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A review of structure-preserving numerical methods for engineering applications

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Abstract

Accurate numerical simulation of dynamical systems is essential in applications ranging from particle physics to geophysical fluid flow to space hazard analysis. However, most traditional numerical methods do not account for the underlying geometric structure of the physical system, leading to simulation results that may suggest nonphysical behavior. The field of geometric numerical integration (GNI) is concerned with numerical methods that respect the fundamental physics of a problem by preserving the geometric properties of the governing differential equations. Research over the past two decades has produced GNI methods that are so accurate that they are now used for benchmarking purposes for long-time simulation of conservative dynamical systems. However, their utility for large-scale engineering problems is still an open question. This paper presents a review of structure-preserving numerical methods with focus on their engineering applications. The purpose of this paper is to provide an overview of different classes of GNI methods for mechanical systems while providing a survey of practical examples from numerical simulation of realistic engineering problems.

Keywords: Structure-preserving numerical methods; Engineering applications; Geometric numerical integration; Variational integrators; Energy–momentum integrators; Lie group methods

1. Introduction

As modern challenges in engineering and science grow in complexity and dimension, the need for sophisticated numerical methods to support model-based design and analysis also grows. With increasing computational power, numerical solutions to increasingly sophisticated problems can be computed over longer time intervals, with millions of time integration steps. For such problems, the qualitative properties of the integrator are critical to the accuracy of the numerical simulation and reliability of long range predictions. In engineering applications, numerical methods for studying dynamical systems are usually designed to give rapid and robust numerical solutions with small overall error. Traditional numerical schemes do not account explicitly for the qualitative features of the underlying physical system, however, incurring error that may suggest nonphysical behavior.

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The field of geometric numerical integration (GNI) is concerned with numerical methods that respect the fundamental physics of a problem by preserving the geometric properties of the governing differential equations. Using ideas from geometric mechanics and differential geometry, the field of GNI has produced a variety of numerical methods for simulating systems described by ordinary differential equations (ODEs), which respect the qualitative features of the dynamical system. GNI methods appeal to physicists, mathematicians, and engineers for many reasons. For physicists, the geometric structure of a dynamical system reveals essential, qualitative features in the system's evolution — features that should appear in an accurate simulation. For mathematicians, numerical methods based on discrete variational principles may exhibit superior numerical stability and structure-preserving capabilities. For engineers, these methods can advance model-based design and analysis by preserving fidelity to the physical, continuous-time system, enabling, for example, more accurate predictions of the energy transfer between subsystems.

Since the emergence of computational methods, fundamental properties such as accuracy, stability, convergence and computational efficiency have been considered crucial for deciding the utility of a numerical algorithm. Recently, various aspects of structure-preservation have emerged as an important addition to these fundamental properties. One of the key ideas of the structure-preserving approach is to treat the numerical method as a discrete dynamical system which approximates the flow of the governing continuous differential equation instead of focusing on numerical approximation of a single trajectory. Such an approach allows a better understanding of the invariants and qualitative properties of the numerical method. Mechanical systems, in particular, often exhibit physically meaningful invariants such as momentum, energy, or vorticity; the behavior of these invariants in simulation provides an important measure of accuracy. Most traditional numerical methods do not account for the underlying geometric structure of the physical system, however, so these methods introduce numerical dissipation and fail to preserve invariants of the system. A structure-preserving numerical method, on the other hand, can ensure that qualitative features, such as invariants of motion or the structure of the configuration space, are reflected in the simulation and they can provide accurate numerical simulation over exponentially long times.

GNI emerged as a major thread in the development of numerical methods in the 1990s. The field has grown steadily due to the efforts of mathematicians concerned with accurately simulating the behavior of solutions to differential equations, and thus with numerical methods that respect the underlying problem structure. These methods have proven quite useful for conservative Lagrangian/Hamiltonian systems; their numerical stability and accurate prediction of the (constant) system energy make them useful tools for studying complicated dynamical systems. In fact, research over the past two decades has produced GNI methods for finite-dimensional, time-invariant mechanical systems subject to conservative forcing that are so accurate for long-time simulation that they are now used for benchmarking purposes. Even for short-term simulations, it has been frequently observed that the structure-preserving approach enjoys smaller errors per time step compared to traditional methods, especially for problems involving finite-time singularities. Since its advent, the structure-preserving approach has become the new benchmark in the simulation of ODEs, while also making substantial progress in the numerical study of partial differential equations (PDEs).

While structure-preserving numerical methods promise considerable benefit for a range of practical problems, their use in engineering applications has been limited. The main goal of this paper is to encourage the broader use of structure-preserving numerical methods in engineering applications by providing an overview of existing GNI methods and their capabilities in an accessible way, while adding perspectives and application examples from the literature. In order to be able to use structure-preserving methods in practice, it is necessary to understand their theoretical bases, numerical properties, limitations and computational complexity. This paper summarizes all these aspects as comprehensibly as possible without delving deep into the mathematical details. In the last two decades the field of structure-preserving methods has grown considerably, with many points of view and intricate subtleties. Since this work is intended to provide a gateway into the field for practitioners, we have attempted to address the underlying principles and ideas in this survey, rather than describing specific algorithms and their numerical implementation.

The remainder of the paper is organized as follows. In Section 2 we give an overview of the geometry and qualitative features of continuous-time dynamical systems with special focus on Lagrangian/Hamiltonian mechanics and mechanical systems evolving on non-Euclidean manifolds. The perspective taken here is to describe in broad brush strokes the different types of qualitative features that can be preserved for mechanical systems found in engineering problems. In Section 3 we provide a brief introduction to the formulation of a variety of structure-preserving methods, including symplectic methods, variational integrators, energy–momentum integrators, and Lie group methods. In Section 4 we give a selection of applications from the literature, that may benefit from a structure-preserving approach based on the requirements of a particular application. Finally, in Section 5 we conclude the paper with a discussion on the perspective offered by the survey and future research directions for broader use of structure-preserving methods.

2. Geometric structure underlying continuous systems

The geometric structure is a property of the governing differential equation which can be defined independently of particular coordinate representations. The structure-preserving approach to numerical simulation views the numerical method as a discrete dynamical system which inherits this geometric structure from the continuous system. Thus, for a better understanding of structure-preserving numerical schemes, we look at the continuous dynamical systems, governing differential equations and their qualitative properties. Although a lot of methods to be discussed in this paper can be applied to a broader class of problems, this work pays special attention to Lagrangian/Hamiltonian mechanical systems evolving on manifolds as they are among the most important class of engineering systems in the context of GNI.

2.1. Basic concepts

The modern formulations of Lagrangian and Hamiltonian mechanics [1–3] utilize the coordinate-free language of differential geometry [4,5] to provide a unifying framework for many disparate engineering systems. Apart from elegance and precise mathematical formulation, use of differential geometry allows applications to mechanical systems evolving on general manifolds. In this subsection we give a quick review of differential geometry concepts used in the Lagrangian mechanics framework. We emphasize the fundamental concepts required for the variational mechanics while suppressing the technical details.

The concept of a smooth manifold is central to the geometric treatment of classical mechanics as it generalizes ideas developed on linear vector spaces to non-Euclidean spaces. Manifolds naturally arise as the configuration spaces for a variety of engineering applications, especially for mechanical systems with restrictions on the allowed motion due to physical constraints. For example, the unit sphere $S^2 = \{(x, y, z) \in \mathbb{R}^3 |\ x^2 + y^2 + z^2 = 1\}$ is the configuration space of a spherical pendulum. The sphere S^2 is a two-dimensional manifold embedded in $\mathbb{R}^3$.

Mathematically, manifolds are topological spaces that are locally equivalent to Euclidean spaces — such as $\mathbb{R}^n$. In simple words, for each point on the n-dimensional manifold, the points in the neighborhood can be labeled using n local coordinates. The important distinction from the vector spaces is that these coordinates are only valid in a small neighborhood of each point and not globally on manifolds. For most of the mechanical systems evolving on manifolds, the configuration manifolds are equipped with differentiable structure allowing calculus on manifolds.

The Lagrangian and Hamiltonian mechanics formulations defined on vector spaces provide local mathematical formulations of mechanics on manifolds using multiple coordinate maps. From the Lagrangian mechanics perspective, there are two basic requirements for studying the dynamics of mechanical systems. First, we need to identify the set of all possible configurations of the system as the configuration manifold. The second requirement is to develop a Lagrangian function which is a real-valued function defined on the state space. For mechanical systems that are most commonly considered, the Lagrangian function is the difference between the kinetic energy of the system and the potential energy of the system. This Lagrangian function is then used in the Hamilton's principle to obtain Euler–Lagrange equations. The Hamiltonian perspective on the other hand utilizes the phase space version of Hamilton's principle to derive the Hamilton's equations.

