of collisions

Organization of the Thesis. In Chapter 2 we first consider the time-continuous situation, and extend the conventional setting of geometric Lagrangian mechanics (see, for example, Marsden and Ratiu [1999]) to include nonsmooth but still continuous trajectories. This allows us to recover the standard jump conditions at impact and to prove that the flow map of the system is symplectic in the extended sense.

To apply the standard geometric mechanical tools in nonsmooth situations, it is necessary to formulate the problem so that the space of admissible trajectories of the system has a smooth manifold structure. To do this, we work in the extended framework where both configuration variables and time are considered as functions of a fixed parameter space. This is the same approach as used in multisymplectic mechanics (see Gotay et al. [1997], Marsden et al. [1998]), where it was introduced to allow the consideration of right, or horizontal, transformations of the system.

Chapter 3 presents a variational approach to nonsmooth multisymplectic field theory. A large collection of nonsmooth dynamical models are considered: rigid-body collisions, material interfaces, elastic collisions, shocks and fluid-solid interactions. This chapter is the PDE extension of the theory developed in Chapter 2 to include continuum mechanics. The results presented in this chapter were published in Fetecau et al. [2003b].

Next, in Chapter 4 we discretize the variational structure presented in Chapter 2, based on the concept of discrete mechanics (see Marsden and West [2001] for an overview and

history), to obtain variational integrators for collision problems. By discretizing the variational structure, rather than some generalized equations of motion, we are able to show that our methods have various geometric properties, including the preservation of momentum maps and symplectic structures.

Finally, in Chapter 5 we consider particular examples of our variational integrators for collision problems and investigate their behavior on a number of sample problems of rigid body collisions. We also discuss briefly about possible use of the nonsmooth calculus approach (see Kane et al. [1999b]) in the context of variational collision integrators. The results presented in Chapters 2, 4 and 5 will appear in Fetecau et al. [2003a].

Chapter 6 is devoted to concluding remarks and future work directions.

Chapter 2

Nonsmooth Classical Mechanics

As noted in the introduction, the basic methodology used here is that of variational mechanics and variational discretizations. Clearly, a generalization to the nonsmooth setting of the autonomous, smooth variational mechanics cannot be done in a straightforward way. One of the major obstacles is that the lack of smoothness for the mappings prevents us from using the differential calculus on the manifold of mappings, as one essentially does in the smooth case (see Marsden and Ratiu [1999]).

The main issue addressed in this chapter is how to overcome this difficulty and how to derive the conservation of quantities such as energy, momentum maps and the symplectic form using a variational approach. The approach we use is to extend the problem to the nonautonomous case, so that both configuration variables and time are functions of a separate parameter τ. This allows the impact to be fixed in τ space while remaining variable in both configuration and time spaces, and it means that the relevant space of configurations will indeed be a smooth manifold, as we shall prove.

To make our variational procedure clear, we initially consider only the frictionless, purely elastic impact problem. In the last section, however, we show how the results can be extended to deal with friction and nonelastic impacts.

2.1 Lagrangian Mechanics in a Nonsmooth Setting

Consider a configuration manifold Q, and a submanifold with boundary $C \subset Q$ which represent the subset of admissible configurations. Let ∂C be called the contact set and let $L : TQ \to \mathbb{R}$ be a regular Lagrangian.

Remark. Similar results are obtained if we considered the configuration Q a manifold with boundary and the contact set to be ∂Q.

Let us now consider the ***path space*** defined by

$$\mathcal{M} = \mathcal{T} \times \mathcal{Q}([0,1], \tau_i, \partial C, Q),$$

where

$$\begin{aligned} \mathcal{T} &= \{c_t \in C^\infty([0,1], \mathbb{R}) \mid c_t' > 0 \text{ in } [0,1]\} \\ \mathcal{Q}([0,1], \tau_i, \partial C, Q) &= \{c_q : [0,1] \to Q \mid c_q \text{ is a } C^0, \text{ piecewise } C^2 \text{ curve}, \\ &\qquad c_q(\tau) \text{ has only one singularity at } \tau_i, c_q(\tau_i) \in \partial C\}. \end{aligned}$$

A path $c \in \mathcal{M}$ is thus a pair $c = (c_t, c_q)$. Given a path we can form the ***associated curve*** $q : [c_t(0), c_t(1)] \to Q$ by

$$q(t) = c_q(c_t^{-1}(t))$$

and we denote by $\mathcal{C}$ the space of all these paths $q(t) \in Q$.

The theory we will develop applies to rigid body impact problems, such as a particle bouncing on a rigid wall or two rigid bodies colliding, where the submanifold ∂C is obtained from the condition that interpenetration of matter cannot occur. The moment of impact τ_i is fixed in the τ space, but is allowed to vary in the t space according to $t_i = c_t(\tau_i)$; thus the setting we suggest is not restrictive in this sense.

We use a nonautonomous formulation of an autonomous mechanical system in order to achieve smoothness of the manifold of mappings, as one can see from the following lemmas.

Lemma 1. *$\mathcal{T}$ is a smooth manifold.*

Proof. $\mathcal{T}$ is an open set in $C^\infty([0,1], \mathbb{R})$, which is a smooth manifold (see Marsden and Ratiu [1999]). Then $\mathcal{T}$ is a submanifold of $C^\infty([0,1], \mathbb{R})$ and thus a manifold. ■

Lemma 2. *$\mathcal{Q}([0,1], \tau_i, \partial C, Q)$ is a smooth manifold.*

Proof. Fix a chart U in Q such that $U \cap \partial C \neq \emptyset$ and $U \cap \partial C$ is a chart in ∂C. Consider the set

$$\mathcal{Q}_U = \mathcal{Q}([0, \tau_i], U) \times \mathcal{Q}([\tau_i, 1], U) \times (U \cap \partial C),$$

where

$$\mathcal{Q}([0,\tau_i],U) = \{q : [0,\tau_i] \to Q \mid q \text{ is a } C^\infty \text{ curve, } q(\tau_i) \in U\}$$

$$\mathcal{Q}([\tau_i,1],U) = \{q : [\tau_i,1] \to Q \mid q \text{ is a } C^\infty \text{ curve, } q(\tau_i) \in U\}.$$

An element $c \in \mathcal{Q}([0,1],\tau_i,\partial C,Q)$ is the inverse image of the origin for some map $g_U : \mathcal{Q}_U \to \mathbb{R}^{2n}$ given by

$$g_U(q_1(\tau),q_2(\tau),q_i) = \begin{pmatrix} q_1(\tau_i) - q_i \\ q_2(\tau_i) - q_i \end{pmatrix},$$

where by n we denote the dimension of Q. One can prove that 0 is a regular value of g_U, and then the set $g_U^{-1}(0)$ is a submanifold of $\mathcal{Q}_U$ and thus it has a manifold structure.

Now $\{g_U^{-1}(0)\}_U$ represents a covering of $\mathcal{Q}([0,1],\tau_i,\partial C,Q)$, where each element of the covering is a manifold. The elements of the covering satisfy the compatibility conditions necessary to assure that $\mathcal{Q}([0,1],\tau_i,\partial C,Q)$ itself is a manifold (see Abraham et al. [1988]). ■

Corollary 1. *$\mathcal{M}$ is a smooth manifold.*

Remark. The theory can be easily extended to a problem involving more than one impact, by simply taking multiple points τ_i at which the trajectory is nonsmooth.

Note that the tangent space at $q \in \mathcal{Q}$ can be written as

$$T_q\mathcal{Q} = \{v : [0,1] \to TQ \mid v \text{ is a } C^0 \text{ piecewise } C^2 \text{ map }, v(\tau_i) \in T_{q(\tau_i)}\partial C\},$$

which will be a convenient form below when we consider variations of trajectories. The tangent space to the path space $\mathcal{M}$ is then given by $T\mathcal{M} = T\mathcal{T} \times T\mathcal{Q}$.

Remark. As we have noted above, fixing the impact point τ_i in τ space allows us to rigorously define what we mean by a variation of the impact point in t space. This is similar to the introduction of a parameterized spacetime in Marsden et al. [1998] and Lew et al. [2002].

The ***action map*** $\mathfrak{G} : \mathcal{M} \to \mathbb{R}$ is given by

$$\mathfrak{G}(c_t, c_q) = \int_0^1 L\left(c_q(\tau), \frac{c_q'(\tau)}{c_t'(\tau)}\right) c_t'(\tau)\, d\tau, \tag{2.1}$$

where c' denotes the derivative with respect to τ.

Remark. $c_q'(\tau)$ does not exist at τ_i, but the definition makes sense nonetheless.

If q is the associated curve for $c \in \mathcal{M}$, by the change of coordinates: $s = c_t(\tau)$ we can also write $\mathfrak{G}$ as

$$\mathfrak{G}(q) = \int_{c_t(0)}^{c_t(1)} L(q(s), \dot{q}(s))ds, \tag{2.2}$$

where $\dot{q}$ denotes the derivative with respect to t.

Define the ***extended configuration manifold*** to be $Q_e = \mathbb{R} \times Q$ and the ***second-order submanifold*** of $T(TQ_e)$ to be

$$\ddot{Q}_e = \{\frac{d^2c}{d\tau^2}(0) \in T(TQ_e) \mid c : [0,1] \to Q_e \text{ is a } C^2 \text{ curve}\}. \tag{2.3}$$

Now we can derive the equations of motions and the jump conditions in a purely variational way, by taking variations of the actions with respect to the path. This leads to the following fundamental theorem:

Theorem 1. *Given a C^k Lagrangian L ,$k \geq 2$, there exists a unique C^{k-2} mapping $EL : \ddot{Q} \to T^*Q_e$ and a unique C^{k-1} 1-form Θ_L on TQ_e, such that for all variations $\delta c \in T_c\mathcal{M}$ of c we have:*

$$d\mathfrak{G}(c) \cdot \delta c = \int_0^{\tau_i} EL(c'') \cdot \delta c\, d\tau + \int_{\tau_i}^1 EL(c'') \cdot \delta c\, d\tau + \Theta_L(c') \cdot \hat{\delta} c|_0^{\tau_i^-} + \Theta_L(c') \cdot \hat{\delta} c|_{\tau_i^+}^1, \tag{2.4}$$

where

$$\hat{\delta} c(\tau) = \left(\left(c(\tau), \frac{\partial c}{\partial \tau}(\tau)\right), \left(\delta c(\tau), \frac{\partial \delta c}{\partial \tau}(\tau)\right)\right).$$

*The mapping EL is called the **Euler-Lagrange derivative** and the 1-form Θ_L is called*

*the **Lagrangian 1-form**. In coordinates they have the expression*

$$EL(c'') = \left[\frac{\partial L}{\partial q}c_t' - \frac{d}{d\tau}\left(\frac{\partial L}{\partial \dot{q}}\right)\right] dc_q + \left[\frac{d}{d\tau}\left(\frac{\partial L}{\partial \dot{q}}\frac{c_q'}{c_t'} - L\right)\right] dc_t \tag{2.5}$$

$$\Theta_L(c') = \left[\frac{\partial L}{\partial \dot{q}}\right] dc_q - \left[\frac{\partial L}{\partial \dot{q}}\frac{c_q'}{c_t'} - L\right] dc_t. \tag{2.6}$$

Proof. Consider $\delta c \in T_c\mathcal{M}$. We calculate $d\mathfrak{G}(c)\cdot\delta c$ using the definition (see Marsden and Ratiu [1999])

$$d\mathfrak{G}(c)\cdot\delta c = \frac{d}{d\lambda}\mathfrak{G}(c^\lambda)\Big|_{\lambda=0}, \tag{2.7}$$

where c^λ is a curve in $\mathcal{M}$ with $c^0 = c$ and $\frac{dc^\lambda}{d\lambda}\Big|_{\lambda=0} = \delta c$. Splitting c^λ into components $c^\lambda = (c_t^\lambda, c_q^\lambda)$, we then have $\left(\frac{d}{d\lambda}c_t^\lambda\big|_{\lambda=0}, \frac{d}{d\lambda}c_q^\lambda\big|_{\lambda=0}\right) = (\delta c_t, \delta c_q)$ and we can calculate

$$d\mathfrak{G}\cdot\delta c = \int_0^1 \left[\frac{\partial L}{\partial q}\delta c_q + \frac{\partial L}{\partial \dot{q}}\left(\frac{\delta c_q'}{c_t'} - \frac{c_q'\delta c_t'}{(c_t')^2}\right)\right] c_t'\, d\tau + \int_0^1 L\delta c_t'\, d\tau.$$

Now we split the integral $\int_0^1$ into $\int_0^{\tau_i} + \int_{\tau_i}^1$ in order to integrate the $\delta c_q'$ and $\delta c_t'$ terms by parts. Some straightforward algebra then leads to equation (2.4). ■

2.2 Hamilton's Principle of Critical Action

Hamilton's principle of critical action tells us that we should consider critical points of the action function. Therefore, let define the ***space of solutions*** $\mathcal{M}_L \subset \mathcal{M}$ to be the set of all paths $c \in \mathcal{M}$ which satisfy $d\mathfrak{G}(c)\cdot\delta c = 0$ for all variations $\delta c \in T_c\mathcal{M}$ which are zero at the boundary points 0 and 1.

Using (2.4) we can see that c is a solution if it satisfies:

$$\int_0^{\tau_i} EL(c'')\cdot\delta c\, d\tau + \int_{\tau_i}^1 EL(c'')\cdot\delta c\, d\tau + \Theta_L(c')\big|_{\tau_i^-}^{\tau_i^+}\cdot\hat{\delta}c(\tau_i) = 0 \tag{2.8}$$

for all variations $\delta c \in T_c\mathcal{M}$.

From equation (2.8) it is clear that c is a solution if and only if the Euler-Lagrange derivative is zero on smooth portions and the Lagrangian 1-form has a zero jump at τ_i.

Splitting $EL(c'')$ into the two components we obtain

$$\frac{\partial L}{\partial q} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) = 0 \quad \text{in} \quad [t_0, t_i) \cup (t_i, t_1] \tag{2.9}$$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\dot{q} - L\right) = 0 \quad \text{in} \quad [t_0, t_i) \cup (t_i, t_1], \tag{2.10}$$

where $t_0 = c_t(0)$, $t_1 = c_t(1)$ and $t_i = c_t(\tau_i)$.

In fact, (2.10) is redundant, as it is a consequence of (2.9). Indeed, if c is a path satisfying (2.9) for all $t \in (t_0, t_i) \cup (t_i, t_1)$, then the second component (2.10) of the Euler-Lagrange equations is identically satisfied. To see this, we may calculate

$$\begin{aligned}
\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\dot{q} - L\right) &= \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right)\dot{q} + \frac{\partial L}{\partial \dot{q}}\ddot{q} - \frac{dL}{dt} \\
&= \left[\frac{\partial L}{\partial q}\dot{q} + \frac{\partial L}{\partial \dot{q}}\ddot{q}\right] - \frac{dL}{dt} \\
&= 0,
\end{aligned}$$

where we used (2.9) to pass from the first to the second line.

The second part (2.10) of the Euler-Lagrange equations represents the conservation of energy for an autonomous system, provided the motion is smooth. The ***energy*** $E : TQ \to \mathbb{R}$ is defined to be

$$E(q, \dot{q}) = \frac{\partial L}{\partial \dot{q}}(q, \dot{q}) \cdot \dot{q} - L(q, \dot{q}).$$

It is not surprising that the second part of the Euler-Lagrange equations (2.10) is redundant, since the first part (2.9) already has the energy evolution built into it.

The previous definition of the energy function allows us to write the Lagrangian 1-form in the compact notation

$$\Theta_L = \frac{\partial L}{\partial \dot{q}} dq - E dt, \tag{2.11}$$

where we use (q, t) to refer to the two components of c. The conservation of the Lagrangian 1-form at the impact time reads:

$$\Theta_L|_{\tau_i^-} = \Theta_L|_{\tau_i^+} \quad \text{on} \quad TQ_e|(\mathbb{R} \times \partial C). \tag{2.12}$$

Splitting this into the two components gives

$$\left.\frac{\partial L}{\partial \dot{q}}\right|_{t=t_i^-} \cdot \delta q = \left.\frac{\partial L}{\partial \dot{q}}\right|_{t=t_i^+} \cdot \delta q \tag{2.13}$$

for any $\delta q \in T_{q(t_i)}\partial C$ and

$$E(q(t_i^-), \dot{q}(t_i^-)) = E(q(t_i^+), \dot{q}(t_i^+)). \tag{2.14}$$

These equations are the Weierstrass-Erdmann type conditions for impact. That is, equation (2.13) states that the linear momentum must be conserved in the tangent direction to ∂C, while equation (2.14) states that the energy must be conserved during an elastic impact.

The system of equations (2.13) and (2.14) must be solved for $\dot{q}(t_i^+)$. An obvious solution is $\dot{q}(t_i^+) = \dot{q}(t_i^-)$, but this is ruled out since the resulting trajectory would no longer lie in the admissible set. That is, it would violate the physical non-interpenetration condition.

Remark. Of course, existence and uniqueness for nonsmooth systems are very deep questions. Here, we will simply remark that for a codimension-one smooth boundary ∂C and quadratic kinetic energy, solutions to the system (2.13), (2.14) exist and are unique locally. The questions of global existence and uniqueness of solutions for more general Lagrangians is left for future works.

2.3 Lagrangian Flows and Conservation of the Symplectic Form

As we have already seen, a path $c \in \mathcal{M}$ is a solution of the variational principle if its associated curve $q(t)$ satisfies the Euler-Lagrange equations (2.9) and the jump conditions (2.13) and (2.14). It is a well-known fact that, in the smooth case, such a trajectory is uniquely determined by an initial condition in TQ. Since we work in a nonsmooth context, we must assume uniqueness of the physical trajectory at the impact point; we have already discussed in the previous section some conditions under which this actually occurs.

Under this hypothesis, the space $\mathcal{C}_L$, defined to be the space of curves $q(t)$ that satisfy (2.9), (2.13) and (2.14) may be identified with the space of initial conditions $(t_0, q_0, \dot{q}_0)$ on $\mathbb{R} \times TQ$.

Based on these remarks, we can define a flow $F_t : \mathbb{R} \times TQ \to \mathbb{R} \times TQ$ as follows

$$F_t(t_0, q_0, \dot{q}_0) = (t_0 + t, q(t_0 + t), \dot{q}(t_0 + t)), \tag{2.15}$$

where $q(t)$ is the unique trajectory in $\mathcal{C}_L$ corresponding to $(t_0, q_0, \dot{q}_0) \in \mathbb{R} \times TQ$. The mapping F_t is called the ***Lagrangian flow***. In the nonsmooth setting, F_t will not necessarily be a smooth map on the whole of its domain. Later, we will restrict attention to the parts of the domain on which F_t is smooth, in order to use the derivatives of F_t with respect to the initial conditions and to time.

Remark. Even though we have worked within an extended configuration manifold formulation up until this point, here we have defined a flow on TQ, rather than taking a flow on TQ_e with initial conditions in TQ_e. The reason for doing this is that the derivative t_0' has no physical meaning, and no mechanical problem has the derivative of time with respect to some parameter as an initial condition.

Next, we will show in which sense the Lagrangian flow F_t is symplectic. We begin by relating the previous approach to the one used in the rest of the chapter.

As we noted above, to any initial condition $(t_0, q_0, \dot{q}_0)$ in $\mathbb{R} \times TQ$ there corresponds a unique trajectory $q(t) \in \mathcal{C}_L$ s.t. $(q(t_0), \dot{q}(t_0)) = (q_0, \dot{q}_0)$. Trajectories in $\mathcal{C}_L$ are unique up to reparameterization in τ. Accordingly, we can define an equivalence relation in $\mathcal{M}_L$ by

$$c^0 \sim c^1 \text{ iff } c_q^0 \circ (c_t^0)^{-1} = c_q^1 \circ (c_t^1)^{-1}, \tag{2.16}$$

where $c^0, c^1 \in \mathcal{M}_L, c^0 = (c_q^0, c_t^0), c^1 = (c_q^1, c_t^1)$. That is, two paths are equivalent if they have the same associated curve, and so to a given trajectory $q(t)$ in $\mathcal{C}_L$ there corresponds an equivalence class $\hat{c}$ of curves in the extended space.

In a similar manner we can define an equivalence relation on TQ_e by

$$(t_0, q_0, t_0', q_0') \sim (t_1, q_1, t_1', q_1') \text{ iff } t_0 = t_1,\ q_0 = q_1 \text{ and } \frac{q_0'}{t_0'} = \frac{q_1'}{t_1'}, \tag{2.17}$$

which is a pointwise version of the previous equivalence relation (2.16).

Now, the quotient space $TQ_e/\sim$ may be identified with the product $\mathbb{R} \times TQ$ and the flow F_t may be regarded not as a flow on TQ_e (which would not be desirable, as explained

in Remark 2.3), but as a flow on the equivalence classes of TQ_e.

To prove symplecticity for the flow F_t in a precise sense we must reinterpret Theorem 1 by slightly modifying the definition of the Lagrangian 1-form Θ_L.

