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Symplectic waveform relaxation methods for Hamiltonian systems

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ABSTRACT

In this literature, a new method called symplectic waveform relaxation method is for the first time proposed to solve Hamiltonian systems. This method is based on waveform relaxation method which makes computation cheaper, and makes use of symplectic method to determine its numerical scheme. Under the guidance of the symplectic method, the discrete waveform relaxation method elegantly preserves the discrete symplectic form. Windowing technique is utilized to accelerate computation. The windowing technique also makes it possible to advance in time, window by window. Convergence results of continuous and discrete symplectic waveform relaxation methods are analyzed. Numerical results show that the symplectic waveform relaxation method with the windowing technique precisely preserves the Hamiltonian function.

1. Introduction

In this paper, we propose a new method to solve the Hamiltonian system

$$\begin{cases} \dfrac{dq}{dt} = H_p, \\ \dfrac{dp}{dt} = -H_q, \end{cases} \tag{1}$$

where $p, q \in \mathbb{R}^d$ are d-dimensional functions to be sought, $H = H(q, p)$ is the Hamiltonian function of the system, and H_p and H_q are partial derivatives of the Hamiltonian function H. According to theoretical physics, the Hamiltonian system (1) is obtained from the Euler–Lagrangian equation by representing system in phase space [9]. Systems of this kind are seen in Mechanics, Klein–Gordon equations [23], and Korteweg–de Vries (KdV) equations [1], and so on. p and q are position and momentum in generalized coordinates, respectively.

Each Hamiltonian system holds a conservation law, that is, the Hamiltonian function $H(q, p)$ is constant with respect to time, i.e.,

$$\frac{dH}{dt} = {H_q}^T \frac{dq}{dt} + {H_p}^T \frac{dp}{dt} = {H_q}^T H_p + {H_p}^T (-H_q) = 0.$$

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For each Hamiltonian system, the **symplectic form**, which is defined as $\omega = dp \wedge dq$, is observed to be a constant. The theory of symmetry geometry leads to the corresponding numerical study. This kind of numerical method is called *symplectic* method. The symplectic method is famous for solving Hamiltonian systems with long term stability [8,11]. It focuses on the conservation of $H(q, p)$ as time evolves, i.e., $H(q_{n+1}, p_{n+1}) = H(q_n, p_n)$, rather than the order of a numerical scheme. This idea brings very good numerical outcomes in the calculation of planetary system.

The well-known symplectic schemes are symplectic Euler method (also known as mid-point Euler method), symplectic Runge–Kutta method, symplectic Runge–Kutta–Nyström method [16,17], symplectic ERKN method [25], Hamiltonian BVM [4], and so on. Study on Hamiltonian also covers two-stage waveform relaxation method [12], non-autonomous Hamiltonian systems [13,29], stochastic Hamiltonian equations [5,7,22], multisymplectic methods [26] and optimal control problems [20] and so on. Furthermore, there is no Runge–Kutta method that is both explicit and symplectic [24].

In this paper, we are going to use waveform relaxation (WR) method [15] to solve this system (1). In order to take advantage of the symplectic method, we use the symplectic method as the numerical tool.

The WR method origins from large scale integrated circuits [19]. It contains two main parts, splitting and iterating. First of all, a splitting function has to be chosen to break the big system into small systems. Then there is a loop. We need to solve the small systems, exchange information between systems, and recursively doing this procedure until convergent. Notable features of the WR method are decoupling and the potential of parallelism.

We call the combination of symplectic method and waveform relaxation method the *symplectic waveform relaxation method* (symplectic WR method). It is a special case of the WR method that makes use of the symplectic structure as a model, and takes advantage of the decoupling feature of WR. On the one hand, the symplectic scheme instructs how to discretize the splitting function. On the other hand, the WR method simplifies the computation.

To solve for a longer time interval, windowing technique [14,18] is introduced. Windowing technique reduces the number of iterations and at the same time does not lose the favor of symplectic method. In [14], the author discussed how big the window size would be. Besides, windowing technique is almost naturally parallel according to [21].

The paper is organized as follows. In Section 2, we analyze the symplectic WR method, and give examples of two discrete symplectic WR schemes. The conservation laws of Hamiltonian function of both continuous and discrete symplectic WR method are analyzed. The windowing technique is used to accelerate symplectic WR method. In Section 3, numerical results are given. Finally, there is a conclusion.

2. Symplectic waveform relaxation methods for Hamiltonian systems

In this section, we analyze the symplectic WR method for Hamiltonian system Eq. (1). Write Eq. (1) as

$$\dot{z} = f(z), \tag{2}$$

where $z = (q; p)$ is the unknown function on $[0, T]$ and $f(z) = (H_p; -H_q)$ is the function on the right hand side of Eq. (1).

The WR method [15] is a mathematical tool that benefits from an idea of integrated circuits. When a system is large in scale, and is hard to compute with current computing resources, we can split it into subsystems that are smaller in scale and easier to compute. To archive this, we choose the splitting function $F(z, y)$ such that $F(z, z) = f(z)$, and replace $f(z)$ with $F(z, y)$ in (1). After choosing a guessed initial value for each subsystem, we compute as if y in $F(z, y)$ is the known function and z is the unknown, which makes the computation easier. However, this computation cannot be exact because the arbitrary choice of the initial value. Then we need an iteration process to ensure its convergence. Often, we write this as $\dot{z}^{k+1} = F(z^{k+1}, z^k)$, where $k = 0, 1, \ldots$ is the step counter.

Regarding the WR method, the splitting function is taken to decouple the system (2). For the WR method, we have the following result.

Theorem 1 [15]**.** *Suppose the splitting function $F(x, y)$ is Lipschitz continuous with respect to x and y in (2), the WR method is convergent.*

2.1. Continuous-time symplectic WR method

The symplectic WR method is internally the classical WR method. So we know that the Theorem 1 holds. Then we take a step further and consider how the Hamiltonian function H behaves with this method.

Theorem 2. *If the symplectic WR method is convergent, and the f in (2) is bounded, then the Hamiltonian function converges to a constant.*

Proof. Denote by H_0 the Hamiltonian function of the system. Since the Hamiltonian H_0 is constant,

$$\frac{dH_0}{dt} = 0.$$

Denote by H^{k+1} the Hamiltonian function in the $(k+1)$th iteration, that is

$$H^{k+1} = H(q^{k+1}, p^{k+1}),$$

where q^{k+1} and p^{k+1} are position and momentum functions in the $(k+1)$th iteration.