Consider a mechanical system evolving on a configuration manifold Q. The tangent space to Q at the configuration $\mathbf{q} \in Q$ is the set of all tangent vectors based at $\mathbf{q}$, denoted by $T_{\mathbf{q}}Q$. The dual space of $T_{\mathbf{q}}Q$, i.e. the set of all linear maps from $T_{\mathbf{q}}Q$ to $\mathbb{R}$, is called the cotangent space and is denoted by $T^*_{\mathbf{q}}Q$. For the path $\mathbf{q}(t)$ on the manifold Q, the velocity $\dot{\mathbf{q}}(t)$ at time t is the tangent vector to Q, based at the point $\mathbf{q}(t) \in Q$. The tangent bundle of Q, denoted by TQ, is the union of all of the tangent spaces to Q. The configuration and velocity $(\mathbf{q}(t), \dot{\mathbf{q}}(t))$ belong to the tangent space to Q at $\mathbf{q}(t)$ and hence the state space is represented by the tangent bundle TQ. On the other hand, the configuration and the momentum $(\mathbf{q}(t), \mathbf{p}(t))$ belong to the cotangent space, and hence the phase space can be identified with the collection of all the cotangent spaces to Q, namely the cotangent bundle T^*Q. Subsequently, the Lagrangian $L : TQ \to \mathbb{R}$ is defined on the tangent bundle TQ whereas the Hamiltonian $H : T^*Q \to \mathbb{R}$ is defined on the cotangent bundle T^*Q.

It is important to recognize that this geometric formulation can be used to describe and analyze dynamical systems globally without resorting to local coordinate maps that may lead to singularities. In fact this representation is both efficient and advantageous for studying qualitative properties of complex dynamical systems but has not been widely used by the engineering community.

2.2. Lagrangian mechanics

In the late seventeenth century, Newton's laws of motion [6] provided a way to study the dynamics for free point masses but this approach did not work that well for more complicated mechanical systems such as rigid bodies or connected bodies. Lagrange [7,8] came up with an elegant way of computing the dynamics of general mechanical systems; he derived a coordinate-invariant formulation of the equations of motion in terms of the Lagrangian. A few decades later Hamilton [9,10] simplified the structure of these equations using the variational principle that bears his name. We closely follow [11] to revisit the variational derivation of the Euler–Lagrange equations and their qualitative properties from the Lagrangian point of view.

Consider a time-invariant Lagrangian mechanical system with a finite-dimensional, smooth configuration manifold Q, state space TQ, and Lagrangian $L : TQ \to \mathbb{R}$. Hamilton's principle [12] states that: The motion of the system between two fixed points from t_i to t_f is such that the action integral has a stationary value for the actual path of the motion. For a conservative Lagrangian system, Hamilton's principle characterizes the path $\mathbf{q}(t)$ which passes through $\mathbf{q}(t_i)$ at $t = t_i$ and $\mathbf{q}(t_f)$ at $t = t_f$ as that which satisfies the following condition:

$$\delta\mathfrak{B}(\mathbf{q}) = \delta \int_{t_i}^{t_f} L(\mathbf{q}(t), \dot{\mathbf{q}}(t))\, dt = \int_{t_0}^{t_f} \left[\frac{\partial L(\mathbf{q}(t), \dot{\mathbf{q}}(t))}{\partial \mathbf{q}(t)} \cdot \delta\mathbf{q}(t) + \frac{\partial L(\mathbf{q}(t), \dot{\mathbf{q}}(t))}{\partial \dot{\mathbf{q}}(t)} \cdot \delta\dot{\mathbf{q}}(t) \right] dt = 0 \tag{1}$$

Using integration by parts and setting the variations at the endpoints equal to zero gives the Euler–Lagrange equations

$$\frac{\partial L(\mathbf{q}(t), \dot{\mathbf{q}}(t))}{\partial \mathbf{q}} - \frac{d}{dt}\left(\frac{\partial L(\mathbf{q}(t), \dot{\mathbf{q}}(t))}{\partial \dot{\mathbf{q}}} \right) = \mathbf{0} \tag{2}$$

Mechanical systems governed by Eq. (2) exhibit important qualitative features. For autonomous Lagrangian systems i.e. no explicit time-dependence in the Lagrangian, the energy is conserved along the solution trajectory. Second, by Noether's theorem [13], there exists an invariant of the motion corresponding to each symmetry that leaves the Lagrangian invariant. Another interesting and useful property is that these Lagrangian mechanical systems conserve a skew-symmetric, bilinear form known as the *symplectic Lagrangian form* along trajectories [1]. For mechanical systems with explicit time-dependence in the Lagrangian, the governing equations and the qualitative features of the nonautonomous system can be studied by utilizing the extended Lagrangian mechanics framework [11]. Unlike standard Lagrangian mechanics, the extended framework accounts for time variations in addition to the configuration variable variations.

The governing equations (2) and their properties discussed above can also be derived from the Hamiltonian point of view by considering Hamilton's principle in phase space. Depending on the problem, some properties can be observed and understood from the Lagrangian perspective and others are easier from the Hamiltonian perspective. For most engineering applications, the Lagrangian is hyperregular and it is possible to obtain the governing equations in the Hamiltonian form from (2) via Legendre transformation. However, for some applications such as interaction between point vortices [14], the Lagrangian is degenerate and no corresponding Hamiltonian formulation exists.

Apart from these two approaches, the Hamilton–Jacobi viewpoint is also very important for developing structure-preserving numerical methods. This theory describes the motion of the system by a characteristic function S that is the solution of a PDE, known as the Hamilton–Jacobi differential equation. This function S is intimately related to construction of any symplectic transformations on the phase space and is also called the generating function. The generating function S satisfying the Hamilton–Jacobi equation leads to the symplectic map of the exact flow for Lagrangian/Hamiltonian systems. Although the governing PDE for obtaining the generating function S is generally nonlinear and a closed form solution is not usually possible, the approximate solutions of this equation played a pivotal role in the early development of symplectic algorithms. This viewpoint is also useful for discovering invariants of the motion for mechanical systems without solving the problem completely.

For an autonomous Lagrangian system with time-independent external forcing $\mathbf{f}_L(\mathbf{q}(t), \dot{\mathbf{q}}(t))$, the Lagrange–d'Alembert principle characterizes trajectories $\mathbf{q}(t) \in Q$ as those satisfying

$$\delta \int_{t_i}^{t_f} L(\mathbf{q}(t), \dot{\mathbf{q}}(t))\, dt + \int_{t_i}^{t_f} \mathbf{f}_L(\mathbf{q}(t), \dot{\mathbf{q}}(t)) \cdot \delta\mathbf{q}\, dt = 0 \tag{3}$$

where the second term accounts for the virtual work done by the external forces when the path $\mathbf{q}(t)$ is varied by $\delta\mathbf{q}(t)$. Using integration by parts and setting the variations at the endpoints equal to zero gives the forced Euler–Lagrange equations

$$\frac{\partial L(\mathbf{q}(t), \dot{\mathbf{q}}(t))}{\partial \mathbf{q}} - \frac{d}{dt}\left(\frac{\partial L(\mathbf{q}(t), \dot{\mathbf{q}}(t))}{\partial \dot{\mathbf{q}}}\right) + \mathbf{f}_L(\mathbf{q}(t), \dot{\mathbf{q}}(t)) = \mathbf{0} \tag{4}$$

Nonconservative external forcing $\mathbf{f}_L$ violates the symplectic structure and the corresponding Lagrangian system does not preserve the symplectic form. This external forcing will generally break the symmetries of the Lagrangian and that will lead to the corresponding momentum as well as the system energy not being conserved. In the special case that the forcing is orthogonal to the symmetry, the corresponding conserved quantity can be derived from the forced Noether's theorem [11]. Although these forced mechanical systems do not, in general, preserve the invariants or the symplectic form, the variational approach reveals how the external forcing alters these properties over time. This is particularly important for developing numerical methods that capture the evolution of energy or momentum accurately.

2.3. Variational formulation of different problems

The variational methodology and the Lagrangian mechanics concepts discussed in Section 2.2 have been successfully extended to a variety of mechanical systems. In this subsection, we summarize the qualitative features and the geometric properties of various classes of mechanical problems that are important for engineering applications. To keep this treatise as simple and direct as possible, we have skipped a lot of mathematical details and focused mainly on the key ideas relevant to structure-preserving discretization. For a thorough exposition, the interested reader may consult the standard textbooks [1,2,15] and the references cited herein.

Holonomic Constraints: The formulation can be extended to mechanical systems with holonomic constraints, i.e. constraints on the configuration manifold, by the augmented approach using the Lagrange multiplier theorem [15]. For a Lagrangian system with holonomic constraints $\phi : Q \to \mathbb{R}^d$, the augmented Lagrangian is $\bar{L}(\mathbf{q}(t), \dot{\mathbf{q}}(t), \lambda(t)) = L(\mathbf{q}(t), \dot{\mathbf{q}}(t)) - \langle \lambda(t), \phi(\mathbf{q}(t)) \rangle$ where the $\langle \cdot, \cdot \rangle$ is the natural pairing between $\mathbb{R}^d$ and its dual space. The configuration $\mathbf{q}(t) \in Q$ along with the Lagrange multipliers $\lambda(t) \in (\mathbb{R}^d)^*$ extremize the action integral corresponding to the augmented Lagrangian $\bar{L}(\mathbf{q}(t), \dot{\mathbf{q}}(t), \lambda(t))$ which leads to constrained Euler–Lagrange equations [11].

