Applied Numerical Mathematics 132 (2018) 35–50

Contents lists available at ScienceDirect

Applied Numerical Mathematics

www.elsevier.com/locate/apnum

Construction and comparison of multidimensional spectral variational integrators and spectral collocation methods

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ARTICLE INFO

Article history:
Received 20 September 2017
Accepted 16 May 2018
Available online 26 May 2018

Keywords:
Lagrangian mechanics
Spectral collocation methods
Spectral variational integrators
Linear stability

ABSTRACT

In this paper, we construct numerical schemes for spectral collocation methods and spectral variational integrators which converge geometrically. We present a systematic comparison of how spectral collocation methods and Galerkin spectral variational integrators perform 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 linear stability of these methods when applied to some classical Hamiltonian systems.

1. Introduction

Hamiltonian systems are omnipresent in scientific and technical applications and play an important role in many different fields, such as celestial mechanics [3], quantum mechanics [11], molecular dynamics [7], control theory [15], etc. Ideally, numerical schemes for the simulation of Hamiltonian systems should not only reproduce the solutions accurately and efficiently, but also preserve as many geometric invariants of the original system as possible. Variational integrators (VI) [12,4] are well-known as they are symplectic, momentum preserving and nearly energy preserving for exponentially long times. Spectral collocation methods (SC) [16,17,10] are a popular choice for the construction of numerical approximations for problems with smooth solutions, as they can achieve geometric rates of convergence and have a relatively small memory footprint. Spectral variational integrators (SVI) [5] inherit almost all the benefits of both methods. Comparisons of Euler methods and Runge–Kutta methods with their corresponding symplectic counterparts are discussed in [4,1,12]. It would be interesting to compare the performance of spectral variational integrators with spectral collocation schemes to see if any additional benefits arise from constructing spectral schemes using a variational approach. The procedures for constructing SVI and SC are illustrated in Fig. 1. The paradigms underlying spectral variational integrators and spectral collocation methods for the numerical solution of dynamical systems are straightforward. Approximate solutions of Lagrangian systems are represented by finite vectors of their values at certain points such as Chebyshev–Gauss–Lobatto points. Each such vector defines a global interpolant and operations on the analytic solutions of the proposed Lagrangian systems are replaced by the corresponding operations on the interpolants. The main difference between the two constructions is that SC performs the

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https://doi.org/10.1016/j.apnum.2018.05.010
0168-9274/

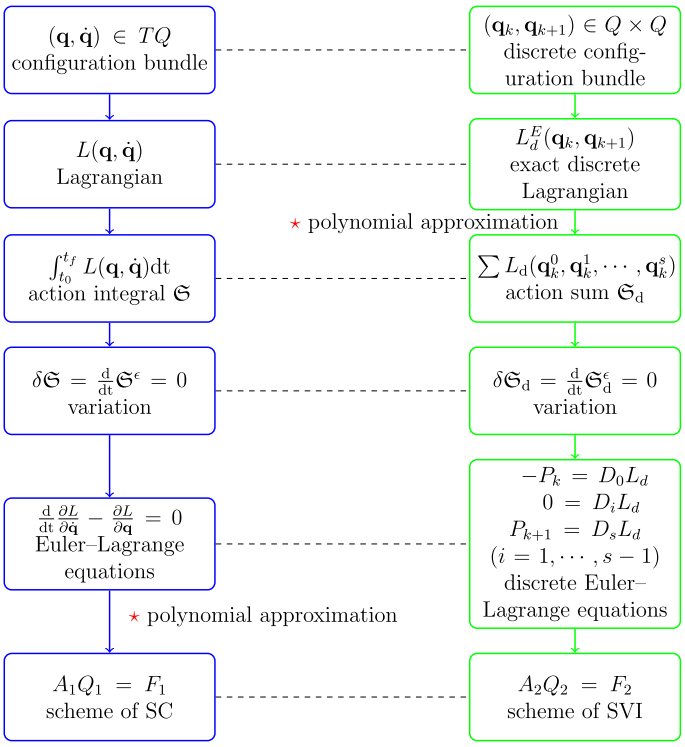

Fig. 1. Construction procedures for SC (left column) and SVI (right column).

variation in Hamilton's principle first and then discretizes the resulting Euler–Lagrange equations, whereas SVI discretizes Hamilton's principle first and then performs the variation of the resulting discrete Hamilton's principle.

1.1. Discrete Lagrangian mechanics and variational integrators

Considering mechanical systems that evolve on an n-dimensional configuration manifold Q with generalized coordinates $q^i, i = 1, ..., n$, the Lagrangian $L : TQ \times \Delta \to \mathbb{R}$ of the proposed mechanical systems are defined as the difference between the kinetic energy and the potential energy, i.e.,

$$L(\mathbf{q}, \dot{\mathbf{q}}, t) = T(\mathbf{q}, \dot{\mathbf{q}}, t) - V(\mathbf{q}, \dot{\mathbf{q}}, t),$$

where Δ represents an interval in the time axis, and where T and V denote the total kinetic and potential energy of the system, respectively. Define the action $\mathfrak{S} : C^2([t_0, T], Q) \to \mathbb{R}$ of the Lagrangian system as the following functional

$$\mathfrak{S} = \int_{t_0}^{T} L(\mathbf{q}(t), \dot{\mathbf{q}}(t), t)\mathrm{d}t,$$

where $(\mathbf{q}, \dot{\mathbf{q}}) \in TQ$ is a smooth curve between states $(\mathbf{q}(t_0), \dot{\mathbf{q}}(t_0))$ and $(\mathbf{q}(T), \dot{\mathbf{q}}(T))$. According to Hamilton's principle, we know that the true trajectory $\mathbf{q} \in C^2([t_0, T], Q)$ is the stationary point of the functional $\mathfrak{S}$ with fixed endpoints $\mathbf{q}(t_0)$ and $\mathbf{q}(T)$, i.e.,

$$\delta\mathfrak{S} = \delta \int_{t_0}^{T} L(\mathbf{q}(t), \dot{\mathbf{q}}(t), t)\mathrm{d}t = 0, \tag{1}$$

which yields the Euler–Lagrange (EL) equations,

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{\mathbf{q}}} - \frac{\partial L}{\partial \mathbf{q}} = 0. \tag{2}$$

The formulation of Lagrangian mechanics in discrete time is mainly based on a discrete analogue of Hamilton's principle. Divide the total time interval $[t_0, T]$ into N subintervals of equal length h. The discrete Lagrangian $L_d : Q \times Q \times \mathbb{R} \to \mathbb{R}$ is an approximation of the exact discrete Lagrangian over each time interval $[kh, (k+1)h]$, i.e.,