Variational Integrators

Melvin Leok
Department of Mathematics, University of California,
San Diego, CA, USA

Mathematics Subject Classification

65P10, 37M15, 70H03

Short Definition

Variational integrators are a class of geometric structure-preserving numerical methods that are based on a discrete Hamilton's variational principle, and are automatically symplectic and momentum preserving.

Description

Introduction

Geometric numerical integrators are numerical methods that preserve the geometric structure of a continuous dynamical system (see, e.g., [8, 11], and references therein), and variational integrators provide a systematic framework for constructing numerical integrators that preserve the symplectic structure and momentum, of Lagrangian and Hamiltonian systems, while exhibiting good energy stability for exponentially long times.

In many problems, the underlying geometric structure affects the qualitative behavior of solutions, and as such, numerical methods that preserve the geometry of a problem typically yield more qualitatively accurate simulations. This qualitative property of geometric integrators can be better understood by viewing a numerical method as a discrete dynamical system that approximates the flow map of the continuous system (see, e.g., [1, 21]), as opposed to the traditional view that a numerical method approximates individual trajectories. In particular, this viewpoint allows questions about long-time stability to be addressed, which would otherwise be difficult to answer.

Variational Integrators

Discrete Lagrangian mechanics [16] is based on a discrete analogue of Hamilton's principle. Given a configuration manifold Q, we introduce the *discrete action sum*, $\mathbb{S}_d : Q^{n+1} \to \mathbb{R}$, which is given by

$$\mathbb{S}_d(q_0, q_1, \ldots, q_n) = \sum_{i=0}^{n-1} L_d(q_i, q_{i+1}),$$

where Q^{n+1} can be viewed as the space of discrete trajectories on Q. The *discrete Hamilton's principle* states that

$$\delta\mathbb{S}_d(q_0, q_1 \ldots, q_n) = 0,$$

when taking variations that leave the endpoints q_0 and q_n fixed. The *discrete Lagrangian*, $L_d : Q \times Q \to \mathbb{R}$, is a generating function of the symplectic flow, and is an approximation to the *exact discrete Lagrangian*,

$$L_d^E(q_0, q_1; h) = \int_0^h L(q_{01}(t), \dot{q}_{01}(t))dt, \qquad (1)$$

where $q_{01}(0) = q_0$, $q_{01}(h) = q_1$, and q_{01} satisfies the Euler–Lagrange equation in the time interval $(0, h)$. The exact discrete Lagrangian is related to

B. Engquist (eds.), *Encyclopedia of Applied and Computational Mathematics*,
DOI 10.1007/978-3-540-70529-1, © Springer-Verlag Berlin Heidelberg 2013

the Jacobi solution of the Hamilton–Jacobi equation. Alternatively, one can characterize the exact discrete Lagrangian in the following way:

$$L_d^E(q_0, q_1; h) = \operatorname*{ext}_{\substack{q \in C^2([0,h],Q) \\ q(0)=q_0, q(h)=q_1}} \int_0^h L(q(t), \dot{q}(t))dt. \tag{2}$$

The exact discrete Lagrangian generates the exact discrete time flow of a Lagrangian system, but cannot be computed explicitly. Instead, these two characterizations of the exact discrete Lagrangian lead to two general approaches for constructing variational integrators.

The discrete variational principle then yields the *discrete Euler–Lagrange (DEL)* equation,

$$D_2 L_d(q_{k-1}, q_k) + D_1 L_d(q_k, q_{k+1}) = 0, \tag{3}$$

where D_i denotes a partial derivative with respect to the i-th argument. This implicitly defines the *discrete Lagrangian map* $F_{L_d} : (q_{k-1}, q_k) \mapsto (q_k, q_{k+1})$ for initial conditions (q_{k-1}, q_k) that are sufficiently close to the diagonal of $Q \times Q$. This is equivalent to the *implicit discrete Euler–Lagrange (IDEL)* equations,

$$p_k = -D_1 L_d(q_k, q_{k+1}), \quad p_{k+1} = D_2 L_d(q_k, q_{k+1}), \tag{4}$$

which implicitly defines the *discrete Hamiltonian map* $\tilde{F}_{L_d} : (q_k, p_k) \mapsto (q_{k+1}, p_{k+1})$, where the discrete Lagrangian is the Type I generating function of the symplectic transformation.