Nonholonomic Constraints: The theory for mechanical systems with nonholonomic constraints [16], i.e. $\phi : TQ \to \mathbb{R}$, uses theory of Ehresmann connections [17] to describe the constraints. The basic idea is to consider a collection of linear subspaces $\mathcal{D}_{\mathbf{q}} \subset T_{\mathbf{q}}Q$ for each $\mathbf{q}(t) \in Q$ which together describe the velocities attainable by the system under the given constraints. The equations of motion for the mechanical system with nonholonomic constraints are given by the Lagrange–d'Alembert principle where we apply (1) with variations of the curve $\mathbf{q}(t)$ satisfying $\delta\mathbf{q}(t) \in \mathcal{D}_{\mathbf{q}}(t)$. The governing equations for the nonholonomic system feature a forcing term which involves the curvature of the connection.

Nonsmooth Problems: The variational approaches discussed so far do not apply directly to nonsmooth problems, such as collision and fragmentation models. This is due to the lack of smoothness of trajectories which prevents the use of differential calculus on manifolds. Using concepts from nonsmooth analysis and extended mechanics framework, the variational approach can be generalized to the nonsmooth setting [18]. Similar to the time-dependent Lagrangian case, the key idea is to treat both configuration variables and time as functions of a fixed parameter space which makes the relevant space of configurations a smooth manifold.

Uncertainty: For mechanical systems with uncertainties, a stochastic action can be defined based on the stochastic flow of randomly perturbed Hamiltonian systems. The stochastic Hamiltonian systems [19] on manifolds extremize a stochastic action defined on the space of manifold-valued semimartingales. Similar to the deterministic case, the stochastic flow is also symplectic [20] and, by the stochastic Noether's theorem [21], preserves the symmetries as well.

Infinite-dimensional Systems: It is important to note that all the governing equations and geometric properties discussed so far are only applicable to mechanical systems evolving on finite-dimensional manifolds. For infinite-dimensional problems, the governing PDEs can be derived through a variational approach by using the covariant field theory [22] where the dynamics is described in terms of finite-dimensional space of fields at a given event in spacetime. The covariant analogue of the symplecticity property is the multisymplectic form formula [23] and the covariant version of Noether's theorem leads to conservation laws for PDEs in the presence of symmetries.

Nonvariational Problems: An obvious limitation of the variational methodology is its limited applicability to Lagrangian/Hamiltonian systems. Although all conservative [24] and a wide variety of nonconservative problems can be modeled using the Lagrangian formalism, it still excludes a lot of interesting systems, for example the problems found in fluid dynamics and thermodynamics. The inverse problem of the calculus of variations [25] deals with the existence and formulation of variational principles for systems of differential equations. The method of formal Lagrangians [26] can embed certain nonvariational systems into a larger system which admits a Lagrangian formulation. This approach extends the applicability of Noether's theorem [27] to a larger class of problems and is particularly useful for the analysis of conservation laws of arbitrary nonvariational differential equations found in fluid dynamics and plasma physics [28].

3. Structure-preserving methods

Traditional numerical integrators for studying dynamical systems usually take an initial condition and move the dynamical system state in the direction specified by the governing differential equations. This approach to numerical discretization ignores the qualitative properties of the continuous-time systems and hence may introduce spurious nonphysical effects leading to incorrect results. On the other hand, GNI methods preserve the underlying geometric structure and provide qualitatively correct numerical results. The philosophy behind this structure-preserving approach is to identify geometric properties of the continuous-time system and then design numerical methods which possess the same properties in the discrete domain. We focus on mechanical integrators — numerical integration methods that preserve some of the invariants of the mechanical system, such as, energy, momentum, or the symplectic form. Other properties that can be important to preserve are phase-space volume, continuous or discrete symmetries, time-reversibility, Casimirs, the correct physical form of dissipation, etc.

In this section, we provide a brief introduction along with a summary of recent developments in numerical integration of Lagrangian/Hamiltonian mechanical systems. Since our focus is on Lagrangian/Hamiltonian systems, we first look at numerical methods which preserve the symplecticity of the flow. In fact, most of the early developments in the field of GNI methods were related to development of numerical integrators that preserved the symplectic nature of the flow. We then look at the two most important classes of mechanical integrators: variational integrators and energy–momentum integrators. We also discuss Lie group methods for mechanical systems evolving on manifolds (see Fig. 1).

3.1. Symplectic methods

As mentioned in Section 2.2, the symplectic property has geometric implications regarding the way in which the Lagrangian flow acts on a set of initial conditions. In simple words, symplecticity describes how all motions starting close to the actual motion are constrained in relation to each other. Based on this observation, Vogelaere [29] first developed numerical integrators that preserved this symplectic property of Hamilton's equations in 1950s. Although the symplectic methods for Lagrangian/Hamiltonian problems have a long history with different approaches, modern efforts can be traced to the generating function based methods of Feng et al. [24] and Ruth [30]. The key idea is to obtain the truncated series expressions for the generating function S from the Hamilton–Jacobi equation and then use these approximate solutions to construct symplectic approximations of the exact flow map. Later, Lasagni [31], Sanz-Serna [32], and Suris [33] showed that certain Runge–Kutta methods preserve symplecticity and they constructed symplectic Runge–Kutta methods from different perspectives. Reich [34] showed that the symplectic Runge–Kutta methods conserve the momentum for Hamiltonian problems with linear symmetries.

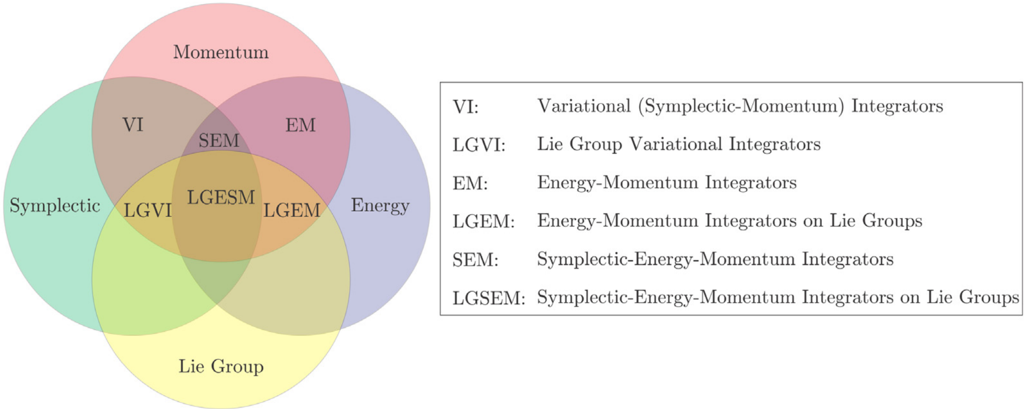


Fig. 1. The taxonomy of structure-preserving methods based on the qualitative features they preserve for a mechanical system.

These methods preserve the symplectic nature of Hamiltonian systems, conserve the momenta and reproduce the dynamic behavior accurately for a long time. The excellent long-time behavior of the symplectic methods can be explained by backward error analysis where instead of asking " What is the numerical error for our problem?", the focus is on "Which nearby problem is solved exactly by our method?". Through backward error analysis of Hamiltonian ODEs, Reich [35] showed that symplectic methods solve a nearby Hamiltonian problem exactly. Thus, despite not conserving the energy of the system exactly, computed trajectories from symplectic methods always remain close to the solution and the energy error remains bounded for an exponentially long time.

Ge and Marsden [36] showed that a fixed time step numerical integrator cannot preserve the symplectic form, momentum, and energy simultaneously for non-integrable systems. Consequently, the structure-preserving fixed time step mechanical integrators can be divided into two categories: (i) energy–momentum and (ii) symplectic-momentum integrators.

3.2. Variational integrators

In comparison to symplectic methods based on the generating functions, variational integrators constitute a more recent approach toward the structure-preserving discretizations of Lagrangian/Hamiltonian mechanical systems. These methods utilize concepts from discrete mechanics, a discrete analogue to continuous-time Lagrangian/Hamiltonian mechanics. Due to their variational nature, these methods can be easily extended to non-conservative mechanical systems by discretizing the Lagrange–d'Alembert principle. The basic idea is to construct a discrete-time approximation of the action integral called the discrete action. Stationary points of this discrete action give discrete-time trajectories of the mechanical system.

Depending on the application, various authors have proposed different versions of discrete mechanics. In fact, discrete-time versions of variational principles are of mathematical interest in their own right. Based on the concept of a difference space, Maeda [37] presented a discrete version of Hamilton's principle and derived discrete Euler–Lagrange equations. Using the same discretization, Maeda [38] later extended Noether's theorem to the discrete setting. Veselov [39,40] pursued these ideas further in the context of integrable systems and showed that these discrete-time systems preserve a symplectic form. Building on these results, Moser and Veselov [41] presented discrete versions of several classical integrable systems including the free rigid body system.

