BIT Numer Math
DOI 10.1007/s10543-011-0355-z

BIT

Quadrature methods for highly oscillatory linear and non-linear systems of ordinary differential equations: part II

Marianna Khanamiryan

Received: 31 December 2009 / Accepted: 23 August 2011

Abstract In this paper we present efficient numerical approximation for systems of highly oscillatory ordinary differential equations with matrices of variable coefficients. We assume that the spectrum of the matrix is purely imaginary and the frequency of oscillation grows large. We develop the *asymptotic* and the *Filon*-type methods for linear systems with time dependent matrices and we integrate oscillatory quadrature rules with *waveform relaxation* methods employing the *WRF* method for non-linear systems. We solve matrix exponential in *Lie* groups employing *Magnus* expansion. The methods are illustrated in several numerical examples of interest.

Keywords High oscillation · Systems of ordinary differential equations · Asymptotic analysis · Filon-type methods · Lie group methods · Magnus method · Waveform relaxation methods · WRF method

Mathematics Subject Classification (2000) 65L05 · 34E05 · 34C15 · 34C60

1 Introduction

In many applications one comes across physical phenomena described by dynamical systems subject to a time dependent perturbation which is localized in space and time. In current work we develop methods for systems of ordinary differential equations (ODEs) with variable coefficients,

$$\boldsymbol{y}'(t) = A_\omega(t)\boldsymbol{y}(t) + \boldsymbol{f}(t, \boldsymbol{y}(t)), \qquad \boldsymbol{y}(0) = \boldsymbol{y}_0 \in \mathbb{R}^d, \quad t \geq 0. \tag{1}$$

Communicated by Syvert Nørsett.

M. Khanamiryan (✉)
Department of Applied Mathematics and Theoretical Physics, University of Cambridge, Wilberforce Road, Cambridge CB3 0WA, UK
e-mail: marianna.khanamiryan@trinity.cantab.net

Published online: 23 September 2011

The following assumptions are hold: the matrix A_ω is time dependent and has large imaginary eigenvalues, $\sigma(A_\omega) \subset i\mathbb{R}$, $\|A_\omega\| \gg 1$, $\|A_\omega^{-1}\| \ll 1$, $\boldsymbol{f} : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$ is a smooth vector-valued function and $\omega \gg 1$ is a real parameter. The solution of this equation becomes highly oscillatory due to the imaginary eigenvalues and increasing values of the parameter ω. Needless to mention that presence of the parameter ω is symbolic. It is a forcing term and its scalar product with the eigenvalues of the matrix A_ω guarantees that the frequency of oscillation in system (1) grows large for $\omega \gg 1$.

It is well known from the classical theory of differential equations, [6], that the analytic solution $\boldsymbol{y}$ of the system of ODEs (1) is described by the variation of parameters formula,

$$\boldsymbol{y}(t) = X_\omega(t)\boldsymbol{y_0} + \int_0^t X_\omega(t-\tau)\boldsymbol{f}(\tau, \boldsymbol{y}(\tau))\mathrm{d}\tau = X_\omega \boldsymbol{y_0} + I[\boldsymbol{f}]. \tag{2}$$

The assumption that matrix A_ω is time dependent, results in a complex solution of a fundamental matrix X_ω, satisfying matrix linear ODE, see [22],

$$X'_\omega = A_\omega X_\omega, \quad X_\omega = \mathrm{e}^{\Omega},$$

where Ω represents the *Magnus* expansion, an infinite recursive series,

$$\begin{aligned}\Omega(t) = &\int_0^t A(t)\mathrm{d}t \\ &+ \frac{1}{2}\int_0^t \left[A(\tau), \int_0^\tau A(\xi)\mathrm{d}\xi\right]\mathrm{d}\tau \\ &+ \frac{1}{4}\int_0^t \left[A(\tau), \int_0^\tau \left[A(\xi), \int_0^\xi A(\zeta)\mathrm{d}\zeta\right]\mathrm{d}\xi\right]\mathrm{d}\tau \\ &+ \frac{1}{12}\int_0^t \left[\left[A(\tau), \int_0^\tau A(\xi)\mathrm{d}\xi\right], \int_0^\tau A(\zeta)\mathrm{d}\zeta\right]\mathrm{d}\tau \\ &+ \cdots .\end{aligned} \tag{3}$$

This solution can be compared to the systems of ODEs with a constant matrix A_ω, considered in [19].

