FINITE ELEMENT METHODS: 1970's AND BEYOND
L.P. Franca (Ed.)

AN OVERVIEW OF VARIATIONAL INTEGRATORS

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To Tom Hughes on the occasion of his 60th birthday.

Tom Hughes has been a friend, collaborator, and colleague to some of us for several decades and has been a major inspiration on many fronts. One aspect of his personality that is held most dear is his clarity of thought and his insistence on understanding things a little more deeply and at a more fundamental level than most. This willingness to take the time to reach back to the foundations of a subject and to scrutinize them closely has of course eventually paid off handsomely in his contributions and his career. It is a real pleasure for us to contribute this small account of some work on integration algorithms for mechanical systems that has been of interest to Tom from time to time throughout his work and was especially important to his dear friend and colleague, the late Juan Simo.

Abstract. The purpose of this paper is to survey some recent advances in variational integrators for both finite dimensional mechanical systems as well as continuum mechanics. These advances include the general development of discrete mechanics, applications to dissipative systems, collisions, spacetime integration algorithms, AVI's (Asynchronous Variational Integrators), as well as reduction for discrete mechanical systems. To keep the article within the set limits, we will only treat each topic briefly and will not attempt to develop any particular topic in any depth. We hope, nonetheless, that this paper serves as a useful guide to the literature as well as to future directions and open problems in the subject.

Key words: mechanical integrators, variational principles, conservation properties, discrete mechanics, symmetry, reduction.

1 VARIATIONAL INTEGRATORS

The idea of variational integrators is very simple: one obtains algorithms by forming a discrete version of Hamilton's variational principle. For conservative systems one uses the usual variational principles of mechanics, while for dissipative or forced systems, one uses the Lagrange–d'Alembert principle.

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Research partially supported by NSF–ITR grant ACI–0204932.

Hamilton's Configuration Space Principle. Let us begin with the case of finite dimensional systems first. We now recall from basic mechanics (see, for example, Marsden and Ratiu [1999]) the *configuration space form of Hamilton's principle*. Let a mechanical system have an n-dimensional configuration manifold Q (with a choice of coordinates denoted by q^i, $i = 1, \ldots, n$) and be described by a Lagrangian $L : TQ \to \mathbb{R}$, denoted in coordinates by $L(q^i, \dot{q}^i)$. Then the principle states that the action integral is stationary for curves in Q with fixed endpoints; this principle is commonly denoted (see Figure 1.1).

$$\delta \int_a^b L(q, \dot{q})\, dt = 0.$$

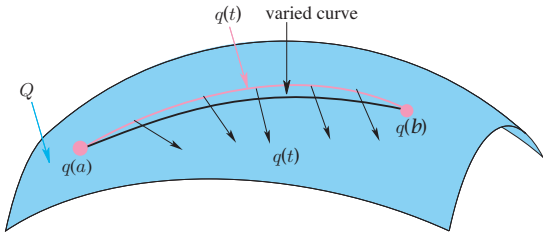


Figure 1.1: The configuration space form of Hamilton's principle

With appropriate regularity assumptions, Hamilton's principle, as is well-known, is equivalent to the *Euler–Lagrange equations*

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i} - \frac{\partial L}{\partial q^i} = 0.$$

Discrete Configuration Space Mechanics. In discrete mechanics from the Lagrangian point of view, which has its roots in discrete optimal control from the 1960's (see Marsden and West [2001] and Lew, Marsden, Ortiz, and West [2004] for accounts of the history and related literature), one first forms a ***discrete Lagrangian***, a function L_d of two points $q_1, q_2 \in Q$ and a time step h by approximating the the action integral along an exact trajectory with a quadrature rule:

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

where $q(t)$ is an *exact solution* of the Euler–Lagrange equations for L joining q_0 to q_1 over the *time step interval* $0 \le t \le h$. Recall that Jacobi's theorem from 1840 states that using the exact value and not an approximation would lead to a solution to the Hamilton–Jacobi equation. This is depicted in Figure 1.2 (a) and points out a key link with Hamilton–Jacobi theory.

Holding h fixed at the moment, we regard L_d as a mapping $L_d : Q \times Q \to \mathbb{R}$. This way of thinking of the discrete Lagrangian as a function of two nearby points (which take the place of a discrete position and velocity) goes back to the origins of Hamilton–Jacobi theory itself, but appears explicitly in the discrete optimal control literature in the 1960s, and was exploited effectively by, for example, Suris [1990];

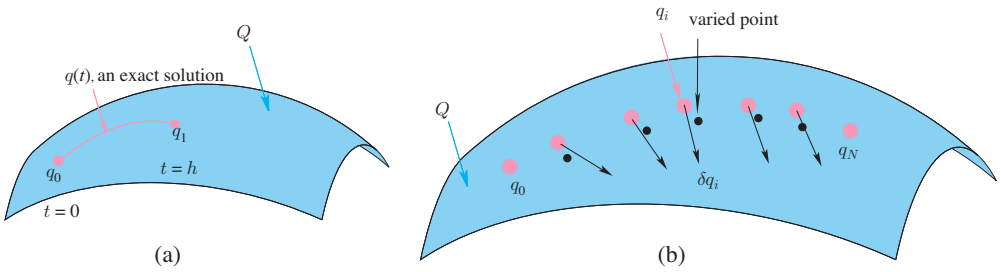


Figure 1.2: The discrete form of the configuration form of Hamilton's principle

Moser and Veselov [1991]; Wendlandt and Marsden [1997]. It is a point of view that is crucial for the development of the theory.