Based on these concepts, Marsden and West [42] developed a theory of discrete mechanics, from both Lagrangian and Hamiltonian perspectives, and derived variational integrators by considering the discrete analogue of variational principles. Although the derivation of variational integrators from discrete variational principles was first given in [43], we closely follow [42] to give a brief review of the construction of variational integrators from the Lagrangian perspective. The idea behind variational integrators is simple: rather than discretize the governing equations (2) or (4), one discretizes the underlying variational principle (1) or (3) (see Fig. 2).

Consider a discrete Lagrangian system with configuration manifold Q and discrete state space $Q \times Q$. For a fixed time step $h = \frac{t_f - t_i}{N}$, the discrete trajectory $\{ \mathbf{q}_k \}_{k=0}^{N}$ is defined by the configuration of the system at the

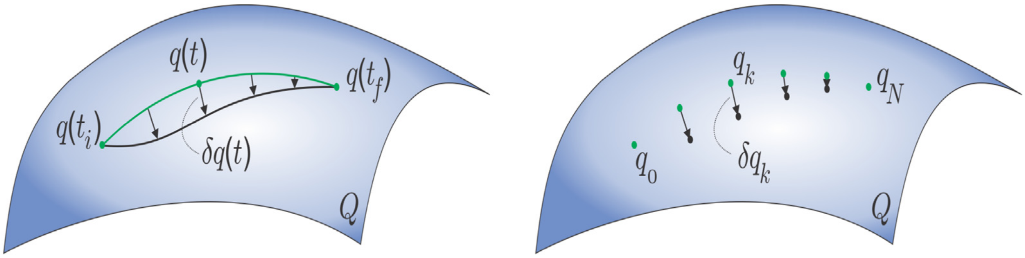


Fig. 2. A cartoon illustrating the continuous time variational mechanics (left) versus the discrete time variational mechanics (right).

sequence of times $\{ \ t_k = t_i + kh \mid k = 0, \ldots, N \}$. We introduce the discrete Lagrangian function $L_d(\mathbf{q}_k, \mathbf{q}_{k+1})$, an approximation of the action integral along the curve from $\mathbf{q}_k$ to $\mathbf{q}_{k+1}$, which approximates the integral of the Lagrangian in the following sense

$$L_d(\mathbf{q}_k, \mathbf{q}_{k+1}) \approx \int_{t_k}^{t_{k+1}} L(\mathbf{q}(t), \dot{\mathbf{q}}(t)) \, dt \tag{5}$$

The discrete analogue of Hamilton's principle seeks curves $\{ \ \mathbf{q}_k \ \}_{k=0}^{N}$ that satisfy

$$\delta \sum_{k=0}^{N-1} L_d(\mathbf{q}_k, \mathbf{q}_{k+1}) = \sum_{k=0}^{N-1} \left[\frac{\partial L_d(\mathbf{q}_k, \mathbf{q}_{k+1})}{\partial \mathbf{q}_k} \cdot \delta \mathbf{q}_k + \frac{\partial L_d(\mathbf{q}_k, \mathbf{q}_{k+1})}{\partial \mathbf{q}_{k+1}} \cdot \delta \mathbf{q}_{k+1} \right] = 0 \tag{6}$$

which gives the discrete Euler–Lagrange equations

$$D_2 L_d(\mathbf{q}_{k-1}, \mathbf{q}_k) + D_1 L_d(\mathbf{q}_k, \mathbf{q}_{k+1}) = \mathbf{0} \qquad k = 1, \ldots, N-1 \tag{7}$$

where D_i denotes differentiation with respect to the ith argument of the discrete Lagrangian L_d. Given $(\mathbf{q}_{k-1}, \mathbf{q}_k)$, the above equations can be solved to obtain $(\mathbf{q}_k, \mathbf{q}_{k+1})$. Thus, the discrete Euler–Lagrange equations can be seen as a numerical integrator of (2) and these equations can be implemented as a variational integrator for autonomous Lagrangian systems. Using the discrete Legendre transform, we can re-write the discrete Euler–Lagrange equations in the Hamiltonian form as follows

$$- D_1 L_d(\mathbf{q}_k, \mathbf{q}_{k+1}) = \mathbf{p}_k \tag{8}$$

$$\mathbf{p}_{k+1} = D_2 L_d(\mathbf{q}_k, \mathbf{q}_{k+1}) \tag{9}$$

where the discrete momentum $\mathbf{p}_k$ converges to its continuous counterpart as the fixed time step h approaches zero. Given $(\mathbf{q}_k, \mathbf{p}_k)$, the above Eqs. (8)–(9) can be solved to obtain $(\mathbf{q}_{k+1}, \mathbf{p}_{k+1})$.

Since the governing discrete equations are derived from the discrete Lagrangian function, the accuracy of trajectories depends on the order of approximation of the discrete Lagrangian. Marsden and West [42] showed that a discrete Lagrangian of order $r+1$ leads to a variational integrator of order r. Regardless of the choice of the discrete Lagrangian, the fixed time step variational integrators are symplectic [44] and momentum-preserving [42,45]. The discrete Lagrangian system preserves a discrete symplectic form [43] and when the discrete system has a symmetry, there is a corresponding conserved quantity at the discrete level. While these fixed time step algorithms do not exactly preserve energy, backward error analysis [35,46] shows that these methods, up to exponentially small errors, exactly integrate a nearby Hamiltonian system. To be more precise, for a small enough fixed time step, the discrete energy computed from the numerical integration will remain close to its initial value for an exponentially long time [44,47]. In practice, the energy error remains bounded without exhibiting drift. As the fixed time step h decreases, the amplitude of energy error oscillations decrease and the discrete energy approaches the continuous system energy. Because of their excellent long-time stability, these variational integrators – also known as symplectic-momentum integrators – are ideal for long-time simulation of conservative dynamical systems.

Marsden and West [42] showed that the discrete Lagrangian function $L_d(\mathbf{q}_k, \mathbf{q}_{k+1})$ is a generating function for the discrete Lagrangian system. Thus, the discrete equations (8)–(9) can be seen as a symplectic method with the corresponding discrete Lagrangian as the approximation to the continuous generating function. This way both symplectic methods and variational integrators belong to the same class of structure-preserving methods but their construction is very different. In contrast to symplectic methods, the variational approach extends easily to nonconservative systems and has more theoretical appeal: the symplectic property as well as the conserved discrete quantities can be derived directly from the variational nature of the algorithm as opposed to the trial and error method. In fact, the variational approach has been useful in explaining the excellent numerical performance of widely used integrators such as Newmark methods [48].

To introduce external forcing, we define two discrete forces $\mathbf{f}_d^{\pm} : Q \times Q \to T^*Q$ which approximate the continuous-time force integral that appears in (3) over one time step in the following sense

$$\mathbf{f}_d^{+}(\mathbf{q}_k, \mathbf{q}_{k+1}) \cdot \delta\mathbf{q}_{k+1} + \mathbf{f}_d^{-}(\mathbf{q}_k, \mathbf{q}_{k+1}) \cdot \delta\mathbf{q}_k \approx \int_{t_k}^{t_{k+1}} \mathbf{f}_L(\mathbf{q}(t), \dot{\mathbf{q}}(t)) \cdot \delta\mathbf{q}\, dt \tag{10}$$

The discrete Lagrange–d'Alembert principle seeks curves $\{ \mathbf{q}_k \}_{k=0}^{N}$ that satisfy

$$\delta \sum_{k=0}^{N-1} L_d(\mathbf{q}_k, \mathbf{q}_{k+1}) + \sum_{k=0}^{N-1} [\mathbf{f}_d^{+}(\mathbf{q}_k, \mathbf{q}_{k+1}) \cdot \delta\mathbf{q}_{k+1} + \mathbf{f}_d^{-}(\mathbf{q}_k, \mathbf{q}_{k+1}) \cdot \delta\mathbf{q}_k] = 0 \tag{11}$$

which yields the following variational integrator for forced Lagrangian systems:

$$-D_1 L_d(\mathbf{q}_k, \mathbf{q}_{k+1}) - \mathbf{f}_d^{-}(\mathbf{q}_k, \mathbf{q}_{k+1}) = \mathbf{p}_k \tag{12}$$

$$\mathbf{p}_{k+1} = D_2 L_d(\mathbf{q}_k, \mathbf{q}_{k+1}) + \mathbf{f}_d^{+}(\mathbf{q}_k, \mathbf{q}_{k+1}) \tag{13}$$

For forced Lagrangian mechanical systems, variational integrators (12)–(13) have been shown to exhibit better energy behavior than traditional numerical integrators [42,48] for weakly dissipative systems. Since the external forcing $\mathbf{f}_L(\mathbf{q}(t), \dot{\mathbf{q}}(t))$ modifies the symplectic structure at every time step, unlike in the conservative case, there are no theoretical results about long-time stable behavior. Despite the lack of theoretical guarantees, the numerical results for a variety of dissipative and forced mechanical systems have demonstrated that variational integrators track the change in energy more accurately compared to traditional methods. Similar to the continuous case, if the discrete forcing is orthogonal to the symmetry of the discrete Lagrangian then the corresponding momentum is conserved based on the discrete forced Noether's theorem [42].