The theory on *Lie* group methods and in particular on Magnus expansion is well developed and we list here only the most relevant literature on the topic: [2–5, 8, 9, 13–15, 25, 30].

The challenge is to evaluate a highly oscillatory integral $I[\boldsymbol{f}]$ in (2) efficiently.

Classical methods based on Gaussian quadrature fail to approximate highly oscillatory integrals for increasing frequency. For the highly oscillatory Fourier-type integral

$$I[f] = \int_a^b f(x)\mathrm{e}^{i\omega g(x)}\mathrm{d}x,$$

with smooth functions $f, g \in \mathbb{C}^\infty$, the error of approximation with a classical quadrature rule is compared to $\mathcal{O}(1)$ for increasing ω, [17, 19]. From this standpoint, con-

sidering that the integral itself is of order $\mathcal{O}(\omega^{-1})$, this result compares to an approximation of the Fourier-type highly oscillatory integral $I[f]$ by zero. Thus it is safe to declare that any approximation that is less accurate than equating the integral to zero is fairly useless. Letting step-size h to depend on the frequency ω on the other hand results in enormous amount of computation for large ω, tremendously reducing the step-size h.

Armed with this information, we first focus on developing numerical methods to solve highly oscillatory integrals with a matrix-valued kernel and next we use our results in numerical approximation of non-linear systems (2).

Given a vector-valued integral over a compact interval $[a, b]$,

$$I[\boldsymbol{f}] = \int_a^b X_\omega(t)\boldsymbol{f}(t)\mathrm{d}t, \qquad X'_\omega = A_\omega X_\omega, \quad X_\omega = \mathrm{e}^{\Omega}, \tag{4}$$

with a time dependant matrix A_ω, such that $\det A_\omega \neq 0$, $\|A_\omega\| \gg 1$, $\|A_\omega^{-1}\| \ll 1$, $\sigma(A_\omega) \subset i\mathbb{R}$, ω is a real parameter and $\boldsymbol{f} \in \mathbb{R}^d$ is a smooth vector-valued function.

In the special case of systems of ODEs with constant matrices A_ω, the task of obtaining the asymptotic expansion for the integral $I[\boldsymbol{f}]$ is fairly straightforward, [19]. Indeed, from the equation $X'_\omega = A_\omega X_\omega$, we derive $X_\omega = A_\omega^{-1} X'_\omega$. The integrals $I[\boldsymbol{f}^{(k)}]$ for $k = 0, 1, 2, \ldots$ are also oscillatory and recursive integration by parts

$$\begin{aligned} I[\boldsymbol{f}] &= A_\omega^{-1}\big[X_\omega(b)\boldsymbol{f}(b) - X_\omega(a)\boldsymbol{f}(a)\big] - A_\omega^{-1}\int_a^b X_\omega(t)\boldsymbol{f}'(t)\mathrm{d}t \\ &= Q_1^A - A_\omega^{-1} I[\boldsymbol{f}'], \end{aligned}$$

leads to the asymptotic expansion of the integral $I[\boldsymbol{f}]$,

$$I[\boldsymbol{f}] \sim -\sum_{m=1}^{\infty}(-A_\omega)^{-m}\big[X_\omega(b)\boldsymbol{f}^{(m-1)}(b) - X_\omega(a)\boldsymbol{f}^{(m-1)}(a)\big].$$

The truncated s-partial sum of the asymptotic expansion represents the asymptotic method Q_s^A, defined as

$$Q_s^A[\boldsymbol{f}] = -\sum_{m=1}^{s}(-A_\omega)^{-m}\big[X_\omega(b)\boldsymbol{f}^{(m-1)}(b) - X_\omega(a)\boldsymbol{f}^{(m-1)}(a)\big].$$

This approach is not valid for a more general oscillator with an arbitrary non-singular matrix A_ω of variable coefficients. Substitution $X_\omega = A_\omega^{-1} X'_\omega$ in $I[\boldsymbol{f}]$ doesn't contribute to a meaningful derivation of the asymptotic expansion,

$$I[\boldsymbol{f}] = \int_a^b A_\omega^{-1}(t) X'_\omega(t)\boldsymbol{f}(t)\mathrm{d}t.$$