Störmer–Verlet Method as a Variational Integrator

The Störmer–Verlet method is an example of a variational integrator, which can also be viewed as a composition method and a splitting method (see, e.g., [7]). As a variational integrator, the Störmer–Verlet method is obtained from the following discrete Lagrangian:

$$L_d(q_0, q_1) = \frac{h}{2}\left[L\left(q_0, \frac{q_1 - q_0}{h}\right) + L\left(q_1, \frac{q_1 - q_0}{h}\right)\right]. \tag{5}$$

This can be interpreted as the trapezoidal rule approximation of the action integral, applied to the linear path that joins the boundary points q_0 and q_1. More generally, we will see that discrete Lagrangians can be constructed with a suitable choice of quadrature formula, and some prescription for specifying the state of the system at the quadrature points, subject to the boundary conditions.

To see that the discrete Lagrangian (5) recovers the Störmer–Verlet method, we consider a Lagrangian given by $L(q, \dot{q}) = \frac{1}{2}\dot{q}^T M \dot{q} - V(q)$, which is the difference of the kinetic and the potential energy. Then, the discrete Euler–Lagrange equations yield

$$\begin{aligned}
0 &= D_2 L_d(q_{k-1}, q_k) + D_1 L_d(q_k, q_{k+1}) \\
&= \frac{h}{2}\left[\frac{1}{h}\frac{\partial L}{\partial \dot{q}}\left(q_{k-1}, \frac{q_k - q_{k-1}}{h}\right) + \frac{\partial L}{\partial q}\left(q_k, \frac{q_k - q_{k-1}}{h}\right) + \frac{1}{h}\frac{\partial L}{\partial \dot{q}}\left(q_k, \frac{q_k - q_{k-1}}{h}\right)\right] \\
&\quad + \frac{h}{2}\left[\frac{\partial L}{\partial q}\left(q_k, \frac{q_{k+1} - q_k}{h}\right) - \frac{1}{h}\frac{\partial L}{\partial \dot{q}}\left(q_k, \frac{q_{k+1} - q_k}{h}\right) - \frac{1}{h}\frac{\partial L}{\partial \dot{q}}\left(q_{k+1}, \frac{q_{k+1} - q_k}{h}\right)\right] \\
&= \frac{h}{2}\left[\frac{2}{h}M\frac{q_k - q_{k-1}}{h} - \nabla V(q_k)\right] + \frac{h}{2}\left[-\nabla V(q_k) - \frac{2}{h}M\frac{q_{k+1} - q_k}{h}\right] \\
&= \frac{M}{h}(-q_{k+1} + 2q_k - q_{k-1}) - h\nabla V(q_k).
\end{aligned}$$

This is equivalent to

$$M(q_{k+1} - 2q_k + q_{k-1}) + h^2 \nabla V(q_k) = 0,$$

which is the two-step formulation of the Störmer–Verlet method with the force given by $f(q) = -M^{-1}\nabla V(q)$.

Desirable Properties of Variational Integrators

Symplecticity

Given a discrete Lagrangian L_d, one obtains a discrete fiber derivative, $\mathbb{F}L_d : (q_0, q_1) \mapsto (q_0, -D_1 L_d(q_0, q_1))$. Variational integrators are symplectic, i.e., the pullback under $\mathbb{F}L_d$ of the canonical symplectic form Ω on the cotangent bundle T^*Q is preserved. Pushing forward the discrete Euler–Lagrange equations yields a symplectic-partitioned Runge–Kutta method.

Momentum Conservation

Noether's theorem states that if a Lagrangian is invariant under the lifted action of a Lie group, then the associated momentum is preserved by the flow. If a discrete Lagrangian is invariant under the diagonal action of a symmetry group, a discrete version of Noether's theorem holds, and the discrete flow preserves the discrete momentum map. For PDEs with a uniform spatial discretization, a backward error analysis implies approximate spatial momentum conservation [19].