Given a discrete Lagrangian L_d, the discrete theory proceeds in its own right as follows. Given a sequence $q_1, \ldots, q_N$ of points in Q, form the ***discrete action sum:***

$$S_d = \sum_{k=0}^{N-1} L_d\left(q_k, q_{k+1}, h_k\right).$$

Then the *discrete Hamilton configuration space principle* requires us to seek a critical point of S_d with fixed end points, q_0 and q_N. Taking the special case of three points q_{i-1}, q_i, q_{i+1}, so the discrete action sum is $L_d\left(q_{i-1}, q_i, h_{i-1}\right) + L_d\left(q_i, q_{i+1}, h_i\right)$ and varying with respect to the middle point q_i gives the *DEL* (***discrete Euler–Lagrange***) equations:

$$D_2 L_d\left(q_{i-1}, q_i, h_{i-1}\right) + D_1 L_d\left(q_i, q_{i+1}, h_i\right) = 0. \tag{1.1}$$

One arrives at exactly the same result using the full discrete variational principle. The equations 1.1 defines, perhaps implicitly, the DEL ***algorithm***: $(q_{i-1}, q_i) \mapsto (q_i, q_{i+1})$.

Example. Let M be a positive definite symmetric $n \times n$ matrix and $V : \mathbb{R}^n \to \mathbb{R}$ be a given potential. Choose a discrete Lagrangian on $\mathbb{R}^n \times \mathbb{R}^n$ of the form

$$L_d(q_0, q_1, h) = h\left[\left(\frac{q_1 - q_0}{h}\right)^T M\left(\frac{q_1 - q_0}{h}\right) - V(q_0)\right], \tag{1.2}$$

which arises in an obvious way from its continuous counterpart by using simply a form of "rectangle rule" on the action integral. For this discrete Lagrangian, the DEL equations are readily worked out to be

$$M\left(\frac{q_{k+1} - 2q_k + q_{k-1}}{h^2}\right) = -\nabla V(q_k),$$

a discretization of Newton's equations, using a simple finite difference rule for the derivative.

Somewhat related to this example, it is shown in Kane, Marsden, Ortiz, and West [2000] that the widely used Newmark scheme (see Newmark [1959]) *is also variational* in this sense as are many other standard integrators, including the midpoint rule, symplectic partitioned Runge–Kutta schemes, etc.; we refer to Marsden

and West [2001] (see also Suris [1990]) for details. Of course, Tom's book (Hughes [1987]) is one of the standard sources for the Newmark algorithm). Some of us have come to the belief that the variational nature of the Newmark scheme is one of the reasons for its excellent performance.

Hamilton's Phase Space Principle. We briefly mention the Hamiltonian point of view; now we are given a Hamiltonian function $H : T^*Q \to \mathbb{R}$, where T^*Q is the cotangent bundle of Q, on which a coordinate choice is denoted $(q^1, \dots q^n, p_1, \dots, p_n)$. In this context one normally uses the *phase space principle of Hamilton*, which states that for curves $(q(t), p(t))$ in T^*Q, with fixed endpoints, that the phase space action integral be stationary:

$$\delta \int_a^b \left(p_i dq^i - H(q^i, p_i) \right) \, dt = 0. \tag{1.3}$$

Of course, $p_i dq^i$ is the coordinate form of the canonical one-form Θ which has the property that $d\Theta = -\Omega = \sum dq^i \wedge dp_i$, the standard symplectic form. Again, under appropriate regularity conditions, this phase space principle is equivalent to Hamilton's equations:

$$\frac{dq^i}{dt} = \frac{\partial H}{\partial p_i}; \quad \frac{dp_i}{dt} = -\frac{\partial H}{\partial q^i}. \tag{1.4}$$

Discrete Hamilton's Phase Space Principle. There are some different choices of the form of the discrete Hamiltonian, corresponding to different forms of generating functions, but perhaps the simplest and most intrinsic one is a function $H_d : T^*Q \times \mathbb{R} \to \mathbb{R}$, where $H_d(q, p, h)$. As in the Lagrangian case, H_d is an approximation of the action integral:

$$H_d(q, p, h) \approx \int_0^h \left(p_i(t) dq^i(t) - H(q^i(t), p_i(t)) \right) \, dt, \tag{1.5}$$

where $(q(t), p(t)) \in T^*Q$ is the unique solution of Hamilton's equations with $(q(0), p(0)) = (q, p)$. We do not discuss the Hamiltonian point of view here, but rather refer to the work of Lall and West [2004] for more information. Many algorithms, such as the midpoint rule and symplectic Runge–Kutta schemes, appear more naturally from the Hamiltonian point of view, as discussed in Marsden and West [2001].

In addition, some problems, such as the dynamics of point vortices discussed in Rowley and Marsden [2002] and below, involved degenerate Lagrangians, but have a nice Hamiltonian formulation. In this case, it seems that there is a definite numerical advantage to using a Hamiltonian formulation directly without going via the Lagrangian formalism. For instance, the discrete Euler–Lagrange equations corresponding to a degenerate continuous Lagrangian may attempt to treat the equations as second order equations, whereas the continuous equations are, in reality, first order. The Lagrangian approach can, for these reasons, lead to potential instabilities due to multi-step algorithms (such as the leapfrog scheme) and so one would have to be very careful in the choice of parameters, as is done in Rowley and Marsden [2002]. It seems that a direct Hamiltonian approach avoids these issues and so is one reason for their usefulness.

2 PROPERTIES OF VARIATIONAL INTEGRATORS

We shall demonstrate through some specific examples that variational integrators work very well for *both* conservative and dissipative or forced mechanical systems in a variety of senses. Some specific properties of variational integrators that make them attractive are given in the following paragraphs.

Structure Preservation. No matter what the choice of the discrete Lagrangian, variational integrators are, for the non-dissipative and non-forced (that is the conservative) case, *symplectic and momentum* conserving. Momentum preserving means that when the discrete system has a symmetry, then there is a discrete Noether theorem that gives a quantity that is exactly conserved at the discrete level. Figure 2.1(a) illustrates the sort of qualitative difference that structure preserving gives in solar system dynamics and in (b) we illustrate that symplectic in the case of two dimensional systems means area preserving, even with large distortions.