In Sect. 3 we develop an alternative approach to derive the asymptotic expansion of $I[\boldsymbol{f}]$ given an arbitrary non-singular matrix A_ω. Armed with the asymptotic expansion, in Sect. 4 we apply the *Filon* method to solve linear systems of highly oscillatory

ODEs with variable coefficients. For the computation of the matrix exponential we apply *Lie* group methods. In particular we choose the *Magnus* method and the *modified Magnus* method bound with the *Filon-type* methods, especially efficient for the oscillatory systems. The natural extension of these ideas is to emulate the Filon-type methods for non-linear highly oscillatory systems of ODEs (1), a generalization that will be exploited in Sect. 5. The non-linearity of the system is handled with the *waveform relaxation* methods, however a clever implication of oscillatory quadrature rules leads to surprisingly good results after only a few of steps of iterations.

2 Asymptotic expansion versus Taylor's expansion for high oscillation

Traditionally, fundamental concepts of numerical analysis of differential equations are based on *Taylor's* theorem. However, we can safely claim that *Taylor's* theorem is incompatible with the numerical analysis of highly oscillatory differential equations. Let us explain the reasons for it.

Suppose f has $n+1$ continuous derivatives on an open interval containing a point a. Employing *Taylor's* theorem, we expand f into its *Taylor* series, for each x in the interval,

$$f(x) = f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f^{(2)}(a)}{2!}(x-a)^2 + \cdots + \frac{f^{(n)}(a)}{n!}(x-a)^n + R_n(x)$$

where

$$R_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x-a)^{n+1}.$$

is the *Lagrange* formula for the remainder for some $\xi \in (a, x)$. For instance, for the *Euler's* method, the truncation error can be examined using *Taylor's* theorem,

$$y(t_{n+1}) = y(t_n) + \Delta t y'(t_n) + \frac{1}{2}\Delta^2 y''(\xi_n), \quad \xi \in [t_n, t_{n+1}].$$

The magnitude of the error arising from the *Euler's* method can be demonstrated by comparison with a *Taylor* expansion of y.

$$y(t_0 + h) = y(t_0) + h y'(t_0) + \frac{1}{2}h^2 y''(t_0) + O(h^3).$$

But *Taylor*'s theorem is a wrong tool for high oscillations. Each time we differentiate, the amplitude is roughly scaled by the frequency of oscillation. This means that in methods based on *Taylor's* reasoning we are compelled to choose a ridiculously small step-size. This is an underlying reason why classical numerical methods fail to approximate highly oscillatory differential equations.

To the contrary to the *Taylor* expansion, *asymptotic expansion* is a more powerful tool in the analysis of highly oscillatory ODEs, since *asymptotic expansion* depends

on and the error term are expressed in terms of inverse powers of the frequency of oscillation. In other words, the error of approximation decays as the frequency of oscillation grows.

For instance, for an intrinsic linear oscillator,

$$\boldsymbol{y}' = A_\omega \boldsymbol{y} + \boldsymbol{f}(t), \quad \text{when } \omega \gg 1,$$

the *asymptotic expansion* is available at any given time point,

$$\boldsymbol{y}(t) \sim \mathrm{e}^{At}\boldsymbol{y}_0 - \sum_{m=1}^{\infty} (-A_\omega)^{-m} (\mathrm{e}^{At}\boldsymbol{f}^{(m-1)}(t) - I\boldsymbol{f}^{(m-1)}(0)),$$

and for the numerical purposes the truncated *asymptotic expansion* can be evaluated for any large time value t. Essentially, the truncation and numerical approximation do not require an introduction of a step-size, since the *asymptotic* method does not depend on a step-size, see Lemma 2. Now, recall that the matrix has pure imaginary spectrum with large eigenvalues describing the frequency of oscillation, $\sigma(A_\omega) \subset i\mathbb{R}$, $\|A_\omega^{-1}\| \leq 1$. Therefore, inverse powers of the matrix A_ω depend on the inverse powers of eigenvalues and hence on the inverse powers of the frequency of oscillation.