Approximate Energy Conservation

While variational integrators do not exactly preserve energy, backward error analysis [1, 5, 6, 20] shows that they preserve a modified Hamiltonian that is close to the original Hamiltonian for exponentially long times. In practice, the energy error is bounded and does not drift. This is the temporal analogue of the approximate momentum conservation result for PDEs, as energy is the momentum map associated with time invariance.

Variational Error Analysis and Discrete Noether's Theorem

The variational integrator approach to constructing symplectic integrators has a few important advantages from the point of view of numerical analysis. In particular, the task of establishing properties of the discrete Lagrangian map $F_{L_d} : Q \times Q \to Q \times Q$ reduces to the simpler task of verifying certain properties of the discrete Lagrangian instead. Here, we summarize the results from Theorems 1.3.3 and 2.3.1 of Marsden and West [16] that relate to the order of accuracy and momentum conservation properties of the variational integrator.

Discrete Noether's Theorem

Given a discrete Lagrangian $L_d : Q \times Q \to \mathbb{R}$ which is invariant under the diagonal action of a Lie group G on $Q \times Q$, then the discrete Lagrangian momentum map, $J_{L_d} : Q \times Q \to \mathfrak{g}^*$, given by

$$J_{L_d}(q_k, q_{k+1}) \cdot \xi = \langle -D_1 L_d(q_k, q_{k+1}), \xi_Q(q_k) \rangle$$

is invariant under the discrete Lagrangian map, i.e., $J_{L_d} \circ F_{L_d} = J_{L_d}$.

Variational Error Analysis

The natural setting for analyzing the order of accuracy of a variational integrator is the variational error analysis framework introduced in Marsden and West [16]. In particular, Theorem 2.3.1 of Marsden and West [16] states that if a discrete Lagrangian, $L_d : Q \times Q \to \mathbb{R}$, approximates the exact discrete Lagrangian, $L_d^E : Q \times Q \to \mathbb{R}$, given in (1) and (2) to order p, i.e.,

$$L_d(q_0, q_1; h) = L_d^E(q_0, q_1; h) + \mathcal{O}(h^{p+1}),$$

then the discrete Hamiltonian map, $\tilde{F}_{L_d} : (q_k, p_k) \mapsto (q_{k+1}, p_{k+1})$, viewed as a one-step method, is order p accurate.

General Techniques for Constructing Variational Integrators

Shooting-Based Variational Integrators

The exact discrete Lagrangian associated with Jacobi's solution (1) can be interpreted as the action integral evaluated on a solution of a two-point boundary-value problem. As such, a computable approximation to the exact discrete Lagrangian can be obtained in two stages: (1) apply a numerical quadrature formula to the action integral, evaluated along the exact solution of the Euler–Lagrange boundary-value problem; (2) replace the exact solution of the Euler–Lagrange boundary-value problem with a numerical solution of the boundary-value problem, in particular, by a converged shooting solution associated with a given one-step method. More generally, the shooting-based solution of the Euler–Lagrange boundary-value problem can also be replaced with approximate solutions based on other numerical schemes, including Taylor integrators, and collocation methods applied to either the Euler–Lagrange vector field or its prolongation.

Given a one-step method $\Psi_h : TQ \to TQ$, and a numerical quadrature formula $\int_0^h f(x)dx \approx h\sum_{i=0}^n b_i f(x(c_i h))$, with quadrature weights b_i and quadrature nodes $0 = c_0 < c_1 < \ldots < c_{n-1} < c_n = 1$, we construct the *shooting-based discrete Lagrangian*,

$$L_d(q_0, q_1; h) = h\sum\nolimits_{i=0}^n b_i L(q^i, v^i),$$

where

$$(q^{i+1}, v^{i+1}) = \Psi_{(c_{i+1}-c_i)h}(q^i, v^i),\ \ q^0 = q_0,\ \ q^n = q_1.$$

These equations, together with the implicit discrete Euler–Lagrange equations (4), can be solved iteratively using a shooting method. If one uses a p-th order accurate one-step method and a q-th order accurate quadrature formula to construct the variational integrator, then the resulting variational integrator will have order of accuracy $\min(p, q)$.