The variational approach to derive mechanical integrators has been successfully extended to a broad class of problems such as:

- **Energy-preserving, adaptive time step variational integrators:** The strong negative result of Ge and Marsden [36] – that integrators with a fixed time step cannot simultaneously preserve energy, the symplectic structure, and conserved quantities for non-integrable systems — led Kane et al. [49] to develop energy-preserving variational integrators with adaptive time stepping for conservative systems. Marsden and West [42] derived the same integrators through a variational approach for a more general case of time-dependent Lagrangian systems. Instead of obtaining the adaptive time step by imposing an additional equation, as in [49], they treated time as a discrete dynamic variable [50] and derived governing discrete equations in the extended Lagrangian mechanics framework. These adaptive time step variational integrators are energy and momentum conserving while also preserving the extended symplectic form. These energy-preserving integrators require solving coupled, nonlinear, ill-conditioned system of equations at every time step and existence of solutions for these discrete trajectories is still an open problem. Shibberu [51] has discussed the well-posedness of these adaptive algorithms and suggested ways to regularize [52] the system of coupled nonlinear discrete equations. Recently, Sharma et al. [53] derived energy-preserving, adaptive time step variational integrators for forced Lagrangian systems and showed that these adaptive algorithms, for forced Lagrangian systems, capture change in energy more accurately than fixed time step variational integrators.
- **Variational integrators for constrained mechanical systems:** Marsden and West extended the variational integrator framework to account for holonomic constraints [42] and these methods have been utilized in applications ranging from molecular dynamics to planetary motion. Their extension to mechanical systems with nonholonomic constraints remained a challenge for some time though. Equations of motion for a nonholonomic system are derived from the Lagrange–d'Alembert principle which means that the nonholonomic flow does not preserve the symplectic flow [54]. Cortes and Martinez [55] obtained nonholonomic integrators by discretizing the Lagrange–d'Alembert principle and they also extended adaptive time step variational integrators to nonholonomic systems using the extended Lagrangian mechanics framework from [42]. Kobilarov et al. [56]

developed nonholonomic integrators for mechanical systems with symmetries and applied it to robotic car and snakeboard examples to demonstrate the advantages compared to standard methods.

- **Stochastic variational integrators:** Based on the foundational work in the field of stochastic geometric mechanics by Bismut [20], Milstein et al. [57,58] developed mean-squared symplectic integrators for stochastic Hamiltonian systems and showed that these integrators capture the correct energy behavior even in presence of dissipation. Bou-Rabee and Owhadi [21] discretized the variational principle for stochastic mechanical systems on manifolds to derive stochastic variational integrators. Similar to their deterministic counterparts, these algorithms are symplectic and satisfy the discrete analogue of Noether's theorem in presence of symmetries. Bou-Rabee and Owhadi [59] also derived constrained, stochastic, variational, partitioned Runge–Kutta methods for stochastic mechanical systems with holonomic constraints. Holm and Tyranwoski [60] utilized the Galerkin type of discretization to derive a more general class of stochastic variational integrators.
- **Variational integrators for impact problems:** Building on the nonsmooth variational mechanics principles, Fetecau et al. [61] developed variational collision integrators. In addition to the discrete trajectory points, this methodology introduces a collision point and the corresponding collision time, which are solved variationally. These algorithms retain the symplectic structure as well as the excellent energy behavior for nonsmooth cases. One of the drawbacks of this approach is that solving for each individual collision becomes cumbersome in situations involving many bodies undergoing collision sequences. For such complex multibody collisions, Johnson et al. [62] developed discontinuous variational integrators by incorporating incremental energy minimization in the discrete mechanics framework.
- **Hamiltonian variational integrators:** As mentioned in Section 2.2, Lagrangian and Hamiltonian dynamics are not equivalent when the system is not hyperregular. For such cases, Lall and West [63] developed discrete Hamiltonian mechanics from the Hamiltonian side, without recourse to the Lagrangian formulation. In contrast to the Lagrangian approach to derive variational integrators, Leok et al. [64] developed Hamiltonian variational integrators from the Hamiltonian point of view by discretizing the Hamiltonian. These Hamiltonian variational integrators are particularly useful for mechanical systems with degenerate Hamiltonian, such as interacting point vortices. In fact, Schmitt and Leok [65] investigated numerical properties of the Hamiltonian variational integrators and showed that, even for the same approximation method, the Lagrangian and Hamiltonian approach may lead to different symplectic-momentum integrators.
- **Multisymplectic variational integrators:** Marsden et al. [23] developed the geometric foundations for variational integrators for variational PDEs. Using ideas from multisymplectic geometry [66], they developed numerical methods that are multisymplectic and preserve discrete momentum maps corresponding to symmetries. Lew et al. [67] developed asynchronous variational integrators for solid mechanics problems. These asynchronous algorithms are based on the spacetime form of the discretized Hamilton's principle and allow the selection of independent time steps in each spatial element. Recently Kraus and Maj [28] extended the variational integrator framework to nonvariational PDEs by utilizing the method of formal Lagrangian.

3.3. Energy–momentum integrators

Conventional numerical methods for ODEs when applied to Lagrangian/Hamiltonian systems conserve the total energy and momenta only up to the order of truncation error. These invariants of motion capture important qualitative features of the long-term dynamics. Aside from their physical significance, from a computational point of view conserved quantities often lead to enhanced numerical stability. For example, algorithmic conservation of energy leads to unconditional stability for nonlinear structural dynamics [68]. In fact, the majority of development on this topic was due to the discovery that numerical methods with unconditional stability for linear dynamics may lose this stability in the non-linear regime [69]. Energy–momentum integrators, in contrast to variational integrators (symplectic-momentum integrators), are designed to preserve the momentum and total energy of the system simultaneously.

Labudde and Greenspan [70–72] developed discrete mechanics based on difference equations and developed energy–momentum conserving algorithms for particle mechanics problems. Simo et al. [73,74] developed a more general methodology to construct energy–momentum integrators for a wide class of mechanical systems. We closely follow [74] to explain the key idea behind these methods.

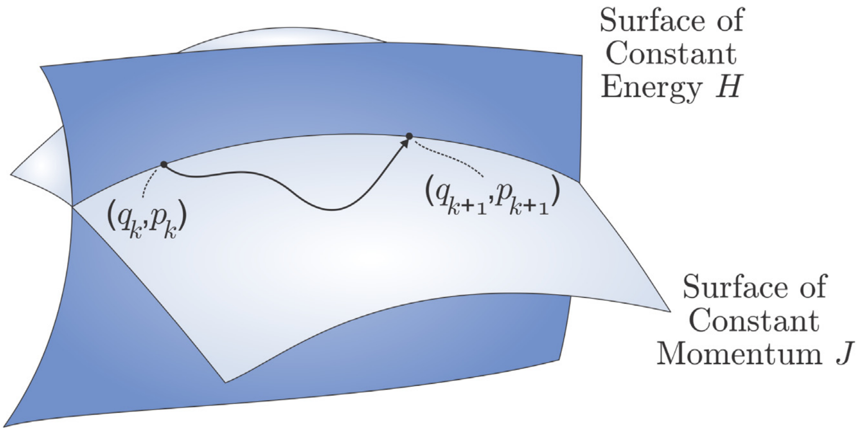


Fig. 3. A cartoon illustrating the use of energy–momentum method where conservation of energy is achieved by an implicit momentum-preserving projection onto the surface of constant energy H.

Consider a finite-dimensional mechanical system with configuration manifold Q and canonical phase space T^*Q. For the simple case of a separable Hamiltonian/Lagrangian system with constant mass matrix M, kinetic energy $K(\mathbf{p}) = \frac{1}{2}\mathbf{p}^T M^{-1}\mathbf{p}$, and potential energy $V(\mathbf{q})$, the governing equations of motion are given by

$$\dot{\mathbf{q}} = M^{-1}\mathbf{p} \qquad \dot{\mathbf{p}} = -\nabla V(\mathbf{q}) \tag{14}$$

It is well-known that the system energy (i.e. the Hamiltonian $H = K + V$) and momentum $J(\mathbf{q},\mathbf{p})$ (corresponding to symmetries) are conserved along the solution trajectory. Given $(\mathbf{q}_k, \mathbf{p}_k)$, the energy–momentum approach designs an approximation $(\mathbf{q}_{k+1}, \mathbf{p}_{k+1})$ such that the system energy $H_{k+1} = H_k$ and momentum $J_{k+1} = J_k$ are conserved. The strategy in the formulation of energy–momentum integrators is to first consider the class of exact momentum conserving schemes and then enforce the additional constraint of exact energy conservation. For the mechanical system described above, the family of exact momentum conserving algorithms, with fixed time step h, given by

$$\mathbf{q}_{k+1} = \mathbf{q}_k + h\kappa_1 M^{-1}\left[\alpha\mathbf{p}_k + (1-\alpha)\mathbf{p}_{k+1}\right] \tag{15}$$

$$\mathbf{p}_{k+1} = \mathbf{p}_k - h\kappa_2 \nabla V\left(\alpha\mathbf{q}_{k+1} + (1-\alpha)\mathbf{q}_k\right) \tag{16}$$

exactly conserve the momentum J corresponding to the symmetry for arbitrary real-valued functions κ_1 and κ_2 and scalar parameter $\alpha \in [0, 1]$. For exact energy conservation, we enforce the law of conservation of energy on the momentum conserving algorithm (15)–(16) (see Fig. 3).