That is, Theorem 1 stands with the same statement and fundamental relation (2.4) if we replace Θ_L with the 1-form $\bar{\Theta}_L$ on $\mathbb{R} \times TQ \cong TQ_e/_\sim$, where $\bar{\Theta}_L$ is given by the same coordinate expression as Θ_L, i.e. relation (2.6). More precisely, (2.4) becomes

$$d\mathfrak{G}(c) \cdot \delta c = \int_0^{\tau_i} EL(c'') \cdot \delta c \, d\tau + \int_{\tau_i}^1 EL(c'') \cdot \delta c \, d\tau \\ + \bar{\Theta}_L(\tilde{c}) \cdot \delta\tilde{c}|_0^{\tau_i^-} + \bar{\Theta}_L(\tilde{c}) \cdot \delta\tilde{c}|_{\tau_i^+}^1, \quad (2.18)$$

where

$$\tilde{c}(\tau) = \left(c_t(\tau), c_q(\tau), \frac{c_q'(\tau)}{c_t'(\tau)} \right)$$
$$\delta\tilde{c}(\tau) = \left(\left(c_t(\tau), c_q(\tau), \frac{c_q'(\tau)}{c_t'(\tau)} \right), \left(\delta c_t(\tau), \delta c_q(\tau), \left(\frac{\delta c_q'}{c_t'} - \frac{c_q' \delta c_t'}{(c_t')^2} \right)(\tau) \right) \right).$$

It is exactly this 1-form $\bar{\Theta}_L$ on $\mathbb{R} \times TQ$ which is preserved by the flow F_t, as we will now show.

To any fixed $(t_0, q_0, \dot{q_0}) \in \mathbb{R} \times TQ$ we associate the integral curve $s \mapsto F_s(t_0, q_0, \dot{q_0})$ for $s \in [0, t]$; the value of $\mathfrak{G}$ on that curve is denoted by $\mathfrak{G}_t$, and again called the ***action***. Thus we define the map $\mathfrak{G}_t : \mathbb{R} \times TQ \to \mathbb{R}$ by

$$\mathfrak{G}_t(t_0, q_0, \dot{q_0}) = \int_{t_0}^{t_0+t} L\left(q(s), \dot{q}(s)\right) ds, \quad (2.19)$$

where $q(t) \in \mathcal{C}_L$ is the solution corresponding to $(t_0, q_0, \dot{q_0})$.

If $c = (c_t, c_q)$ is any representative in the equivalence class $\hat{c}$ corresponding to q, we can write

$$F_t(t_0, q_0, \dot{q_0}) = \left(c_t(\tau), c_q(\tau), \frac{c_q'(\tau)}{c_t'(\tau)} \right), \quad (2.20)$$

where $\tau = c_t^{-1}(t_0 + t)$.

Consider now an arbitrary curve $\lambda \mapsto (t_0^\lambda, q_0^\lambda, \dot{q}_0^\lambda)$ in $\mathbb{R} \times TQ$ which passes through $(t_0, q_0, \dot{q}_0)$ at $\lambda = 0$. Denote by $q^\lambda(t)$ the unique trajectories in $\mathcal{C}_L$ corresponding to $(t_0^\lambda, q_0^\lambda, \dot{q}_0^\lambda)$ and by $\hat{c}^\lambda$ their equivalence classes in $\mathcal{M}_L$ (at $\lambda = 0$ they reduce to $q(t)$ and $\hat{c}$,

respectively). We pick representatives $(c_t^\lambda, c_q^\lambda)$ in $\hat{c}^\lambda$ such that for any $\lambda \geq 0$ we have

$$(c_t^\lambda)^{-1}(t_0^\lambda + t) = \text{const}, \tag{2.21}$$

for some $t > 0$; we denote this common value by τ.

Then, using (2.20) and (2.21), the fundamental equation (2.18) becomes

$$\begin{aligned} d\mathfrak{G}_t((t_0, q_0, \dot{q}_0)) \cdot (\delta t_0, \delta q_0, \delta \dot{q}_0) = \bar{\Theta}_L(F_t(t_0, q_0, \dot{q}_0)) \cdot \frac{d}{d\lambda} F_t(t_0^\lambda, q_0^\lambda, \dot{q}_0^\lambda)\Big|_{\lambda=0} \\ - \bar{\Theta}_L(t_0, q_0, \dot{q}_0) \cdot \frac{d}{d\lambda}(t_0^\lambda, q_0^\lambda, \dot{q}_0^\lambda)\Big|_{\lambda=0}, \end{aligned} \tag{2.22}$$

where $(\delta t_0, \delta q_0, \delta \dot{q}_0) = \frac{d}{d\lambda}|_{\lambda=0}(t_0^\lambda, q_0^\lambda, \dot{q}_0^\lambda)$.

Taking the exterior derivative of (2.22) we derive

$$0 = dd\mathfrak{G}_t = F_t^*(d\bar{\Theta}_L) - d\bar{\Theta}_L. \tag{2.23}$$

Defining the ***Lagrangian symplectic form*** by $\Omega_L = -d\bar{\Theta}_L$ we now see that relation (2.23) gives the symplecticity of the flow in the extended sense

$$F_t^* \Omega_L = \Omega_L. \tag{2.24}$$

Thus, we derived conservation of the canonical symplectic structure in the extended sense (see Kane et al. [1999a]), namely,

$$\Omega_L = \omega_L + dE \wedge dt, \tag{2.25}$$

where $\omega_L = -d\theta_L$ is the canonical symplectic form. Here, θ_L represents the component of the Lagrangian 1-form given by (2.11)

$$\theta_L = \frac{\partial L}{\partial \dot{q}} dq. \tag{2.26}$$

It is the term $dE \wedge dt$ that distinguishes the nonautonomous structure used here from the autonomous approach, for which the symplectic structure is given only by the canonical symplectic form ω_L.

2.4 Noether's Theorem

Suppose that a Lie group G, with Lie algebra $\mathfrak{g}$, acts on Q by the (left or right) action $\Phi : G \times Q \to Q$. Consider the tangent lift of this action to $T\Phi : G \times TQ \to TQ$ given by $(T\Phi)_g(v_q) = T(\Phi_g) \cdot v_q$ and for $\xi \in \mathfrak{g}$ define the ***infinitesimal generators*** $\xi_Q : Q \to TQ$ and $\xi_{TQ} : TQ \to T(TQ)$ by

$$\xi_Q(q) = \frac{d}{dt}_{|_{t=0}} \exp(t\xi) \cdot q$$
$$\xi_{TQ}(v_q) = \frac{d}{dt}_{|_{t=0}} T_q\phi_t(v_q),$$

where ϕ_t is the flow of the vector field ξ_Q.

In this section we will not use the extended configuration manifold setting with variations in both time and configuration variables, as is done in the rest of the chapter. This means that we are restricted to symmetries of the configuration variables, which do not involve altering the time variable. This allows us to deal with most of the interesting physical problems, while still keeping the theory relatively simple. For a full account of the conservation of momentum maps in the extended setting see Marsden and West [2001].

For a fixed initial time $t_0 \in \mathbb{R}$, define the flow map $\tilde{F}_t : TQ \to TQ$ by

$$\tilde{F}_t(q_0, \dot{q}_0) = (q(t_0 + t), \dot{q}(t_0 + t)), \tag{2.27}$$

where $q(t)$ is the unique trajectory in $\mathcal{C}_L$ corresponding to $(q_0, \dot{q}_0) \in TQ$, as initial condition at t_0.

In the autonomous setting the Lagrangian 1-form $\bar{\Theta}_L$ reduces to the configuration component θ_L given by (2.26) and the action $\mathfrak{G}_t$ from (2.19) becomes the map $\bar{\mathfrak{G}}_t : TQ \to \mathbb{R}$ defined by

$$\bar{\mathfrak{G}}_t(q_0, \dot{q}_0) = \int_{t_0}^{t_0+t} L\left(q(s), \dot{q}(s)\right) ds. \tag{2.28}$$

Define the ***Lagrangian momentum map*** $J_L : TQ \to \mathfrak{g}^*$ to be

$$J_L(v_q) \cdot \xi = \theta_L \cdot \xi_{TQ}(v_q).$$

We will now show that when the group action is a symmetry of both the Lagrangian and

the submanifold ∂C, then the momentum maps are conserved quantities of the flow.

A Lagrangian $L : TQ \to \mathbb{R}$ is said to be ***infinitesimally invariant*** under the lift of the group action $\Phi : G \times Q \to Q$ if $dL \cdot \xi_{TQ} = 0$ for all $\xi \in \mathfrak{g}$, and in this case the group action is said to be a ***symmetry*** of the Lagrangian.

In proving the following theorem we will essentially use the assumption that the group action Φ leaves the boundary ∂C of the collision set invariant (locally). An example where this assumption is valid is the case of two or more irregular bodies (for example binary asteroids) moving in space under gravitational forces. In this case the collision set is invariant to translations and rotations ($G = SE(3)$).

Theorem 2 (Noether's Theorem). *Consider a Lagrangian system $L : TQ \to \mathbb{R}$ which is infinitesimally invariant under the lift of the (left or right) group action $\Phi : G \times Q \to Q$. In the assumption that the group action leaves ∂C invariant (locally), then the corresponding Lagrangian momentum map $J_L : TQ \to \mathfrak{g}^*$ is a conserved quantity of the flow, so that $J_L \circ \tilde{F}_t = J_L$ for all times t.*

Proof. The group action of G on Q induces a group action of G on the space $\mathcal{C}$ of paths $q(t)$ in Q by pointwise action, so that $\Phi_g(q)(t) = \Phi_g(q(t))$. The tangent lift of Φ acting on $\mathcal{C}$ will thus be the pointwise group action of the tangent lift of Φ group action on Q. From this we derive

$$d\mathfrak{G}(q) \cdot \xi_{\mathcal{C}}(q) = \int_{t_0}^{t_1} dL \cdot \xi_{TQ} \, dt$$

and so, symmetries of the Lagrangian induce symmetries of the action. This implies that Φ_g leaves the space of solutions $\mathcal{C}_L$ of the Euler-Lagrange equations invariant, and so we may restrict Φ_g to $\mathcal{C}_L$.

Furthermore, the flow map $\tilde{F}_t : TQ \to TQ$ commutes with the tangent lift of Φ on $\mathcal{C}$: $\tilde{F}_t \circ T\Phi_g = T\Phi_g \circ \tilde{F}_t$. Differentiating this with respect to g in the direction ξ gives

$$T(\tilde{F}_t) \cdot \xi_{TQ} = \xi_{TQ} \circ \tilde{F}_t.$$

We now follow the same idea used to prove symplecticity of the flow map F_t and identify the space of solutions $\mathcal{C}_L$ with the space of initial conditions TQ. For an initial condition

$v_q \in TQ$ and corresponding solution curve $q \in \mathcal{C}_L$ we thus have

$$\begin{aligned} d\mathfrak{G}(q) \cdot \xi_{\mathcal{C}}(q) &= d\bar{\mathfrak{G}}_t(v_q) \cdot \xi_{TQ}(v_q) \\ &= ((\tilde{F}_t)^*(\theta_L) - \theta_L)(v_q) \cdot \xi_{TQ}(v_q) \end{aligned} \tag{2.29}$$

from (2.22).

To derive (2.29) one uses the assumption that the group action Φ leaves ∂C invariant (locally). More precisely, it is essential that the path curves $q^\lambda \in \mathcal{C}$ corresponding to $v_q^\lambda = \eta_\lambda(v_q)$ (by η_λ we denote the flow of ξ_{TQ} on TQ) have exactly the same impact time t_i as the curve q. We conclude this from the relation

$$q^\lambda(t_i) = \Phi_{\exp(\lambda\xi)}(q)(t_i) = \exp(\lambda\xi) \cdot q(t_i),$$

as well as the assumption on the group action and the condition that $q(t_i) \in \partial C$.

As the left-hand side of (2.29) is always zero, the previous identity gives

$$(\theta_L \cdot \xi_{TQ}) \circ \tilde{F}_t = \theta_L \cdot \xi_{TQ},$$

which is the definition of conservation of the momentum map. This argument is valid for any time $t \in \mathbb{R}$, giving Noether's theorem. ■

2.5 Forcing and Friction

In this section we extend the theory developed so far to include forcing and friction. To do this in the variational framework, we turn from using Hamilton's principle to the Lagrange-d'Alembert extension of it.

The usual force field description of impact dynamics contains a given external force, a normal contact force field over the area in contact and a friction force field required to be self-equilibrated and tangential to the surfaces in contact.

Following Marsden and Ratiu [1999], we define the ***exterior force field*** as a fiber-preserving map $F : TQ_e \to T^*Q_e$ over the identity, which we write in coordinates as

$$F : (c, c') \mapsto (c, F(c, c')). \tag{2.30}$$

We use a unified treatment of contact forces (the normal and the frictional forces) by defining the ***contact force field*** to be a map $f^{\text{con}} : TQ_e|(\partial C \times \mathbb{R}) \to T^*(\partial C \times \mathbb{R})$.

Given a Lagrangian L and the exterior and contact force fields defined as above, the ***integral Lagrange-d'Alembert principle*** for a curve $c \in \mathcal{M}$ states that

$$\delta \int_0^1 L\left(c_q(\tau), \frac{c_q'(\tau)}{c_t'(\tau)}\right) c_t'(\tau)\, d\tau + \int_0^1 F(c(\tau), c'(\tau)) \cdot \delta c(\tau)\, d\tau + f^{\text{con}}(c(\tau_i), c'(\tau_i)) \cdot \delta c(\tau_i) = 0, \quad (2.31)$$

for all admissible variations δc vanishing at the endpoints.

Using integration by parts and notations from Section 2.1 one can show that (2.31) is equivalent to

$$\int_0^{\tau_i} \left[EL(c'') + F(c')\right] \cdot \delta c\, d\tau + \int_{\tau_i}^1 (EL(c'') + F(c')) \cdot \delta c\, d\tau + \Theta_L(c')|_{\tau_i^-}^{\tau_i^+} \cdot \hat{\delta} c(\tau_i) + f^{\text{con}}(c(\tau_i), c'(\tau_i)) \cdot \delta c(\tau_i) = 0. \quad (2.32)$$

From (2.32) we obtain the ***extended forced Euler-Lagrange equations***, which have coordinate expressions

$$\frac{d}{d\tau}\left(\frac{\partial L}{\partial \dot{q}}\right) - \frac{\partial L}{\partial q} c_t' = F_q \text{ in } [0, \tau_i) \cup (\tau_i, 1] \quad (2.33)$$

$$-\frac{d}{d\tau}\left(\frac{\partial L}{\partial \dot{q}}\dot{q} - L\right) = F_t \text{ in } [0, \tau_i) \cup (\tau_i, 1], \quad (2.34)$$

where (F_t, F_q) denote the corresponding components of F.

However, the first part (2.33) of the extended forced Euler-Lagrange equations has the energy evolution built into it, as can be seen from

$$\begin{aligned} \frac{dE}{dt} &= \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\dot{q} - L\right) \\ &= \left(\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) - \frac{\partial L}{\partial q}\right)\dot{q} \\ &= \frac{F_q}{c_t'}\dot{q}, \end{aligned} \quad (2.35)$$

where we used (2.33) to pass from the first to the second line.

Therefore, from (2.34), the time component F_t of the exterior force field must necessarily

be of the form

$$F_t = -F_q \cdot \dot{q}. \tag{2.36}$$

This compatibility condition is a consequence of the fact that the mechanical system is autonomous and the equations must depend only on the associated curve $q(t)$. The nonautonomous approach is relevant only in the context of nonsmooth mechanics and it is not surprising that there is no particular gain of this approach wherever the motion is smooth.

Now we turn to (2.32) and write the remaining terms on the left hand side in components, to obtain

$$\left.\frac{\partial L}{\partial \dot{q}}\right|_{t_i^-}^{t_i^+} \cdot \delta q + f_q^{\text{con}} \cdot \delta q = 0, \tag{2.37}$$

for any $\delta q \in T_{q(t_i)}\partial C$, and

$$E(q(t_i^+), \dot{q}(t_i^+)) - E(q(t_i^-), \dot{q}(t_i^-)) - f_t^{\text{con}} = 0. \tag{2.38}$$

The equations (2.37) and (2.38) represent the standard jump conditions for an inelastic impact with friction. The equation (2.37) gives the jump in the tangential component of the linear momentum due to the frictional forces acting on the tangent plane of the contact submanifold ∂C. The energy dissipation, given by (2.38), is due to the tangential frictional forces, as well as to the normal reaction force exerted by the constraint. For frictionless collisions, f_t^{con} plays the same role as the coefficient of restitution from the measure differential inclusion formulation of contact dynamics (Kunze and Marques [2000]; Stewart [2000]).

Chapter 3

Nonsmooth Continuum Mechanics

The purpose of this chapter is to combine the ideas of the variational collision theory and algorithms with the multisymplectic theory and algorithms to produce a variational theory for PDE's in mechanics that allow for material interfaces, elastic collisions, shocks and fluid-solid interactions. In Section 3.4.2 we classify a collection of nonsmooth dynamic models that we will study.

To lay the variational and multisymplectic foundations for nonsmooth continuum mechanics we will rely on the smooth case studied from this perspective in Marsden et al. [2001]. We plan to merge this work with variational algorithms and discrete mechanics in our future work on the topic. The results presented in this chapter were published in Fetecau et al. [2003b].

3.1 Multisymplectic Geometry

In this section we will review some aspects of basic covariant field theory in the framework of multisymplectic geometry. The multisymplectic framework is a PDE generalization of classical non-relativistic mechanics (or particle mechanics) and has diverse applications, including to electromagnetism, continuum mechanics, gravity, bosonic strings, etc.

The traditional approach to the multisymplectic geometric structure closely follows the derivation of the canonical symplectic structure in particle mechanics. The derivation first defines the field theoretic analogues of the tangent and cotangent bundles (called the first jet bundle and the dual jet bundle, respectively). It then introduces a canonical multisymplectic form on the dual jet bundle and pulls it back to the Lagrangian side using the covariant Legendre transform. As an alternative, Marsden et al. [1998] gave a very elegant approach

of deriving the multisymplectic structure by staying entirely on the Lagrangian side, which we will use here.

We start by reviewing the main concepts of the multisymplectic field-theoretic setting.

Let X be an oriented manifold, which in many examples is spacetime, and let $\pi_{XY} : Y \to X$ be a finite-dimensional fiber bundle called the ***covariant configuration bundle***. The physical fields will be sections of this bundle, which is the covariant analogue of the configuration space in classical mechanics.

The role of the tangent bundle is played by J^1Y (or $J^1(Y)$), the ***first jet bundle*** of Y. We identify J^1Y with the *affine* bundle over Y whose fiber over $y \in Y_x = \pi_{XY}^{-1}(x)$ consists of those linear maps $\gamma : T_xX \to T_yY$ satisfying

$$T\pi_{XY} \circ \gamma = \mathrm{Id}_{T_xX}.$$

We let $\dim X = n+1$ and the fiber dimension of Y be N. Coordinates on X are denoted $x^\mu, \mu = 1, 2, \ldots, n, 0$, and fiber coordinates on Y are denoted by $y^A, A = 1, \ldots, N$. These induce coordinates $v^A\mu$ on the fibers of J^1Y. For a section $\varphi : X \to Y$, its tangent map at $x \in X$, denoted $T_x\varphi$, is an element of $J^1Y_{\varphi(x)}$. Thus, the map $x \mapsto T_x\varphi$ is a local section of J^1Y regarded as a bundle over X. This section is denoted $j^1(\varphi)$ or $j^1\varphi$ and is called the first jet of φ. In coordinates, $j^1(\varphi)$ is given by

$$x^\mu \mapsto (x^\mu, \varphi^A(x^\mu), \partial_\nu\varphi^A(x^\mu)), \tag{3.1}$$

where $\partial_\nu = \frac{\partial}{\partial x^\nu}$.

We will study Lagrangians defined on J^1Y and derive the Euler-Lagrange equations by a procedure similar to that used in Lagrangian mechanics on the tangent bundle of a configuration manifold (see Marsden and Ratiu [1999]). We thus consider theories for which Lagrangians depend at most on the fields and their *first* derivatives (first-order field theories). For a geometric-variational approach to second-order field theories we refer the reader to Kouranbaeva and Shkoller [2000].

Higher order jet bundles of Y, J^mY, can be defined as $J^1(\cdots(J^1(Y)))$ and are used in the higher order field theories. In this work we will use only J^1Y and a specific subbundle Y'' of J^2Y which we will define below.

Let $\gamma \in J^1Y$ so that $\pi_{X,J^1Y}(\gamma) = x$. Analogous to the tangent map of the projection π_{Y,J^1Y}, $T\pi_{Y,J^1Y} : TJ^1Y \to TY$, we may define the jet map of this projection which takes J^2Y onto J^1Y:

$$J\pi_{Y,J^1Y} : \mathrm{Aff}(T_xX, T_\gamma J^1Y) \to \mathrm{Aff}(T_xX, T\pi_{Y,J^1Y} \cdot T_\gamma J^1Y).$$

We define the subbundle Y'' of J^2Y over X which consists of second-order jets so that on each fiber

$$Y''_x = \{s \in J^2Y_\gamma \mid J\pi_{Y,J^1Y}(s) = \gamma\}. \tag{3.2}$$

In coordinates, if $\gamma \in J^1Y$ is given by $(x^\mu, y^A, v^A{}_\mu)$, and $s \in J^2Y_\gamma$ is given by $(x^\mu, y^A, v^A{}_\mu, w^A{}_\mu, k^A{}_{\mu\nu})$, then s is a second-order jet if $v^A{}_\mu = w^A{}_\mu$. Thus, the second jet of a section φ, $j^2(\varphi)$, given in coordinates by the map $x^\mu \mapsto (x^\mu, \varphi^A, \partial_\nu\varphi^A, \partial_\mu\partial_\nu\varphi^A)$, is an example of a second-order jet.