Galerkin Variational Integrators

The variational characterization of the exact discrete Lagrangian (2) leads to a class of Galerkin variational integrators, where one replaces the integral with a quadrature formula and replaces the space of C^2 curves with a finite-dimensional function space.

Let $\{\psi_i(\tau)\}_{i=1}^s$, $\tau \in [0, 1]$, be a set of basis functions for a s-dimensional function space C_d^s, and choose a numerical quadrature formula with quadrature weights b_i and quadrature nodes c_i. Then, a Galerkin variational integrator is given by,

$$\begin{aligned}
q_1 &= q_0 + h\sum_{i=1}^s B_i V^i,\\
p_1 &= p_0 + h\sum_{i=1}^s b_i \frac{\partial L}{\partial q}(Q^i, \dot{Q}^i),\\
Q^i &= q_0 + h\sum_{j=1}^s A_{ij} V^j, && i = 1, \ldots, s\\
0 &= \sum_{i=1}^s b_i \frac{\partial L}{\partial \dot{q}}(Q^i, \dot{Q}^i)\psi_j(c_i) - p_0 B_j\\
&\quad - h\sum_{i=1}^s (b_i B_j - b_i A_{ij})\frac{\partial L}{\partial q}(Q^i, \dot{Q}^i), && j = 1, \ldots, s\\
0 &= \sum_{i=1}^s \psi_i(c_j) V^i - \dot{Q}^j, && j = 1, \ldots, s
\end{aligned}$$

where (b_i, c_i) are the quadrature weights and quadrature points, $B_i = \int_0^1 \psi_i(\tau)d\tau$, $A_{ij} = \int_0^{c_i} \psi_j(\tau)d\tau$. When the chosen basis functions satisfy a Kronecker delta property, the last equation states that $V^i = \dot{Q}^i$, and the method reduces to a *symplectic-partitioned Runge–Kutta method*.

While variational integrators are typically described in terms of the Lagrangian, an analogous theory of variational integrators formulated in terms of the Hamiltonian was developed in Leok and Zhang [13]. When the Lagrangian and Hamiltonian are hyperregular, these two approaches yield equivalent variational integrators, but the Hamiltonian approach remains valid in the case of degenerate Hamiltonian systems, for which there is no Lagrangian analogue.

Generalizations of Variational Integrators

Lie Group and Homogeneous Space Variational Integrators

Lie groups are smooth manifolds that have a group structure. More explicitly, a Lie group can be locally identified with Euclidean space, and it has a smooth group operation. Such manifolds often arise as configuration spaces in applications involving robotics and other modern engineering systems. The basic idea of Lie group integrators is to express the update map on a Lie group G in terms of the group operation:

$$g_{k+1} = g_k \circ f_k, \tag{6}$$

where $g_k, g_{k+1} \in G$ are configuration variables, $f_k \in G$ is the incremental update, and the group operation is denoted by $\circ$. Since the group element is updated by a group operation, the group structure is preserved automatically without the need for local parameterizations, explicit constraints, or reprojection. This is in contrast to conventional numerical integrators that update group elements using addition, which does not preserve the Lie group structure, since the addition operation on the embedding linear space is not closed when restricted to the Lie group.

On a Lie group G that acts on the left, one uses the exponential map, which is a local diffeomorphism, to obtain an open neighborhood $U \subset G$ of e such that $\exp_e^{-1} : U \to \mathfrak{u} \subset \mathfrak{g}$. This yields a natural chart $\psi_g : L_g U \to \mathfrak{u}$ at $g \in G$ given by $\psi_g = \exp_e^{-1} \circ L_{g^{-1}}$. Consider an interpolatory function at the level of the Lie algebra $\mathfrak{g}$ that is described by a set of control points $\xi^\nu = \psi_{g^0}^{-1}(g^\nu)$ at control times $0 = d_0 < d_1 <$