In this work we develop numerical methods based on the *asymptotic* expansion for solving systems of highly oscillatory ODEs. We show that our methods have a remarkable advantage once applied to equations with a large frequency of oscillation. The accuracy of approximation improves as the frequency of oscillation grows. For small frequencies our methods are comparable with classical methods with Gaussian node points. Our algorithms are implemented in Matlab and the symbolic calculation is implemented in Maple symbolic package. Efficiency of the methods was tested and compared with Magnus nested integrals evaluated exactly. The superior performance of our methods is illustrated in numerical examples. Not only we built our methods with a relatively large step-size, but we also use very little information about function, essentially working with end-points only. Moreover, our methods do not require explicit availability of the derivatives, for instance for the interval [0, 1] one can substitute a sequence $\frac{1}{\omega}$ around the zero and a sequence $1 - \frac{1}{\omega}$ for the values around point one.

3 The asymptotic method

In this section we show how applying some matrix transformations in $I[\boldsymbol{f}]$ leads to its explicit asymptotic expansion.

Given,

$$I[\boldsymbol{f}] = \int_a^b X_\omega(t)\boldsymbol{f}(t)\mathrm{d}t, \qquad X'_\omega = A_\omega X_\omega, \quad X_\omega = \mathrm{e}^{\Omega}, \tag{5}$$

with a matrix valued kernel X_ω depending on a real parameter $\omega \gg 1$ and satisfying matrix linear differential equation (5). We assume that A_ω is a non-singular matrix

with variable coefficients, $\sigma(A_\omega) \subset i\mathbb{R}$, $\|A_\omega^{-1}\| \ll 1$ and $\boldsymbol{f} \in \mathbb{R}^d$ is a smooth vector-valued function.

Current representation of the integral $I[\boldsymbol{f}]$ in (5) is not suitable for obtaining its asymptotic expansion due to a more general choice of a matrix A_ω. Once we substitute $X_\omega = A_\omega^{-1} X'_\omega$ in $I[\boldsymbol{f}]$,

$$I[\boldsymbol{f}] = \int_a^b A_\omega^{-1}(t) X'_\omega(t) \boldsymbol{f}(t) \mathrm{d}t,$$

we realise that the flexibility of the matrix X_ω is now limited and the rule of integration by parts is not applicable at this stage.

To overcome this issue and obtain a more flexible representation of the integral (5) we suggest to transform $I[\boldsymbol{f}]$ into an equivalent integral, written in a more convenient form for our purposes. Below we describe that transformation.

We first vectorize the matrix X_ω,

$$X_\omega = \begin{pmatrix} x_{11} & x_{12} & \dots & x_{1d} \\ x_{21} & x_{22} & \dots & x_{2d} \\ \vdots & \ddots & \ddots & \vdots \\ x_{d1} & x_{d2} & \dots & x_{dd} \end{pmatrix}$$

into $\boldsymbol{X}_\omega$,

$$\boldsymbol{X}_\omega = [\bar{\boldsymbol{x}}_1, \bar{\boldsymbol{x}}_2, \dots, \bar{\boldsymbol{x}}_d],$$

whereby each entry element $\bar{\boldsymbol{x}}_i$ is a column vector from the matrix X_ω above,

$$\bar{\boldsymbol{x}}_i = \begin{bmatrix} x_{1i} \\ x_{2i} \\ \vdots \\ x_{di} \end{bmatrix}.$$

Further, we take the transpose of the vector $\boldsymbol{X}_\omega$ obtaining a corresponding $d^2 \times 1$ vector $\bar{\boldsymbol{X}}_{\boldsymbol{\omega}}$,

$$\bar{\boldsymbol{X}}_{\boldsymbol{\omega}} = [\bar{\boldsymbol{x}}_1, \bar{\boldsymbol{x}}_2, \dots, \bar{\boldsymbol{x}}_d]^\intercal = \boldsymbol{X}_\omega^\intercal.$$

Definition 1 The matrix direct sum of n matrices constructs a block diagonal matrix from a set of square matrices,

$$\bigoplus_{i=1}^{d} A_i = \operatorname{diag}(A_1, A_2, \dots, A_n) = \begin{pmatrix} A_1 & 0 & \dots & 0 \\ 0 & A_2 & \dots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \dots & A_n \end{pmatrix}.$$