Next we introduce the field theoretic analogue of the cotangent bundle. We define the ***dual jet bundle*** J^1Y^* to be the *vector* bundle over Y whose fiber at $y \in Y_x$ is the set of affine maps from J^1Y_y to $\Lambda^{n+1}(X)_x$, the bundle of $(n+1)$-forms on X. A smooth section of J^1Y^* is therefore an affine bundle map of J^1Y to $\Lambda^{n+1}(X)$ covering π_{XY}.

Fiber coordinates on J^1Y^* are $(p, p_A{}^\mu)$, which correspond to the affine map given in coordinates by

$$v^A{}_\mu \mapsto (p + p_A{}^\mu v^A{}_\mu) d^{n+1}x, \tag{3.3}$$

where

$$d^{n+1}x = dx^1 \wedge \cdots \wedge dx^n \wedge dx^0.$$

Analogous to the canonical one- and two-forms on a cotangent bundle, there are canonical $(n+1)$- and $(n+2)$-forms on the dual jet bundle J^1Y^*. We will omit here the intrinsic definitions of these canonical forms (see Gotay et al. [1997] for details). In coordinates, with $d^nx_\mu = \partial_\mu \lrcorner\, d^{n+1}x$, these forms are given by

$$\Theta = p_A{}^\mu dy^A \wedge d^nx_\mu + p d^{n+1}x \tag{3.4}$$

and

$$\Omega = dy^A \wedge dp_A{}^\mu \wedge d^nx_\mu - dp \wedge d^{n+1}x. \tag{3.5}$$

A ***Lagrangian density*** $\mathcal{L} : J^1Y \to \Lambda^{n+1}(X)$ is a smooth bundle map over X. In coordinates, we write

$$\mathcal{L}(\gamma) = L(x^\mu, y^A, v^A_\mu)d^{n+1}x. \tag{3.6}$$

The covariant Legendre transform for $\mathcal{L}$ is a fiber preserving map over Y, $\mathbb{F}\mathcal{L} : J^1Y \to J^1Y^*$, expressed intrinsically as the first-order vertical Taylor approximation to $\mathcal{L}$:

$$\mathbb{F}\mathcal{L}(\gamma) \cdot \gamma' = \mathcal{L}(\gamma) + \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \mathcal{L}(\gamma + \epsilon(\gamma' - \gamma)), \tag{3.7}$$

where $\gamma, \gamma' \in J^1Y_y$.

The coordinate expression of $\mathbb{F}\mathcal{L}$ is given by

$$p^\mu_A = \frac{\partial L}{\partial v^A{}_\mu}, \quad \text{and} \quad p = L - \frac{\partial L}{\partial v^A{}_\mu} v^A{}_\mu \tag{3.8}$$

for the multimomenta p^μ_A and the covariant Hamiltonian p.

Now we can use the covariant Legendre transform to pull back to the Lagrangian side the multisymplectic canonical structure on the dual jet bundle. We define the ***Cartan form*** as the $(n+1)$-form $\Theta_\mathcal{L}$ on J^1Y given by

$$\Theta_\mathcal{L} = (\mathbb{F}\mathcal{L})^*\Theta \tag{3.9}$$

and the $(n+2)$-form $\Omega_\mathcal{L}$ by

$$\Omega_\mathcal{L} = -d\Theta_\mathcal{L} = (\mathbb{F}\mathcal{L})^*\Omega, \tag{3.10}$$

with local coordinate expressions

$$\Theta_\mathcal{L} = \frac{\partial L}{\partial v^A_\mu} dy^A \wedge d^n x_\mu + \left(L - \frac{\partial L}{\partial v^A_\mu} v^A_\mu\right) d^{n+1}x \tag{3.11}$$

and

$$\Omega_\mathcal{L} = dy^A \wedge d\left(\frac{\partial L}{\partial v^A_\mu}\right) \wedge d^n x_\mu - d\left(L - \frac{\partial L}{\partial v^A_\mu} v^A_\mu\right) \wedge d^{n+1}x. \tag{3.12}$$

To lay the groundwork for the following sections we introduce the concept of jet prolongations. We will show how automorphisms of Y lift naturally to automorphisms of J^1Y and we will construct the covariant analogue of the tangent map.

Let $\eta_Y : Y \to Y$ be a π_{XY}-bundle automorphism covering a diffeomorphism $\eta_X : X \to$

X. If $\gamma : T_xX \to T_yY$ is an element of J^1Y, let $\eta_{J^1Y}(\gamma) : T_{\eta_X(x)}X \to T_{\eta_Y(y)}Y$ be defined by

$$\eta_{J^1Y}(\gamma) = T\eta_Y \circ \gamma \circ T\eta_X^{-1}. \tag{3.13}$$

The π_{Y,J^1Y}-bundle automorphism $j^1(\eta_Y)$, also denoted η_{J^1Y}, is called the ***first jet extension*** or ***prolongation*** of η_Y to J^1Y and has the coordinate expression

$$\eta_{J^1Y}(\gamma) = \left(\eta_X^\mu(x), \eta_Y^A(x,y), \left[\partial_\nu \eta_Y^A + \left(\partial_B \eta_Y^A\right) v^B{}_\nu\right] \partial_\mu \left(\eta_X^{-1}\right)^\nu\right), \tag{3.14}$$

where $\gamma = (x^\mu, y^A, v^A{}_\mu)$.

If V is a vector field on Y whose flow is η_λ, so that

$$V \circ \eta_\lambda = \frac{d\eta_\lambda}{d\lambda},$$

then its ***first jet extension*** or ***prolongation***, denoted $j^1(V)$ or V_{J^1Y}, is the vector field on J^1Y whose flow is $j^1(\eta_\lambda)$; that is

$$j^1(V) \circ j^1(\eta_\lambda) = \frac{d}{d\lambda} j^1(\eta_\lambda). \tag{3.15}$$

In coordinates, $j^1(V)$ has the expression

$$j^1(V) = \left(V^\mu, V^A, \frac{\partial V^A}{\partial x^\mu} + \frac{\partial V^A}{\partial y^B} v_\mu^B - v_\nu^A \frac{\partial V^\nu}{\partial x^\mu}\right). \tag{3.16}$$

We note that one can also view V as a section of the bundle $TY \mapsto Y$ and take its first jet in the sense of (3.1). Then one obtains a section of $J^1(TY) \mapsto Y$ which is not to be confused with $j^1(V)$ as defined by (3.15) and (3.16); they are two different objects.

This is the differential-geometric formulation of the multisymplectic structure. However, as we mentioned before, there is a very elegant and interesting way to construct $\Theta_{\mathcal{L}}$ directly from the variational principle, staying entirely on the Lagrangian side. It is this variational approach that we will use in the next sections to extend the multisymplectic formalism to the nonsmooth context.

3.2 Variational Multisymplectic Geometry in a Nonsmooth Setting

We now consider the variational approach to multisymplectic field theory of Marsden et al. [1998] and formulate it a nonsmooth setting. A novelty of this variational approach is that it considers *arbitrary* and not only *vertical* variations of sections. The motivation for such a generalization is that, even though both the vertical and arbitrary variations result in the same Euler-Lagrange equations, the Cartan form obtained from the vertical variations is missing one term (corresponding to the $d^{n+1}x$ form). However, the horizontal variations account precisely for this extra term and make the Cartan form complete.

We reconsider the need for horizontal variations in the nonsmooth context and adapt the formalism developed in Marsden et al. [1998] to give a rigorous derivation of the jump conditions when fields are allowed to be nonsmooth.

3.2.1 Nonsmooth Multisymplectic Geometry

Let U be a manifold with smooth closed boundary. In the smooth context, the configuration space is the infinite-dimensional manifold defined by an appropriate closure of the set of smooth maps

$$\mathcal{C}^\infty = \{\phi : U \to Y \mid \pi_{XY} \circ \phi : U \to X \text{ is an embedding}\}.$$

In the the nonsmooth setting, we must also introduce a codimension 1 submanifold $D \subset U$, called the ***singularity submanifolds*** across which the fields ϕ may have singularities. For example, the submanifold D may be the spacetime surface separating two regions of a continuous medium or, in the case of two elastic bodies colliding, D may be the spacetime contact set.

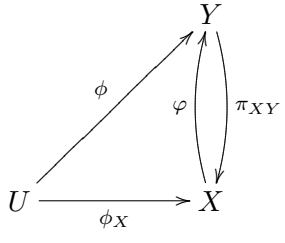
For the smooth case, the observation that the configuration space is a smooth manifold enables the use of differential calculus on the manifold of mappings as required by variational principles (see Marsden and Ratiu [1999], Marsden et al. [1998]). In this subsection we will present various types of configuration spaces that one must consider in the nonsmooth context and discuss their manifold structure.

Configuration spaces The applications that we present in the next sections require different configuration spaces, according to the type of singularities that we allow across the singularity submanifold D.

Case (a). Continuous but nonsmooth For the first examples presented in this chapter (such as rigid-body dynamics with impact and propagating singular surfaces within a continuum medium), the configuration space is the set of continuous maps

$$\begin{aligned}\mathcal{C}^a = \{\phi : U \to Y \mid \pi_{XY} \circ \phi : U \to X \text{ is an embedding,} \\ \phi \text{ is } C^0 \text{ in } U \text{ and of class } C^2 \text{ in } U \setminus D\}.\end{aligned} \tag{3.17}$$

For each $\phi \in \mathcal{C}^a$, we set $\phi_X = \pi_{XY} \circ \phi$ and $U_X = \pi_{XY} \circ \phi(U)$, $D_X = \pi_{XY} \circ \phi(D)$, so that $\phi_X : U \to U_X$ and its restriction to D are diffeomorphisms. We also denote the section $\phi \circ {\phi_X}^{-1}$ by φ, as in



The submanifold D separates the interior of U into two disjoint open subsets U^+ and U^-, that is $\text{int}(U) = U^+ \cup U^- \cup (U \cap D)$ and we let $U_X^+ = \phi_X(U^+)$ and $U_X^- = \phi_X(U^-)$ be their corresponding images in X. It follows that $\text{int}(U_X) = U_X^+ \cup U_X^- \cup (U_X \cap D_X)$.

Remark 1. *For particle mechanics, the formalism reduces to the spacetime formulation that we developed in Chapter 2 (see also Fetecau et al. [2003a]) to study nonsmooth rigid-body dynamics. We will discuss this example in detail in Section 3.3.*

Case (b). Discontinuous without separation (slip) For problems such as propagation of free surfaces in fluids or interaction of an elastic body and a fluid, the configuration map ϕ is no longer continuous. We must therefore choose a new configuration space to include these cases. Observe that in such problems the fluid-fluid and the solid-fluid boundaries are material surfaces, in the sense that particles which are on the separating surface at a given time remain on the surface at later times.

Let U_S and U_F be two open subsets of U such that $\partial U_S = \partial U_F = D$ is a codimension 1 submanifold in U. We adopt the subscripts S and F because one of the applications of this general setting will be solid-fluid interactions; U_S, U_F and D will be interpreted as the spacetime regions of the solid, the fluid and of the surface separating the two materials, respectively. For fluid-fluid boundaries, D is the spacetime free surface.

The requirement that there be no flow across the material interface is expressed by considering the configuration space

$$\begin{aligned}\mathcal{C}^b = \{&\phi : U \to Y \mid \pi_{XY} \circ \phi : U \to X \text{ is an embedding,} \\ &\phi \text{ is of class } C^2 \text{ in } U_S \cup U_F \text{ and } \overline{\phi_S}(D) = \overline{\phi_F}(D) = \phi(D)\},\end{aligned} \tag{3.18}$$

where ϕ_S, ϕ_F are the restrictions of the map ϕ on U_S, U_F, respectively, and the notation $\overline{f}$ represents the continuous extension of the map f to the closure of its domain.

Remark 2. *One may alternatively denote U_S and U_F by U^+ and U^-, respectively. This will be particularly useful in §3.2.2, where we retain only these notations for the domains where there are no singularities. As in case (a), we denote by U_X^+, U_X^- and D_X the images in X of U^+, U^- and D, under ϕ_X,.*

Case (c). Discontinuous with separation (collisions) Collisions of elastic bodies may exhibit both of the features of the two classes of configuration maps presented so far. The mechanical impact of two solids generates stress waves that propagate through their bodies, reflect on the boundaries and then return to the contact interface. At the instant when a returning wave first reaches the contact surface, the release begins and separation will eventually occur. Because of the complicated, non-linear structure of the governing equations, little of a general nature may be presented for impact problems. We refer to Graff [1991] for a detailed discussion on the longitudinal impact of two elastic rods and on the impact of an elastic sphere with a rod, to demonstrate some of the complexities encountered in such problems.

We will consider the frictionless impact with slipping of two elastic bodies. The analog of D from the previous paragraphs will be the spacetime contact set. However, to the contact set in the spatial configuration, there correspond two distinct surfaces in the reference configuration. In the multisymplectic formalism we consider two disjoint open sets U_1 and

U_2 in U and $D_1 \subset \partial U_1$, $D_2 \subset \partial U_2$ two codimension 1 submanifolds. We consider the following set as the configuration space for collision problems

$$\begin{aligned}\mathcal{C}^c = \{\phi : U \to Y \mid \pi_{XY} \circ \phi : U \to X \text{ is an embedding,} \\ \phi \text{ is of class } C^2 \text{ in } U \text{ and } \overline{\phi}(D_1) = \overline{\phi}(D_2)\},\end{aligned} \tag{3.19}$$

where the notation $\overline{f}$ represents, as before, the continuous extension of the map f.

Remark 3. *The set $\overline{\phi}(D_1)$ (or equivalently, $\overline{\phi}(D_2)$) must be interpreted as a* subset *of the spacetime contact set. The subset does not contain points which belong to other types of discontinuity surfaces (such as, for example, the points on the interface at the very moment of impact, which also belong to $\mathcal{C}^a$ type waves that are generated by the mechanical impact and propagate through the bodies). Intersections of different types of discontinuity surfaces are extremely important and we intend to treat this subject in our future work on this topic. We will thus not discuss this point further here.*

Remark 4. *For a more unified presentation and to include all three cases a-c in the general result from Section 3.2.2, we will refer later to U_1 and U_2 as U^+ and U^-.*

Remark 5. *For purposes of connecting this work with PDE methods, one can consider the closure of either of $\mathcal{C}^{a-c}$ in the topology of a larger space such as $H^s(U, Y)$ or $\mathcal{C}^\infty(U^+, Y) \times \mathcal{C}^\infty(U^-, Y)$. This enables one to regard $\mathcal{C}^{a-c}$ as subsets in a manifold of mappings of the appropriate Sobolev class, as in Palais [1968] and Ebin and Marsden [1970].*

Remark 6. *In the remainder of the chapter we will write $\mathcal{C}^{a-c}$ to indicate the appropriate configuration space with the manifold structure obtained by the procedure explained above. However, whenever we state a general result which applies to all configuration manifolds a-c, we will write $\mathcal{C}$ to mean any of the three.*

Variations and tangent spaces We will account for general variations of maps $\phi \in \mathcal{C}$ induced by a family of maps ϕ^λ defined by the action of some Lie group. More precisely, let $\mathcal{G}$ be a Lie group of π_{XY}-bundle automorphism η_Y covering diffeomorphisms η_X, with Lie algebra $\mathfrak{g}$, acting on $\mathcal{C}$ by $\Phi : \mathcal{G} \times \mathcal{C} \to \mathcal{C}$, where

$$\Phi(\eta_Y, \phi) = \eta_Y \circ \phi. \tag{3.20}$$

Now let $\lambda \mapsto \eta_Y^\lambda$ be an arbitrary smooth path in $\mathcal{G}$ such that $\eta_Y^0 = \mathrm{Id}_Y$, and let $V \in T_\phi \mathcal{C}$ be given by

$$V = \frac{d}{d\lambda}\bigg|_{\lambda=0} \Phi(\eta_Y^\lambda, \phi), \quad \text{and} \quad V_X = \frac{d}{d\lambda}\bigg|_{\lambda=0} \eta_X^\lambda \circ \phi_X. \tag{3.21}$$

We define the vertical component $V_y Y$ of the tangent space at y to be

$$V_y Y = \{\mathcal{V} \in T_y Y \mid T\pi_{XY} \cdot \mathcal{V} = 0\}. \tag{3.22}$$

Using this, we can naturally split the tangent space at each point $y = \phi(u)$ in the image of ϕ into vertical and horizontal components, $T_y Y = V_y Y \oplus H_y Y$, where

$$H_y Y = T_u \phi \cdot T_u U.$$

This decomposition of $T_y Y$ induces a decomposition of $T_\phi \mathcal{C}$, so that any vector $V \in T_\phi \mathcal{C}$ may be decomposed as $V = V^h + V^v$, where

$$V^h = T(\phi \circ \phi_X^{-1}) \cdot V_X, \tag{3.23}$$

and by (3.21), $V_X = T\pi_{XY} \cdot V$.

Case (a). For $\phi \in \mathcal{C}^a$, it is easy to show that the tangent space $T_\phi \mathcal{C}^a$ is given by

$$\begin{aligned} T_\phi \mathcal{C}^a = \{&V : U \to TY \mid V \text{ is } C^0 \text{ in } U \text{ and of class } C^2 \text{ in } U \setminus D, \\ &\pi_{Y,TY} \circ V = \phi \text{ and } T_{\pi_{XY}} \circ V = V_X \text{ is a vector field on } X\}. \end{aligned} \tag{3.24}$$

Case (b). In the multisymplectic description of a continuum medium, the bundle Y over X is trivial. It consists of a fiber manifold M (also called the ambient space) attached to each point of the spacetime $X = B \times \mathbb{R}$ (B is called the reference configuration). The fiber components of the points $\phi(u)$ with $u \in D$ (the interface in the reference configuration) constitute the image of the interface in the spatial configuration.

By constructing variations of maps $\phi \in \mathcal{C}^b$ as in (3.20), we can prove the following lemma

Lemma 3. *Let N_A be the outward unit normal of the current configuration interface and $V = (V^\mu, V^A)$ be a tangent vector obtained by (3.21). Then, $[\![V^A(u)]\!] N_A = 0$, for all $u \in D$.*

Proof. Let us first explain the sense in which the jump condition of this lemma must be interpreted. A point $y \in D$ is mapped by ϕ to a point $\phi(y) \in Y$ and denote by y the fiber component of $\phi(y)$ (y is a point on the current interface). By definition (3.18), there exist two points $y_S, y_F \in D$ such that $\overline{\phi_S}(y_S) = \overline{\phi_F}(y_F) = \phi(y)$.

Consider now a variation of a map $\phi \in \mathcal{C}^b$ given by $\phi^\lambda = \eta_Y^\lambda \circ \phi$, where η_Y^λ are π_{XY}-bundle automorphisms covering diffeomorphisms η_X and $\eta_Y^0 = \mathrm{Id}_Y$. By $[\![V(x)]\!]$ we mean

$$[\![V(u)]\!] = \left.\frac{d}{d\lambda}\right|_{\lambda=0} \overline{\phi_S^\lambda}(u_S) - \left.\frac{d}{d\lambda}\right|_{\lambda=0} \overline{\phi_F^\lambda}(u_F), \tag{3.25}$$

where ϕ_S^λ, ϕ_F^λ are the restrictions of the map ϕ^λ on U_S, U_F, respectively. The two terms in the right-hand side of (3.25) are vectors in $T_{\phi(u)}Y$, so the addition operation makes sense.

Since $\phi^\lambda \in \mathcal{C}^b$, there exists a point $u_F^\lambda \in D$ such that

$$\overline{\phi_S^\lambda}(u_S) = \overline{\phi_F^\lambda}(u_F^\lambda).$$

We note that $u_F^0 = u_F$. Then, we can derive

$$\left.\frac{d}{d\lambda}\right|_{\lambda=0} \overline{\phi_S^\lambda}(u_S) = \left.\frac{d}{d\lambda}\right|_{\lambda=0} \overline{\phi_F^\lambda}(u_F) + T\overline{\phi_F}(u_F) \cdot v, \tag{3.26}$$

where

$$v = \left.\frac{d}{d\lambda}\right|_{\lambda=0} u_F^\lambda \in T_{u_F} D. \tag{3.27}$$

By using (3.26), (3.25) becomes

$$[\![V(u)]\!] = T\overline{\phi_F}(u_F) \cdot v. \tag{3.28}$$

Now, (3.27) and (3.28) prove the lemma. ■

Using the same notation as before, we thus proved

$$\begin{aligned} T_\phi \mathcal{C}^b = \{V : U \to TY \mid V \text{ is of class } C^2 \text{ in } U_S \cup U_F, \pi_{Y,TY} \circ V = \phi, \\ T_{\pi_{XY}} \circ V = V_X \text{ is a vector field on } X, \text{ and } [\![V^A]\!] N_A = 0 \text{ on } D\}. \end{aligned} \tag{3.29}$$

Case (c). A result very similar to Lemma 3 will hold for case (c) as well. More precisely, consider two points $u_1 \in D_1$ and $u_2 \in D_2$ such that $\overline{\phi}(u_1) = \overline{\phi}(u_2) = y$. By an argument

similar to the one used in the proof of Lemma 3, we can prove

$$V(u_2) - V(u_1) = T\overline{\phi}(u_1) \cdot v, \tag{3.30}$$

where $v \in T_{u_1} D_1$. Then, $V(u_2) - V(u_1) \in T_y Y$ and, if we denote by N_A the components of the outward unit normal of the contact set in the current configuration, we abuse the notation and write

$$[\![V^A]\!] N_A = 0.$$

Hence, the tangent space $T_\phi \mathcal{C}^c$ is given by

$$\begin{aligned} T_\phi \mathcal{C}^c = \{V : U \to TY \mid V \text{ is of class } C^2 \text{ in } U_1 \cup U_2, \pi_{Y,TY} \circ V = \phi, \\ T_{\pi_{XY}} \circ V = V_X \text{ is a vector field on } X \text{ and } [\![V^A]\!] N_A = 0 \text{ on } D\}, \end{aligned} \tag{3.31}$$

where the jump relation has the interpretation explained before.