$d_2 < \ldots < d_{s-1} < d_s = 1$. Lifting this curve to the Lie group yields the following G-equivariant interpolant,

$$\varphi(g^\nu; \tau h) = \psi_{g^0}^{-1}\Big(\sum\nolimits_{\nu=0}^{s} \psi_{g^0}(g^\nu)\tilde{l}_{\nu,s}(\tau)\Big),$$

where $\tilde{l}_{\nu,s}(t)$ denote the Lagrange polynomials associated with the control times d_ν. A quadrature approximation of the integral then yields the following discrete Lagrangian:

$$L_d(g_0, g_1) = \underset{g^\nu \in G; g^0 = g_0; g^s = g_0^{-1} g_1}{\operatorname{ext}} h \sum\nolimits_{i=1}^{s} b_i L(T\varphi(\{g^\nu\}_{\nu=0}^{s}; c_i h)).$$

This can be expressed in terms of the Lie algebra element $\xi^\nu = \psi_{g_0}(g^\nu)$ associated with the ν-th control point g^ν, which yields the following expression for the discrete Lagrangian:

$$\begin{aligned} L_d(g_0, g_1) = \underset{\xi^\nu \in \mathfrak{g}; \xi^0 = 0; \xi^s = \psi_{g_0}(g_1)}{\operatorname{ext}} h \sum\nolimits_{i=1}^{s} b_i L\Big(& L_{g_0} \exp(\xi(c_i h)), \\ & T_{\exp(\xi(c_i h))} L_{g_0} \cdot T_e L_{\exp(\xi(c_i h))} \cdot \operatorname{dexp}_{\operatorname{ad}_{\xi(c_i h)}}(\dot{\xi}(c_i h))\Big). \end{aligned}$$

The extremal conditions for the Lie algebra elements can be explicitly computed to give

$$L_d(g_0, g_1) = h \sum\nolimits_{i=1}^{s} b_i L\Big(L_{g_0} \exp(\xi(c_i h)), T_{\exp(\xi(c_i h))} L_{g_0} \cdot T_e L_{\exp(\xi(c_i h))} \cdot \operatorname{dexp}_{\operatorname{ad}_{\xi(c_i h)}}(\dot{\xi}(c_i h))\Big)$$

with $\xi^0 = 0$, $\xi^s = \psi_{g_0}(g_1)$, and the other Lie algebra elements are implicitly defined by,

$$\begin{aligned} 0 = h \sum\nolimits_{i=1}^{s} b_i \Bigg[& \frac{\partial L}{\partial g}(c_i h) T_{\exp(\xi(c_i h))} L_{g_0} \cdot T_e L_{\exp(\xi(c_i h))} \cdot \operatorname{dexp}_{\operatorname{ad}_{\xi(c_i h)}} \tilde{l}_{\nu,s}(c_i) \\ & + \frac{1}{h} \frac{\partial L}{\partial \dot{g}}(c_i h) T^2_{\exp(\xi(c_i h))} L_{\exp(\xi(c_i h))} \cdot T_e^2 L_{\exp(\xi(c_i h))} \cdot \operatorname{ddexp}_{\operatorname{ad}_{\xi(c_i h)}} \dot{\tilde{l}}_{\nu,s}(c_i) \Bigg], \end{aligned}$$

for $\nu = 1, \ldots, s-1$, and where $\operatorname{dexp}_w = \sum_{n=0}^{\infty} \frac{w^n}{(n+1)!}$, and $\operatorname{ddexp}_w = \sum_{n=0}^{\infty} \frac{w^n}{(n+2)!}$. These conditions are analogous to the internal stages of a Runge–Kutta method. The expression for the Lie group discrete Lagrangian yields a *Lie group variational integrator* [9].

Another important related class of manifolds are homogeneous spaces, which are manifolds with a transitive Lie group action. Given a homogeneous space H and a Lie group G, a curve $h : \mathbb{R} \to H$ on the homogeneous space can be lifted to a curve

$g : \mathbb{R} \to G$, where $h(t) = g(t) \cdot h(0)$, and $g(0) = e$. One complication is that the lifting is not unique, due to the presence of isotropy, which are elements of the Lie group G that fix a given point of the homogeneous space. The lifted curve can be made unique if we choose a connection and require that the lifted curve is horizontal with respect to this connection. This procedure allows one to develop *homogeneous space variational integrators* [10], by relating them to flows on Lie groups, and applying Lie group variational integrators.