Definition 2 Kronecker product, or direct product, denoted by $\bigotimes$, is an operation on two matrices of arbitrary size resulting in a block matrix. It gives the matrix of the

tensor product with respect to a standard choice of basis. If A is an $m \times n$ matrix and B is a $p \times q$ matrix, then the Kronecker product is the $mp \times nq$ block matrix,

$$A \otimes B = \begin{pmatrix} a_{11}B & \dots & a_{1n}B \\ \vdots & \ddots & \vdots \\ a_{m1}B & \dots & a_{mn}B \end{pmatrix}$$

with elements defined by

$$c_{\alpha\beta} = a_{ij}b_{kl},$$

where

$$\alpha = p(i-1)+k,$$
$$\beta = q(j-1)+l.$$

It is easy to verify that $\bar{\boldsymbol{X}}_{\boldsymbol{\omega}}$ satisfies a linear differential equation $\bar{\boldsymbol{X}}'_{\omega} = B_{\omega}\bar{\boldsymbol{X}}_{\omega}$, with $B_{\omega} = \bigoplus_{i=1}^{d} A_{\omega}$ representing a direct d-tuple sum of the original matrix A_{ω}. We also scale an identity matrix I by taking its direct product with the vector-valued function $\boldsymbol{f} := \boldsymbol{f}^{\intercal} = [f_1, f_2, \dots, f_d]$, $\boldsymbol{F} = \boldsymbol{f}_{1\times d} \otimes I_{d\times d}$. For instance, take

$$f = [f_1, f_2] \quad \text{and} \quad I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Direct product $\boldsymbol{F} = f \otimes I$ results in the following matrix,

$$\boldsymbol{F} = \begin{pmatrix} f_1 & 0 & f_2 & 0 \\ 0 & f_1 & 0 & f_2 \end{pmatrix}.$$

Definition 3 Let $\{\boldsymbol{A}_i\}$ be arbitrary matrices of the size $m \times n_i$, $i = 1, 2, \dots, k$. Define the matrix union $\boldsymbol{F}$ of the size $m \times \sum_{i=1}^{k} n_i$ by $\boldsymbol{F} = \bigcup_{i=1}^{d} \boldsymbol{A}_i$, where

$$\boldsymbol{F} = [A_1, A_2, \dots, A_k].$$

In general, $\boldsymbol{F}$ represents a tensor uniting the following matrices F_i, namely, $\boldsymbol{F} = \bigcup_{i=1}^{d} F_i$, where each entry matrix is a diagonal matrix with the corresponding element f_i on the diagonal,

$$F_i = \begin{pmatrix} f_i & 0 & \dots & 0 \\ 0 & f_i & \dots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & f_i \end{pmatrix}.$$

These transformations result in equality $X_{\omega}\boldsymbol{f} = \boldsymbol{F}\bar{\boldsymbol{X}}_{\omega}$, and appear to be suitable for integration by parts and representation of the asymptotic expansion of the integral (5).

Example 1 Let

$$X_\omega = \begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{pmatrix}, \qquad A_\omega = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \quad \text{and} \quad \boldsymbol{f} = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix}.$$

Then

$$\bar{\boldsymbol{X}}_\omega = \begin{bmatrix} x_{11} \\ x_{21} \\ x_{12} \\ x_{22} \end{bmatrix}, \qquad B_\omega = \begin{pmatrix} a_{11} & a_{12} & 0 & 0 \\ a_{21} & a_{22} & 0 & 0 \\ 0 & 0 & a_{11} & a_{12} \\ 0 & 0 & a_{21} & a_{22} \end{pmatrix}$$

and

$$\boldsymbol{F} = \begin{pmatrix} f_1 & 0 & f_2 & 0 \\ 0 & f_1 & 0 & f_2 \end{pmatrix}.$$

Hence,

$$X_\omega \boldsymbol{f} = \boldsymbol{F} \bar{\boldsymbol{X}}_\omega = \begin{bmatrix} x_{11} f_1 + x_{12} f_2 \\ x_{21} f_1 + x_{22} f_2 \end{bmatrix},$$

and $\bar{\boldsymbol{X}}'_\omega = B_\omega \bar{\boldsymbol{X}}_\omega$, once $X'_\omega = A_\omega X_\omega$.

