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Spectral-collocation variational integrators

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ABSTRACT

Spectral methods are a popular choice for constructing numerical approximations for smooth problems, as they can achieve geometric rates of convergence and have a relatively small memory footprint. In this paper, we introduce a general framework to convert a spectral-collocation method into a shooting-based variational integrator for Hamiltonian systems. We also compare the proposed spectral-collocation variational integrators to spectral-collocation methods and Galerkin spectral variational integrators in terms of their ability to reproduce accurate trajectories in configuration and phase space, their ability to conserve momentum and energy, as well as the relative computational efficiency of these methods when applied to some classical Hamiltonian systems. In particular, we note that spectrally-accurate variational integrators, such as the Galerkin spectral variational integrators and the spectral-collocation variational integrators, combine the computational efficiency of spectral methods together with the geometric structure-preserving and long-time structural stability properties of symplectic integrators.

1. Introduction

Symplectic integrators have long played an important role in the long-time simulation of mechanical systems [2,3], and the characterization of symplectic integrators in terms of variational integrators [16] has proven to be very fruitful. Additionally, variational integrators can be applied to the discretization of optimal control problems in robotics and aeronautics [7,10,11,21]. The basic idea of a variational integrator is to construct the numerical scheme by discretizing the appropriate variational principle, e.g., Hamilton's principle for conservative systems, and the Lagrange–d'Alembert principle for dissipative or forced systems. The resulting integrators exhibit clear advantages when compared with conventional numerical integration algorithms. They are symplectic, momentum-preserving, and exhibit near energy conservation for exponentially long times. Moreover, they can be easily extended to a large class of problems, such as Lagrangian and Hamiltonian PDEs [14], Lie–Poisson dynamical systems [17], and optimal control problems [10,21]. A comparison of spectral-collocation methods and symplectic methods when applied to Hamiltonian systems was conducted in [8], and in this paper, we will discuss methods for constructing spectrally-accurate variational integrators that combine the geometric convergence of spectral methods and the geometric structure-preserving properties of symplectic integrators.

There are two general methods for constructing higher-order variational integrators, the first is the Galerkin construction [13,18], and the other is the shooting-based construction [12,19]. The construction of Galerkin variational integrators relies on a variational characterization of the exact discrete Lagrangian, which is then approximated through the choice of a

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finite-dimensional function space and a sufficiently accurate quadrature formula. The shooting-based approach relies on the characterization of the exact discrete Lagrangian in terms of Jacobi's solution of the Hamilton–Jacobi equation, which involves evaluating the action integral on the solution of the Euler–Lagrange boundary value problem. This is approximated by constructing a numerical approximation of the solution of the Euler–Lagrange boundary value problem by using the shooting method and approximating the action integral with a numerical quadrature formula.

In this paper, we first present a brief overview of Lagrangian and Hamiltonian mechanics and variational integrators in Section 1. In Section 2, we introduce the construction and convergence analysis of shooting-based variational integrators derived from spectral-collocation methods. In Section 3, practical numerical algorithms for implementing spectral-collocation variational integrators are presented, and numerical examples are given in Section 4. In Section 5, we make some concluding remarks and comment on possible future directions.

1.1. Lagrangian and Hamiltonian mechanics

Lagrangian mechanics Consider a mechanical system on an n-dimensional configuration manifold Q with generalized coordinates $q^i, i = 1, ..., n$, which is described by a Lagrangian $L : TQ \to \mathbb{R}$ that is given by the kinetic energy minus the potential energy. The action $\mathfrak{S} : C^2([a, b], Q) \to \mathbb{R}$ is given by

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

Then, Hamilton's principle states that the action is stationary for curves $q \in C^2([a, b], Q)$ with fixed endpoints, i.e.,

$$\delta\mathfrak{S}(q) = \delta \int_a^b L(q, \dot{q})dt = 0, \tag{1}$$

where $\delta q(a) = \delta q(b) = 0$. By the fundamental theorem of the calculus of variations, we have

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i} - \frac{\partial L}{\partial q^i} = 0, \tag{2}$$

which are referred to as the Euler–Lagrange equations.

Hamiltonian mechanics Alternatively, the mechanical system can be described by a Hamiltonian $H : T^*Q \to \mathbb{R}$ given by

$$H(q, p) = p_i\dot{q}^i - L(q, \dot{q}),$$

where the velocities on the right-hand side are implicitly defined in terms of the momenta by the Legendre transformation $p_i = \frac{\partial L}{\partial \dot{q}^i}$, and there is an implicit summation over the index i. This leads to Hamilton's principle in phase space,

$$\delta \int [p_i\dot{q}^i - H(q, p)]dt = 0,$$

where we again assume that the variations in q vanish at the endpoints, i.e., $\delta q(a) = \delta q(b) = 0$. By the fundamental theorem of the calculus of variations,

$$\dot{q}^i = \frac{\partial H}{\partial p_i}, \qquad \dot{p}_i = -\frac{\partial H}{\partial q^i}, \qquad i = 1, \ldots, n, \tag{3}$$

which are Hamilton's canonical equations.

1.2. Discrete mechanics and variational integrators

Discrete Lagrangian mechanics [16] is based on a discrete analogue of Hamilton's principle. We first consider a discrete Lagrangian, $L_d : Q \times Q \to \mathbb{R}$, and construct the discrete action sum, $\mathfrak{S}_d : Q^{n+1} \to \mathbb{R}$, which is given by

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

Then, the discrete Hamilton's principle states that

$$\delta\mathfrak{S}_d = 0$$

for variations that vanish at the endpoints, i.e., $\delta q_0 = \delta q_n = 0$. This yields the discrete Euler–Lagrange (DEL) equation,