Multisymplectic Variational Integrators

The variational principle for Lagrangian PDEs involves a multisymplectic formulation [17, 18]. The *base space* $\mathcal{X}$ consists of independent variables, denoted by $(x^0, \ldots, x^n) \equiv (t, x)$, where $x^0 \equiv t$ is time, and $(x^1, \ldots, x^n) \equiv x$ are space variables. The dependent field variables, $(y^1, \ldots, y^m) \equiv y$, form a fiber over each spacetime basepoint. The independent and field variables form the *configuration bundle*, $\pi : Y \to \mathcal{X}$. The configuration of the system is specified by a *section* of Y over $\mathcal{X}$, which is a continuous map $\phi : \mathcal{X} \to Y$, such that $\pi \circ \phi = 1_{\mathcal{X}}$. This means that for every $(t, x) \in \mathcal{X}$, $\phi((t, x))$ is in the fiber over (t, x), which is $\pi^{-1}((t, x))$.

For ODEs, the Lagrangian depends on position and its time derivative, which is an element of the tangent bundle TQ, and the action is obtained by integrating the Lagrangian in time. In the multisymplectic case, the Lagrangian density is dependent on the field variables and the partial derivatives of the field variables with respect to the spacetime variables, and the action integral is obtained by integrating the Lagrangian density over a region of spacetime. The multisymplectic analogue of the tangent bundle is the *first jet bundle* J^1Y, consisting of the configuration bundle Y, and the first partial derivatives of the field variables with respect to the independent variables. In coordinates, we have $\phi(x^0, \ldots, x^n) = (x^0, \ldots x^n, y^1, \ldots y^m)$, which allows us to denote the partial derivatives by $v^a_\mu = y^a{}_{,\mu} = \partial y^a / \partial x^\mu$. We can think of J^1Y as a fiber bundle over $\mathcal{X}$. Given a section $\phi : \mathcal{X} \to Y$, we obtain its *first jet extension*, $j^1\phi : \mathcal{X} \to J^1Y$, that is given by

$$j^1\phi(x^0, \ldots, x^n) = \big(x^0, \ldots, x^n, y^1, \ldots, y^m, \\ y^1{}_{,0}, \ldots, y^m{}_{,n}\big),$$

which is a section of the fiber bundle J^1Y over $\mathcal{X}$. The *Lagrangian density* is a map $L : J^1Y \to \Omega^{n+1}(\mathcal{X})$. Given the action functional, $\mathcal{S}(\phi) = \int_{\mathcal{X}} L(j^1\phi)$, Hamilton's principle states that the physical solutions are extremals of the functional $\mathcal{S}$, i.e., $\delta\mathcal{S} = 0$.

With the generalization of Hamilton's principle to Lagrangian field theories, one can develop variational integrators for PDEs. A discrete action $\mathcal{S}_d$ is constructed by choosing a finite-dimensional approximation of the space of sections of the configuration bundle, e.g., spacetime finite elements or spectral expansions, and integrating the Lagrangian density over spacetime with a suitable quadrature formula. The discrete Hamilton's principle, which states that $\delta\mathcal{S}_d = 0$ for variations of the discrete sections that fix the boundary conditions, leads to a multisymplectic variational integrator. This is a more general framework than applying a symplectic integrator to a semidiscretized Lagrangian PDE, since it allows for discretizations of spacetime that are not tensor products. This flexibility is used in *asynchronous variational integrators* [14], where each element may have a different timestep. Analogous to the ODE case, variational integrators for Lagrangian PDEs preserve a multisymplectic form, and for problems with symmetries, a multimomentum map is preserved as well.