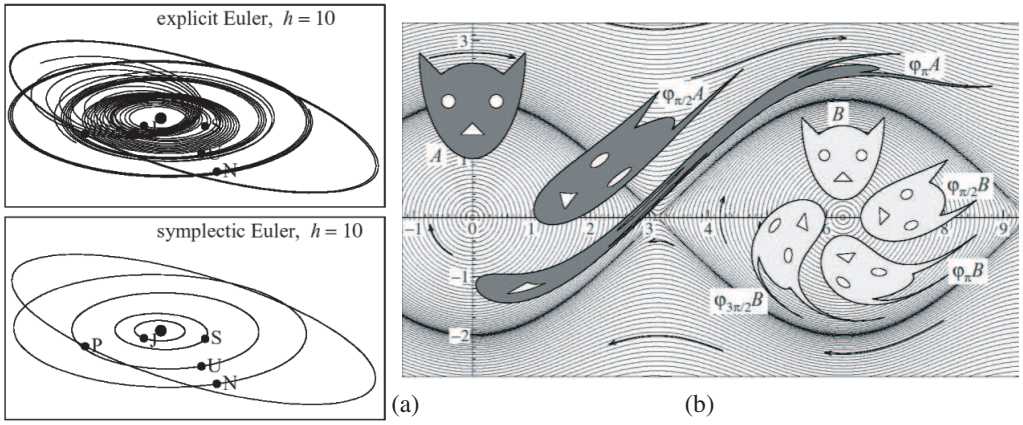


Figure 2.1: (a) Variational integrators give good qualitative behavior for comparable computational effort. (b) Variational integrators preserve the symplectic form in phase space (area in two dimensions). These figures are due to Hairer, Lubich, and Wanner [2001], to which we refer for further information.

Marsden and West [2001] give a detailed discussion of discrete mechanics in the finite dimensional case, the associated numerical analysis and for a variational proof of the symplectic property and the discrete conservation laws. We also note that this theory shows the sense in which, for example, the Newmark scheme is symplectic; some people have searched in vain *by hand* to try to discover a conserved symplectic form for the Newmark algorithm—but it is hidden from view and it is the variational technique that evokes it!

One can check the conservation properties by direct computation (see Wendlandt and Marsden [1997]) or what is more satisfying, one can derive them directly from the variational nature of the algorithm. In fact, the symplectic nature of the algorithm results from the boundary terms in the variational principle when the endpoints are allowed to vary. This argument is due to Marsden, Patrick, and Shkoller [1998].

Another remark is in order concerning both the symplectic nature as well as the Noether conserved quantities. In the continuous theory, the conserved symplectic structure is given, in the Lagrangian picture, by the differential two-form $\Omega = dq^i \wedge dp_i$, where a sum on i is understood and $p_i = \partial L/\partial \dot{q}^i$. One has to be careful about

what the discrete counterpart of Ω is. Trial and error, which has been often used, is of course very inefficient. Fortunately, the theory *produces automatically* the correct conserved form, a two-form on $Q \times Q$, just from the variational nature of the problem by mimicking the continuous proof. Similar remarks apply to the case of the Noether conserved quantities.

It should be also noted that there are deep links between the variational method for discrete mechanics and integrable systems. This area of research was started by Moser and Veselov [1991] and was continued by many others, notably by Bobenko and Suris; we refer the reader to the book Suris [2003] for further information. The main and very interesting example studied by Moser and Veselov [1991] was to find an integrable discretization of the n-dimensional rigid body, an integrable system; see also Bloch, Crouch, Marsden, and Ratiu [2002] for further insight into the discretization process in this case.

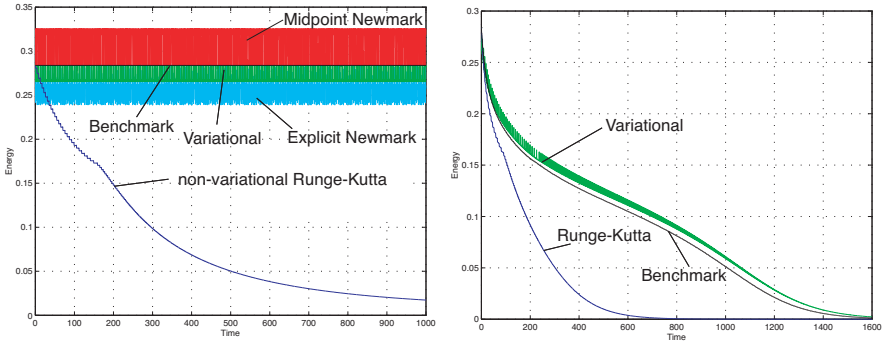
A bit more history that touches Tom personally is perhaps in order at this point. We need to recall, first of all, that Tom has had a long interest in energy preserving schemes, for example, in his work with Caughey (see Chorin, Hughes, Marsden, and Mccracken [1978] and references therein). We also need to recall that a result of Ge and Marsden [1988] states that typically integrators with a fixed time step cannot simultaneously preserve energy, the symplectic structure and conserved quantities. "Typically" means for instance that integrable systems can be an exception to this rule. This result led to a dichotomy in the literature between symplectic-momentum and energy-momentum integrators; the late Juan Simo was a champion of the energy-momentum approach, as discussed in, for instance Simo, Tarnow, and Wong [1992], Gonzalez and Simo [1996], and Gonzalez [1996]. On the other hand, one can "have it all" if one uses adaptive schemes, as in Kane, Marsden, and Ortiz [1999]. However, for reasons of numerical efficiency and because of the remarkable energy behavior of symplectic schemes (discussed below), it seems that symplectic-momentum methods are the methods of choice at the moment, although adaptation is a key issue discussed further in the context of AVI methods below.