3.2.2 Variational Approach

We will show next how to derive the equations of motion and the jump conditions directly from the variational principle, staying entirely on the Lagrangian side.

The ***action function*** $S : \mathcal{C} \to \mathbb{R}$ is defined by

$$S(\phi) = \int_{U_X} \mathcal{L}(j^1(\phi \circ \phi_X^{-1})). \tag{3.32}$$

We say that $\phi \in \mathcal{C}$ is a ***stationary point*** or ***critical point*** of S if

$$\left.\frac{d}{d\lambda}\right|_{\lambda=0} S(\Phi(\eta_Y^\lambda, \phi)) = 0 \tag{3.33}$$

for all curves η_Y^λ with $\eta_Y^0 = \mathrm{Id}_Y$.

Using the infinitesimal generators defined in (3.21), we compute:

$$\begin{aligned} dS_\phi \cdot V &= \left.\frac{d}{d\lambda}\right|_{\lambda=0} S(\Phi(\eta_Y^\lambda, \phi)) \\ &= \left.\frac{d}{d\lambda}\right|_{\lambda=0} \int_{\eta_X^\lambda(U_X)} \mathcal{L}(j^1(\Phi(\eta_Y^\lambda, \phi))) \\ &= \int_{U_X} \left.\frac{d}{d\lambda}\right|_{\lambda=0} \mathcal{L}(j^1(\Phi(\eta_Y^\lambda, \phi))) + \int_{U_X} \mathfrak{L}_{V_X} \left[\mathcal{L}(j^1(\phi \circ \phi_X^{-1}))\right]. \end{aligned}$$

In Marsden et al. [1998] the following lemma is proved.

Lemma 4. *For any $V \in T_\phi \mathcal{C}$,*

$$dS_\phi \cdot V^h = \int_{\partial U_X} V_X \lrcorner \left[\mathcal{L}(j^1(\phi \circ \phi_X^{-1}))\right], \tag{3.34}$$

and

$$dS_\phi \cdot V^v = \int_{U_X} \left.\frac{d}{d\lambda}\right|_{\lambda=0} \mathcal{L}(j^1(\Phi(\eta_Y^\lambda, \phi))). \tag{3.35}$$

The previous lemma leads to the following fundamental theorem.

Theorem 3. *Given a Lagrangian density $\mathcal{L} : J^1Y \to \Lambda^{n+1}(X)$, which is smooth away from the discontinuity, there exists a unique smooth section $D_{EL}\mathcal{L} \in C^\infty(Y'', \Lambda^{n+1}(X) \otimes T^*Y))$ and a unique differential form $\Theta_\mathcal{L} \in \Lambda^{n+1}(J^1Y)$ such that for any $V \in T_\phi \mathcal{C}$ which is compactly supported in U and any open subset U_X such that $\overline{U_X} \cap \partial X = \emptyset$,*

$$\begin{aligned} dS_\phi \cdot V = &\int_{U_X^+} D_{EL}\mathcal{L}(j^2(\phi \circ \phi_X^{-1})) \cdot V + \int_{U_X^-} D_{EL}\mathcal{L}(j^2(\phi \circ \phi_X^{-1})) \cdot V \\ &+ \int_{U_X \cap D_X} [\![j^1(\phi \circ \phi_X^{-1})^* \left(j^1(V) \lrcorner \Theta_\mathcal{L}\right)]\!], \end{aligned} \tag{3.36}$$

where $[\![\cdot]\!]$ denotes the jump.

Furthermore,

$$D_{EL}\mathcal{L}(j^2(\phi \circ \phi_X^{-1})) \cdot V = j^1(\phi \circ \phi_X^{-1})^*[j^1(V) \lrcorner \Omega_\mathcal{L}]. \tag{3.37}$$

In coordinates, the action of the ***Euler-Lagrange derivative*** $D_{EL}\mathcal{L}$ *on* Y'' *is given by*

$$\begin{aligned} D_{EL}\mathcal{L}(j^2(\phi\circ\phi_X^{-1})) = \Bigg[&\frac{\partial L}{\partial y^A}(j^1(\phi\circ\phi_X^{-1})) - \frac{\partial^2 L}{\partial x^\mu \partial v^A{}_\mu}(j^1(\phi\circ\phi_X^{-1})) \\ &- \frac{\partial^2 L}{\partial y^B \partial v^A{}_\mu}(j^1(\phi\circ\phi_X^{-1}))\cdot(\phi\circ\phi_X^{-1})^B_{,\mu} \\ &- \frac{\partial^2 L}{\partial v^B{}_\mu \partial v^A{}_\nu}(j^1(\phi\circ\phi_X^{-1}))\cdot(\phi\circ\phi_X^{-1})^B_{,\mu\nu}\Bigg] d^{n+1}x\otimes dy^A, \end{aligned} \tag{3.38}$$

while the form $\Theta_{\mathcal{L}}$ *matches the definition of the* ***Cartan form*** *obtained via the Legendre transform and has the coordinate expression*

$$\Theta_{\mathcal{L}} = \frac{\partial L}{\partial v^A{}_\mu} dy^A \wedge d^n x_\mu + \left(L - \frac{\partial L}{\partial v^A{}_\mu} v^A{}_\mu\right) d^{n+1}x. \tag{3.39}$$

Proof. We choose $U_X = \phi_X(U)$ small enough so that it is contained in a coordinate chart O. In the coordinates on O, let $V = (V^\mu, V^A)$ so that along $\phi\circ\phi_X^{-1}$, the decomposition (3.23) can be written as

$$V_X = V^\mu \frac{\partial}{\partial x^\mu} \text{ and } V^v = (V^v)^A \frac{\partial}{\partial y^A} = \left(V^A - V^\mu \frac{\partial(\phi\circ\phi_X^{-1})^A}{\partial x^\mu}\right)\frac{\partial}{\partial y^A}.$$

Now, we use (3.35) to obtain

$$\begin{aligned} dS_\phi \cdot V^v = \int_{U_X} \Bigg[&\frac{\partial L}{\partial y^A}(j^1(\phi\circ\phi_X^{-1}))\cdot(V^v)^A \\ &+ \frac{\partial L}{\partial v^A{}_\mu}(j^1(\phi\circ\phi_X^{-1}))\cdot\frac{\partial (V^v)^A}{\partial x^\mu}\Bigg] d^{n+1}x. \end{aligned} \tag{3.40}$$

We split the integral $\int_{U_X}$ into $\int_{U_X^+} + \int_{U_X^-}$ and integrate by parts to obtain

$$\begin{aligned} dS_\phi \cdot V^v = &\int_{U_X^+}\left[\frac{\partial L}{\partial y^A}(j^1(\phi\circ\phi_X^{-1})) - \frac{\partial}{\partial x^\mu}\frac{\partial L}{\partial v^A{}_\mu}(j^1(\phi\circ\phi_X^{-1}))\right] \\ &\qquad\cdot (V^v)^A d^{n+1}x \\ &+ \int_{U_X^-}\left[\frac{\partial L}{\partial y^A}(j^1(\phi\circ\phi_X^{-1})) - \frac{\partial}{\partial x^\mu}\frac{\partial L}{\partial v^A{}_\mu}(j^1(\phi\circ\phi_X^{-1}))\right] \\ &\qquad\cdot (V^v)^A d^{n+1}x \\ &+ \int_{U_X\cap D_X}\left[\!\!\left[\frac{\partial L}{\partial v^A{}_\mu}(j^1(\phi\circ\phi_X^{-1}))\cdot(V^v)^A\right]\!\!\right] d^n x_\mu. \end{aligned} \tag{3.41}$$

The jump arises from the different orientations of D_X when we use Stokes theorem in U_X^+ and U_X^-. Additionally, from (3.34) we obtain the horizontal contribution

$$dS_\phi \cdot V^h = \int_{U_X \cap D_X} [\![V^\mu L]\!] d^{n+1}x. \tag{3.42}$$

We note that the terms corresponding to $\int_{\partial U_X}$ vanish in both (3.41) and (3.42) since V is compactly supported in U. Now, we can combine (3.41) and (3.42) to obtain

$$\begin{aligned} dS_\phi \cdot V = \int_{U_X^+ \cup U_X^-} \left\{ \left[\frac{\partial L}{\partial y^A} - \frac{\partial}{\partial x^\mu} \frac{\partial L}{\partial v_\mu^A} \right] (j^1(\phi \circ \phi_X^{-1})) \right\} d^{n+1}x \otimes dy^A \cdot V \\ + \int_{U_X \cap D_X} \Bigg[\!\!\Bigg[V \lrcorner \left\{ \frac{\partial L}{\partial v_\mu^A} (j^1(\phi \circ \phi_X^{-1})) dy^A \wedge d^n x_\mu \right. \\ \left. + \left[L - \frac{\partial L}{\partial v_\mu^A} (j^1(\phi \circ \phi_X^{-1})) \frac{\partial (\phi \circ \phi_X^{-1})^A}{\partial x^\mu} \right] d^{n+1}x \right\} \Bigg]\!\!\Bigg]. \end{aligned} \tag{3.43}$$

Let α be the n-form in the jump brackets of the integrand of the boundary integral in (3.43). Then, $\int_{U_X \cap D_X} \alpha = \int_{j^1(\phi \circ \phi_X^{-1})(U_X \cap D_X)} \alpha$, since α is invariant under this lift. Moreover, the vector V in the second term of (3.43) (now written as an integral over $j^1(\phi \circ \phi_X^{-1})(U_X \cap D_X)$) may be replaced by $j^1(V)$ since $\pi_{Y,J^1(Y)}$-vertical vectors are in the kernel of the form that V is acting on. Now we can pull back the integrand with $j^1(\phi \circ \phi_X^{-1})^*$ to get an n-form on $U_X \cap D_X$. To summarize, we proved that the boundary integral in (3.43) can be written as

$$\int_{U_X \cap D_X} [\![j^1(\phi \circ \phi_X^{-1})^* \left(j^1(V) \lrcorner \Theta_{\mathcal{L}} \right)]\!],$$

where $\Theta_{\mathcal{L}} \in \Lambda^{n+1}(J^1(Y))$ has the coordinate expression given by (3.39).

The integrand of the first integral in (3.43) defines the coordinate expression of the Euler-Lagrange derivative $D_{EL}\mathcal{L}$. However, if we choose another coordinate chart O', the coordinate expressions of $D_{EL}\mathcal{L}$ and $\Theta_{\mathcal{L}}$ must agree on the overlap $O \cap O'$ since the left hand side of (3.36) is intrinsically defined. Thus, we have uniquely defined $D_{EL}\mathcal{L}$ and $\Theta_{\mathcal{L}}$.

Now, we can define intrinsically $\Omega_{\mathcal{L}} = -d\Theta_{\mathcal{L}}$ and check that (3.37) holds, as both sides have the same coordinate expressions. ■

We now use Hamilton's principle of critical action and look for those paths $\phi \in \mathcal{C}$ which

are critical points of the action function. More precisely, we call a field $\phi \in \mathcal{C}$ a ***solution*** if

$$dS(\phi) \cdot V = 0, \tag{3.44}$$

for all vector fields $V \in T_\phi \mathcal{C}$ which vanish on the boundary ∂U.

From Theorem 3 it follows that a field ϕ is a solution if and only if the Euler-Lagrange derivative (evaluated at $j^2(\phi \circ \phi_X^{-1})$) is zero on U_X^+ and U_X^- and the n-form $j^1(\phi \circ \phi_X^{-1})^* \left[j^1(V) \lrcorner \Theta_{\mathcal{L}} \right]$ has a zero jump across $U_X \cap D_X$.

We thus obtain the Euler-Lagrange equations in U_X^+ and U_X^-, away from the singularities. In coordinates, they read

$$\frac{\partial L}{\partial y^A}(j^1(\phi \circ \phi_X^{-1})) - \frac{\partial}{\partial x^\mu} \frac{\partial L}{\partial v^A{}_\mu}(j^1(\phi \circ \phi_X^{-1})) = 0 \quad \text{in} \quad U_X^+ \cup U_X^-. \tag{3.45}$$

Finally, the intrinsic jump condition

$$\int_{U_X \cap D_X} \left[\!\!\left[j^1(\phi \circ \phi_X^{-1})^* \left(j^1(V) \lrcorner \Theta_{\mathcal{L}} \right) \right]\!\!\right] = 0 \tag{3.46}$$

has the following coordinate expression

$$\begin{aligned} \int_{U_X \cap D_X} \Bigg(& \left[\!\!\left[\frac{\partial L}{\partial v^A{}_\mu}(j^1(\phi \circ \phi_X^{-1})) \cdot V^A \right]\!\!\right] \\ & + \left[\!\!\left[L V^\mu - \frac{\partial L}{\partial v^A{}_\mu}(j^1(\phi \circ \phi_X^{-1})) \frac{\partial (\phi \circ \phi_X^{-1})^A}{\partial x^\nu} V^\nu \right]\!\!\right] \Bigg) d^n x_\mu = 0. \end{aligned} \tag{3.47}$$

In the next section we will write the jump conditions (3.47) for the particle and continuum mechanics multisymplectic models and give their physical interpretations. Here, we simply note that by taking vertical variations only ($V^\mu = 0$) we obtain a jump condition involving only momenta $p_A{}^\mu$; this will represent the jump in linear momentum condition. Horizontal variations will in turn give the correct energy jump and a kinematic compatibility condition.

3.3 Classical Mechanics

For a classical mechanical system (such as particles or rigid bodies) with configuration space Q, let $X = \mathbb{R}$ (parameter time) and $Y = \mathbb{R} \times Q$, with π_{XY} the projection onto the first factor. The first jet bundle $J^1 Y$ is the bundle whose holonomic sections are tangents of

sections $\phi : X \to Y$, so we can identify $J^1Y = \mathbb{R} \times TQ$. Using coordinates (t, q^A) on $\mathbb{R} \times Q$, the induced coordinates on J^1Y are the usual tangent coordinates (t, q^A, v^A).

We will apply the multisymplectic formalism described in Section 3.1 to nonsmooth rigid-body dynamics. We are particularly interested in the problem of rigid-body collisions, for which the velocity, acceleration and forces are all nonsmooth or even discontinuous. The multisymplectic formalism will elegantly recover the spacetime formulation of nonsmooth Lagrangian mechanics from Chapter 2 (see Fetecau et al. [2003a]).

In Chapter 2, a mechanical system with configuration manifold Q is considered, but with the dynamics restricted to a submanifold with boundary $C \subset Q$, which represents the subset of admissible configurations. The boundary ∂C is called the contact set; for rigid body collision problems, the submanifold ∂C is obtained from the condition that interpenetration of matter cannot occur. The dynamics is specified by a regular Lagrangian $L : TQ \to \mathbb{R}$. We note that the multisymplectic framework allows us to consider time dependent Lagrangians as well (see the general definition of a Lagrangian density in Section 3.1), but we will restrict our discussion here to only autonomous systems.

To apply the multisymplectic formalism for such systems, we choose U to be the interval $[0, 1]$ and D the set containing only one element $\tau_i \in [0, 1]$. The set $\mathcal{C}^a$ from (3.17) becomes

$$\begin{aligned} \mathcal{C}' = \{\phi : [0,1] \to \mathbb{R} \times Q \mid \phi \text{ is a } C^0, PW\ C^2 \text{ curve }, \\ \phi(\tau) \text{ has only one singularity at } \tau_i\}. \end{aligned} \tag{3.48}$$

Now let $U_X = [t_0, t_1]$ be the image in $X = \mathbb{R}$ of the embedding $\phi_X = \pi_{XY} \circ \phi$. The section $\varphi = \phi \circ \phi_X^{-1} : [t_0, t_1] \to \mathbb{R} \times Q$ can be written in coordinates as $t \mapsto (t, q^A(t))$. Let $t_i = \phi_X(\tau_i)$ be the the moment of impact, so that $q(t_i) \in \partial C$. We note that, even though the singularity parameter time τ_i is fixed, it is allowed to vary in the t space according to $t_i = \phi_X(\tau_i)$ and thus, the setting is not restrictive in this sense.

Hence, the map $\phi_X : [0, 1] \to [t_0, t_1]$ is just a time reparametrization. The need for a nonautonomous formulation of an autonomous mechanical system is explained in the following remarks.

Remark 7. *In the smooth context, the dynamics of a mechanical system can be described by sections of smooth fields $\varphi : [t_0, t_1] \to Q$. As we noted in the general setting, the key observation that the set of such smooth fields is a C^∞ infinite-dimensional manifold enables*

the use of differential calculus on the manifold of mappings (see Marsden and Ratiu [1999]). However, generalization to the nonsmooth setting is not straightforward and this is one of the main issues addressed in Fetecau et al. [2003a].

Remark 8. *The approach used in Chapter 2 is to extend the problem to the nonautonomous case, so that both configuration variables and time are functions of a separate parameter τ. This allows the impact to be fixed in τ space while remaining variable in both configuration and time spaces, and it means that the relevant space of configurations will indeed be a smooth manifold, as proved in Chapter 2. The nonsmooth multisymplectic formalism applied to this problem leads to essentially the same extended formulation.*

The Cartan form (3.39) becomes the extended Lagrange 1-form of particle mechanics, with coordinate expression

$$\Theta_{\mathcal{L}} = \frac{\partial L}{\partial \dot{q}^A} dq^A + \left(L - \frac{\partial L}{\partial \dot{q}^A} \dot{q}^A \right) dt. \tag{3.49}$$

Define the ***energy*** $E : TQ \to \mathbb{R}$ by

$$E(q, \dot{q}) = \frac{\partial L}{\partial \dot{q}}(q, \dot{q}) \cdot \dot{q} - L(q, \dot{q}),$$

which allows us to write the Lagrangian 1-form in the compact notation

$$\Theta_{\mathcal{L}} = \frac{\partial L}{\partial \dot{q}} dq - E dt. \tag{3.50}$$

Let $V \in T_\phi \mathcal{C}$ be a tangent vector constructed as in (3.21) with coordinates $V = (V^0, V^A)$. As the fiber component of $\varphi(t_i)$ is varied in ∂C, we can write the jump condition (3.46) as

$$\Theta_{\mathcal{L}}|_{t_i^-} = \Theta_{\mathcal{L}}|_{t_i^+} \text{ on } \mathbb{R} \times TQ|\partial C. \tag{3.51}$$

In coordinates, the jump condition (3.51) reads

$$V^A \left. \frac{\partial L}{\partial \dot{q}^A} \right|_{t_i^-}^{t_i^+} + V^0 \left(L - \frac{\partial L}{\partial \dot{q}^A} \dot{q}^A \right) \Bigg|_{t_i^-}^{t_i^+} = 0. \tag{3.52}$$

Splitting this into the two components gives

$$\left.\frac{\partial L}{\partial \dot{q}}\right|_{t=t_i^-} \cdot \delta q = \left.\frac{\partial L}{\partial \dot{q}}\right|_{t=t_i^+} \cdot \delta q \tag{3.53}$$

for any $\delta q = V^A \frac{\partial}{\partial q^A} \in T_{q(t_i)}\partial C$ and

$$E(q(t_i^-), \dot{q}(t_i^-)) = E(q(t_i^+), \dot{q}(t_i^+)). \tag{3.54}$$

These equations are the Weierstrass-Erdmann type conditions for impact. That is, equation (3.53) states that the linear momentum must be conserved in the tangent direction to ∂C, while equation (3.54) states that the energy must be conserved during an elastic impact.

Hence, horizontal variations (V^0) give conservation of energy and vertical variations (V^A) give conservation of the Lagrange 1-form on $T\partial C$.

3.4 Continuum Mechanics

3.4.1 Multisymplectic Formulation of Continuum Mechanics

Configuration Spaces in the Multisymplectic Formalism We will use here the formalism constructed in Marsden et al. [2001] to describe the configurations of a continuous medium. Let (B, G) be a smooth n-dimensional compact oriented Riemannian manifold with smooth boundary and let (M, g) be a smooth N-dimensional compact oriented Riemannian manifold. The space (B, G) will represent what is traditionally called the ***reference configuration***, while (M, g) will denote the ***ambient space***.