As discussed in [74], this constraint can be implemented via a number of different ways. The projection methods, fix the collocation parameter to $\alpha = \frac{1}{2}$ and obtain κ_1 and κ_2 such that the energy constraint is satisfied. From a geometric point of view, the resulting energy–momentum integrator can be seen as an implicit projection of the mid-point rule from the level set of conserved momentum onto the constant energy surface. The collocation methods, on the other hand, fix the real valued constants $\kappa_1 = \kappa_2 = 1$ and solve the energy constraint equation for the collocation parameter $\alpha \in [0, 1]$.

It is important to note that the energy–momentum approach requires solving an implicit equation and the stability of these methods depends on the solvability of the energy equation. Assuming the energy equation is solvable, the resulting algorithms are exactly energy and momentum preserving. In addition to the favorable conservation properties, these algorithms are unconditionally stable in the nonlinear regime. Simo and Gonzalez [75] showed that the unresolved high frequencies are controlled by exact energy conservation whereas the symplectic-momentum approach can lead to instability in such cases. These numerical properties make the energy–momentum integrators ideal for numerical simulation of highly oscillatory mechanical systems. Since the early development of energy–momentum integrators was based on the idea of modifying the midpoint rule, all of the energy–momentum conserving algorithms were symmetric. Hairer et al. [44] showed that the good long-time behavior of energy–momentum integrators was due to their reversibility and not the conserving properties. They also numerically demonstrated that the non-symmetric energy–momentum integrators do not exhibit good long-time behavior.

Betsch and Steinmann [76,77] presented a unifying approach to derive energy–momentum integrators by discretizing the weighted residual of Hamilton's equations using continuous Galerkin methods. Unlike the finite difference approach taken by Simo and colleagues, they employed the finite element method for the temporal discretization process and devised quadrature rules that lead to energy–momentum integrators. Betsch and Steinmann [78] also extended this Galerkin-based approach to mechanical systems with holonomic constraints by introducing the mixed Galerkin method based on mixed finite elements in time. Later, Groß et al. [79] modified the continuous Galerkin method and derived higher order energy–momentum integrators for multi-dimensional mechanical systems.

For dynamic problems involving high frequency content such as constrained, flexible, multi-body problems, the high frequency oscillations can lead to convergence issues for the energy–momentum integrators due to their lack of high frequency numerical dissipation. Armero and Petocz [80] introduced numerical dissipation in the energy–momentum integrators to derive modified energy–momentum integrators. These "energy decaying" schemes eliminate the energy associated with vibratory motions at high frequency while still preserving the momentum. Instead of satisfying a discrete energy conservation law, the energy decaying schemes are based on the energy decay inequality given by Hughes [81]. Kuhl and Crisfield [82] proposed an alternate strategy based on controllable numerical dissipation to derive generalized energy–momentum integrators. This generalization of the energy conserving/decaying algorithms allows larger time steps, due to numerical damping characteristics and these algorithms are easier to extend to adaptive time-stepping.

3.4. Discrete gradient methods

The construction of energy–momentum integrators is related to the concept of discrete gradients. The discrete gradient method is a general technique for deriving integral-preserving integrators. Gonzalez [83] introduced discrete Hamiltonian systems as formal abstractions of conserving algorithms based on the idea of discrete directional derivatives. Using this discrete derivative idea, McLachlan et al. [84] developed the discrete gradient methods for the more general case of dynamical systems with a Lyapunov function.

The discrete gradient methods are applicable to systems with differential equation $\dot{y} = A(y)\nabla H(y)$ where $A(y)$ is a skew-symmetric matrix. For Lagrangian/ Hamiltonian mechanical systems, the vector $y = (\mathbf{q}, \mathbf{p})$ belongs to the phase space with the constant symplectic matrix J as the skew-symmetric matrix $A(y)$ and the Hamiltonian of the system as the energy function $H(y)$. The discrete gradient methods are of the form

$$y_{k+1} = y_k + h\bar{A}(y_{k+1}, y_k)\bar{\nabla} H(y_{k+1}, y_k) \tag{17}$$

where $\bar{A}(\hat{y}, y)$ is a skew-symmetric matrix for all $\hat{y}$, y, and $\bar{\nabla} H(\hat{y}, y)$ is the discrete gradient satisfying

$$\bar{\nabla} H(\hat{y}, y)^T(\hat{y} - y) = H(\hat{y}) - H(y) \qquad \bar{\nabla} H(y, y) = \nabla H(y) \tag{18}$$

These numerical methods are symmetric and are both energy- and momentum-preserving. It has been shown that the projection method approach to derive energy–momentum integrators is a special case of discrete gradient methods. In fact, the symmetric nature of discrete gradient methods played an important role in explaining the good long-time behavior of energy–momentum integrators. For Hamiltonian systems with holonomic constraints, Gonzalez [85] applied the discrete gradient approach to the governing differential–algebraic equations to derive energy–momentum integrators for constrained mechanical systems. Recently, Celledoni [86] applied the discrete gradient approach to numerical integration of nonholonomic systems. The resulting algorithms exhibit exact energy preservation while ensuring the nonholonomic constraints are satisfied. For PDEs, McLachlan and Quispel [87] showed that discrete gradient methods preserve energy conservation laws and conserve the energy exactly when the symplectic structure is constant. Celledoni et al. [88] applied these methods to PDEs with constant dissipative structure and the numerical results demonstrated that the algorithms capture the correct monotonic decrease in energy.

3.5. Lie group methods

In many engineering applications, the governing differential equations evolve on a non-Euclidean manifold and there are two main numerical approaches for such problems, embedded and intrinsic methods. In the first of these approaches, as the name suggests, one embeds the manifold in $\mathbb{R}^n$ and applies a traditional numerical integration

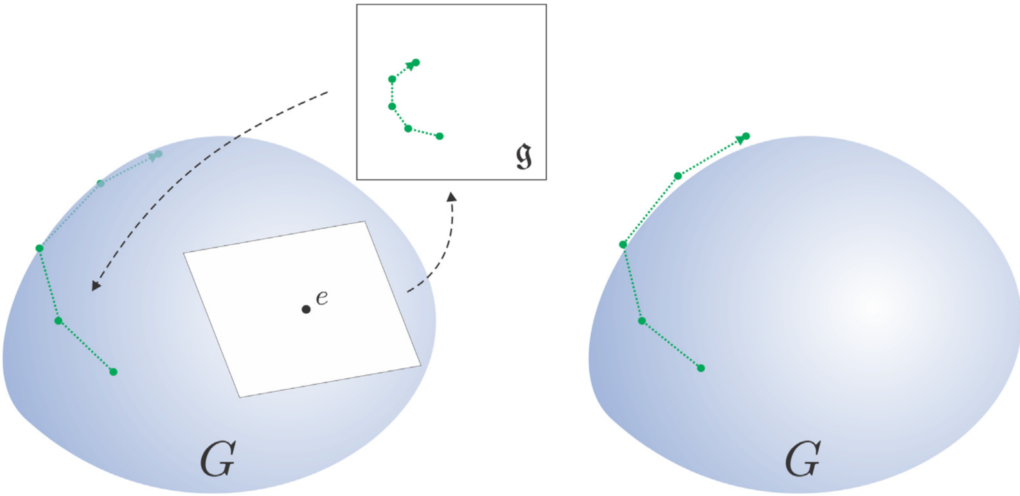


Fig. 4. A cartoon illustrating the use of a Lie group method (left) versus a conventional method (right) in the case $\mathcal{M} = \mathcal{G}$. (The Lie algebra $\mathfrak{g}$ is the tangent space to $\mathcal{G}$ at the identity $e \in \mathcal{G}$).

scheme. The drawback of this approach is that, except in special cases, traditional numerical methods are unlikely to provide solutions that remain exactly on the correct manifold. The alternative approach uses intrinsic operations on the group to make sure the computed trajectories are guaranteed to lie on the manifold.

From a mathematical point of view, a Lie group G is a group which is also a differentiable manifold, and for which the group operation $G \times G \to G$ and inverse operation are smooth maps. The tangent space $\mathfrak{g} = T_I G$ at the identity of a Lie group G is closed under commutation of its elements making it an algebra, the Lie algebra $\mathfrak{g}$ of the Lie group G. For a differential equation on Lie group G, the continuous trajectory remains on the Lie group for any initial condition on G and the flow map of the system can be seen as group operation. For example, the attitude dynamics of a rigid body can be described as differential equations on the special orthogonal group $\mathsf{SO}(3)$, the group of proper orthogonal linear transformations.