Integrator Design. A nice feature of the variational approach to symplectic integrators is that it leads to a systematic construction of *higher-order* integrators, which is much easier than finding approximate solutions to the Hamilton–Jacobi equation, which is the original methodology (discussed in, for example, De Vogelaére [1956], Ruth [1983] and Channell and Scovel [1990]). For instance, by taking appropriate Gauss–Lobatto quadrature approximations of the action function, one arrives in a natural way at the SPARK (symplectic partitioned adaptive Runge–Kutta) methods of Jay [1996] (see also Belytschko [1981] and Grubmüller et. al. [1991]); this is shown in Marsden and West [2001]. It is also notable that these integrators are *flexible*, they include explicit or implicit algorithms; thus, in the design, there is no bias towards either type of integrator. In addition, the variational methodology has led to the important notion of *multisymplectic integrators*, discussed below.

Accuracy and Energy Behavior. In Marsden and West [2001] it is shown that the order of approximation of the action integral is reflected in the corresponding order of approximation for the algorithm. For instance, this is the general reason that the Newmark algorithm is second order accurate and why the SPARK schemes

can be designed to be higher order accurate. A corresponding statement for the PDE case is given in Lew, Marsden, Ortiz, and West [2004]. The notion of Γ-*convergence* is also emerging as a very important notion for variational integrators and this aspect is investigated in Müller and M. Ortiz [2004].

Variational integrators have remarkably good energy behavior in both the conservative and dissipative cases (for the latter, recall that one discretizes the Lagrange-d'Alembert principle); consider, for example, the system described in Figure 2.2, namely a particle moving in the plane.



(a) Conservative mechanics (b) Dissipative mechanics

Figure 2.2: Showing the excellent energy behavior for both conservative and dissipative systems: a particle in $\mathbb{R}^2$ with a radially symmetric polynomial potential (left); with small dissipation of the standard sort (proportional to the velocity) (right).

This figure illustrates the fact that variational integrators have long time energy stability (as long as the time step is reasonably small). This is a key property, but it is also a deep one from the theoretical point of view and is observed to hold numerically in many cases when the theory cannot strictly be verified; the key technique is known as *backward error analysis* and it seeks to show that the algorithm is, up to exponentially small errors, the exact time integration of a nearby Hamiltonian system, an idea going back to Neishtadt [1984]. See, for instance, Hairer and Lubich [2000] for an excellent analysis.

But there are many unanswered questions. For instance, apart from the numerical evidence, a corresponding theory for the dissipative case is not known at the present time. Some progress is being made on the PDE case, but the theory still has a long way to go; see, for instance Oliver, West, and Wulff [2004]. For this example, in the absence of dissipation the variational algorithms are *exactly symplectic and angular momentum preserving*—if one were to plot a measure of these quantities, one would just see a horizontal line, confirming the theory that this is indeed always the case.

Computing Statistical Quantities. Variational integrators have some other interesting properties having to do with the accurate computation of statistical quantities. One should not think that individual trajectories are necessarily computed accurately in a chaotic regime, but it does seem that important statistical quantities are computed correctly. In other words, these integrators somehow "get the physics right".

We give two examples of such behavior. The first of these (see Figure 2.3), taken from Rowley and Marsden [2002], is the computation of chaotic invariant

sets in the four point vortex dynamics in the plane. As mentioned previously, the Lagrangian for this problem is degenerate and so one has to be careful with both the formulation and the numerics. As mentioned previously, if one uses Hamilton's phase space principle directly on this problem, things are somewhat improved. The figure shows a Poincaré section for this problem in a chaotic regime. It clearly shows that variational integrators produce the structure of the chaotic invariant set more accurately than (non symplectic) Runge–Kutta algorithms, even more accurate ones.

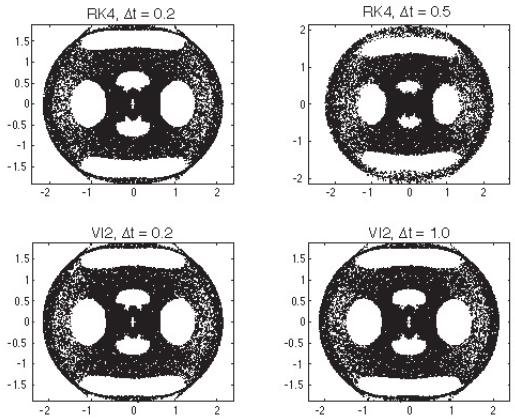


Figure 2.3: Variational integrators capture well the structure of chaotic sets; RK4 is a fourth order Runge–Kutta algorithm, while VI2 is a second order accurate variational integrator. The time step is $h = \Delta t$. Both schemes produce clear Poincaré sections for $h = 0.2$, but for $h = 0.5$, scheme RK4 produces a blurred section, while the section from scheme VI2 remains crisp even for $h = 1.0$. For $h = 1.0$, scheme RK4 deviates completely, and transitions into a spurious quasiperiodic state.

Another interesting statistical quantity is the computation of the *"temperature"* (strictly speaking, the "heat content", or the time average of the kinetic energy) of a system of interacting particles, taken from Lew, Marsden, Ortiz, and West [2004] and shown in Figure 2.4. Of course the "temperature" is not associated with any conserved quantity and nevertheless variational integrators give a well defined temperature over what appears to be an indefinite integration time, while standard integrators eventually deviate and again give spurious results.

