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COMPARISON OF A SPECTRAL COLLOCATION METHOD AND SYMPLECTIC METHODS FOR HAMILTONIAN SYSTEMS

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Abstract. We conduct a systematic comparison of a spectral collocation method with some symplectic methods in solving Hamiltonian dynamical systems. Our main emphasis is on non-linear problems. Numerical evidence has demonstrated that the proposed spectral collocation method preserves both energy and symplectic structure up to the machine error in each time (large) step, and therefore has a better long time behavior.

Key Words. Hamiltonian systems, spectral method, collocation, symplectic structure, energy conservation.

1. Introduction

Hamiltonian systems typically arise as models of conservative physical systems and have many applications in classical mechanics, molecular dynamics, hydrodynamics, electrodynamics, plasma physics, relativity, astronomy, and other scientific fields [29, 30]. They are an alternative and equivalent formalism of Newtonian and Lagrangian formalisms and become one of the most useful tools in the mathematical theory of physical and engineering sciences. Almost all real physical processes with negligible dissipation can be described in some way or another by Hamiltonian formalism [1].

The canonical system

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}, \quad \frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}; \qquad i = 1, 2, \ldots, n \tag{1}$$

with given Hamiltonian function $H(p_1, \ldots, p_n; q_1, \ldots, q_n)$ was first introduced by Hamilton in 1824. Since then, many famous scientists, such as Poincaré, Jacobi, Birkhoff, Weyl, Kolmogorov, and Arnold, studied the subject [1].

In addition to its elegance and symmetry, the Hamiltonian system has some remarkable properties, most important among which are its symplectic structure and optimality for energy preservation. Any good numerical scheme should be able to replicate as many of these physical properties as possible. The symplectic structure is in nature volume-preserving. Traditional ODE solvers such as Runge-Kutta, multi-step methods usually do not preserve the symplectic structure and energy, and as a consequence, numerical trajectories tend to gradually drift away from the true solution trajectories in a phenomenon called phase shift. The idea of developing numerical methods that maintain the symplectic structure was first studied in a general setting by Feng in the 1980' [10]. This was followed by a successful systematic study of designing so-called symplectic algorithms [11, 12,

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13, 14, 15, 16, 17, 26, 33]. But, none of these symplectic algorithms is energy-preserving in general. Indeed, it was proved that there exists no energy preserving symplectic algorithm for general non-linear Hamiltonian systems [19, 9]. On the other hand, Galerkin type methods such as finite element methods are well-known to preserve energy. Now we face a dilemma and have to choose between preserving energy and preserving symplectic structure. Some argue that for highly oscillatory problems, preserving energy may be more important than the symplectic structure [7, 8, 32, 4, 18].

In this paper, we introduce an algorithm based on spectral collocation to preserve both energy and volume (symplectic structure) up to numerically negligible error terms. If the error term is so small that it reaches the machine epsilon – the computer round-off error, then the algorithm is practically energy and volume preserving. We shall use a series numerical benchmark problems to demonstrate that our methods are effective and much accurate than symplectic methods with the similar computational cost.

There have been some recent attempts in using spectral method [35] and spectral collocation method [22] to solve ODEs. In this work, we carry on a systematic comparison between the proposed spectral collocation method and symplectic methods. For more references regarding spectral and spectral collocation methods, the reader is referred to [2, 3, 5, 6, 20, 21, 27, 31, 34, 37] and references therein.

2. The algorithm

To simplify the discussion, we use the case $n = 1$ in (1) to illustrate the idea. Consider the nonlinear Hamiltonian system

$$p' = -\frac{\partial H}{\partial q} = f(p,q), \quad q' = \frac{\partial H}{\partial p} = g(p,q), \qquad p(0) = p_0, \quad q(0) = q_0,$$

where f and q are nonlinear functions. We use either the Chebyshev-Gauss-Lobatto or the Legendre-Gauss-Lobatto collocation methods to solve it. We solve the system on $[0, r]$ first, then use the obtained values $(p(r), q(r))$ as an initial condition to repeat the process on $[r, 2r]$, and so on .... Here r could be large, a convenient choice is $r = 2$.

Let $t_0 < t_1 < \cdots t_N$ be collocation points where $t_0 = 0$ and $t_N = r$. We interpolate p and q as

$$p_N(t) = \sum_{j=0}^{N} p(t_j)\ell_j(t), \quad q_N(t) = \sum_{j=0}^{N} q(t_j)\ell_j(t),$$

where ℓ_j is the Lagrange nodal basis function satisfying $\ell_j(t_i) = \delta_{ij}$.

We are seeking numerical approximations of $(p(t_j), q(t_j))$, denoted as (p_j, q_j). In the literature of the spectral method, the explicit form of the differentiation matrix $D = (d_{ij})_{i,j=0}^{N}$ is known [2, 3, 5, 6, 21, 34] with $d_{ij} = \ell_j'(t_i)$. Note that the rank of the $(N+1) \times (N+1)$ matrix D is N. Therefore, we may solve the system

$$\begin{aligned}
d_{11}p_1 + d_{12}p_2 + \cdots d_{1N}p_N &= f(p_1, q_1) - d_{10}p_0 \\
&\vdots \\
d_{N1}p_1 + d_{N2}p_2 + \cdots d_{NN}p_N &= f(p_N, q_N) - d_{N0}p_0 \\
d_{11}q_1 + d_{12}q_2 + \cdots d_{1N}q_N &= g(p_1, q_1) - d_{10}q_0 \\
&\vdots \\
d_{N1}q_1 + d_{N2}q_2 + \cdots d_{NN}q_N &= g(p_N, q_N) - d_{N0}q_0
\end{aligned}$$