Consider a dynamical system whose configuration evolves on a differentiable manifold $\mathcal{M}$ subject to the action of some Lie group $\mathcal{G}$. Given an initial condition $y_0 \in \mathcal{M}$, rather than ask "What is the state y at time t?", the Lie group approach asks an equivalent question [89]: "What is the group action that takes the system from y_0 to $y(t)$?". Posing the question in terms of the group action helps one relate it to the underlying Lie algebra, which is a linear space. Thus, Lie group methods include an intrinsic and consistent strategy for the parametrization of the nonlinear manifold $\mathcal{M}$ in their algorithmic structure. In simple words: Instead of solving the original ODE on $\mathcal{M}$, Lie group methods solve the corresponding problem in the Lie algebra, ensuring that the solution remains on the manifold $\mathcal{M}$ (see Fig. 4).

For dynamical systems evolving on non-Euclidean manifolds, the governing differential equations are intimately connected to Lie groups. Although the mathematical properties of differential equations on manifolds were well understood already by early twentieth century, it is only in last few decades that numerical methods utilizing these aspects have been developed. Crouch and Grossman [90] wrote an influential paper on numerical integrators for ODEs on manifolds where they computed the numerical solution by computing flows of vector fields in the Lie algebra. Munthe-Kaas [91] constructed generalized Runge–Kutta methods on general Lie groups, now known as the Runge–Kutta–Munthe–Kaas (RKMK) methods, and then derived RKMK methods of arbitrarily high order [92] on homogeneous manifolds. The essential aspects of Lie group methods can be reviewed in [93] and a recent survey paper by Celledoni et al. [94] covers the more recent developments and potential applications.

Although the Lie group methods are applicable to any dynamical system evolving on a manifold, for this particular review, we focus on Lie group methods in the context of mechanical systems. The energy–momentum or variational integrators developed for mechanical systems evolving on vector spaces in general will not retain their conservation properties when applied to systems with nonlinear configuration space of a non-Euclidean manifold. For engineering applications, there are two important classes of conserving schemes for mechanical systems evolving on non-Euclidean manifolds: variational (symplectic-momentum) integrators and energy–momentum integrators.

Simo et al. [74] extended the exact energy–momentum methods to classical rigid body dynamics for which the configuration manifold is the rotation group $\mathsf{SO}(3)$. They exploited knowledge of the Lie group's role in rigid body motion, using the exponential map from the Lie algebra to the Lie group in order to numerically integrate the dynamic equations. Lewis and Simo [95] developed energy–momentum and symplectic integrators for the general case of Hamiltonian systems evolving on Lie groups i.e. nonlinear configuration spaces with a group structure.

Bobenko and Suris [96] extended the discrete mechanics ideas in [41] to the Lie group setting. Variational integrators for the reduced dynamics of a mechanical system with a Lie group symmetry were first derived by Marsden et al. [97]. By incorporating ideas from Lie group methods in the variational integrator framework, Leok [64] developed the general theory of Lie group variational integrators. Lee et al. [98–100] adapted the Lie group variational integrators to rigid body dynamics applications. As the name "Lie group variational integrator" suggests, these methods essentially combine the structure-preserving features of Lie group methods and variational integrators. The resulting integrators are thus symplectic and momentum-preserving *and* they preserve the structure of the configuration space. Lie group variational integrators have recently been extended to the infinite-dimensional setting of beam and plate dynamics by Demoures et al. [101–103].

Lie group methods discussed so far, in addition to preserving the nonlinear configuration space structure and momentum, conserve either the energy or the symplectic form. These Lie group methods cannot preserve all three elements – energy, momentum and symplectic form – simultaneously. For the special case of a rigid body system, Lewis and Simo [95] presented a strategy for deriving algorithms that preserve energy, momentum and symplectic form while also making sure the computed trajectory lies on the correct manifold. Based on the strong negative result for fixed step algorithms by Ge and Marsden [36], we know that this approach does not work for the more general case of non-integrable systems. Recently, Sharma et al. [104,105] developed the extended Lagrangian mechanics framework on $\mathsf{SO}(3)$ and $\mathsf{SE}(3)$, and derived energy-preserving, adaptive time step Lie group variational integrators for rigid body dynamics.

4. Science and engineering applications

The numerical methods covered in Section 3 have been successfully applied to a wide range of problems in engineering (see Fig. 5). In this section, we give examples from the literature where these structure-preserving methods have been utilized in physics, mechanics and dynamics.

4.1. Celestial mechanics and dynamical astronomy

Celestial mechanics and dynamical astronomy apply the principles of classical mechanics to solve problems concerning the motion of objects in space. These problems involve determining long-term trajectories of bodies such as stars, planets, and asteroids as well as computing spacecraft trajectories, from launch through atmospheric re-entry, including the orbital maneuvers. Similarly, interplanetary trajectory and planetary protection applications also require accurate long-time numerical simulations. Symplectic methods due to their symplectic and momentum-preserving nature along with long-time stability are ideal for numerical simulation of such problems.

Based on the symplectic method proposed by Ruth [30], various symplectic algorithms for canonical integration of Hamiltonian systems were proposed by Feng and Qin [106], Channell and Scovel [107], and Forest and Routh [108]. Wisdom and Holman [109], building on the previous work by Wisdom [110,111], developed symplectic algorithms for N-body problems with a large central mass such as planetary systems or satellite dynamics. Yoshida [112] applied symplectic methods to study the motion of minor bodies in the solar system and the long-term evolution of outer planets. These methods came to the attention of the celestial mechanics [113] and dynamical astronomy [114] community in the early 1990s and have now become the benchmark in the study of orbit propagation [115], close encounters [116], asteroid [117,118] dynamics, cometary orbits [119,120], long-term formation flight dynamics [121] and N-body dynamics [109,122].

Since the development of discrete mechanics and variational integrators, a variety of symplectic algorithms, derived from the variational point of view, have been applied to celestial mechanics, spacecraft dynamics and orbital propagation problems. Farr and Bertschinger [123] developed adaptive variational integrators for N-body problems with superior symplecticity and momentum preservation. Lee et al. applied Lie group variational integrators to study the complex dynamics of a tethered spacecraft system [124] and spacecraft with imbalanced reaction wheels [125]. Hall and Leok [126] applied spectral variational integrators to solar system simulation and obtained closed, extremely stable and precession free orbits, even for large time steps. Recently, Palacios and Gurfil [127] developed variational integrators for satellite relative orbit propagation including atmospheric drag.

4.2. Elastodynamics

Formulation of dynamic problems in nonlinear solid mechanics is built on energy and momentum conservation laws and these fundamental properties of the continuum dynamics play a key role in many engineering applications. Customary temporal and spatial finite difference/finite element discretizations of the continuum dynamics do not always inherit the conservation properties. The construction of robust spacetime discretizations of these problems has been a long-standing goal in the field of computational mechanics.

For nonlinear elastodynamics problems, especially stiff systems possessing high-frequency contents, energy–momentum schemes are known to possess enhanced numerical stability properties in the nonlinear regime [69]. In most of the applications, the semidiscrete equations resulting from a finite element discretization are viewed as a finite-dimensional Hamiltonian system with symmetry and are solved in time using energy–momentum integrators. In the context of nonlinear elastodynamics, Simo and Tarnow [73] first developed numerical methods for Saint Venant-Kirchhoff model and later, Simo and Gonazalez [128,129] extended these methods to the more general case of hyperelastic materials. Based on this pioneering work, a variety of energy–momentum algorithms have been designed for structural elements such as beams [130], plates [131] and shells [132].

Unlike the energy–momentum integrator applications, variational integrators use the spacetime approach for elastodynamics problems. Lew et al. [67] developed asynchronous variational integrators (AVI) for nonlinear elastodynamics that permit independent time steps in each spatial element. Based on this work, Lietz et al. [101] developed AVIs for geometrically exact beam and plate dynamics. Lew [133] used AVIs to study rotor blade dynamics and contained detonation of a highly-explosive material. Kale and Lew [134] developed scalable parallel AVI algorithms and applied them to study the interaction dynamics involved in atomic force microscopy.

4.3. Multibody dynamics

Multibody dynamics applications often involve a system consisting of rigid bodies and elastic bodies undergoing large displacements and rotations and the numerical simulation of these systems require advanced modeling strategies. Space discretization for these problems usually results in stiff, nonlinear, differential–algebraic equations and energy–momentum schemes are well-suited for such nonlinear systems due to their algorithmic conservation and numerical stability properties. A variety of energy preserving/decaying schemes were presented in the late 1990s by a number of authors for multibody systems.

Ordern and Goicolea [135] utilized discrete gradient ideas to develop energy–momentum integrators for constrained dynamics of flexible multibody systems. Betsch and Lyndecker [136] developed energy–momentum integrators in the discrete null space setting for multibody dynamics and later Leyendecker et al. [137] applied these methods to flexible multibody dynamics. Based on the work by Betsch and Steinmann [138], Betsch and Uhlar [139] developed a rotationless formulation for energy–momentum conserving integration of multibody systems. Uhlar and Betsch [140] extended this method to nonconservative systems and applied it to a double wishbone suspension of a car.