Discrete Reduction Theory. Reduction theory is an indispensable tool in the study of many aspects of mechanical systems with symmetry, such as stability of relative equilibria by the energy–momentum method. See Marsden and Weinstein [2001] for a review of the many facets of this theory and for references. It is natural to seek discrete analogs of this theory. Motivated by the work of Moser and Veselov [1991], the first version of discrete reduction that was developed was the discrete analog of Euler–Poincaré reduction, which reduces second-order Euler–Lagrange equations on a Lie group G to first order dynamics on its Lie algebra $\mathfrak{g}$. Examples of this sort of reduction are the Euler equations for a rigid body and the Euler equations for an ideal fluid. The discrete version of this gives the DEL or *Discrete Euler–Lagrange* equations. These equations were investigated by Marsden, Pekarsky, and Shkoller [1999, 2000] and Bobenko and Suris [1999,?] (who also made some interesting links with integrable structures and semi-direct products).

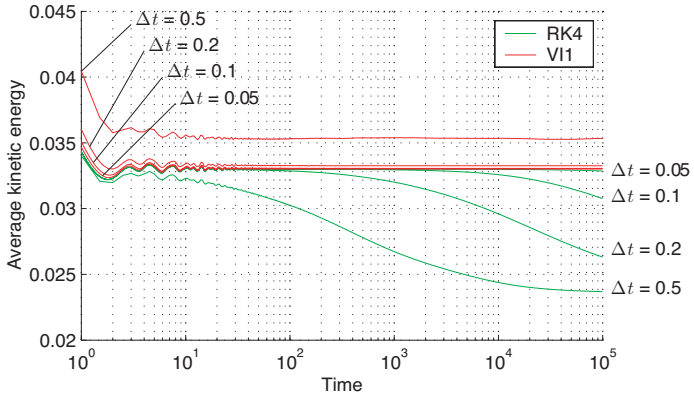


Figure 2.4: Variational integrators capture statistically significant quantities, such as the heat content of a chaotic system. The average kinetic energy as a function of the integration run T for a nonlinear spring–mass lattice system in the plane, using a first order variational integrator (VI1) and a fourth order Runge–Kutta method (RK4) and a range of timesteps Δt. Observe that the Runge–Kutta method suffers substantial numerical dissipation, unlike the variational method.

Another step forward was made by Jalnapurkar, Leok, Marsden, and West [2004] who developed discrete reduction for the case of Routh reduction; that is, one fixes the value of the momentum conjugate to cyclic variables and drops the dynamics to the quotient space. This was applied to the case of satellite dynamics for an oblate Earth (the J_2 problem) and to the double spherical pendulum. Already this case is interesting because these examples exhibit geometric phases and the reduction allows one to "separate out" the phase shift and thereby avoid any spurious numerical phases.

It is clear that discrete reduction should continue to develop. For instance, in addition to the nonabelian case of Routh reduction (due to Marsden, Ratiu, and Scheurle [2000]), one should develop the DLP (Discrete Lagrange–Poincaré) and DHP (Discrete Hamilton–Poincaré) equations. The continuous LP and HP equations are discussed in Cendra, Marsden, and Ratiu [2001, 2003]. Of course, counterparts on the Hamiltonian side should also be developed.

3 MULTISYMPLECTIC AND AVI INTEGRATORS

One of the beautiful and simple things about the variational approach is that it suggests an extension to the PDE case. Namely one should discretize, in space-time, the variational principle for a given field theory, such as elasticity. This variational formulation of elasticity is well known and is described in many books, such as Marsden and Hughes [1983]. The idea is to extend the discrete formulation of Hamilton's principle discussed at the beginning of this article to an analogous discretization of a field theory. One replaces the discrete time points with a mesh in *spacetime* and replaces the points in Q with clusters of points (so that one can represent the needed derivatives of the fields) of field values.

Another historical note involving Tom is relevant here. Tom was always interested in and pushed the idea that one should ultimately do things in spacetime and not just in space with fixed time steps. He explored this idea in various papers, such as Masud and Hughes [1997] and Hughes and Stewart [1996] and even going back to Hughes and Hulbert [1988]. The AVI method is developed in the same spirit.

The Setting of AVI Methods. The basic set up and feasibility of this idea in a variational multisymplectic context was first demonstrated in Marsden, Patrick, and Shkoller [1998] who used the sine-Gordon equation to illustrate the method numerically. The paper also showed that there were discrete field theoretic analogs of all the structures one has in finite dimensional mechanics with some modifications; the symplectic structure gets replaced by a multisymplectic structure (using differential forms of higher degree) and analogs of discrete Noether quantities. As in the case of finite dimensional mechanics, all of these properties follow from the fact that one has a discrete variational principle. The appropriate multisymplectic formalism setting that set the stage for discrete elasticity was given in Marsden, Pekarsky, Shkoller, and West [2001]. Motivated by this work, Lew, Marsden, Ortiz, and West [2003] developed the theory of AVIs (Asynchronous Variational Integrators) along with an implementation for the case of elastodynamics. These integrators are based on the introduction of spacetime discretizations allowing different time steps for different elements in a finite element mesh along with the derivation of time integration algorithms in the context of discrete mechanics, i. e., the algorithm is given by a spacetime version of the Discrete Euler–Lagrange (DEL) equations of a discrete version of Hamilton's principle.

The spacetime bundle picture provides an elegant generalization of Lagrangian mechanics, including temporal, material and spatial variations and symmetries as special cases. This unites energy, configurational forces and the Euler–Lagrange equations within a single picture. The geometric formulation of the continuous theory is used to guide the development of discrete analogues of the geometric structure, such as discrete conservation laws and discrete (multi)symplectic forms. This is one of the most appealing aspects of this methodology.

To reiterate the main point, the AVI method provides a general framework for asynchronous time integration algorithms, allowing each element to have a different time step, similar in spirit to subcycling (see, for example, Neal and Belytschko [1989]), but with no constraints on the ratio of time step between adjacent elements.

