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Preservation of stability properties near fixed points of linear Hamiltonian systems by symplectic integrators

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ABSTRACT

Based on reasonable testing model problems, we study the preservation by symplectic Runge–Kutta method (SRK) and symplectic partitioned Runge–Kutta method (SPRK) of structures for fixed points of linear Hamiltonian systems. The structure-preservation region provides a practical criterion for choosing step-size in symplectic computation. Examples are given to justify the investigation.

1. Introduction and preliminaries

Consider the n-degree-of-freedom (d.o.f) Hamiltonian system

$$\dot{\mathbf{z}} = J\nabla H(\mathbf{z}), \quad J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}, \tag{1.1}$$

where H is a smooth scalar function of the extended phase space variables $\mathbf{z} \in \mathbb{R}^{2n}$, denoting the Hamiltonian, and J is the Poisson matrix with I the $n \times n$ identity matrix. By introducing the canonically conjugate variables, $\mathbf{z} = (q,p)$, the above system can be rewritten as

$$\dot{q} = \partial H/\partial p, \quad \dot{p} = -\partial H/\partial q, \tag{1.2}$$

where $q \in \mathbb{R}^n$ represents the configuration coordinates of the system and their canonically conjugate momenta $p \in \mathbb{R}^n$ represents the impetus gained by movement. As is well-known, Hamiltonian systems are introduced as a type of system for which the existence of conservative quantities are automatic. System (1.2) possesses two remarkable properties:

(1) the solutions preserve the Hamiltonian, i.e.,

$$\frac{dH}{dt} = 0; \tag{1.3}$$

(2) the corresponding flow is symplectic, i.e.,

$$\frac{d}{dt}[dp \wedge dq] = 0. \tag{1.4}$$

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In the last two decades, enormous attention has been paid to numerical methods which preserve the symplecticity, namely, symplectic integrators for Hamiltonian systems; we refer to the monographs Hairer et al. [1] and Sanz-Serna & Calvo [9] for details and related literature. Theoretical analysis together with numerous numerical experiments has shown that symplectic integrator not only produces improved qualitative numerical behaviors, but also allows for a more accurate long-time scale computation than with general-purpose methods. In the symplectic integration study, a widely recognized fact is that the symplecticity of a numerical integrator has little to do with its step-size. Particularly, for SRK and SPRK methods, their symplecticities are only related to the coefficients (see Section 2 below). Therefore, in practical computations, one usually resorts to the classical stability analyses to find a suitable range for choosing numerical step-sizes. However, in a recent paper [3], it is shown that in some cases even the step-size of the symplectic Euler method satisfies the classical linear stability requirements, one can still get periodic-two numerical solutions, or even chaotic solutions. That means, we need to require more stringent conditions on step-sizes in addition to the classical stability considerations in simulations of Hamiltonian flows, even for symplectic integrators. In order to gains some insights into this aspect, we shall investigate the influences induced by the numerical discretization on the equilibrium structure of the underlying Hamiltonian system. The study would also provide practical criteria for choosing step-sizes for symplectic integrators. It is recalled that for a general ODE of the form

$$\dot{\mathbf{z}} = f(\mathbf{z}), \quad \mathbf{z} \in \mathbb{R}^m, \quad f : \mathbb{R}^m \mapsto \mathbb{R}^m,$$

it may admit the presence of equilibrium point, namely, $\bar{\mathbf{z}} \in \mathbb{R}^m$ such that $f(\bar{\mathbf{z}}) = 0$, and the eigenvalues of the corresponding stability matrix $\nabla_{\mathbf{z}} f(\bar{\mathbf{z}})$ determine the type of the equilibrium point and its stability property. We would like to mention that in [7], the preservation of stability for implicit midpoint and leapfrog methods applied to harmonic oscillator is considered. In this paper, we shall present a more systematic study for general SRK and SPRK methods.

In the sequel, we are mainly concerned with the Runge–Kutta (RK) methods and partitioned Runge–Kutta (PRK) methods. Henceforth, we customarily refer to an s-stage RK method by the triple $\mathcal{R}_s = (A, b, c)$, with $A = (a_{ij})_{i,j=1}^s, b = (b_i)_{i=1}^s$ and $c = (c_i)_{i=1}^s$ being, respectively, the coefficient matrix, weights and abscissae, and an s-stage PRK method by the pair $\mathcal{R}_s^{(1)} - \mathcal{R}_s^{(2)}$. Next, we would like to review some of the classical linear stability concepts and by tracing the origins we can thus draw forth our motivations for the current work. The probably most well known A-stability is introduced by Dahlquist in 1960s (see, e.g., [2]). Applying $\mathcal{R}_s$ to the famous Dahlquist test equation

$$y' = \lambda y, \quad \lambda \in \mathbb{C}, \quad \Re\lambda < 0, \tag{1.5}$$

we get the following scheme

$$y_{l+1} = R(z) y_l, \quad l = 0, 1, 2, \ldots, \text{ and } z = \lambda h, \tag{1.6}$$

with $R(z)$ the stability function of $\mathcal{R}_s$ (see, Chapter IV.3, [2]). It is noted that the solution to (1.5) asymptotically decays to zero as $t \to \infty$, and in order for the numerical scheme (1.6) to yield such qualitative behavior without any restriction on the step size h, we naturally require that

$$|R(z)| < 1, \quad \text{for any} \quad h > 0. \tag{1.7}$$

Methods satisfying (1.7) are called A-stable, and this concept has been playing an indispensable role in the numerical field. Apparently, one can derive the same conclusion (1.7) for $\mathcal{R}_s$ when applying it to the following equation

$$y' = \bar{\lambda} y, \tag{1.8}$$

where $\bar{\lambda} \in \mathbb{C}$ is the complex conjugate to λ in Eq. (1.5). If we set $\lambda = \alpha + \mathrm{i}\beta$ with $\alpha, \beta \in \mathbb{R}$ and $\alpha < 0$, it is easy to see that Eqs. (1.5) and (1.8) are equivalent to the following system of ODE,

$$\begin{cases} \dot{x} = \alpha x - \beta y, \\ \dot{y} = \beta x + \alpha y. \end{cases} \tag{1.9}$$

System (1.9) has an equilibrium point $(0,0)$ and its corresponding stability matrix is given by

$$\mathbf{J} = \begin{bmatrix} \alpha & -\beta \\ \beta & \alpha \end{bmatrix},$$

which has two eigenvalues $\lambda_{1,2} = \alpha \pm \mathrm{i}\beta$. Now, we apply $\mathcal{R}_s$ to (1.9) and get

$$\begin{bmatrix} x_{l+1} \\ y_{l+1} \end{bmatrix} = Q \begin{bmatrix} R(z) & 0 \\ 0 & R(\bar{z}) \end{bmatrix} Q^{-1} \begin{bmatrix} x_l \\ y_l \end{bmatrix}, \tag{1.10}$$

with

$$z = \lambda h, \quad \bar{z} = \bar{\lambda} h, \quad \lambda = \alpha + \mathrm{i}\beta \text{ and } Q = \frac{1}{\sqrt{2}} \begin{bmatrix} i & -1 \\ 1 & -i \end{bmatrix}.$$

Introducing the forward difference operators

$$\delta_t^+ x_l = \frac{x_{l+1} - x_l}{h}, \quad \delta_t^+ y_l = \frac{y_{l+1} - y_l}{h},$$