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ESSENTIALLY SYMPLECTIC BOUNDARY VALUE METHODS FOR LINEAR HAMILTONIAN SYSTEMS*[1)]

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Abstract

In this paper we are concerned with finite difference schemes for the numerical approximation of linear Hamiltonian systems of ODEs. Numerical methods which preserves the qualitative properties of Hamiltonian flows are called *symplectic integrators*. Several symplectic methods are known in the class of Runge-Kutta methods. However, no high order symplectic integrators are known in the class of Linear Multistep Methods (LMMs). Here, by using LMMs as Boundary Value Methods (BVMs), we show that symplectic integrators of arbitrary high order are also available in this class. Moreover, these methods can be used to solve both initial and boundary value problems. In both cases, the properties of the flow of Hamiltonian systems are "essentially" maintained by the discrete map, at least for linear problems.

1. Introduction

In many areas of physics, mechanics, etc., Hamiltonian systems of ODEs play a very important role. Such systems have the following general form:

$$y' = J_{2m}^T \bigtriangledown H(y,t), \quad t \in [t_0, T], \quad y(t_0) = y_0 \in \mathbb{R}^{2m}, \tag{1}$$

where, by denoting with O_m and I_m the null matrix and the identity matrix of order m, respectively,

$$J_{2m} = \begin{pmatrix} O_m & I_m \\ -I_m & O_m \end{pmatrix}.$$

Simple properties of the matrix J_{2m} are the following ones:

$$J_{2m}^{-1} = J_{2m}^T = -J_{2m}, \qquad \det(J_{2m}) = 1.$$

In equation (1) $\bigtriangledown H(y,t)$ is the gradient of a scalar function $H(y,t)$, usually called *Hamiltonian.* In the case where $H(y,t) = H(y)$, then the value of this function remains constant along the solution $y(t)$, that is:

$$H(y(t)) = H(y_0), \qquad \text{for all} \quad t \geq t_0.$$

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In particular, we shall consider the simpler case where

$$H(y) = \frac{1}{2} y^T S y, \qquad S = S^T \in \mathbb{R}^{2m \times 2m}. \tag{2}$$

In this case, problem (1) is linear:

$$y' = J_{2m}^T S y, \quad t \in [t_0, T], \qquad y(t_0) = y_0. \tag{3}$$

In the following, we assume the matrix S to be nonsingular.

Another important feature of problem (3) is that oriented areas are preserved by the flow. This because the exponential $e^{J_{2m}^T S}$ is symplectic, that is:

$$(e^{J_{2m}^T S})^T J_{2m} e^{J_{2m}^T S} = J_{2m}.$$

We now want to look for numerical schemes which satisfy the following two requirements:

1. they define a symplectic map and
2. they preserve the quadratic form (2).

Such methods are usually called *symplectic* or *canonical* integrators.

The known symplectic methods are essentially Runge-Kutta schemes[13,19,20,21], while it seems that they are rare in the class of LMMs. This apparent weakness of LMMs has been recently overcome by using them as Boundary Value Methods (BVMs). We shall recall the main facts about BVMs in Section 2. In Section 3 we shall examine one step methods, while in Section 4 we shall consider multistep methods. In Section 5 we shall analyze three classes of symplectic BVMs and, finally, in Section 6 some numerical examples are reported.

2. Boundary Value Methods

In this section we briefly recall the basic results on BVMs[3,7,8]. Let us then consider the IVP

$$y' = f(t, y), \quad t \in [t_0, T], \qquad y(t_0) = y_0. \tag{4}$$

To approximate its solution, we consider the k-step LMM

$$\sum_{i=0}^{k} \alpha_i y_{n+i} = h \sum_{i=0}^{k} \beta_i f_{n+i}, \tag{5}$$

used over the partition

$$t_i = t_0 + ih, \quad i = 0, \cdots, N + k_2 - 1, \qquad h = \frac{T - t_0}{N + k_2 - 1},$$

where $0 \le k_2 < k$. As usual, y_{n+i} and f_{n+i} denote the approximations to $y(t_{n+i})$ and $f(t_{n+i}, y(t_{n+i}))$, respectively. It is known that the discrete problem (5) needs k