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Adiabatic Filon-type methods for highly oscillatory second-order ordinary differential equations

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ABSTRACT

In this paper, we study efficient numerical integrators for linear and nonlinear systems of highly oscillatory second-order ordinary differential equations. The systems are reformulated as a first-order system, which is then transformed to adiabatic variables. The solution of the transformed system is a smoother function which is more accessible to numerical approximation than the original system. We develop Filon-type methods for linear systems by approximating the integral as a linear combination of function values and derivatives. We then present a special combination of Filon-type methods and waveform relaxation methods for nonlinear systems. Both types of methods can be used with far larger step sizes than those required by traditional schemes and their performance drastically improves as frequency grows, as are illustrated by numerical experiments.

1. Introduction

Highly oscillatory differential equations arise frequently in celestial mechanics, chemistry, biology, classical and quantum mechanics, and engineering. The integration of such systems has been a numerical challenge for a long time (see, e.g., [1,2]). To approximate the solution with sufficient accuracy, one usually has to take step sizes far smaller than the smallest period of the oscillations with standard numerical methods. Gauthschi [3] proposed trigonometric integrators for differential equations of the form $\ddot{x} + \omega^2 x = g(t, x)$ with a fixed large frequency ω. These methods might be regarded as the earliest approach to take larger time steps in oscillatory problems and are then extended to $\ddot{x} + Ax = g(t, x)$ with a constant, symmetric, positive semi-definite matrix A of large norm. For this type of systems, García-Archilla et al. [4] proposed and analysed the mollified impulse method, Hochbruck & Lubich [5] analysed the Gautschi-type integrators, and Grimm & Hochbruck [6] provided an error analysis for a family of exponential integrators. Sanz-Serna [7] introduced a family of impulse like methods for the integration of highly oscillatory second-order differential equations $M\ddot{x} = f(x) + g(x)$, where M is a symmetric positive-definite mass matrix and the forces are split into a fast part f and a slow part g. Khanamiryan [8] presented asymptotic and Filon-type methods for highly oscillatory first-order initial problems $\dot{x}(t) = Ax(t) + f(t, x(t))$, where A is a constant non-singular $d \times d$ matrix with large eigenvalues. Wang et al. [9] analysed a Filon-type asymptotic approach for highly oscillatory second-order initial value problems $\ddot{x}(t) + Mx(t) = f(t, x(t), x'(t))$ using the variation-of-constants formula, where M is a non-singular and diagonalizable matrix having large eigenvalues. Numerical methods for second-order differential equations with high time-dependent frequencies have also been studied (see, e.g., [10–14]).

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In this paper, we are concerned with numerical integration of second-order differential equations

$$\ddot{x}(t) + Ax(t) = g(t, x, \dot{x}), \quad t \in [0, T], \qquad x(0) = x_0, \qquad \dot{x}(0) = \dot{x}_0, \tag{1.1}$$

where $x(t) : \mathbb{R} \to \mathbb{R}^d$, $g(t, x, \dot{x}) : \mathbb{R} \times \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$ is a smooth function, A is a symmetric and positive definite $d \times d$ constant matrix with large eigenvalues, $\|A\|_2 \gg 1$ and $\|A^{-1}\|_2 \ll 1$. We are interested in deriving numerical methods with the property that their accuracy improves with the increase of the frequencies of A.

The paper is organized as follows. In Section 2, we reformulate the system (1.1) into a first-order system and then transformed to adiabatic variables. The solution of the transformed system is a smoother function and may be more accessible to numerical approximation. In Section 3, we construct adiabatic Filon-type methods for linear systems by approximating the integral as a linear combination of function values and derivatives, and provide error bounds for the methods. We extend and present a special combination of the Filon-type methods and waveform relaxation methods for nonlinear systems in Section 4. In Section 5, numerical experiments are carried out to show the effectiveness of our proposed methods by comparing with some existing algorithms in the literature. A conclusion is included in Section 6.

2. Adiabatic transformation

We first transform (1.1) into a first-order system instead of considering the original one directly. The approach adopted here was proposed in [15,16,14].

Suppose that the real symmetric and positive definite matrix A in (1.1) is decomposed into

$$A = Q\Omega^2 Q^T, \tag{2.1}$$

where Q is a real orthogonal $d \times d$ matrix and $\Omega = \mathrm{diag}(\omega_k)$ a diagonal $d \times d$ matrix. We assume that $\omega_k \gg 1,\ k = 1, 2, \ldots, d$ throughout the paper. Denote $B = A^{\frac{1}{2}} = Q\Omega Q^T$ and let $\dot{x}(t) = By(t)$. Then (1.1) is equivalent to the following first-order system

$$\begin{pmatrix} \dot{x}(t) \\ \dot{y}(t) \end{pmatrix} = M \begin{pmatrix} x(t) \\ y(t) \end{pmatrix} + \begin{pmatrix} 0 \\ B^{-1} g(t, x(t), By(t)) \end{pmatrix}, \tag{2.2}$$

where

$$M = \begin{pmatrix} 0 & B \\ -B & 0 \end{pmatrix}.$$

Meanwhile, the skew-symmetric matrix M in (2.2) can be decomposed into

$$M = U \mathrm{i} \Lambda U^*$$

with

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & \mathrm{i} \\ \mathrm{i} & 1 \end{pmatrix} \otimes Q, \qquad \Lambda = \begin{pmatrix} \Omega & 0 \\ 0 & -\Omega \end{pmatrix}, \tag{2.3}$$

where i is the imaginary unit, U is a unitary matrix, and U^* is the conjugate transpose of U. Note that Λ is a $2d \times 2d$ diagonal matrix with $\|\Lambda\|_2 \gg 1$ and $\|\Lambda^{-1}\|_2 \ll 1$.

We now introduce a new variable

$$\eta(t) = e^{-\mathrm{i}\Lambda t} U^* \begin{pmatrix} x(t) \\ y(t) \end{pmatrix}. \tag{2.4}$$

So

$$\begin{pmatrix} x(t) \\ y(t) \end{pmatrix} = U e^{\mathrm{i}\Lambda t} \eta(t) = S(t)\eta(t), \tag{2.5}$$

where

$$S(t) = U e^{\mathrm{i}\Lambda t} = \frac{1}{\sqrt{2}} \begin{pmatrix} Q e^{\mathrm{i}\Omega t} & \mathrm{i} Q e^{-\mathrm{i}\Omega t} \\ \mathrm{i} Q e^{\mathrm{i}\Omega t} & Q e^{-\mathrm{i}\Omega t} \end{pmatrix}. \tag{2.6}$$

Set

$$S(t) = \begin{pmatrix} S^{11}(t) & S^{12}(t) \\ S^{21}(t) & S^{22}(t) \end{pmatrix}, \qquad S^{ij}(t) \in \mathbb{R}^{d \times d}, \quad i, j = 1, 2. \tag{2.7}$$

From (2.5) and (2.7), we have

$$x(t) = (S^{11}(t), S^{12}(t))\eta(t), \tag{2.8}$$