Structure-Preserving SAV-RK*s* Spectral Methods for Nonlinear Hamiltonian System

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Abstract. It is well-established that high-order symplectic Runge–Kutta methods cannot preserve polynomial energy of Hamiltonian systems beyond degree two. However, the scalar auxiliary variable (SAV) approach, which was originally proposed for gradient flow systems, offers an effective strategy to overcome this limitation, albeit with a modified energy. In this paper, we study high-order Runge–Kutta methods for solving general Hamiltonian systems without imposing a lower bound on the high-order part of the energy functional. By integrating a symplectic Runge–Kutta method with a new SAV strategy, we develop a class of high-order nonlinear structure-preserving *s*-stage Runge–Kutta SAV (SAV-RK*s*) spectral methods, and prove that the nonlinear semi-discrete scheme can preserve the Hamiltonian energy and other conservative quantities such as mass/momentum (if they exist). In addition, we design a tailored fast Newton iteration algorithm to efficiently solve the resulting nonlinear algebraic system. Finally, we carry out extensive numerical simulations on several benchmark problems, including cases where the energy functional is either bounded or unbounded, to validate the accuracy and robustness of the proposed algorithms.

1 Introduction

Hamiltonian systems play a pivotal role in the study of classical mechanics and have found extensive applications in various fields, including quantum mechanics and statis-

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tical mechanics. A Hamiltonian system is characterized by a scalar function known as the Hamiltonian, which typically represents the total energy of the system and remains unchanging over time.

In this paper we are concerned with a class of Hamiltonian systems in the form of

$$\partial_t u = \mathcal{D}\frac{\delta H}{\delta u}, \quad t \in (0,T], \tag{1.1}$$

where $\mathcal{D}$ is a skew-adjoint operator, u is a function defined on $\mathbb{V}$ ($\mathbb{V} = \mathbb{C}$ or $\mathbb{R}$), and $\frac{\delta H}{\delta u}$ represents the variational derivative of H with respect to u. The Hamiltonian energy $H := H[u]$ satisfies

$$H := H_L + H_N,$$

where

$$\frac{\delta H_L}{\delta u} = \mathcal{L}u, \quad \frac{\delta H_N}{\delta u} = \mathcal{N}u$$

with $\mathcal{L}$ and $\mathcal{N}$ representing linear and nonlinear operators, respectively.

The system (1.1) encompasses many important equations in classical mechanics, quantum physics and nonlinear optics. Notable examples include the Camassa–Holm (CH) equation [3], the Korteweg–de Vries (KdV) equation [32], the nonlinear Schrödinger (NLS) equation [10], the derivative nonlinear Schrödinger (DNLS) equation [4,24], which play significant roles in the field of the nonlinear optics [30,33,34,41], among others.

Due to the antisymmetry of the operator $\mathcal{D}$, it is straightforward to deduce that the system (1.1) conserves the Hamiltonian energy, i.e.,

$$\frac{\mathrm{d}}{\mathrm{d}t}H = \left(\frac{\delta H}{\delta u}, \partial_t u\right) = \left(\frac{\delta H}{\delta u}, \mathcal{D}\frac{\delta H}{\delta u}\right) = 0. \tag{1.2}$$

The invariant

$$\frac{\mathrm{d}}{\mathrm{d}t}(u,1) = 0 \tag{1.3}$$

is also conserved provided that $\mathcal{D}$ is a linear differential operator. In addition, Hamiltonian systems may conserve other quantities such as mass/momentum, etc. We shall assume that the solution of the system (1.1) also satisfies

$$\frac{\mathrm{d}}{\mathrm{d}t}(u, \mathcal{B}u) = 0, \tag{1.4}$$

where $\mathcal{B}$ is a linear symmetric (algebraic or differential) operator. Some specific examples will be provided in the next section. Preserving these invariant properties in a numerical scheme is highly desirable, as it ensures that the discrete solution preserves the essential features of the original differential equation.

Over the past few decades, significant efforts have been devoted to developing efficient and accurate numerical methods capable of preserving as many conservation laws