Although the multibody dynamics field has mainly used energy–momentum integrators for computational studies, recently some researchers have also used variational integrators and Lie group methods in the context of multibody dynamics. Leyendecker et al. [141] adapted the discrete null space method to the discrete mechanics framework and applied the variational discrete null space method to a kinematic chain of rigid bodies and flexible multibody systems. Leyendecker and Ober-Blöbaum [142] applied multirate variational integrators to study constrained systems with dynamics on strongly varying time scales. For systems with large displacements and rotations, various Lie group methods for complex flexible multibody dynamics have been developed by Bruls et al. [143,144], Park and Chung [145], and Terze et al. [146].

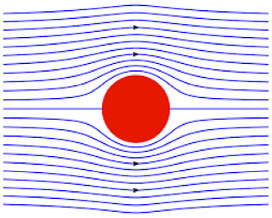
4.4. Fluid dynamics

Computational methods for fluid dynamics problems typically discretize the governing equations through finite volume, finite element or finite difference methods and are rarely designed with structure preservation in mind, leading to spurious numerical artifacts such as energy and circulation drift. In sharp contrast to these traditional methods, structure-preserving methods based on the geometric nature of Euler fluids (adiabatic and inviscid)

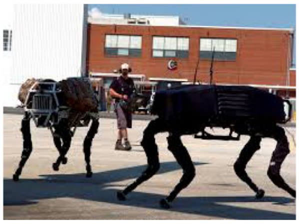
(a) Wheelbone suspension [140]

(b) Tethered dynamics [125]

(c) Helicopter blade dynamics [67]



(d) Fluid flow animation [152]



(e) Little dog robot [157]

Fig. 5. GNI applications from literature .

have recently become popular in the context of numerical methods for fluid dynamics. Perot et al. [147] studied conservation properties of unstructured staggered mesh schemes and constructed numerical methods that conserve kinetic energy, vorticity, and momentum in 2D. Elcott et al. [148] proposed numerically stable integrators for fluids that satisfy the discrete version of Kelvin's circulation theorem.

Based on the pioneering work by Arnold [149], Euler fluids have been extensively studied in the literature from the geometric–differential standpoint. Cotter et al. [150] provided multisymplectic formulation of fluid dynamics using the inverse map approach. In the variational description of fluid dynamics [151], the configuration space is defined as the volume-preserving diffeomorphisms, and Kelvin's circulation theorem is seen as a consequence of Noether's theorem associated with the particle relabeling symmetry. This variational formulation provides a powerful framework to construct structure-preserving methods for fluid dynamics.

Mullen et al. [152] constructed time-reversible integrators that preserve energy for inviscid fluids (or capture the correct energy decay for viscous fluids) and are particularly useful for fluid animation by maintaining the liveliness of fluid motion without recourse to corrective devices. Pavlov et al. [153] derived fluid mechanics equations from Hamilton's principle and derived Lie group variational integrators for incompressible Euler fluids by constructing a finite-dimensional approximation to the volume-preserving diffeomorphism group for the discretization. The resulting scheme exhibits energy conservation over long simulations, time reversibility, and circulation preservation. Using similar ideas, Gawlik et al. [154] derived variational discretizations of continuum theories arising in fluid dynamics, magnetohydrodynamics (MHD), and the dynamics of complex fluids. Kraus and his colleagues [28] have utilized the formal Lagrangian approach to develop variational integrators for a variety of MHD models. Similarly, Desbrun et al. [155] developed structure-preserving space–time discretization schemes for rotating and/or stratified flows which are relevant for modeling large-scale atmospheric or oceanic flows. Recently, Bauer et al. [156] have developed a framework for geometric variational discretization of compressible fluids in the context of rotating shallow water equations.

4.5. Optimal control

The optimal control of a mechanical system is an important engineering problem in application areas such as space mission design, robotics and biomechanics. The numerical solution to the optimal control problem involves the discretization of the infinite-dimensional optimization problem and one has to repeatedly solve a sequence of nearby systems approximately. Using the discrete mechanics framework on the dynamic level in the optimal control problem leads to structure-preserving time-stepping equations and these equations act as equality constraints on the final finite-dimensional nonlinear optimization problem. Besides the structure-preserving aspect, both optimal control and variational mechanics have their roots in calculus of variations. Junge et al. [157] exploited this connection and developed the Discrete Mechanics and Optimal Control (DMOC) method, in which both the dynamics and optimization are discretized variationally.

Building on this work, Ober-Blöbaum et al. [158] showed that the DMOC approach is equivalent to time discretization of Hamilton's equations using a symplectic method and utlilized the structure-preserving nature of discretization to provide proof of convergence. Leyendecker et al. [159] formulated the dynamics subject to holonomic constraints and controls by applying a constrained version of Lagrange–d'Alembert principle for the optimal control of constrained systems. Kobilarov and Sukhatme [160] applied the DMOC framework to nonholonomic mechanical systems using nonholonomic variational integrators and later Kobilarov et al. [56] also extended the framework to mechanical systems with symmetries. Betsch and Becker [161] presented an optimal control version of Noether's theorem for mechanical systems with rotational symmetries and developed momentum-preserving optimal control schemes based on both symplectic-momentum and energy–momentum integrators. Manns and Mombaur [162] showed that the DMOC method offers competitive performance for complex models with large degrees of freedom by taking advantage of the parallel computer architecture.

Although the DMOC method is relatively new, since its introduction it has been utilized in a variety of problems from diverse fields. In spaceflight mechanics, the DMOC method has been applied to problems like low thrust orbital transfer [163], attitude maneuvers of spacecraft [164] and formation flying satellites [157]. For robotics applications, the DMOC method has been applied successfully to simultaneous path planning and trajectory optimization [165], periodic gait optimization [166,167] and robot planning [168] problems. Manchester et al. [169,170] have developed trajectory optimization algorithms using the DMOC framework and applied them in handling the contact constraints found in robot planning problems. Apart from these, the DMOC method has also been used for problems like hybrid systems control [171], vibration suppression control of a film [167], and image analysis [172].

5. Discussion

This paper presents a review of structure-preserving numerical methods along with a survey of engineering applications. Based on the review, we find that prior research efforts in the field of geometric numerical integration have demonstrated the advantage of structure-preserving integration methods largely through comparison with traditional integrators (e.g., the non-structure-preserving Runge–Kutta method) for "toy" problems. While this approach is useful to demonstrate the advantages of structure-preservation, it does not provide a fair assessment for practitioners.

We believe more work is needed on the applications of structure-preserving methods with a focus on large-scale systems from specific engineering applications. Furthermore, it is of interest to know how these methods compare with traditional methods in terms of the computational cost. Recently, Johnson and Murphey [173] utilized the tree-based structure to develop scalable variational integrators. Using ideas from the recursive Newton–Euler algorithm and articulated body algorithm, Lee et al. [174] developed a linear-time variational integrator for multibody systems, and Fan et al. [175] developed linear-time higher order variational integrators. A key topic related to this is the issue of solvability of geometric methods as most of these methods for nonlinear systems are implicit and require the solution of a system of nonlinear equations at every iteration. The connection between time step selection and solvability of implicit methods has not received enough attention in the context of structure-preserving methods. Kobilarov [176] studied the solvability of geometric integrators and developed bounds on the fixed time step which guarantee convergence of the root-finding problem of the system of nonlinear equations. Future work along these directions will play a key role in broader use of structure-preserving methods for engineering applications.

From the reviewed literature, we also find that the majority of research published in the field of geometric numerical integration compares the results of proposed/developed structure-preserving methods with traditional methods that are not designed to respect the underlying geometric structure. In the growing literature on structure-preserving methods, apart from few exceptions [75,177,178], there is very little work focusing on comparison between different classes of structure-preserving methods. For example, both variational (symplectic-momentum) and energy–momentum integrators respect the qualitative features of mechanical systems. On one hand, energy conservation guarantees, a priori, that the numerical solution is restricted to a codimension 1 submanifold of the configuration manifold whereas variational integrators through symplectic structure preservation, ensure a more global and multi-dimensional behavior. From an engineering perspective, this points to a very important question:

For a given mechanical system, should one use variational (symplectic-momentum) or energy–momentum methods to numerically simulate it? In order to answer this question, a detailed comparison of the numerical performance of both methods for benchmark problems from various types of mechanical systems is required. We believe research work in this direction will help practitioners understand which class of structure-preserving numerical methods is best suited to a given mechanical system.

Finally, most of the mechanical systems in engineering applications are subject to non-conservative external forcing. It is of interest to understand which class of methods performs better for nonconservative systems where the external forcing drives the dynamics such as highly oscillatory systems found in biolocomotion or aeroelasticity applications. Also of interest is the extent to which the long-time stability advantages of structure preservation for conservative dynamical systems can carry over to mechanical systems with external forcing.

Most of the research so far has been done for PDEs with variational structure [23,47]. Going further the research challenge is to consider nonvariational PDEs [28] and develop/extend structure-preserving algorithms for a wider class of PDEs.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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