We choose $X = B \times \mathbb{R}$; the coordinates on X are $x^\mu = (x^i, x^0) = (x^i, t)$, with $\mu = 0, \ldots, n,\ i = 1, \ldots, n$. Let $Y = X \times M$ be a trivial bundle over X with M being a fiber at each point and let $\pi_{XY} : Y \to X$; $(x, t, y) \mapsto (x, t)$ be the projection on the first factor ($y \in M$ is the fiber coordinate). Let $y^A,\ A = 1, \ldots, N$ be fiber coordinates; they induce the coordinates on J^1Y denoted $\gamma = (x^\mu, y^A, v^A{}_\mu)$. We denote the fiber coordinates on J^1Y^* by $(\Pi, p_A{}^\mu)$; they correspond to the affine map given in coordinates by $v^A{}_\mu \mapsto (\Pi + p_A{}^\mu v^A{}_\mu) d^{n+1}x$.

A section $\varphi : X \to Y$ of π_{XY} has coordinate representation $\varphi(x) = (x^\mu, \varphi^A(x))$, while

its first jet $j^1\varphi$ is given by

$$x^\mu \mapsto (x^\mu, \varphi^A(x), \partial_\mu \varphi^A(x)), \tag{3.55}$$

where $\partial_0 = \frac{\partial}{\partial t}$ and $\partial_k = \frac{\partial}{\partial x^k}$.

We note that we introduced two different Riemannian structures on the spatial part of the base manifold X and on the fiber M. Thus, the formalism is general enough to apply for continuum models where the metric spaces (B, G) and (M, g) are essentially different (rods, shells models, fluids with free boundary). However, for classical 2-D or 3-D elasticity or for fluid dynamics in a domain with fixed boundaries, the two Riemannian structures may coincide.

Define the function $J : J^1Y \to \mathbb{R}$ with coordinate expression

$$J(x, t, y, v) = \det[v]\sqrt{\frac{\det[g(y)]}{\det[G(x)]}}. \tag{3.56}$$

For a section φ, $J(j^1(\varphi))$ represents the Jacobian of the linear transformation $D\varphi_t$. We note that, even in the cases where the metrics G and g coincide, there is no cancellation in (3.56), as the metric tensors are evaluated at different points ($g(y)$ is different from $G(x)$ unless $y = x$ or both tensors are constant).

Lagrangian dynamics To describe the dynamics of a particular continuum medium in the variational multisymplectic framework, one needs to specify a Lagrangian density $\mathcal{L}$. The Lagrangian density $\mathcal{L} : J^1Y \to \Lambda^{n+1}X$ is defined as a smooth bundle map

$$\begin{aligned}\mathcal{L}(\gamma) = L(\gamma)d^{n+1}x = \mathbb{K} - \mathbb{P} = \frac{1}{2}\sqrt{\det[G]}\rho(x)g_{AB}v^A{}_0 v^B{}_0 d^{n+1}x \\ - \sqrt{\det[G]}\rho(x)W(x, G(x), g(y), v^A{}_j)d^{n+1}x,\end{aligned} \tag{3.57}$$

where $\gamma \in J^1Y$, $\rho : B \to \mathbb{R}$ is the mass density and W is the ***stored energy function***.

The first term in (3.57), when restricted to first jet extensions, represents the kinetic energy, as $v^A{}_0$ becomes the time derivative $\partial_t\varphi^A$ of the section φ. The second term represents the potential energy and different choices of the function W specify particular models of continuous media. Typically, for elasticity, W depends on the field's partial derivatives through the Green deformation tensor C (see Marsden and Hughes [1983], for example), while for ideal fluid dynamics, W is only a function of the Jacobian J (3.56).

The Lagrangian density (3.57) determines the Legendre transformation $\mathbb{F}\mathcal{L} : J^1Y \to J^1Y^*$. The conjugate momenta are given by

$$p_A{}^0 = \frac{\partial L}{\partial v^A{}_0} = \rho g_{AB} v^B{}_0 \sqrt{\det[G]}, \quad p_A{}^j = \frac{\partial L}{\partial v^A{}_j} = -\rho \frac{\partial W}{\partial v^A{}_j} \sqrt{\det[G]},$$

and

$$\Pi = L - \frac{\partial L}{\partial v^A{}_\mu} v^A{}_\mu = \left[-\frac{1}{2} g_{AB} v^A{}_0 v^B{}_0 - W + \frac{\partial W}{\partial v^A{}_j} v^A{}_j \right] \rho \sqrt{\det[G]}.$$

We define the ***energy density*** e by

$$e = \frac{\partial L}{\partial v^A{}_0} v^A{}_0 - L \quad \text{or, equivalently} \quad e\, d^{n+1}x = \mathbb{K} + \mathbb{P}. \tag{3.58}$$

The Cartan form on J^1Y can be obtained either by using the Legendre transformation and pulling back the canonical $(n+1)$-form on the dual jet bundle as in (3.9), or by a variational route as in Theorem 3. The resulting coordinate expression is given by

$$\begin{aligned} \Theta_{\mathcal{L}} = {} & \rho g_{AB} v^B{}_0 \sqrt{\det[G]} dy^A \wedge d^n x_0 - \rho \frac{\partial W}{\partial v^A{}_j} \sqrt{\det[G]} dy^A \wedge d^n x_j \\ & + \left[-\frac{1}{2} g_{AB} v^A{}_0 v^B{}_0 - W + \frac{\partial W}{\partial v^A{}_j} v^A{}_j \right] \rho \sqrt{\det[G]} d^{n+1}x. \end{aligned} \tag{3.59}$$

Substituting the Lagrangian density (3.57) into equation (3.45) we obtain the Euler-Lagrange equations for a continuous medium

$$\begin{aligned} \rho g_{AB} \left(\frac{D_g \dot{\varphi}}{Dt} \right)^B - \frac{1}{\sqrt{\det[G]}} \frac{\partial}{\partial x^k} \left(\rho \frac{\partial W}{\partial v^A_k} (j^1\varphi) \sqrt{\det[G]} \right) & \\ = -\rho \frac{\partial W}{\partial g_{BC}} \frac{\partial g_{BC}}{\partial y^A} (j^1\varphi), & \end{aligned} \tag{3.60}$$

where

$$\left(\frac{D_g \dot{\varphi}}{Dt} \right)^A = \frac{\partial \dot{\varphi}^A}{\partial t} + \gamma^A_{BC} \dot{\varphi}^B \dot{\varphi}^C \tag{3.61}$$

is the covariant time derivative, and

$$\gamma^A_{BC} = \frac{1}{2} g^{AD} \left(\frac{\partial g_{BD}}{\partial y^C} + \frac{\partial g_{CD}}{\partial y^B} - \frac{\partial g_{BC}}{\partial y^D} \right)$$

are the Christoffel symbols associated with the metric g.

Given a potential energy W which specifies the material, equation (3.60) is a system of PDE's to be solved for a section $\varphi(x,t)$. We remark that all terms in this equation are functions of x and t and hence have the interpretation of material quantities. In particular, (3.61) corresponds to ***material acceleration***.

We define the multisymplectic analogue of the ***Cauchy stress tensor*** σ by

$$\sigma^{AB}(\varphi, x) = \frac{2\rho(x)}{J}\frac{\partial W}{\partial g_{AB}}(j^1\varphi(x)). \tag{3.62}$$

Equation (3.62) is known in the elasticity literature as the Doyle-Ericksen formula. We make the important remark that the balance of angular momentum

$$\sigma^T = \sigma$$

follows from the definition (3.62) and the symmetry of the metric tensor g.

In the case of Euclidean manifolds with constant metrics g and G, equation (3.60) simplifies to the familiar expression

$$\rho\frac{\partial^2\varphi_A}{\partial t^2} = \frac{\partial}{\partial x^k}\left(\rho\frac{\partial W}{\partial v^A{}_k}(j^1\varphi)\right). \tag{3.63}$$

Next we will describe the multisymplectic formalism for the two main application of the theory we developed: elasticity and ideal fluid dynamics.

Elasticity As we noted before, for the theory of elasticity the reference configuration (B, G) and the ambient space (M, g) are generally different. The spatial part B of the base manifold X has the interpretation of the reference configuration and the extra dimension of X corresponds to time. Later configurations of the elastic body are captured by a section φ of the bundle Y. For a fixed time t, the sections φ_t play the role of ***deformations***; they map the reference configuration B onto the spatial configuration, which is a subset of the ambient space M.

The fiber coordinates of the first jet $j^1\varphi$ of a section φ, as defined by (3.55), consist of the time derivative of the deformation $\dot{\varphi}^A$ and the ***deformation gradient*** F_i^A given by

$$F_i^A(x,t) = \frac{\partial\varphi^A}{\partial x^i}. \tag{3.64}$$

Hence, the first jet of a section φ has the local representation

$$j^1\varphi : (x,t) \mapsto ((x,t), \varphi(x,t), \dot{\varphi}(x,t), F(x,t)).$$

For a given section φ, the ***first Piola-Kirchhoff stress tensor*** $\mathcal{P}_A{}^j$ is defined by

$$\mathcal{P}_A{}^j(\varphi, x) = \rho(x) \frac{\partial W}{\partial v^A{}_j}(j^1\varphi(x)). \tag{3.65}$$

We also define ***the Green deformation tensor*** (also called the right Cauchy-Green tensor) C by $C = \varphi_t^*(g)$; in coordinates we have

$$C_{ij}(x,t) = g_{AB} F_i^A F_j^B. \tag{3.66}$$

Using definitions (3.62) and (3.65), the Euler-Lagrange equations (3.60) become

$$\rho g_{AB} \left(\frac{D_g \dot{\varphi}}{Dt} \right)^B = \mathcal{P}_A{}^i{}_{|i} + \gamma_{AC}^B (\mathcal{P}_B^j F_j^C - J g_{BD} \sigma^{DC}), \tag{3.67}$$

where we have introduced the ***covariant divergence*** defined by

$$\mathcal{P}_A{}^i{}_{|i} = \mathrm{DIV}\mathcal{P} = \frac{\partial \mathcal{P}_A^i}{\partial x^i} + \mathcal{P}_A^j \Gamma_{jk}^k - \mathcal{P}_B^i \gamma_{AC}^B F_i^C. \tag{3.68}$$

Here, the Γ_{jk}^i are the Christoffel symbols corresponding to the base metric G.

We note that in (3.67) there is no a priori relationship between the first Piola-Kirchhoff stress tensor and the Cauchy stress tensor, as W is assumed to have the most general form $W(x, G, g, v)$. However, such a relationship can be derived by imposing material frame indifference on the energy function. This assumption will imply that the energy function W depends on the deformation gradient F (equivalently, on v) and on the field metric g only through the Green deformation tensor given by (3.66), that is $W = W(C(v, g))$. For this particular form of W, definitions (3.62) and (3.65) lead to

$$\mathcal{P}_A^i = J(\sigma F^{-1})_A^i. \tag{3.69}$$

Relation (3.69) is known as the Piola transformation law. Substituting it into (3.67), one

obtains the Euler-Lagrange equations for the standard elasticity model

$$\rho g_{AB}\left(\frac{D_g\dot{\varphi}}{Dt}\right)^B = \mathcal{P}_A^{\ i}{}_{|i}. \tag{3.70}$$

For elasticity in a Euclidean space, this equation simplifies to

$$\rho\frac{\partial^2\varphi^A}{\partial t^2} = \frac{\partial\mathcal{P}^{Ai}}{\partial x^i}. \tag{3.71}$$

Barotropic Fluids For ideal fluid dynamics we have the same multisymplectic bundle picture as that described for elasticity. For fluids moving in a fixed region we set $B = M$ and call it the ***reference fluid container***. However, for fluid dynamics with free boundary, the structures (B, G) and (M, g) are generally different. Configurations of the fluid are captured by a section φ of the bundle Y, which has the interpretation of the particle placement field. In coordinates, the spatial point $y \in Y_{(x,t)}$ corresponds to a position $y = \varphi(x, t)$ of the fluid particle x at time t.

For standard models of barotropic fluids, the potential energy of the fluid depends only on the Jacobian of the deformation, that is $W = W(J(g, G, v))$. The ***pressure*** function is defined to be

$$P(\varphi, x) = -\rho(x)\frac{\partial W}{\partial J}(j^1\varphi(x)). \tag{3.72}$$

For a given section φ, $P(\varphi) : X \to \mathbb{R}$ has the interpretation of the material pressure which is a function of the material density. Using (3.72), the Cauchy stress tensor (3.62) becomes

$$\sigma^{AB}(x) = \frac{2\rho}{J}\frac{\partial W}{\partial J}\frac{\partial J}{\partial g_{AB}}(j^1\varphi) = -P(x)g^{AB}(y(x)). \tag{3.73}$$

We refer to Marsden et al. [2001] for a discussion on how the pressure function arises in both the compressible and incompressible models. We also remark here that one could also consider (3.73) as a defining equation for pressure, from which (3.72) would follow.

With these notations, the Euler-Lagrange equations (3.60) become

$$\rho g_{AB}\left(\frac{D_g\dot{\varphi}}{Dt}\right)^B = -\frac{\partial P}{\partial x^k}J\left(\left(\frac{\partial\varphi}{\partial x}\right)^{-1}\right)_A^k. \tag{3.74}$$

We introduce the ***spatial density*** $\rho_{\text{sp}} = \rho/J$ and define the ***spatial pressure*** $p(y)$ by

$p(y(x)) = P(x)$; then (3.74) can be re-written in the familiar form

$$\frac{D_g\dot{\varphi}}{Dt}(x,t) = -\frac{1}{\rho_{\text{sp}}}\ \text{grad}\ p \circ \varphi(x,t). \tag{3.75}$$

3.4.2 Propagating Singular Surfaces within an Elastic Body

In this subsection we apply the theory developed in Section 3.2.1 to investigate the motion of a singular surface of order 1 within a compressible elastic body. The ***order*** of a singular surface is given by the lowest order of the derivatives of the configuration map $\phi(x,t)$ that suffer a non-zero jump across the surface. For a singular surface of order 1, the configuration map $\phi(x,t)$ is continuous, but its first-order derivatives (the velocity $\dot{\phi}$ and the deformation gradient F) may suffer jump discontinuities upon the surface. Thus, the configuration space for this problem belongs to class (a) of the classification considered in Section 3.2.1.

The multisymplectic formalism will lead to the derivation of the correct jumps in linear momentum and energy across the discontinuity surface. Moreover, spatial horizontal variations will lead to a kinematic condition known as the Maxwell compatibility condition.

We use the same notation as previously, so let U be diffeomorphic to an open subset of the spacetime X and let D be a codimension 1 submanifold in U representing a discontinuity surface in spacetime, moving within the elastic body. The configuration space $\mathcal{C}$ is given by (3.17) and all the results from Section 3.2 apply for this example.

We note first that Theorem 3 implies that the Euler-Lagrange equations (3.67) will be satisfied on either side of the discontinuity.

Now let $V \in T_\phi\mathcal{C}$ be a tangent vector with coordinates (V^μ, V^A) and consider initially only *vertical* variations ($V^\mu = 0$). From (3.47) we obtain the jump conditions

$$\int_{D_X} \left[\!\!\left[\frac{\partial L}{\partial v^A{}_\mu}(j^1(\phi \circ \phi_X^{-1})) \right]\!\!\right] \cdot V^A d^n x_\mu = 0, \tag{3.76}$$

where we used the continuity of the vector field V.

For simplicity, consider the Euclidean case, where $G_{\mu\nu} = \delta_{\mu\nu}$ and $g_{AB} = \delta_{AB}$. The jump relation (3.76) becomes

$$\int_{D_X} \left[\!\!\left[\rho(x)\frac{\partial \varphi^A}{\partial t} \right]\!\!\right] \cdot V^A d^n x_0 + \int_{D_X} [\![\mathcal{P}_A^{\ j}]\!] \cdot V^A d^n x_j = 0, \tag{3.77}$$

where, as before, φ denotes the section $\varphi = \phi \circ \phi_X^{-1}$.

The 1-forms dt and dx^j, $j = 1, \ldots, n$, on D_X are not independent. More precisely, if D_X is given locally by $f(t, x^1, \ldots, x^n) = 0$, then by differentiating we obtain

$$\partial_j f \, dx^j + \partial_t f \, dt = 0. \tag{3.78}$$

Define N_j by $N_j = \partial_j f / |\nabla_x f|$ and define the propagation speed U by

$$U = -\frac{\partial_t f}{|\nabla_x f|}, \tag{3.79}$$

where $|\cdot|$ represents the Euclidean norm. This speed is a measure of the rate at which the moving surface traverses the material; it also gives the excess of the normal speed of the surface over the normal speed of the particles comprising it. Then (3.77) becomes

$$\int_{D_X} \left(\left[\!\!\left[\rho U \frac{\partial \varphi^A}{\partial t} \right]\!\!\right] + \left[\!\!\left[\mathcal{P}_A^{\ j} \right]\!\!\right] N_j \right) \cdot V^A d^n x_0 = 0. \tag{3.80}$$

By a standard argument in the calculus of variations we can pass to the local form and recover the standard jump of linear momentum across a propagating singular surface of order 1, which is

$$\left[\!\!\left[\rho U \frac{\partial \varphi^A}{\partial t} \right]\!\!\right] + \left[\!\!\left[\mathcal{P}_A^{\ j} \right]\!\!\right] N_j = 0. \tag{3.81}$$

An alternative approach to derive the jump in linear momentum uses the balance of linear momentum for domains traversed by singular surfaces (see Truesdell and Toupin [1960], pg. 545 for example). For such derivations, the jump conditions are usually expressed in spatial coordinates, where the propagation speed U and the Piola-Kirchhoff stress tensor are replaced by a local propagation speed and the Cauchy stress tensor, respectively.

Remark 9. *The conservation of mass implies the following jump relation, known as the Stokes-Christoffel condition (see Truesdell and Toupin [1960], pg. 522)*

$$\left[\!\!\left[\rho U \right]\!\!\right] = 0. \tag{3.82}$$

In Courant and Friedrichs [1948], the continuous quantity ρU is denoted by m and is called

the mass flux *through the surface. Using (3.82), we can re-write (3.81) as*

$$\rho U \left[\!\!\left[\frac{\partial \varphi^A}{\partial t} \right]\!\!\right] + [\![\mathcal{P}_A^j]\!] N_j = 0. \tag{3.83}$$

Remark 10. *In the terminology of Truesdell and Toupin [1960], the singular surfaces that have a non-zero propagation speed are called* propagating *singular surfaces or* waves. *We first note that this definition excludes material surfaces, for which $U = 0$. Moreover, Truesdell and Toupin [1960] classifies the singular surfaces with non-zero jump in velocity into two categories: surfaces with transversal discontinuities ($[\![U]\!] = 0$), called* ***vortex sheets****, and surfaces with arbitrary discontinuities in velocity ($[\![U]\!] \neq 0$), called* ***shock surfaces****. One can conclude that there are no material shock surfaces, i.e., shock surfaces are always waves. Also, there is a nonzero mass flux ($m \neq 0$) through a shock surface or through a vortex sheet which is not material.*

Remark 11. *In the context of gas dynamics, Courant and Friedrichs [1948] define a* ***shock front*** *as a discontinuity surface across which there is a non-zero gas flow ($m \neq 0$). Then, a shock surface in the sense of Truesdell and Toupin [1960] is also a shock front.*

The linear momentum jump was derived by taking vertical variations of the sections. Next we will focus on *horizontal* variations ($V^\mu \neq 0$) and derive the corresponding jump laws. Using (3.81), the jump conditions (3.47) become

$$\int_{D_X} \left[\!\!\left[LV^\mu - \frac{\partial L}{\partial v_\mu^A} (j^1(\phi \circ \phi_X^{-1})) \frac{\partial (\phi \circ \phi_X^{-1})^A}{\partial x^\nu} V^\nu \right]\!\!\right] d^n x_\mu = 0. \tag{3.84}$$

Consider first only time component variations ($V^0 \neq 0$, $V^j = 0$ for $j = 1, \ldots, n$); then (3.84) gives

$$\begin{aligned} &\int_{D_X} \left[\!\!\left[L - \frac{\partial L}{\partial v_0^A} \frac{\partial (\phi \circ \phi_X^{-1})^A}{\partial t} \right]\!\!\right] V^0 d^n x_0 \\ &\quad - \int_{D_X} \left[\!\!\left[\frac{\partial L}{\partial v_j^A} \frac{\partial (\phi \circ \phi_X^{-1})^A}{\partial t} \right]\!\!\right] V^0 d^n x_j = 0. \end{aligned} \tag{3.85}$$

Using (3.65), (3.78) and (3.79), (3.85) becomes

$$\int_{D_X} \left([\![Ue]\!] + \left[\!\!\left[\mathcal{P}_A^j \frac{\partial \varphi^A}{\partial t} \right]\!\!\right] N_j \right) V^0 d^n x_0 = 0. \tag{3.86}$$

From (3.86) we recover the standard jump of energy (see Truesdell and Toupin [1960], pg. 610 for example),

$$[\![Ue]\!] + \left[\!\!\left[\mathcal{P}_A^j \frac{\partial \varphi^A}{\partial t} \right]\!\!\right] N_j = 0. \tag{3.87}$$

Finally we consider space component variations ($V^j \neq 0$) in (3.84) and use (3.86) to obtain

$$\begin{aligned} &\int_{D_X} \left[\!\!\left[\frac{\partial L}{\partial v_0^A} \frac{\partial (\phi \circ \phi_X^{-1})^A}{\partial x^j} V^j \right]\!\!\right] d^n x_0 \\ &\quad - \int_{D_X} \left[\!\!\left[L V^j - \frac{\partial L}{\partial v_j^A} \frac{\partial (\phi \circ \phi_X^{-1})^A}{\partial x^k} V^k \right]\!\!\right] d^n x_j = 0. \end{aligned} \tag{3.88}$$

Then, by using (3.65), (3.78), (3.79) and (3.82), (3.88) becomes

$$\int_{D_X} \left(\rho U \left[\!\!\left[F^A{}_j \frac{\partial \varphi^A}{\partial t} \right]\!\!\right] + [\![L]\!] N_j + [\![F^A{}_j \mathcal{P}_A{}^k]\!] N_k \right) V^j d^n x_0 = 0. \tag{3.89}$$

Since the components V^j are arbitrary we conclude that

$$\rho U \left[\!\!\left[F_j^A \frac{\partial \varphi^A}{\partial t} \right]\!\!\right] + [\![L]\!] N_j + [\![F_j^A \mathcal{P}_A^k]\!] N_k = 0. \tag{3.90}$$

Even though (3.90) does not resemble any standard conservation law, after some algebraic manipulations using (3.81) and (3.87), (3.90) can be rewritten, for continuous U, as

$$U\, [\![F_j^A]\!] + \left[\!\!\left[\frac{\partial \varphi^A}{\partial t} \right]\!\!\right] N_j = 0, \tag{3.91}$$

which is the statement of the Maxwell compatibility condition (see Jaunzemis [1967], Chapter 2 or Truesdell and Toupin [1960], Chapter C.III. for the derivation of the kinematical conditions of compatibility from Hadamard's lemma).