A local discrete energy balance equation is obtained in a natural way in the AVI formalism. This equation is expected to be satisfied by adjusting the elemental time steps. However, as was mentioned before, it is sometimes computationally expensive to do this exactly and from simulations (such as the one given below), it seems to be unnecessary. That is, the phenomenon of near energy conservation indefinitely in time appears to hold, just as in the finite dimensional case. As was mentioned already, the full theory of a backward error analysis in the PDE context is in its infancy (see Oliver, West, and Wulff [2004]).

Elastodynamics Simulation. The formulation and implementation of a sample algorithm (explicit Newmark for the time steps) is given in this framework. An important issue is how it is decided which elements to update next consistent with hyperbolicity (causality) and the CFL condition. In fact, this is a nontrivial issue and it is accomplished using the notion of a *priority queue* borrowed from computer science. Figure 3.1 shows one snapshot of the dynamics of an elastic L-beam (the beam is undergoing oscillatory deformations). The smaller elements near the edges are updated much more frequently than the larger elements.

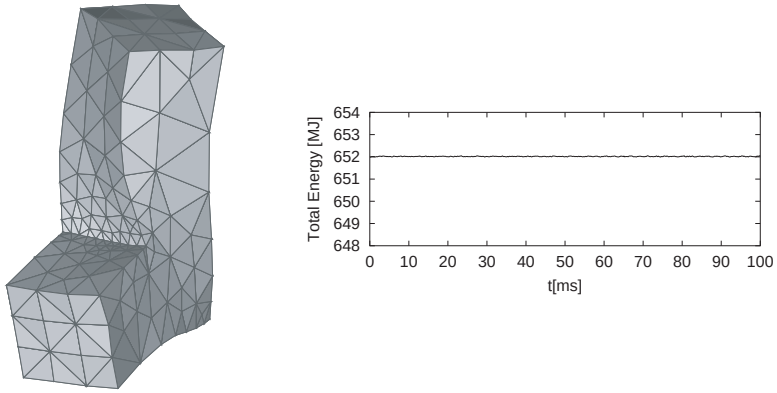


Figure 3.1: AVI methods are used to simulate the dynamics of an elastic L-beam. The energy of the L-beam is nearly constant after a long integration run with millions of updates of the smallest elements.

The figure also shows the very favorable energy behavior for the L-beam obtained with AVI techniques; the figure shows the total energy, but it is important to note that also the local energy balance is excellent—that is, there is no spurious energy exchange between elements as can be obtained with other elements. In fact, by computing the discrete Euler–Lagrange equation for the discrete action sum corresponding to each elemental time step, a local energy equation is obtained. This equation is not generally enforced, and the histogram in Figure 3.2 shows the distribution of maximum relative error in satisfying the local energy equation on each element for a two-dimentsional nonlinear elastodynamics simulation. The relative error is defined as the absolute value of the quotient between the residual of the the local energy equation and the instantaneous total energy in the element. More than 50% of the elements have a maximum relative error smaller than 0.1%, while 97.5% of the elements have a maximum relative error smaller that 1%. This test shows that the local energy behavior of AVI is excellent, even though it is not exactly enforced.

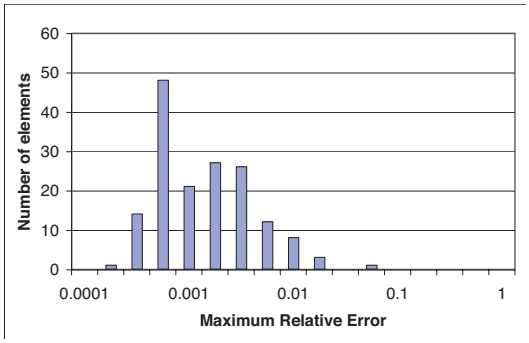


Figure 3.2: Local energy conservation for a two-dimensional nonlinear elastodynamics simulation.

These issues of small elements (sliver elements) are even more pronounced in other examples such as rotating elastic helicopter blades (without the hydrodynamics) which have also been simulated in some detail. The Helicopter blade is one of the examples that was considered by the late Juan Simo who showed that standard (and

even highly touted) algorithms can lead to troubles of various sorts. For example, if the modeling is not done carefully, then it can lead to spurious softening and also, even though the algorithm may be energy respecting, it can be very bad as far as angular momentum conserving is concerned. The present AVI techniques suffer from none of these difficulties. This problem is discussed in detail in Lew [2003] and West [2004].

Networks and Optimization. One of the main points of the AVI methodology is that it is spatially distributed in a natural way and hence it suggests that one should seek a unification of its ideas with those used in network optimization, where in the primal–dual methodology, there is an iteration between local updates for optimization and then message passing. For example, this is one of the main things going on in TCP/IP protocols, which in reality are AVI methods! This aspect of the theory is currently under development in Lall and West [2004] and represents a very exciting direction of current research.

4 COLLISIONS

Another major success of variational methods is in collision problems, both finite dimensional (particles, rigid bodies, etc) and elastic (elastic solids as well as). We refer to Fetecau, Marsden, Ortiz, and West [2003] for the complex history of the subject. In fact, most of the prior approaches to the problem are based on smoothing, on penalty methods or on weak formulations. All of these approaches suffer from difficulties of one sort or another. Our approach, in contrast, is based on a variational methodology that goes back to Young [1969]. For the algorithms, we combine this variational approach with the discrete discrete Lagrangian principle together with the introduction of a collision point and a collision time, which are solved for variationally. This variational methodology allows one to retain the symplectic nature as well as the remarkable near energy preserving properties (or correct decay in the case of dissipative problems–inelastic collisions) even in the non-smooth case.