Conclusions

Variational integrators provide a systematic framework for leveraging existing knowledge in approximation theory, one-step numerical methods, and quadrature rules, to construct a large class of geometric structure-preserving numerical integrators that are applicable to a wide range of problems. In particular, this leads to methods for PDEs [14], nonsmooth collisions [4], stochastic systems [2], nonholonomic systems [3], and constrained systems [15]. Furthermore, generalizations involving Dirac structures and mechanics [12] allow one to consider interconnections between discrete Lagrangian systems, which will potentially provide a unified approach for multiphysics systems.

References

1. Benettin, G., Giorgilli, A.: On the Hamiltonian interpolation of near to the identity symplectic mappings with application to symplectic integration algorithms. J. Stat. Phys. **74**, 1117–1143 (1994)

2. Bou-Rabee, N., Owhadi, H.: Stochastic variational integrators. IMA J. Numer. Anal. **29**(2), 421–443 (2009)
3. Cortés, J., Martínez. S.: Non-holonomic integrators. Nonlinearity **14**(5), 1365–1392 (2001)
4. Fetecau, R., Marsden, J., Ortiz, M., West, M.: Nonsmooth Lagrangian mechanics and variational collision integrators. SIAM J. Appl. Dyn. Syst. **2**(3), 381–416 (2003)
5. Hairer, E.: Backward analysis of numerical integrators and symplectic methods. Ann. Numer. Math. **1**, 107–132 (1994)
6. Hairer, E., Lubich, C.: The life-span of backward error analysis for numerical integrators. Numer. Math. **76**, 441–462 (1997)
7. Hairer, E., Lubich, C., Wanner, G.: Geometric numerical integration illustrated by the Störmer-Verlet method. Acta. Numer. **12**, 399–450 (2003)
8. Hairer, E., Lubich, C., Wanner, G.: Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations. Springer Series in Computational Mathematics, vol 31, 2nd edn. Springer, Berlin (2006)
9. Lee, T., Leok, M., McClamroch, N.: Lie group variational integrators for the full body problem. Comput. Method. Appl. Mech. Eng. **196**(29–30), 2907–2924 (2007)
10. Lee, T., Leok, M., McClamroch, N.: Lagrangian mechanics and variational integrators on two-spheres. Int. J. Numer. Method Eng. **79**(9), 1147–1174 (2009)
11. Leimkuhler, B., Reich, S.: Simulating Hamiltonian Dynamics. Cambridge Monographs on Applied and Computational Mathematics, vol 14. Cambridge University Press, Cambridge (2004)
12. Leok, M., Ohsawa, T.: Variational and geometric structures of discrete Dirac mechanics. Found. Comput. Math. (2011). doi:10.1007/s10208-011-9096-2
13. Leok, M., Zhang, J.: Discrete Hamiltonian variational integrators. IMA J. Numer. Anal. (2011). doi:10.1093/imanum/drq027
14. Lew, A., Marsden, J., Ortiz, M., West, M.: Asynchronous variational integrators. Arch. Ration. Mech. Ana. **167**(2), 85–146 (2003)
15. Leyendecker, S., Marsden, J., Ortiz, M.: Variational integrators for constrained mechanical systems. ZAMM Angew. Math. Mech. **88**, 677–708 (2008)
16. Marsden, J., West, M.: Discrete mechanics and variational integrators. Acta Numer. **10**, 317–514 (2001). Cambridge University Press
17. Marsden, J., Patrick, G., Shkoller, S.: Multisymplectic geometry, variational integrators, and nonlinear PDEs. Commun. Math. Phys. **199**(2), 351–395 (1998)
18. Marsden, J., Pekarsky, S., Shkoller, S., West, M.: Variational methods, multisymplectic geometry and continuum mechanics. J. Geom. Phys. **38**(3–4), 253–284 (2001)
19. Oliver, M., West, M., Wulff, C.: Approximate momentum conservation for spatial semidiscretizations of nonlinear wave equations. Numer. Math. **97**, 493–535 (2004)
20. Reich, S.: Backward error analysis for numerical integrators. SIAM J. Numer. Anal. **36**, 1549–1570 (1999)
21. Tang, Y.: Formal energy of a symplectic scheme for Hamiltonian systems and its applications (I). Comput. Math. Appl. **27**, 31–39 (1994)