To summarize, the *vertical* variations of the sections led us to derive the jump in linear momentum, while *horizontal* time and space variations accounted for the energy balance and the kinematic compatibility condition, respectively.

3.4.3 Free Surfaces in Fluids and Solid-fluid Boundaries

Now, we investigate in the multisymplectic framework a different type of discontinuous motion that will illustrate the case (b) of the classification from Section 3.2.1. We consider two types of discontinuity surfaces, namely, *free surfaces* in fluids and *solid-fluid boundaries*.

A free surface or a free boundary is a surface separating two immiscible fluids or two regions of the same fluid in different states of motion (Karamcheti [1966]). The second type of discontinuity considers the interaction of a deformable elastic body with a surrounding barotropic fluid.

As we already noted in Section 3.2.1, these types of discontinuous surfaces have one feature in common, namely, they are material surfaces (particles which are on the surface at a given time remain on the surface at later times). Equivalently, there is no flow across the discontinuity and the surface is stationary relative to the medium. Hence, in the reference configuration, the surface D_X is given locally by $f(x^1, \ldots, x^n) = 0$ (no dependence of the function f on t). Moreover, from (3.79) we have that the propagation speed U for such surfaces is zero. In the terminology of Truesdell and Toupin [1960], these surfaces are material vortex sheets of order 0.

Free Surfaces in Fluids Theorem 3 implies that Euler-Lagrange equations of type (3.74) will be satisfied on either side of the surface separating the two fluid regions. Next, we will show that Theorem 3 gives the correct force balance on the separating surface and the other physical conditions that must be satisfied on such boundaries.

Let $V \in T_\phi \mathcal{C}$ be a tangent vector with coordinates (V^μ, V^A). We consider first only *vertical* variations ($V^\mu = 0$); from (3.47) we obtain the following jump conditions

$$\int_{D_X} \left[\!\!\left[\frac{\partial L}{\partial v_\mu^A}(j^1(\phi \circ \phi_X^{-1})) \cdot V^A \right]\!\!\right] d^n x_\mu = 0. \tag{3.92}$$

For simplicity, we will consider Euclidean geometries, that is, $G_{\mu\nu} = \delta_{\mu\nu}$ and $g_{AB} = \delta_{AB}$. We recall that for fluids, $W = W(J)$; this relation and the stationarity of the discontinuity surface ($U = 0$ on D_X) simplifies the jump relation (3.92) to

$$\int_{D_X} \left[\!\!\left[\rho \frac{\partial W}{\partial J} \frac{\partial J}{\partial v_j^A} N_j \cdot V^A \right]\!\!\right] d^n x_0 = 0, \tag{3.93}$$

where $N_j = \frac{\partial_j f}{|\nabla_x f|}$ is the normal vector to D_X. From the definition of the Jacobian J (3.56), one can derive

$$\frac{\partial J}{\partial v_j^A} = J(v^{-1})_A^j.$$

We use this relation and the definition of the material pressure (3.72) to re-write (3.93) as

$$\int_{D_X} \left[\!\!\left[PJ \left(\left(\frac{\partial \varphi}{\partial x} \right)^{-1} \right)_A^j N_j V^A \right]\!\!\right] d^n x_0 = 0. \tag{3.94}$$

We notice that in (3.94), the term $J \left(\left(\frac{\partial \varphi}{\partial x} \right)^{-1} \right)_A^j N_j d^n x_0$ represents the A-th component of the area element in the spatial configuration, as given by the formula of Nanson (see Truesdell and Toupin [1960], pg. 249 or Jaunzemis [1967], pg. 154, for example). Hence, substituting $y = \varphi_t(x)$ in (3.94) and then passing to the local form we can obtain the jump relation

$$[\![pV^A N_A]\!] = 0, \tag{3.95}$$

where p is the spatial pressure defined by $p(y(x)) = P(x)$. Now, we combine (3.95) with the property that the vector field V has a zero normal jump (see (3.29)), to obtain

$$[\![p]\!] = 0, \tag{3.96}$$

which is the standard pressure balance at a free surface.

We take now horizontal variations $V^\mu \neq 0$ such that $V^0 \neq 0$ and $V^j = 0$, for $j = 1, \ldots, n$. Then, (3.47) simplifies to

$$\int_{D_X} \left[\!\!\left[\frac{\partial L}{\partial v_j^A} \frac{\partial (\phi \circ \phi_X^{-1})^A}{\partial t} N_j V^0 \right]\!\!\right] d^n x_0 = 0. \tag{3.97}$$

Furthermore, using the continuity of V^0 and the particular form of $W = W(J)$ in the Lagrangian (3.57), we can write (3.97) as

$$\int_{D_X} \left[\!\!\left[PJ \left(\left(\frac{\partial \varphi}{\partial x} \right)^{-1} \right)_A^j \frac{\partial \varphi^A}{\partial t} N_j \right]\!\!\right] V^0 d^n x_0 = 0. \tag{3.98}$$

As before, we use the formula of Nanson, substitute $y = \varphi_t(x)$ in (3.98), and then pass to the local form to obtain

$$\left[\!\!\left[p \frac{\partial \varphi^A}{\partial t} N_A \right]\!\!\right] = 0. \tag{3.99}$$

Using the pressure continuity (3.96), the jump condition (3.99) becomes

$$\left[\!\left[\frac{\partial \varphi^A}{\partial t} N_A\right]\!\right] = 0. \tag{3.100}$$

We can also use the continuity of the normal vector to write (3.100) as

$$\left[\!\left[\frac{\partial \varphi^A}{\partial t}\right]\!\right] N_A = 0. \tag{3.101}$$

The jump condition (3.100) is a kinematic condition which restricts the possible jumps of the fluid velocity only to tangential discontinuities (the normal component is continuous). In the literature, this condition may appear either as a boundary condition (see Karamcheti [1966]) or as a definition for vortex sheets (see Truesdell and Toupin [1960]). However, we recover it through a variational procedure, as a consequence of the general theorem of the Section 3.2.2, using the particular form of the space of configurations (3.18) and of its admissible variations (3.29).

Finally, let consider only space component horizontal variations ($V^0 = 0$ and $V^j \neq 0$, for $j = 1, \ldots, n$). The vector field $V^j \frac{\partial}{\partial x^j}$ on X is lifted by $T(\phi \circ \phi_X^{-1})$ to a horizontal vector field on Y (see decomposition (3.23)) with coordinates

$$V^A = \frac{\partial (\phi \circ \phi_X^{-1})^A}{\partial x^j} V^j. \tag{3.102}$$

Then, by using the previous jump conditions (3.96), (3.47) simplifies to

$$\int_{D_X} \left[\!\left[\frac{\partial L}{\partial v_k^A} \frac{\partial (\phi \circ \phi_X^{-1})^A}{\partial x^j} N_k V^j\right]\!\right] d^n x_0 = 0, \tag{3.103}$$

where we also used that $V^j N_j = 0$ for material surfaces. Using (3.102) and the definition of the material pressure (3.72), (3.103) becomes exactly (3.94), so it will provide the already known jump condition (3.96).

Solid-fluid Boundaries We again apply Theorem 3 to find that the Euler-Lagrange equations (3.67) will be satisfied in the domain occupied by the elastic body, while the fluid dynamics in the outer region will be described by (3.74). As for free surfaces, the boundary terms in Theorem 3 will give the correct pressure-traction balance on the boundary of the

elastic body, as well as restrictions on the jumps in velocity.

For vertical variations only, the jump conditions are those given by (3.92). For Euclidean geometries, these conditions become

$$\int_{D_X} \left[\mathcal{P}_A^j N_j (V^A)^+ - PJ \left(\left(\frac{\partial \varphi}{\partial x} \right)^{-1} \right)_A^j N_j (V^A)^- \right] d^n x_0 = 0, \tag{3.104}$$

where we adopt the usual notation with superscript $+$ and $-$ for the limit values of a discontinuous function at a point on the singular surface by approaching the point from each side of the discontinuity.

Using the Piola transformation (3.69) and the formula of Nanson we can make the substitution $y = \varphi_t(x)$ in (3.104) and then pass to the local form; we obtain

$$\sigma^{AB} N_B (V^A)^+ - p N_A (V^A)^- = 0. \tag{3.105}$$

We use the property of the vector field V from (3.29),

$$(V^A)^+ N_A - (V^A)^- N_A = 0,$$

to write (3.105) as

$$(\sigma^{AB} N_B - p N_A) \cdot (V^A)^+ = 0. \tag{3.106}$$

As there are no restrictions on $(V^A)^+$, we have

$$\sigma^{AB} N_B - p N_A = 0. \tag{3.107}$$

Moreover, by denoting by $t^A = \sigma^{AB} N_B$ the stress vector, we obtain

$$t^A N_A - p = 0, \tag{3.108}$$

which is the pressure-traction balance on the boundary of the elastic body.

We now consider horizontal variations $V^\mu \neq 0$ such that $V^0 \neq 0$ and $V^j = 0$, for $j = 1, \ldots, n$. Using the previous result (3.108), the general jump conditions (3.47) reduce

to

$$\int_{D_X} \left[\!\!\left[\frac{\partial L}{\partial v_j^A} \frac{\partial (\phi \circ \phi_X^{-1})^A}{\partial t} N_j V^0 \right]\!\!\right] d^n x_0 = 0. \tag{3.109}$$

For solid-fluid interactions, the jump conditions (3.109) become

$$\int_{D_X} \left[\mathcal{P}_A^j N_j \left(\frac{\partial \varphi^A}{\partial t} \right)^+ - PJ \left(\left(\frac{\partial \varphi}{\partial x} \right)^{-1} \right)_A^j N_j \left(\frac{\partial \varphi^A}{\partial t} \right)^- \right] V^0 d^n x_0 = 0, \tag{3.110}$$

By using the Piola transformation (3.69) and Nanson's formula, we make the substitution $y = \varphi_t(x)$ in (3.110) and then pass to the local form to get

$$\sigma^{AB} N_B \left(\frac{\partial \varphi^A}{\partial t} \right)^+ - p N_A \left(\frac{\partial \varphi^A}{\partial t} \right)^- = 0. \tag{3.111}$$

Now, from (3.107) and (3.111) we can derive

$$\left[\!\!\left[\frac{\partial \varphi^A}{\partial t} \right]\!\!\right] N_A = 0, \tag{3.112}$$

which implies the continuity of the normal component of the velocity. Thus, only tangential discontinuities in the velocity are possible. We emphasize again that we obtain this restriction as a consequence of the choice of the configuration space (see (3.18) and (3.29)) and not by prescribing it as a boundary condition.

By an argument similar to the one used for fluid-fluid interfaces, we can show that the space component horizontal variations do not provide new jump conditions; they will lead in fact to the jump condition (3.105), from which the pressure-traction balance (3.108) can be derived.

3.4.4 Collisions of Elastic Bodies

We now illustrate the last category of the classification of configuration spaces from Section 3.2.1. We will apply the general formalism to investigate the collision of two elastic bodies, where the configuration manifold is given by $\mathcal{C}^c$ defined in (3.19) and the analog of the singular surfaces from the previous subsections is the codimension 1 spacetime contact surface. The interface is a material surface, so it has a zero propagation speed $U = 0$. By the choice of the configuration space $\mathcal{C}^c$ we allow the elastic bodies to slip on each other during the collision, but they do so without friction.

If we consider only vertical variations, the jump conditions will be given by (3.92). In the Euclidean case these conditions become

$$\int_{D_X} [\![\mathcal{P}_A^{\ j} N_j V^A]\!] d^n x_0 = 0. \tag{3.113}$$

By making the change of variables $y = \phi_t(x)$ in (3.113) and using the Piola transformation (3.69), we can write the integral in the spatial configuration and then pass to the local form to obtain

$$[\![\sigma^{AB} N_B V^A]\!] = 0, \tag{3.114}$$

where N_A are the components of the outward unit normal to the contact set in the current configuration.

Let $t^A = \sigma^{AB} N_B$ denote the stress vector, as before. By using the jump restriction on V from (3.31) we can derive

$$[\![t^A N_A]\!] = 0, \tag{3.115}$$

which represents the balance of the normal tractions on the contact set during a collision. From the derivation of (3.115) we also obtain that the tangential tractions are zero on the contact surface.

Let us consider now time component horizontal variations ($V^0 \neq 0$ and $V^j = 0$, for $j = 1, \ldots, n$); the general jump conditions (3.47) reduce to (3.109), which in turn become

$$\int_{D_X} \left[\!\!\left[\mathcal{P}_A^{\ j} N_j \left(\frac{\partial \varphi^A}{\partial t} \right) \right]\!\!\right] V^0 d^n x_0 = 0. \tag{3.116}$$

By the same procedure used before, we can pass to the local form in the spatial configuration and obtain

$$\left[\!\!\left[t^A \frac{\partial \varphi^A}{\partial t} \right]\!\!\right] = 0. \tag{3.117}$$

From (3.115) and (3.117) we can derive

$$\left[\!\!\left[\frac{\partial \varphi^A}{\partial t} N_A \right]\!\!\right] = 0, \tag{3.118}$$

which gives the continuity of the normal components of the velocities, once the contact is established. However, the tangential discontinuity in velocities, due to slipping, may be

arbitrary.

The space component horizontal variations will not provide new jump conditions; we can show this by the same procedure used in Section 3.4.3.

Chapter 4

Variational Collision Integrators

We now turn to considering discrete models of contact problems, in which the continuous time variable is replaced with a discrete time index. The equations of motion are thus algebraic rather than differential equations, and they can be regarded as an integrator for the continuous system.

The approach we use is based on discrete variational mechanics (see Marsden and West [2001]), in which the variational principle is discretized and the discrete equations and their conservation properties are derived as in the continuous case. This has the advantage of automatically capturing much of the geometric structure of the true problem even in the approximate discrete setting.

4.1 Discrete Configurations and Equations of Motion

Disregard for the moment the continuous formulation of the Chapter 2 and introduce a fixed ***timestep*** $h \in \mathbb{R}$. Consider a ***discrete Lagrangian*** $L_d : Q \times Q \to \mathbb{R}$ which is a function of two configuration points and the timestep, so that $L_d = L_d(q_0, q_1, h)$. The discrete Lagrangian will be chosen to approximate the continuous action integral over an interval of length h, so that

$$L_d(q_0, q_1, h) \approx \int_0^h L(q, \dot{q}) dt,$$

where $q : [0, h] \to \mathbb{R}$ is an exact solution of the Euler-Lagrange equations for L satisfies the boundary conditions $q(0) = q_0$ and $q(h) = q_1$.

We now consider an increasing sequence of times

$$t_k = kh \text{ for } k = 0, \ldots, N$$

and we also fix $\tilde{\alpha} \in [0,1]$ and we let $\tilde{\tau} = t_{i-1} + \tilde{\alpha}h$ denote the fixed impact time (corresponding to τ_i from the continuous model) and $\tilde{t} = t_{i-1} + \alpha h$ denote the actual impact time (corresponding to t_i). We take $\alpha = t_d(\tilde{\alpha})$, where t_d is some strictly increasing function which maps $[0,1]$ onto $[0,1]$. Thus, we only assumed that the step at which the impact occurs, is known, and not the impact time $\tilde{t}$, which is allowed to vary according to variations in α.

The ***discrete path space*** is defined by

$$\mathcal{M}_d = \mathcal{T}_d \times \mathcal{Q}_d(\tilde{\alpha}, \partial C, Q), \tag{4.1}$$

where

$$\mathcal{T}_d = \{t_d(\tilde{\alpha}) \mid t_d \in C^\infty([0,1],[0,1]), t_d \text{ onto}, t_d' > 0 \text{ in} [0,1]\} \tag{4.2}$$

$$\mathcal{Q}_d(\tilde{\alpha}, \partial C, Q) = \{q_d : \{t_0, \ldots, t_{i-1}, \tilde{\tau}, t_i, \ldots, t_N\} \to Q, q_d(\tilde{\tau}) \in \partial C\}. \tag{4.3}$$

Remark. The set $\mathcal{T}_d$ is actually the real interval $[0,1]$, but we used (4.2) to define it in order to emphasize the analogy with the continuous case.

We identify the discrete trajectory with its image

$$(\alpha, q_d) = (\alpha, \{q_0, \ldots, q_{i-1}, \tilde{q}, q_i, \ldots, q_N\}),$$

where $q_k = q_d(t_k)$ for $k \in \{0, \ldots, N\}$, $\tilde{q} = q_d(\tilde{\tau})$ and $\alpha = t_d(\tilde{\alpha})$. Thus a discrete trajectory can be regarded as a sequence of points in Q, one of which must be in ∂C, and a single real number $\alpha \in [0,1]$. The portion of the discrete trajectory around the impact is illustrated graphically in Figure 4.1.

The ***discrete action map*** $\mathfrak{G}_d : \mathcal{M}_d \to \mathbb{R}$ is defined by

$$\mathfrak{G}_d(\alpha, q_d) = \sum_{k=0}^{i-2} L_d(q_k, q_{k+1}, h) + \sum_{k=i}^{N-1} L_d(q_k, q_{k+1}, h) + L_d(q_{i-1}, \tilde{q}, \alpha h) + L_d(\tilde{q}, q_i, (1-\alpha)h) \tag{4.4}$$

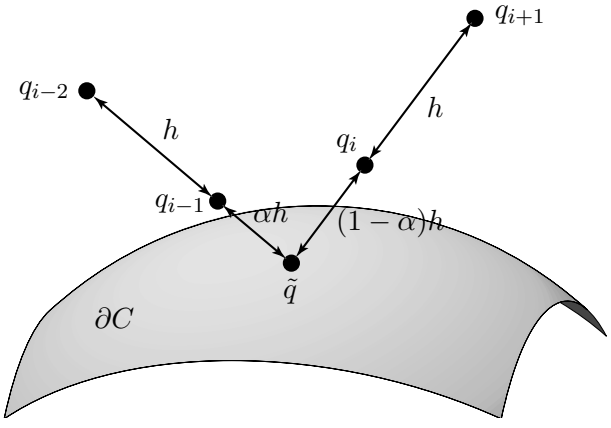


Figure 4.1: The discrete variational principle for collisions

As the discrete path space $\mathcal{M}_d$ is isomorphic to $[0,1] \times Q \times \cdots \times \partial C \times \cdots \times Q$ (N copies of Q), it can be given a smooth manifold structure.

For $q_d \in \mathcal{Q}_d(\tilde{\alpha}, \partial C, Q)$ the tangent space $T_{q_d}\mathcal{Q}_d(\tilde{\alpha}, \partial C, Q)$ is the set of all maps $v_{q_d} : \{t_0, \ldots, t_{i-1}, \tilde{\tau}, t_i, \ldots, t_N\} \to TQ$ such that $\pi_Q \circ v_{q_d} = q_d$ and $v_{q_d}(\tilde{\tau}) \in T_{\tilde{q}}\partial C$. For simplicity we will identify v_{q_d} with its image in TQ.

The tangent space to the full discrete path space is now $T\mathcal{M}_d = T\mathcal{T}_d \times T\mathcal{Q}_d$. At a given point $(\alpha, q_d) \in \mathcal{M}_d$ we will write a tangent vector in $T_{(\alpha,q_d)}\mathcal{M}_d$ as

$$(\delta\alpha, \delta q_d) = (\delta\alpha, \{\delta q_0, \ldots, \delta q_{i-1}, \delta\tilde{q}, \delta q_i, \ldots \delta q_N\}).$$

Define the ***discrete second-order manifold*** to be

$$\ddot{Q}_d = Q \times Q \times Q,$$

which has the same information content as the continuous second-order manifold $\ddot{Q}$.

We now proceed, as in the continuous case, to derive the discrete equations of motion and the conservation laws from Hamilton's principle of critical action. We take variations of the discrete action sum with respect to the discrete path and to the parameter α, as stated in the following theorem.