A key first step is to introduce, for the time continuous case, a space of configuration trajectories including curve parametrizations as variables, so that the traditional approach to the calculus of variations can be applied. This extended setting enables one to give a rigorous interpretations to the sense in which the flow map of a mechanical system subjected to dissipationless impact dynamics is symplectic in a way that is consistent with Weierstrass–Erdmann type conditions for impact, in terms of energy and momentum conservation at the contact point. The discrete variational formalism leads to symplectic-momentum preserving integrators consistent with the jump conditions and the continuous theory. The basic idea is shown in Figure 4.1 in which the points q_i are varied in the discrete action sum, just as in the general DEL algorithm, but in addition, the point $\tilde{q}$ is inserted on the boundary and the variable time of collision through the parameter α are introduced. One has just the right number of equations to solve for $\tilde{q}$ and α from the variational principle.

An important issue is how nonsmooth analysis techniques—based on the Clarke calculus (see Clarke [1983] and Kane, Repetto, Ortiz, and Marsden. [1999])—can be incorporated into the variational procedure for elastic collisions, such that the integrator can cope with nonsmooth contact geometries (corner to corner collisions,

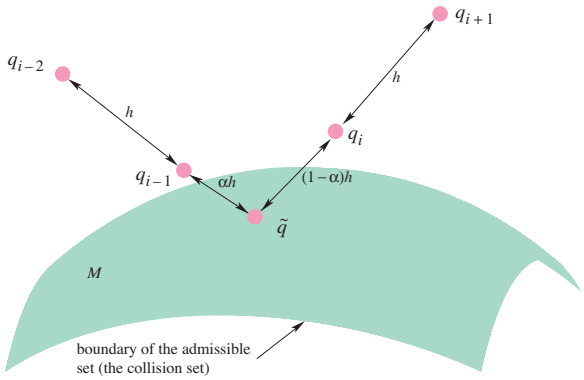


Figure 4.1: The basic geometry of the collision algorithm.

for instance). This is a case which most existing algorithms cannot handle very well (the standard penalty methods simply fail since no proper gap function can be defined for such geometries). We should also note that friction can be incorporated into these methods using, following our general methodology, the Lagrange-d'Alembert principle or similar optimization methods for handling dissipation. This is given in Pandolfi, Kane, Marsden, and Ortiz [2002].

Closely related methods have been applied to the difficult case of shell collisions in Cirak and West [2004], which are handled using a combination of ideas from AVI, subdivision, velocity decompositions and collision methods similar to those described above, along with some important spatially distributed parallelization techniques for computational efficiency. We show an example of such a collision between two thin shells in Figure 4.2. Similar methods have been applied to the case of colliding beams and to airbag inflation. In such problems, the numerous near coincidental self collisions presented a major hurdle.

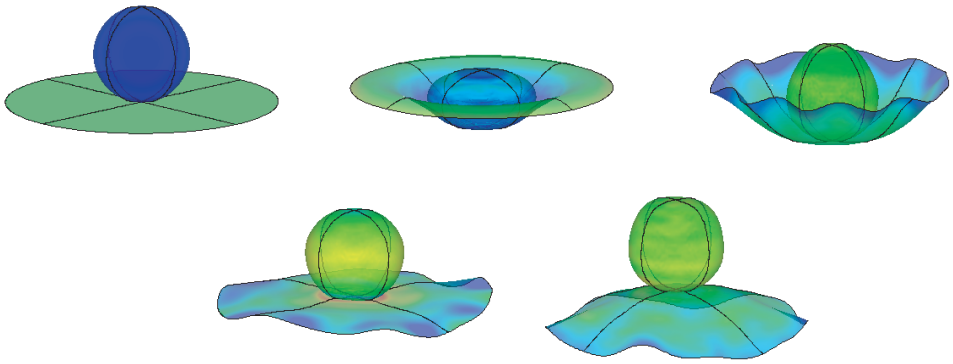


Figure 4.2: AVI methodology: collision between an elastic sphere and a plate (Cirak and West [2004].

5 SHOCK CAPTURING FOR A CONTAINED EXPLOSION

Lew [2003] has applied the AVI methodology to the case of shocks in high explosives. The detonation is initiated by impacting one of the planar surfaces of the set canister-explosive. The time steps of the elements are dynamically modified to track the front of the detonation wave and capture the chemical reaction time scales.

Figure 5.1 (parts I and II) shows the evolution of the number of elemental updates during a preset time interval (lower half of each snapshot) and the pressure contours (upper half of each snapshot), both in the explosive and in the surrounding solid. The plots of the number of elemental updates only show values on a plane of the cylinder that contains its axis, and can be roughly described as composed of three strips. The central strip, which lies in the explosive region, has fewer elemental updates than the two thin lateral strips, which lie in the solid canister region. This corresponds to having neighboring regions with different sound speeds and therefore different time steps given by the Courant condition.

