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VON NEUMANN STABILITY ANALYSIS OF SYMPLECTIC INTEGRATORS APPLIED TO HAMILTONIAN PDEs*[1)]

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Abstract

Symplectic integration of separable Hamiltonian ordinary and partial differential equations is discussed. A von Neumann analysis is performed to achieve general linear stability criteria for symplectic methods applied to a restricted class of Hamiltonian PDEs. In this treatment, the symplectic step is performed prior to the spatial step, as opposed to the standard approach of spatially discretising the PDE to form a system of Hamiltonian ODEs to which a symplectic integrator can be applied. In this way stability criteria are achieved by considering the spectra of linearised Hamiltonian PDEs rather than spatial step size.

Key words: symplectic integration, Hamiltonian PDEs, linear stability, von Neumann analysis.

1. Introduction

Symplectic integration schemes are numerical methods for solving Hamiltonian ordinary differential equations (ODEs). They differ from many other types of numerical integration schemes because they preserve the differential 2-form with each iteration (time step) of Hamiltonian ODEs. Symplectic schemes are the preferred method of numerical integration of Hamiltonian ODEs because they approximate the flow of the system. As a result, they inhibit artificial dissipation and other undesirable effects often introduced with the use of non-symplectic numerical methods (see [1]) and error growth is qualitatively and comparatively small [1, 2, 3].

Symplectic integration of Hamiltonian partial differential equations (PDEs) has traditionally been a matter of applying symplectic methods to a system of Hamiltonian ODEs resulting from a spatial discretisation of the PDE. This has been the case for applications to the sine-Gordon equation, the KdV equation, the "good" Boussinesq equation, Fisher's equation, the nonlinear Schrödinger equation and others [4, 5, 6, 7, 8, 9]. The usual procedures are to spatially discretise the Hamiltonian operator and the Hamiltonian separately, using a finite difference method or a spectral method, and then form the resultant ODEs, or to directly discretise the PDE in conservative form. This is followed by applying a symplectic integrator to the resultant system of ODEs.

In this paper we will investigate the linear stability of symplectic methods applied to Hamiltonian PDEs. We restrict consideration to separable Hamiltonian PDEs in canonical form. For these types of equations the Hamiltonian operator is linear and constant. Hence, the preservation of Hamiltonian structure is ensured when the Hamiltonian operator and the Hamiltonian are spatially discretised separately or when the PDE is discretised directly in conservative form [10].

In this paper, the symplectic integration scheme is applied directly to the PDEs in conservative form. The application of symplectic integrators to Hamiltonian PDEs in function space

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results in systems of equations which fit naturally into a von Neumann stability analysis. The result is a general method for determining stability criteria for symplectic methods applied directly to linearised Hamiltonian PDEs, independent of spatial discretisation.

2. Explicit and Implicit Symplectic Integrators

We first consider separable and autonomous Hamiltonian ODEs of the form $H(p,q) = T(p) + V(q)$, with Hamiltonian vector field $X_H = X_T + X_V$. Hamilton's equations are

$$\frac{d}{dt}\begin{pmatrix} p \\ q \end{pmatrix} = \begin{pmatrix} -\frac{\partial V}{\partial q} \\ \frac{\partial T}{\partial p} \end{pmatrix} = J\nabla H. \tag{1}$$

In this paper we will consider explicit and implicit symplectic integration schemes as constructed by the method of generating functions and composition [11, 12, 13, 14, 15], or by conditions imposed on Rung-Kutta schemes [2, 16, 17, 18, 19]). A general explicit symplectic method is

$$p_i = p_{i-1} - d_i\tau\frac{\partial V}{\partial q}(q_i), \qquad q_i = q_{i-1} + c_i\tau\frac{\partial T}{\partial p}(p_{i-1}), \tag{2}$$

where $i = 1, \ldots, k$, $(p_0, q_0) = (p(t_0), q(t_0))$ represent the initial conditions at time $t = t_0$ and $(p_k, q_k) = (p', q') = (p(t_0+\tau), q(t_0+\tau))$ is the approximation of the position and momentum after one time step of length τ. In terms of an exponential product, an explicit n-th order symplectic integrator can be expressed as

$$\begin{pmatrix} p' \\ q' \end{pmatrix} = \prod_{i=1}^{k} \mathrm{e}^{c_i\tau X_T}\mathrm{e}^{d_i\tau X_V}\begin{pmatrix} p_0 \\ q_0 \end{pmatrix} = S_n(\tau)\begin{pmatrix} p_0 \\ q_0 \end{pmatrix}. \tag{3}$$

Table 1 includes a selection of explicit symplectic methods constructed via a method of generating functions and composition (after [4]). Details of the calculation of the coefficients c_i and d_i can be found in [11, 12, 20, 13, 14, 15]. Table 2 contains 4th, 5th and 6th order Runge-Kutta-Nyström (RKN) methods constructed in [2, 19]. RKN methods are applicable only when the kinetic energy, $T(p)$, in the Hamiltonian is quadratic.

Implicit symplectic methods can be obtained by imposing conditions on already existing Runge-Kutta (RK) methods. When Hamilton's equations are of the form (1), an s-stage symplectic RK method can be expressed as

$$\begin{aligned} p' &= p_0 - \tau\sum_{i=1}^{s} b_i\frac{\partial V}{\partial q}(Q_i), \qquad q' = q_0 + \tau\sum_{i=1}^{s} b_i\frac{\partial T}{\partial p}(P_i), \\ P_i &= p_0 - \tau\sum_{j=1}^{s} a_{ij}\frac{\partial V}{\partial q}(Q_j), \qquad Q_i = q_0 + \tau\sum_{j=1}^{s} a_{ij}\frac{\partial T}{\partial p}(P_j). \end{aligned} \tag{4}$$

The necessary and sufficient conditions for an s-stage Runge-Kutta method to be symplectic [16, 21] are $b_ib_j - b_ia_{ij} - b_ja_{ji} = 0, i, j \leq s$. If $a_{ij} = 0$ for $i \leq j$ these methods are explicit, otherwise they are implicit.

Gaussian Runge-Kutta (GRK) methods are implicit even-order RK methods that are always symplectic [17]. Coefficients a_{ij}, b_j, are determined using methods specific to Gauss collocation, described in [17] and [18]. Coefficients for the 2nd order implicit midpoint rule (MP2), and the 4th, 6th, 8th and 10th order Gauss method (GRK4,6,8,10 respectively) appear in [17, 18, 22].

3. Linear Stability

3.1. Hamiltonian Ordinary Differential Equations

As an introduction to linear stability theory of symplectic maps we'll look at the stability of symplectic integrators applied to linear ODEs, as provided in [4] and [23], and then tackle the more complicated case of Hamiltonian PDEs.