Theorem 4. *Given a C^k discrete Lagrangian $L_d : Q \times Q \times \mathbb{R} \to \mathbb{R}$, $k \geq 1$, there exists a unique C^{k-1} mapping $EL_d : \ddot{Q}_d \to T^*Q$ and unique C^{k-1} 1-forms $\Theta^-_{L_d}$ and $\Theta^+_{L_d}$ on the discrete Lagrangian phase space $Q \times Q$, such that for all variations $(\delta\alpha, \delta q_d) \in T_{(\alpha,q_d)}\mathcal{M}_d$*

of (α, q_d) *we have*

$$\begin{aligned}
&d\mathfrak{G}_d(\alpha, q_d)\cdot(\delta\alpha, \delta q_d)\\
&\quad= \sum_{k=1}^{i-2} EL_d(q_{k-1}, q_k, q_{k+1})\cdot\delta q_k + \sum_{k=i+1}^{N-1} EL_d(q_{k-1}, q_k, q_{k+1})\cdot\delta q_k\\
&\quad\quad+ \Theta^+_{L_d}(q_{N-1}, q_N)\cdot(\delta q_{N-1}, \delta q_N) - \Theta^-_{L_d}(q_0, q_1)\cdot(\delta q_0, \delta q_1)\\
&\quad\quad+ \left[D_2L_d(q_{i-2}, q_{i-1}, h) + D_1L_d(q_{i-1}, \tilde{q}, \alpha h)\right]\cdot\delta q_{i-1}\\
&\quad\quad+ h\left[D_3L_d(q_{i-1}, \tilde{q}, \alpha h) - D_3L_d(\tilde{q}, q_i, (1-\alpha)h)\right]\cdot\delta\alpha\\
&\quad\quad+ i^*(D_2L_d(q_{i-1}, \tilde{q}, \alpha h) + D_1L_d(\tilde{q}, q_i, (1-\alpha)h))\cdot\delta\tilde{q}\\
&\quad\quad+ \left[D_2L_d(\tilde{q}, q_i, (1-\alpha)h) + D_1L_d(q_i, q_{i+1}, h)\right]\cdot\delta q_i,
\end{aligned} \tag{4.5}$$

where $i^* : T^*Q \to T^*\partial C$ *is the cotangent lift of the embedding* $i : \partial C \to Q$.

The map EL_d *is called the* ***discrete Euler-Lagrange derivative*** *and the 1-forms* $\Theta^+_{L_d}$ *and* $\Theta^-_{L_d}$ *are the* ***discrete Lagrangian 1-forms****. In coordinates these have the expressions*

$$EL_d(q_{k-1}, q_k, q_{k+1}) = \left[D_2L_d(q_{k-1}, q_k, h) + D_1L_d(q_k, q_{k+1}, h)\right]dq_k \tag{4.6}$$

for $k \in \{1, \ldots, i-2, i, \ldots, N-1\}$ *and*

$$\begin{aligned}
\Theta^+_{L_d}(q_k, q_{k+1}) &= D_2L_d(q_k, q_{k+1}, h)\,dq_{k+1}\\
\Theta^-_{L_d}(q_k, q_{k+1}) &= -D_1L_d(q_k, q_{k+1}, h)\,dq_k.
\end{aligned}$$

Proof. The formula is derived by straightforward algebra, by computing the derivative of the discrete action map and by some rearrangement of the summation. This rearrangement corresponds to a discrete version of integration by parts, resulting in two boundary terms which are interpreted as the discrete Lagrangian 1-forms. ■

By using the discrete version of Hamilton's principle we consider the paths (α, q_d) which are critical points of the discrete action. Therefore, we define the ***discrete space of solutions*** to be the set of all paths which satisfy $d\mathfrak{G}_d(\alpha, q)\cdot(\delta\alpha, \delta q) = 0$ for all variations $(\delta\alpha, \delta q_d) \in T_{(\alpha,q_d)}\mathcal{M}_d$ which are zero at the boundary points 0 and N.

From (4.5) we conclude that (α, q_d) is a solution if and only if the discrete Euler-Lagrange

derivative is zero at all k other than $\{0, i-1, i, N\}$. This statement at an arbitrary k reads

$$D_2L_d(q_{k-1}, q_k, h) + D_1L_d(q_k, q_{k+1}, h) = 0 \tag{4.7}$$

and is known as ***discrete Euler-Lagrange equations***. These describe the motion of the system away from the impact point, by implicitly defining a map $(q_{k-1}, q_k) \mapsto (q_k, q_{k+1})$.

Near the point of impact, the discrete Hamilton's principle gives three additional sets of equations, namely,

$$D_2L_d(q_{i-2}, q_{i-1}, h) + D_1L_d(q_{i-1}, \tilde{q}, \alpha h) = 0 \tag{4.8a}$$

$$\tilde{q} \in \partial C, \tag{4.8b}$$

which is a system of $n+1$ equations to be solved for $\tilde{q}$ and α, and

$$D_3L_d(q_{i-1}, \tilde{q}, \alpha h) - D_3L_d(\tilde{q}, q_i, (1-\alpha)h) = 0 \tag{4.9a}$$

$$i^*(D_2L_d(q_{i-1}, \tilde{q}, \alpha h) + D_1L_d(\tilde{q}, q_i, (1-\alpha)h)) = 0, \tag{4.9b}$$

which is a system of n equations for the unknown q_i. Finally, we also have

$$D_2L_d(\tilde{q}, q_i, (1-\alpha)h) + D_1L_d(q_i, q_{i+1}, h) = 0, \tag{4.10}$$

which gives n equations to be solved for q_{i+1}.

A discrete trajectory can thus be formed by starting from an initial condition (q_0, q_1), using (4.7) to solve successively for the q_k until the impact time is reached, and then solving the systems (4.8), (4.9) and (4.10) in turn to obtain $\tilde{q}$, α and then q_i and q_{i+1}, before once again continuing with (4.7) to complete the trajectory.

Remark. The discrete energy conservation through the collision depends critically on exactly resolving the collision time with the parameter α. This is also the key feature of the recent improvements of Pandolfi et al. [2002] to the nonsmooth collision methods developed by Kane et al. [1999b].

4.2 Relationship between Discrete and Continuous Models

Having established the basic discrete variational mechanics, we now consider how the discrete model can be regarded as an approximation to the continuous model.

At first glance it appears that the discrete Euler-Lagrange equations are defined only in terms of pairs of configuration positions. We will now see, however, that they can also be interpreted as defining a mapping on the cotangent bundle T^*Q. Define the ***discrete Legendre transforms*** or ***discrete fiber derivatives*** $\mathbb{F}^+L_d, \mathbb{F}^-L_d : Q \times Q \to T^*Q$ as given by

$$\begin{aligned}\mathbb{F}^+L_d(q_0, q_1) \cdot \delta q_1 &= D_2L_d(q_0, q_1, h) \cdot \delta q_1 \\ \mathbb{F}^-L_d(q_0, q_1) \cdot \delta q_0 &= -D_1L_d(q_0, q_1, h) \cdot \delta q_0,\end{aligned}$$

where h is the timestep in between q_0 and q_1. We note the implicit dependence on the timestep of the definition above. This dependence is completely neglected in the constant timestep discrete variational mechanics or rigorously treated in the nonautonomous setting (using adaptive timesteps) and we refer to Marsden and West [2001] for a complete account of these ideas.

These also can be written

$$\mathbb{F}^+L_d : (q_0, q_1) \mapsto (q_1, p_1) = (q_1, D_2L_d(q_0, q_1, h)) \tag{4.11a}$$

$$\mathbb{F}^-L_d : (q_0, q_1) \mapsto (q_0, p_0) = (q_0, -D_1L_d(q_0, q_1, h)). \tag{4.11b}$$

If both discrete fiber derivatives are locally isomorphisms, then we say that L_d is ***regular***. We will generally assume that we are working with regular discrete Lagrangians.

We introduce the notation

$$p^+_{k,k+1} = p^+(q_k, q_{k+1}, h) = \mathbb{F}^+L_d(q_k, q_{k+1}) \tag{4.12a}$$

$$p^-_{k,k+1} = p^-(q_k, q_{k+1}, h) = \mathbb{F}^-L_d(q_k, q_{k+1}) \tag{4.12b}$$

for the momentum at the two endpoints of each interval $[k, k+1]$.

We can now use definitions (4.11a) and (4.12) of the discrete fiber derivatives and of the

discrete momenta to see that the discrete Euler-Lagrange equations (4.7) can be written as

$$\mathbb{F}^+ L_d(q_{k-1}, q_k) = \mathbb{F}^- L_d(q_k, q_{k+1}) \tag{4.13}$$

or simply

$$p^+_{k-1,k} = p^-_{k,k+1}. \tag{4.14}$$

That is, the discrete Euler-Lagrange equations enforce the condition that the momentum at time k should be the same when evaluated from the lower interval $[k-1, k]$ or the upper interval $[k, k+1]$.

In this interpretation, equation (4.9b) represents conservation of the projection of momentum (by i^*, on $T^*\partial C$) at the moment of impact

$$i^* p^+(q_{i-1}, \tilde{q}, \alpha h) = i^* p^-(\tilde{q}, q_i, (1-\alpha)h), \tag{4.15}$$

which is a discrete version of the jump condition (2.13) from the continuous case.

To give an interpretation of the discrete equations around the impact time, we define the ***discrete energy*** to be

$$E_d(q_k, q_{k+1}, h) = -D_3 L_d(q_k, q_{k+1}, h). \tag{4.16}$$

Using this, we can write equation (4.9a) as

$$E_d(q_{i-1}, \tilde{q}, \alpha h) = E_d(\tilde{q}, q_i, (1-\alpha)h), \tag{4.17}$$

so this equations simply represents conservation of discrete energy at the impact time, a discrete analog of (2.14).

Remark. The discrete energy defined in this way is used in Kane et al. [1999a] and can be motivated in several ways; first of all, for Lagrangians of the form of kinetic minus potential energy, and with the choice of discrete Lagrangians given by

$$L_d(q_0, q_1, h) = L\left(\gamma q_0 + (1-\gamma)q_1, \frac{q_1 - q_0}{h}\right), \tag{4.18}$$

where $\gamma \in [0,1]$ is an interpolation parameter, the discrete energy gets the usual expression

$$E_d(q_0, q_1, h) = \frac{1}{2}\left(\frac{q_1 - q_0}{h}\right)^T M \left(\frac{q_1 - q_0}{h}\right) + V(\gamma q_0 + (1-\gamma)q_1). \tag{4.19}$$

A second motivation is the fact that the discrete energy becomes exactly the Hamiltonian when one uses the exact discrete Lagrangian L_d^E–that is, the discrete Lagrangian is equal to the action integral taken along exact solutions of the Euler–Lagrange equations.

4.3 Symplecticity of the Flow

Define the ***discrete Lagrangian map*** $F_{L_d} : Q \times Q \to Q \times Q$ by

$$(q_0, q_1) \mapsto (q_1, q_2), \tag{4.20}$$

where q_2 is obtained by using the algorithm from Section 4.1. A solution $(\alpha, q_d) \in \mathcal{M}_d$ is formed by iteration of the map F_{L_d} and it is uniquely determined by the initial condition $(q_0, q_1) \in Q \times Q$ and the choice of timestep h. Hence, we parameterize the discrete solutions of the variational principle by the initial conditions (q_0, q_1), and we consider the restriction of $\mathfrak{G}_d$ to that solution space.

The discrete fiber derivatives enables us to push the discrete Lagrangian map $F_{L_d} : Q \times Q \to Q \times Q$ forward to T^*Q. We define the ***discrete Hamiltonian map*** $\tilde{F}_{L_d} : T^*Q \to T^*Q$ by

$$\tilde{F}_{L_d} = \mathbb{F}^+ L_d \circ F_{L_d} \circ (\mathbb{F}^+ L_d)^{-1}, \tag{4.21}$$

with the coordinate expression

$$\tilde{F}_{L_d} : (q_0, p_0) \mapsto (q_1, p_1). \tag{4.22}$$

We note that the discrete Hamiltonian map can be equivalently defined using the other discrete Legendre transform

$$\tilde{F}_{L_d} = \mathbb{F}^- L_d \circ F_{L_d} \circ (\mathbb{F}^- L_d)^{-1}. \tag{4.23}$$

Define the ***restricted discrete action map*** $\hat{\mathfrak{G}}_d : Q \times Q \to \mathbb{R}$ to be $\hat{\mathfrak{G}}_d(q_0, q_1) =$

$\mathfrak{G}_d(\alpha, q_d)$, where (α, q_d) is the corresponding solution in $\mathcal{M}_d$ such that $(q_d(t_0), q_d(t_1)) = (q_0, q_1)$. Then, equation (4.5) becomes

$$d\hat{\mathfrak{G}}_d = (F_{L_d}^N)^* \Theta_{L_d}^+ - \Theta_{L_d}^-. \tag{4.24}$$

Taking a further derivative of this expression, and using the fact that $d^2\hat{\mathfrak{G}}_d = 0$, we obtain

$$(F_{L_d}^N)^*(\Omega_{L_d}) = \Omega_{L_d}, \tag{4.25}$$

where $\Omega_{L_d} = d\Theta_{L_d}^+ = d\Theta_{L_d}^-$ is the unique ***discrete Lagrangian symplectic form***, with coordinate expression

$$\Omega_{L_d}(q_0, q_1) = \frac{\partial^2 L_d}{\partial q_0^i \partial q_1^j} dq_0^i \wedge dq_1^j. \tag{4.26}$$

We have thus proven that the discrete evolution map exactly preserves a discrete symplectic structure, so regarding F_d as an integrator for the continuous system we see that it is automatically a symplectic method.

Note that the discrete Lagrangian symplectic form is the pullback under either discrete Legendre transform of the canonical symplectic form on T^*Q. The discrete Hamiltonian map $\tilde{F}_{L_d} : T^*Q \to T^*Q$ thus preserves the canonical symplectic form and the canonical momentum maps on T^*Q.

4.4 Discrete Noether Theorem

Consider the (left or right) group action $\Phi : G \times Q \to Q$ of a Lie group G on Q, with infinitesimal generator as defined in Section 2.4. This action can be lifted to $Q \times Q$ by the product $\Phi_g(q_0, q_1) = (\Phi_g(q_0), \Phi_g(q_1))$, which has the ***infinitesimal generator*** $\xi_{Q\times Q} : Q \times Q \to T(Q \times Q)$ given by

$$\xi_{Q\times Q}(q_0, q_1) = (\xi_Q(q_0), \xi_Q(q_1)). \tag{4.27}$$

The two ***discrete Lagrangian momentum maps*** $J^+_{L_d}, J^-_{L_d} : Q \times Q \to g^*$ are

$$J^+_{L_d}(q_0, q_1) \cdot \xi = \Theta^+_{L_d} \cdot \xi_{Q\times Q}(q_0, q_1) \tag{4.28a}$$

$$J^-_{L_d}(q_0, q_1) \cdot \xi = \Theta^-_{L_d} \cdot \xi_{Q\times Q}(q_0, q_1). \tag{4.28b}$$

As in the continuous approach to the Noether's theorem from Section 2.4, we are restricted to symmetries of the configuration variables only. We consider symmetries which do not involve altering the time variable and thus consider the timestep h to be a fixed constant.

If a discrete Lagrangian $L_d : Q \times Q \to \mathbb{R}$ is such that $dL_d \cdot \xi = 0$, then L_d is said to be ***infinitesimally invariant*** under the group action, and Φ is said to be a ***symmetry*** of the discrete Lagrangian. Note that

$$dL_d \cdot \xi = (\Theta^+_{L_d} - \Theta^-_{L_d}) \cdot \xi_{Q\times Q}$$

and so, when L_d is infinitesimally invariant under the group action Φ, the two discrete momentum maps are equal. In such cases we will use the notation $J_{L_d} : Q \times Q \to \mathfrak{g}^*$ for the unique single ***discrete Lagrangian momentum map***.

Theorem 5. (Discrete Noether's theorem) *Consider a discrete Lagrangian system $L_d : Q \times Q \times \mathbb{R} \to \mathbb{R}$ which is infinitesimally invariant under the lift of the (left or right) action $\Phi : G \times Q \to Q$. If we assume that the action leaves ∂C invariant (locally), then the corresponding discrete Lagrangian momentum map $J_{L_d} : Q \times Q \to \mathfrak{g}^*$ is a conserved quantity of the discrete Lagrangian map $F_{L_d} : Q \times Q \to Q \times Q$, so that $J_{L_d} \circ F_{L_d} = J_{L_d}$.*

Proof. We introduce an action of G on the discrete path space $\mathcal{M}_d$ by pointwise action on the configuration components, so that $\Phi_g : \mathcal{M}_d \to \mathcal{M}_d$ is given by $\Phi_g(\alpha, q_d) = (\alpha, \Phi_g(q_d))$. Then, the infinitesimal generator $\xi_{\mathcal{M}_d} : \mathcal{M}_d \to T\mathcal{M}_d$ is given by

$$\xi_{\mathcal{M}_d}(\alpha, q_d) = (0, \xi_Q(q_0), \ldots, \xi_Q(q_{i-1}), \xi_Q(\tilde{q}), \xi_Q(q_i), \ldots, \xi_Q(q_N)).$$

From (4.4) we derive

$$d\mathfrak{G}_d(\alpha, q_d) \cdot \xi_{\mathcal{M}_d}(\alpha, q_d) = \sum_{k=0}^{N-1} dL_d \cdot \xi \tag{4.29}$$

and so the space of solutions of the discrete Euler-Lagrange is invariant under the action of G, and the Lagrangian map $F_{L_d} : Q \times Q \to Q \times Q$ commutes with the lifted action $\Phi_g : Q \times Q \to Q \times Q$.

Identifying the space of solutions with the space of initial conditions $Q \times Q$ and using (4.24) we obtain

$$\begin{aligned} d\mathfrak{G}_d(\alpha, q_d) \cdot \xi_{\mathcal{M}_d}(\alpha, q_d) &= d\hat{\mathfrak{G}}_d(q_0, q_1) \cdot \xi_{Q\times Q}(q_0, q_1) \\ &= ((F^N_{L_d})^*(\Theta^+_{L_d}) - \Theta^-_{L_d})(q_0, q_1) \cdot \xi_{Q\times Q}(q_0, q_1). \end{aligned}$$

From (4.29) and the invariance of the discrete Lagrangian, the left hand side of the previous equation is zero, and so we have

$$(\Theta^+_{L_d} \cdot \xi_{Q\times Q}) \circ F^N_{L_d} = \Theta^-_{L_d} \cdot \xi_{Q\times Q}. \tag{4.30}$$

The last relation is simply the statement of preservation of the discrete momentum map, given that for symmetry actions there is only a single unique discrete momentum map and that the above argument holds for all subintervals, including a single timestep. ■

Observe that J_{L_d} is the pullback under $\mathbb{F}^{\pm}L_d$ of the canonical momentum map J_H on T^*Q, and that J_H is thus preserved by $\tilde{F}_{L_d}$.

Chapter 5

Numerical Examples

In this chapter we will choose a particular discrete Lagrangian and illustrate the performance of the algorithm from the previous chapter on two simple conservative systems. We are particularly interested here in the extent to which the variational integrator preserves the energy for very long time simulations.

The examples that we present simplify very much the issues regarding grazing impacts and multiple nearby solutions, such as one would encounter in complex collisions (simulation studies of powder flows for example). Our algorithm, as presented in this chapter, is limited to relatively simple situations, when one can readily identify and resolve the impacts. However, considerable progress has already been made in extending these methods to more practical schemes which are demonstrated on examples involving very complicated collision sequences (see Cirak and West [2003]).

5.1 The Discrete Algorithm

For systems of the form

$$L(q, \dot{q}) = \frac{1}{2}\dot{q}^T M \dot{q} - V(q), \tag{5.1}$$

where M is a mass matrix and V is a potential function, the Euler-Lagrange equations are given by

$$M\ddot{q} = -\nabla V(q),$$

which is simply Newton's equation of mass times acceleration equals force. We consider the second-order discrete Lagrangian

$$L_d(q_0, q_1, h) = \frac{h}{2}\left(\frac{q_1 - q_0}{h}\right)^T M \left(\frac{q_1 - q_0}{h}\right) - h\left(\frac{V(q_0) + V(q_1)}{2}\right), \tag{5.2}$$

which is clearly an approximation to the action integral over an interval of length h. The discrete energy function for this choice of discrete Lagrangian is

$$E_d(q_0, q_1, h) = \frac{1}{2}\left(\frac{q_1 - q_0}{h}\right)^T M \left(\frac{q_1 - q_0}{h}\right) + \left(\frac{V(q_0) + V(q_1)}{2}\right) \tag{5.3}$$

and the discrete Euler-Lagrange equations are

$$M\frac{q_{k+2} - 2q_{k+1} + q_k}{h^2} = -\nabla V(q_{k+1}). \tag{5.4}$$

Using the discrete Legendre transform (4.11a), we can push forward this algorithm on T^*Q and obtain a map

$$(q_k, p_k) \mapsto (q_{k+1}, p_{k+1})$$

given by

$$\begin{aligned} q_{k+1} &= q_k + hM^{-1}p_k - \frac{h^2}{2}M^{-1}\nabla V(q_k) \\ p_{k+1} &= p_k - \frac{h}{2}\left(\nabla V(q_k) + \nabla V(q_{k+1})\right). \end{aligned}$$

The integrator defined by the previous set of equations is called the leapfrog/Verlet integrator and is one of the most popular integration scheme in molecular dynamics. It is a second-order accurate integrator, as one can also infer from the fact that the discrete Lagrangian is second order (see Marsden and West [2001] for details about this theory).