As a result, we have obtained the following equality for the two integrals,

$$I[\boldsymbol{f}] = \int_a^b X_\omega(t) \boldsymbol{f}(t) \mathrm{d}t = \int_a^b \boldsymbol{F}(t) \bar{\boldsymbol{X}}_\omega(t) \mathrm{d}t = I[\boldsymbol{F}],$$

where matrix X_ω and vector $\bar{\boldsymbol{X}}_\omega$ satisfy linear ODEs,

$$X'_\omega = A_\omega X_\omega \quad \text{and} \quad \bar{\boldsymbol{X}}'_\omega = B_\omega \bar{\boldsymbol{X}}_\omega$$

respectively. This means that now we can approximate integral $I[\boldsymbol{F}]$ and thus $I[\boldsymbol{f}]$. Allowing integration by parts we can now obtain the asymptotic expansion for the integral $I[\boldsymbol{f}]$,

$$\begin{aligned} I[\boldsymbol{f}] &= \int_a^b \boldsymbol{F}(t) \bar{\boldsymbol{X}}_\omega(t) \mathrm{d}t = \int_a^b \boldsymbol{F}(t) B_\omega^{-1}(t) \bar{\boldsymbol{X}}'_\omega(t) \mathrm{d}t \\ &= \left[\boldsymbol{F}(t) B_\omega^{-1}(t) \bar{\boldsymbol{X}}_\omega(t) \right]_a^b - \int_a^b \left(\boldsymbol{F}(t) B_\omega^{-1}(t) \right)' \bar{\boldsymbol{X}}_\omega(t) \mathrm{d}t. \end{aligned}$$

Hereafter we refer to [29] for the notation on matrix functions asymptotics depending on a real parameter ω. For the entirety of the paper, all norms are L^∞ norms, for vectors, matrices and functions. The norm of a function is taken over the finite interval $[a, b]$.

We say that $f = \mathcal{O}(\tilde{f})$ for an arbitrary function f and non-negative constant $\tilde{f}$, which depend on a real parameter ω, if the norm of f and its derivatives are all

of order $O(\tilde{f})$ as $\omega \to \infty$, namely $\|f^{(m)}\| = O(\tilde{f})$ for $m = 0, 1, \ldots$. For arbitrary two $n \times m$ matrices $A(x) = (a_{ij}(x))$ and $\tilde{A} = (\tilde{a}_{ij})$, $\tilde{a}_{ij} \geq 0$, depending on a real parameter ω, we can thus posit $A(x) = \mathcal{O}(\tilde{A})$, if $a_{ij}(x) = \mathcal{O}(\tilde{a}_{ij})$ element-wise as $\omega \to \infty$. We may also say that $f = \mathcal{O}(1)$, if f and its derivatives remain bounded on $[a, b]$, as $\omega \to \infty$. Let $\mathbf{1} = \{1_{ij}\}$ stand for a matrix with all entries one. This allows us to write $A(x) = \mathcal{O}(\mathbf{1})$, if $a_{ij}(x) = \mathcal{O}(1)$ element-wise as $\omega \to \infty$. And finally, if $A = \mathcal{O}(\tilde{A})$ and $B = \mathcal{O}(\tilde{B})$, then the integration and multiplication properties are $\int_a^b A(x)\mathrm{d}x = O(\tilde{A})$ and $AB = \mathcal{O}(\tilde{A}\tilde{B})$.

Letting

$$\begin{aligned} \sigma_0 &= \boldsymbol{F}, \\ \sigma_{k+1} &= (\sigma_k B_\omega^{-1})', \quad k = 0, 1, \ldots \end{aligned}$$

we define *asymptotic* method as

$$Q_s^A[\boldsymbol{f}] = \sum_{k=0}^{s-1} (-1)^k \left(\sigma_k(b) B_\omega^{-1}(b) \bar{\boldsymbol{X}}_\omega(b) - \sigma_k(a) B_\omega^{-1}(a) \bar{\boldsymbol{X}}_\omega(a) \right).$$

Below we state the two statements, Theorem 1 from [29] and Lemma 1 from [19]. Subsequently, in Theorem 2 we generalise these results for a matrix-valued kernel X_ω, a vector-valued function $\boldsymbol{f}$ and a time dependant matrix A_ω in $I[\boldsymbol{f}]$, (5).