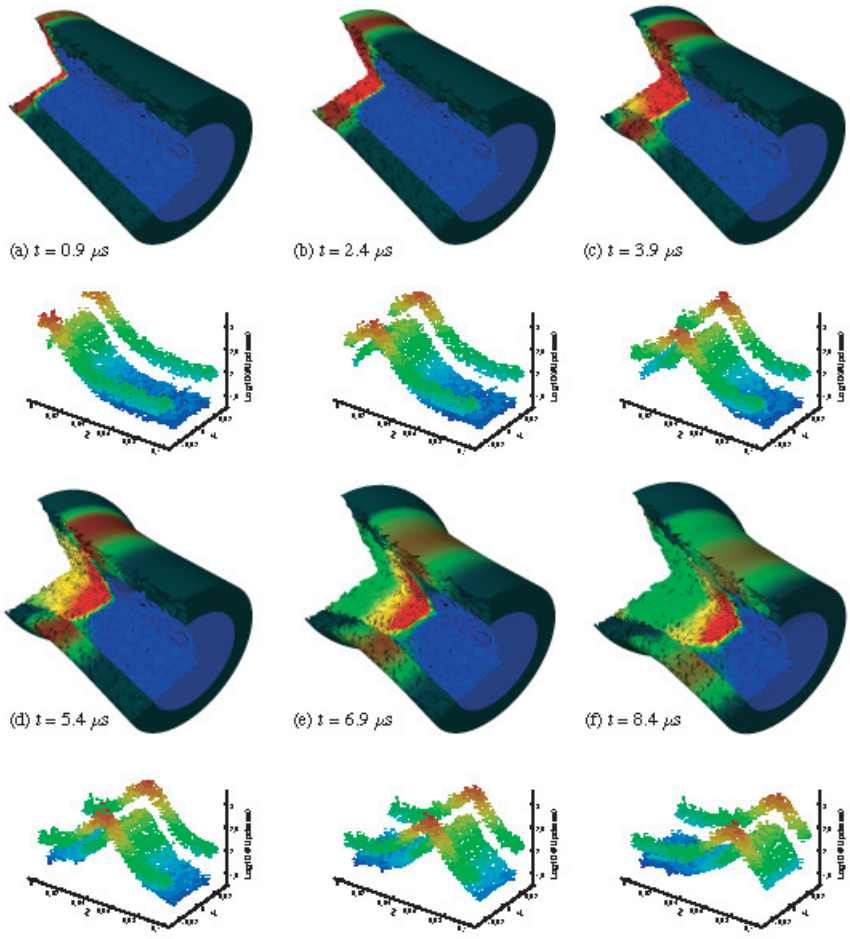


Figure 5.1 (part I): Evolution of a detonation wave within a nonlinear solid canister.

6 ADDITIONAL REMARKS AND CONCLUSIONS

It is perhaps worth pointing out that AVI methods are (perhaps without some of the users realizing it) are already being used in molecular dynamics; see, for example, Tuckerman, Berne, and Martyna [1992], Grubmüller et. al. [1991], Skeel and Srinivas [2000] and Skeel, Zhang, and Schlick [1997]. Again, we believe that some of these schemes, like the Newmark scheme have shown their value partly because of their variational and AVI nature.

One of the main problems with the current approach to molecular dynamics is one of modeling: molecular dynamics simulations are clearly inadequate for simulating

biomolecules and so one must find good ways to reduce the computational complexity. There have been many proposals for doing so, but one that is appealing to us is to use a localized KL (Karhunen–Loève or Proper Orthogonal Decomposition) method based on the hierarchical ideas used in CHARMS (see Krysl, Grinspun, and Schröder [2003]) so that these model reduction methods can be done dynamically on the fly and of course to combine them with AVI methods using the basic ideas of Lagrangian model reduction (see Lall, Krysl, and Marsden [2003]).

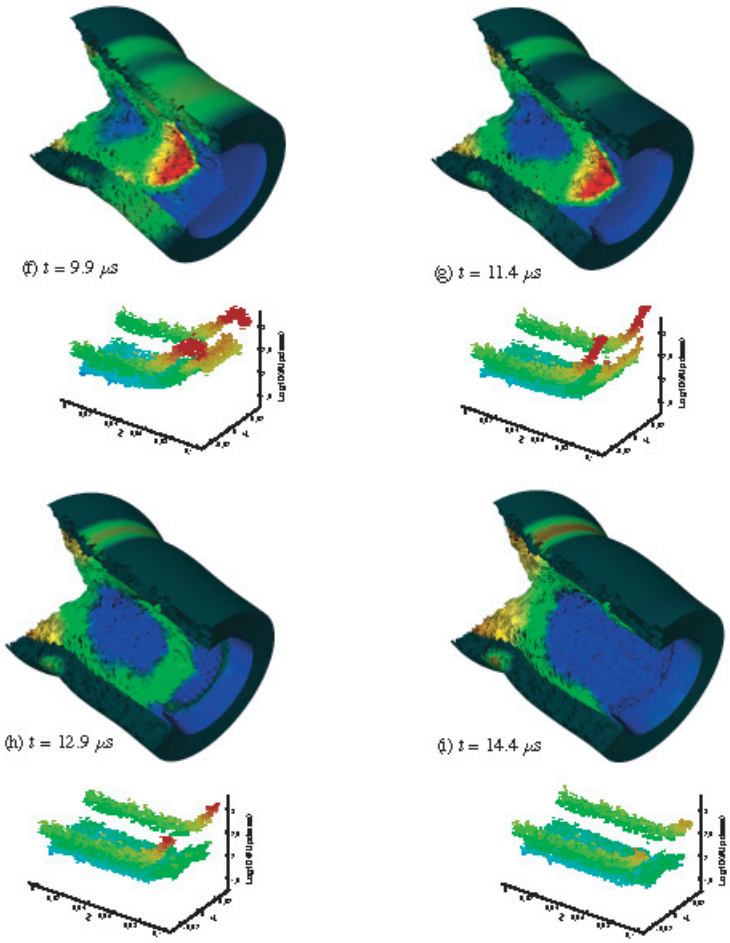


Figure 5.1 (part II): Evolution of a detonation wave within a nonlinear solid canister—continued.

Amongst the many other possible future directions, one that is currently emerging as being very exciting is that of combining AVI's with DEC *Discrete Exterior Calculus*; see, for instance, Desbrun, Hirani, Leok, and Marsden [2004] for a history and for additional references to the mechanics, geometry and graphics literature on DEC. For example, it is known in computational electromagnetism (see, for instance Bossavit [1998]) that one gets spurious modes if the usual grad–div–curl relation is violated on the discrete level. Similarly, in the mimetic differencing literature, it is known that various calculations also require this. A nice example of this are the computations used for the *EPDiff equation* (the n-dimensional generalization of the Camassa–Holm equation and also agreeing with the template matching equation of

computer vision). Such computations are given in Holm and Staley [2003] (for the general theory of the EPDiff equation, and further references, see Holm and Marsden [2004]). A theory that combines AVI and DEC techniques would be a natural topic for future research.

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