This equation describes the motion of the discrete system away from the point of impact. Given a point (q_{i-1}, p_{i-1}) just before impact, we must then solve (4.8) for $\tilde{q}$ and α, which are

$$M\frac{\tilde{q} - q_{i-1}}{\alpha h} - M\frac{q_{i-1} - q_{i-2}}{h} + (1+\alpha)\frac{h}{2}\nabla V(q_{i-1}) = 0 \tag{5.5a}$$

$$\tilde{q} \in \partial C. \tag{5.5b}$$

Next we solve (4.9) for q_i, which reads

$$\frac{1}{2}\left(\frac{q_i-\tilde{q}}{(1-\alpha)h}\right)^T M\left(\frac{q_i-\tilde{q}}{(1-\alpha)h}\right)-\frac{1}{2}\left(\frac{\tilde{q}-q_{i-1}}{\alpha h}\right)^T M\left(\frac{\tilde{q}-q_{i-1}}{\alpha h}\right) + \frac{1}{2}(V(q_i)-V(q_{i-1}))=0 \tag{5.6a}$$

$$i^*\left(M\frac{q_i-\tilde{q}}{(1-\alpha)h}-M\frac{\tilde{q}-q_{i-1}}{\alpha h}+\frac{h}{2}\nabla V(\tilde{q})\right)=0. \tag{5.6b}$$

To implement the system (5.6) we write (5.6b) in a form using Lagrange multipliers. More precisely, we consider ∂C to have a local representation $\partial C=\phi^{-1}(0)\subset Q$, where 0 is a regular point of the constraint function $\phi: Q\to\mathbb{R}$. Then we solve (5.6a) together with the system

$$M\frac{q_i-\tilde{q}}{(1-\alpha)h}-M\frac{\tilde{q}-q_{i-1}}{\alpha h}+\frac{h}{2}\nabla V(\tilde{q})+\lambda\nabla\phi(\tilde{q})=0 \tag{5.7}$$

for the unknowns $q_i\in\mathbb{R}^n$ and $\lambda\in\mathbb{R}$.

Finally, we solve for q_{i+1} by (4.10), which is

$$M\frac{q_{i+1}-q_i}{h}-M\frac{q_i-\tilde{q}}{(1-\alpha)h}+(2-\alpha)\frac{h}{2}\nabla V(q_i)=0 \tag{5.8}$$

and we then continue integrating with equation (5.4) above.

We can also handle multiple impacts within a single timestep by dividing the impact step in as many substeps as we need and solving sequentially (5.5) and (5.6) for any constraint involved in the impact. We will explicitly derive the equations for the case of two impacts solved within the timestep (t_{i-1},t_i); generalization to an arbitrary number would be immediate.

If multiple impacts are realized in the timestep (t_{i-1},t_i), then the system (5.6) will return a solution q_i which is not admissible ($q_i\notin C$). Let's assume that there is only one additional impact in the subinterval $(\tilde{t},t_i)$ which occurs at the contact point $\tilde{q}'\in\partial C$ and time $\tilde{t}'=\tilde{t}+\beta h$, with $0<\beta\leq 1-\alpha$. Then, conservation of the discrete energy and momentum at the impact point $\tilde{q}$, in addition with the condition that $\tilde{q}'$ must lie on ∂C

give the following system of $n+1$ equations

$$\frac{1}{2}\left(\frac{\tilde{q}'-\tilde{q}}{\beta h}\right)^T M\left(\frac{\tilde{q}'-\tilde{q}}{\beta h}\right)-\frac{1}{2}\left(\frac{\tilde{q}-q_{i-1}}{\alpha h}\right)^T M\left(\frac{\tilde{q}-q_{i-1}}{\alpha h}\right) + \frac{1}{2}(V(\tilde{q}')-V(q_{i-1}))=0 \tag{5.9a}$$

$$i^*\left(M\frac{\tilde{q}'-\tilde{q}}{\beta h}-M\frac{\tilde{q}-q_{i-1}}{\alpha h}+(\alpha+\beta)\frac{h}{2}\nabla V(\tilde{q})\right)=0 \tag{5.9b}$$

$$\tilde{q}'\in\partial C \tag{5.9c}$$

to be solved for $\tilde{q}'$ and β.

Next, the analogous versions of (5.9a) and (5.9b) for the second impact point $\tilde{q}'$ give n equations for q_i

$$\frac{1}{2}\left(\frac{q_i-\tilde{q}'}{(1-\alpha-\beta)h}\right)^T M\left(\frac{q_i-\tilde{q}'}{(1-\alpha-\beta)h}\right)-\frac{1}{2}\left(\frac{\tilde{q}'-\tilde{q}}{\beta h}\right)^T M\left(\frac{\tilde{q}'-\tilde{q}}{\beta h}\right) + \frac{1}{2}(V(q_i)-V(\tilde{q}))=0 \tag{5.10a}$$

$$i^*\left(M\frac{q_i-\tilde{q}'}{(1-\alpha-\beta)h}-M\frac{\tilde{q}'-\tilde{q}}{\beta h}+(1-\alpha)\frac{h}{2}\nabla V(\tilde{q}')\right)=0. \tag{5.10b}$$

The case of an arbitrary number of impacts is treated in a similar manner, by dividing the timestep (t_{i-1},t_i) in as many substeps as needed and solving sequentially systems of type (5.9) to find all the contact points and times. Finally, we solve a system of type (5.10) for q_i and then we revert to the standard discrete Euler-Lagrange equations to continue away from the impact.

In the numerical examples, we solve the implicit sets of equations (5.5) and (5.6) with nested Newton loops.

5.2 Particle Colliding with a Rigid Surface

The first example we consider consists of a particle with unit mass moving under gravity in the (x,y) plane and successively colliding and bouncing on a horizontal rigid floor located at $y=0$. This simple system has two degrees of freedom (the coordinates of the particle) $q=(x,y)$, the configuration manifold is $Q=\mathbb{R}^2$ and the contact submanifold ∂C is the line $y=0$. The particle moves with trajectory $q(t)\in\mathbb{R}^2$ in the admissible set $y\geq 0$.

The Lagrangian describing this problem is in the form (5.1), where M is the diagonal

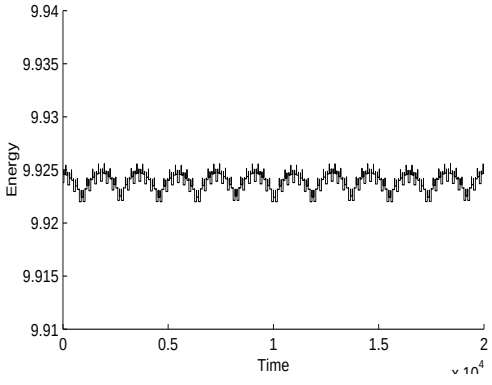


Figure 5.1: The longtime energy behavior for a particle bouncing on a rigid floor

2×2 mass matrix with diagonal elements (m, m) (m denotes the mass of the particle) and V is the gravitational potential given by

$$V(q) = mgy. \tag{5.11}$$

Here, g denotes the gravitational acceleration.

The discretization we use is (5.2), the one for which the variational collision integrator was explicitly derived in the last section. The integrator in run with a step size of $h = 0.01$; the initial conditions we used in the simulation are $q_0 = (0, 1)$ and $\dot{q}_0 = (-2, 0)$. We considered a unitary mass particle ($m = 1$).

The energy behavior in this case is shown in Figure 5.1 for a relatively large number of impacts (1000 impacts). The same pattern is observed if the simulation is carried out for essentially arbitrarily long times. This fluctuating energy behavior in typical of symplectic methods. A detailed account on how the variational symplectic methods perform on smooth conservative systems can be found in Kane et al. [2000].

5.3 Rotating Nonconvex Rigid Body Colliding with a Rigid Surface

Now consider a sequence of collisions and bounces on a horizontal rigid floor for a three degree of freedom system, namely, a rotating four point, star shaped rigid body (see Figure 5.2) moving in a plane. The convex hull of the star shaped body is a square with sides

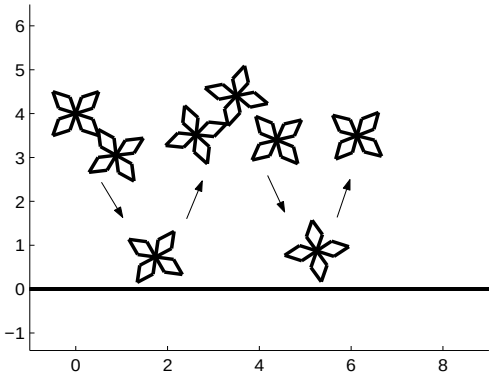


Figure 5.2: A rotating four-point, star-shaped rigid body colliding and bouncing on a horizontal rigid floor

of length L. The rigid body moves under the gravitational force field in the vertical (x, y) plane. The configuration manifold Q is $SE(2)$ with local coordinates $q = (x, y, \theta)$, where $(x, y) \in \mathbb{R}^2$ stand for the coordinates of the center of mass and $\theta \in [0, 2\pi]$ for the oriented angle that a line moving rigidly with the body makes with the horizontal axis. The contact set ∂C given by the non-penetration condition is given explicitly by

$$y = \frac{L}{2} \left(|\sin\theta| + |\cos\theta| \right). \tag{5.12}$$

The subset of points where $y \geq \frac{L}{2} \left(|\sin\theta| + |\cos\theta| \right)$ represents the admissible set $C \subset Q$ and contact occurs whenever the relation becomes an equality.

The Lagrangian describing this problem has the expression (5.1), where V is the gravitational potential (5.11) and M is the diagonal 3×3 mass matrix with diagonal elements (m, m, I), where m is the mass of the body and I is the moment of inertia of the star shaped body with respect to the z axis through its center of symmetry. In terms of m and L, I is given by $I = \frac{29}{192} m L^2$.

We use again the discretization given by (5.2) and run the variational collision integrator from Section 5.1 with a timestep $h = 0.005$ and initial conditions $q_0 = (0, 3.5, 0)$ and $\dot{q}_0 = (-2, 0, 5)$. We considered the body to have unitary mass $m = 1$ and a square convex hull of size $L = 1$. A longtime (1,500 impacts) energy plot is shown in Figure 5.3. The longtime energy behavior appears to be reasonably stable. It is not clear from these numerical experiments whether this is an indication of a nearby conserved energy, as exists for variational integrators applied to smooth systems, or simply a fairly stable random walk.

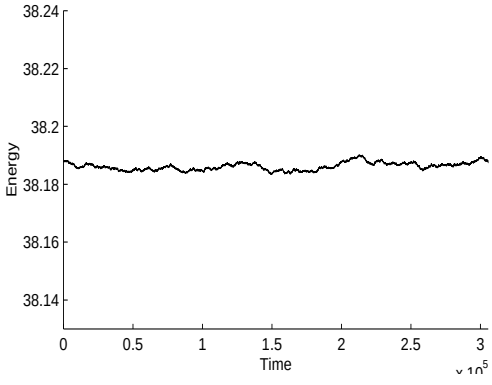


Figure 5.3: The longtime energy behavior for a star-shaped rigid body bouncing on a rigid floor. Note the fluctuating energy behavior typical of symplectic methods

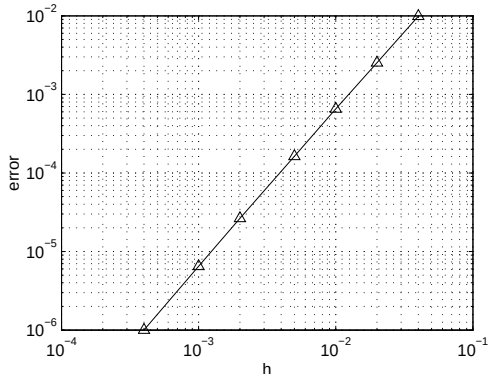


Figure 5.4: Log-log error diagram for the method in the star bounce example, after one collision. The 2nd order accuracy of the integrator from the smooth setting is preserved through collision. In this case a nonlinear gravity was used to avoid the degeneracy of the exactly integrable linear gravitational potential

More numerical investigations and analytical work is needed to resolve this question.

We checked numerically the order of accuracy of the algorithm for the star bounce example. A log-log error diagram after one collision is presented in Figure 5.4. The numerical results show that the integrator is 2nd order accurate, i.e., the order of the method is the same as the order of the discrete Lagrangian L_d. This is in fact a fundamental property of the variational integrators developed in smooth settings (see Marsden and West [2001]) and we believe that it extends to the nonsmooth setting as well. In our future work on the subject we intend to formulate and prove such results for the variational collisional algorithms presented in this work.

5.4 Nonsmooth Analysis Approach

The purpose of this section is to discuss collisions with multibody nonsmooth contact geometries when the contact set ∂C has a large number of singularities. For example, in granular flows or fragmentation of brittle solids there are a large number of fragments undergoing complex collision sequences. For these collisions, situations like corner to corner contact are very likely to occur and the variational algorithm from Section 4.1 cannot cope with contact in singular points of the contact set ∂C.

However, the nonsmooth analysis (see Clarke [1983]) provides an efficient analytical tool to formulate and treat algorithmically complex contact situations, as shown in Kane et al. [1999b]. The goal of this section is to combine discrete Lagrangian mechanics with nonsmooth calculus to derive a variational formulation of the nonsmooth contact (in the sense of nonsmooth admissible configuration sets). The symplectic nature of such an algorithm is poorly understood, but one can conjecture that future theory on that would depend on approaches like this one.

If C is the admissible set (possibly nonsmooth and nonconvex) of the system, we must have $q(t) \in C$ for all times or, in the discrete case, $q_k \in C$ for all k. These constraints may be enforced by adding to the Lagrangian the indicator function I_C of C defined by

$$I_C(x) = \begin{cases} 0 & \text{if } x \in C \\ \infty & \text{otherwise.} \end{cases} \tag{5.13}$$

In the discrete context this translates into defining a constrained discrete Lagrangian $\tilde{L}_d$ by adding contributions from the indicator function. One particular way to do this is

$$\tilde{L}_d(q_k, q_{k+1}, h) = L_d(q_k, q_{k+1}, h) - \frac{1}{2}\left[I_C(q_k) + I_C(q_{k+1})\right]. \tag{5.14}$$

We use, as before, the variational principle of Hamilton to derive the discrete equations of motions. Thus, the discrete Euler-Lagrange equations become

$$D_2 L_d(q_{k-1}, q_k, h) + D_1 L_d(q_k, q_{k+1}, h) - \partial I_C(q_k) \ni 0, \tag{5.15}$$

where ∂I_C denotes the generalized gradient of the indicator function.

For points q in the interior of C, $\partial I_C(q) = \{0\}$, while for points on the boundary of C, $\partial I_C(q) = N_C(q)$, where $N_C(q)$ represents the normal cone to C at q defined in the nonsmooth analysis framework (see Clarke [1983] for a complete account of the nonsmooth calculus used here). However, if q is a convex point, $N_C(q)$ reduces to the normal cone in the usual convex analysis sense.

The constrained discrete equations (5.15) are thus the usual discrete Euler-Lagrange equations (4.7) away from the impact. The generalized gradient ∂I_C is not trivial only for $\tilde{q} \in \partial C$. If we specialize (5.15) for points $q_{i-1}, \tilde{q}$ and q_{i+1}, then we obtain

$$D_2 L_d(q_{i-1}, \tilde{q}, \alpha h) + D_1 L_d(\tilde{q}, q_{i+1}, (1-\alpha)h) - \partial I_C(\tilde{q}) \ni 0, \tag{5.16}$$

which is a natural generalization of (4.9b) in the case when $\tilde{q}$ is a singular point of ∂C.

Alternatively, using the previous notations for discrete momenta (4.12), (5.16) can be written as

$$p^+(q_{i-1}, \tilde{q}, \alpha h) - p^-(\tilde{q}, q_{i+1}, (1-\alpha)h) \in N_C(\tilde{q}), \tag{5.17}$$

where we used $\partial I_C(\tilde{q}) = N_C(\tilde{q})$ for $\tilde{q} \in \partial C$. Therefore, (5.17) generalizes (4.15) in the case when $\tilde{q}$ is a corner of ∂C and we cannot define a tangent plane at that point.

For Lagrangians consisting of only kinetic energy and for the particular discretization (4.18), the momentum conservation (5.16) leads to a very interesting geometrical interpretation. Indeed, for a unitary mass matrix, (5.16) becomes

$$\frac{\tilde{q} - q_{i-1}}{\alpha h} - \frac{q_i - \tilde{q}}{(1-\alpha)h} - \partial I_C(\tilde{q}) \ni 0. \tag{5.18}$$

The inclusion (5.18) can be rewritten in the following form

$$(1-\alpha) q_{i-1} + \alpha q_i \in (I - \partial I_C)(\tilde{q}). \tag{5.19}$$

Now we will connect (5.19) with the concept of the ***closest point projection***. First recall the definition of the ***resolvent*** of the set-valued operator ∂I_C as

$$R = (I + \partial I_C)^{-1}. \tag{5.20}$$

It is a well-known fact that the resolvent of the subgradient of the indicator function of a

convex set is the closest-point projection onto that set (see Rockafellar [1970]). Under the assumption that $\bar{C}$, the complement of C, is a convex set (see Figure 5.5), the inclusion (5.19) can be written as

$$\tilde{q} = P_{\bar{C}}(q_{i-\alpha}), \tag{5.21}$$

where $P_{\bar{C}}$ represents the closest-point projection operator onto $\bar{C}$ and $q_{i-\alpha}$ is the convex combination of the points q_{i-1} and q_i

$$q_{i-\alpha} = (1-\alpha)q_{i-1} + \alpha q_i.$$

We will conclude this section by the following two remarks which re-emphasize the particular benefit of the nonsmooth calculus approach.

Remark. Besides its theoretical attractiveness, the nonsmooth analysis approach has a great advantage over the standard penalty formulation methods in dealing with complex nonsmooth contact geometries (see Kane et al. [1999b]), where neither normals nor gap functions may be defined. Indeed, for such problems penalty methods simply fail.

Remark. The nonsmooth approach also gives the natural framework for constructing time-adaptive variational integrators for collisions (see Kane et al. [1999a] and Marsden and West [2001]), but we will leave the development and illustration of such contact algorithms for future work.

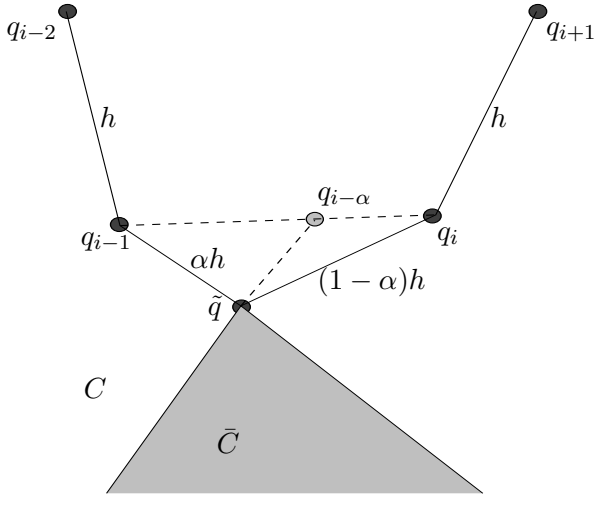


Figure 5.5: Collision at a singular point of the contact set ∂C

Chapter 6

Concluding Remarks and Future Directions

Concluding Remarks. The main goal of this thesis was to develop a geometric computational approach to collisions and free boundary problems. By using a variational methodology we gain insights and new perspectives on these problems from both theoretical and computational viewpoints. Regarded from a PDE/functional analysis point of view, this thesis may seem to lack hard mathematical analysis results on existence and uniqueness theory. This is indeed a theory which we do not address. For the interested reader, we provide a brief literature survey on such alternative approaches (measure differential inclusions, sweeping processes) to rigid-body dynamics with impact—see the introduction. For recent progress on existence and uniqueness for free boundary problems we refer the reader to Coutand and Shkoller [2003] and references therein.

Future Directions. There are several directions to pursue in the future to complete the foundations laid in this work. Perhaps the most important task is to develop algorithms and a discrete mechanics for nonsmooth multisymplectic variational mechanics and to take advantage of the current algorithms that are already developing in this direction.

Another task is to further develop the theory of shock waves by combining the geometric approach here with more analytical techniques, such as those used in hyperbolic systems of conservation laws, as well as incorporating appropriate thermodynamic notions. Alternatively, a possible direction is to link the nonsmooth multisymplectic theory developed in this work with Lagrangian averaging regularization techniques used in alpha models (see Holm et al. [1998]). The Lagrangian averaging technique is an intrinsic regularization method

for the high wave modes of the Euler equations such that all the geometrical structure of the fluid dynamics is preserved. Possible usage of the multisymplectic formalism into this context will be investigated in our future work.

For some systems, there will be surface tension and other boundary effects; for some of these systems a Hamiltonian structure is already understood (see Lewis et al. [1986] and references therein), but not a multisymplectic structure.

Here we have only considered isolated discontinuities, but there may be degeneracies caused by the intersections of different types and dimensions of discontinuity surfaces that require further attention.

Finally, as in Kane et al. [2000], friction (or other dissipative phenomena) and forcing need to be included in the multisymplectic formalism.

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