Theorem 1 [29] *Suppose that $\mathbf{y}$ satisfies the differential equation,*

$$\mathbf{y}'(x) = A(x)\mathbf{y}(x),$$

in the interval $[a, b]$, for some invertible matrix-valued function A such that $A^{-1} = \mathcal{O}(\hat{A})$, for $\omega \to \infty$. Assume that

$$I[\boldsymbol{f}] = \int_a^b \boldsymbol{f}^\intercal(x)\mathbf{y}(x)\mathrm{d}x,$$

where $\boldsymbol{f} \in \mathbb{R}^d$ is a smooth vector-valued function and $\mathbf{y} \in \mathbb{R}^d$ is a smooth, highly oscillatory vector-valued function. Define

$$Q_s^A[f] = \sum_{k=0}^{s-1} (-1)^k [\sigma_k^\intercal(b) A^{-1}(b)\mathbf{y}(b) - \sigma_k^\intercal(a) A^{-1}(a)\mathbf{y}(a)],$$

where

$$\sigma_0 \equiv f, \qquad \sigma_{k+1} = (A^{-\intercal}\sigma_k)', \quad k = 0, 1, \ldots.$$

If $f = O(\tilde{f})$ and $\mathbf{y}(x) = O(\tilde{\mathbf{y}})$ for $a \leq x \leq b$, then

$$I[f] - Q_s^A[f] = (-1)^s \int_a^b \sigma_s^\intercal \mathbf{y}\mathrm{d}x = O(\tilde{\boldsymbol{f}}^\intercal \hat{A}^{s+1} \tilde{\mathbf{y}}), \quad \text{as } \omega \to \infty.$$

Lemma 1 [19] *Let*

$$I[\boldsymbol{f}]=\int_a^b X_\omega(t)\boldsymbol{f}(t)\mathrm{d}t,\qquad X'_\omega=A_\omega X_\omega,$$

where the matrix kernel X_ω satisfies linear matrix ODE as above, A_ω is a constant non-singular matrix, $\|A_\omega^{-1}\|\ll 1$ and $\boldsymbol{f}:\mathbb{R}\to\mathbb{R}^d$ is a smooth vector-valued function. Then, for $\omega\gg 1$,

$$I[\boldsymbol{f}]\sim-\sum_{m=1}^{\infty}(-A_\omega)^{-m}\big[X_\omega(b)\boldsymbol{f}^{(m-1)}(b)-X_\omega(a)\boldsymbol{f}^{(m-1)}(a)\big].$$

For $\psi=\max\{\|\boldsymbol{f}^{(s)}\|,\|\boldsymbol{f}^{(s+1)}\|\}$,

$$Q_s^A[\boldsymbol{f}]-I[\boldsymbol{f}]\sim\mathcal{O}(\|A_\omega^{-s-1}\|\|X_\omega\|\psi),\quad as\ \omega\to\infty.$$

If $X_\omega=\mathcal{O}(\hat{X}_\omega)$ and $\boldsymbol{f}=\mathcal{O}(\tilde{\boldsymbol{f}})$, then

$$Q_s^A[\boldsymbol{f}]-I[\boldsymbol{f}]=\mathrm{O}(A_\omega^{-s-1}\hat{X}_\omega\tilde{\boldsymbol{f}}),\quad as\ \omega\to\infty,$$

element wise.

Theorem 2 *Postulate that*

$$I[\boldsymbol{f}]=\int_a^b X_\omega(t)\boldsymbol{f}(t)\mathrm{d}t,\quad and\quad X'_\omega=A_\omega(t)X_\omega,$$

where A_ω is an arbitrary non-singular matrix, $\sigma(A_\omega)\subset i\mathbb{R}$, ω is a real parameter and $\boldsymbol{f}\in\mathbb{R}^d$ is a smooth vector-valued function.

If $\boldsymbol{F}_\omega=\mathcal{O}(\hat{\boldsymbol{F}})$, $B_\omega^{-1}=\mathcal{O}(\hat{B})$ and $\bar{\boldsymbol{X}}_\omega=\mathcal{O}(\hat{\boldsymbol{X}}_\omega)$, then

$$I[\boldsymbol{f}]-Q_s^A[\boldsymbol{f}]=(-1)^s\int_a^b\sigma_s(t)\bar{\boldsymbol{X}}_{\boldsymbol{\omega}}(t)\mathrm{d}t=\mathrm{O}(\hat{\boldsymbol{F}}\hat{B}^{s+1}\hat{\boldsymbol{X}}),\quad as\ \omega\to\infty.$$

Proof We first prove the identity by induction,

$$\begin{aligned}I[\boldsymbol{F}]&=\Big[\boldsymbol{F}(t)B_\omega^{-1}(t)\bar{\boldsymbol{X}}_\omega(t)\Big]_a^b-\int_a^b\Big(\boldsymbol{F}(t)B_\omega^{-1}(t)\Big)'\bar{\boldsymbol{X}}_\omega(t)\mathrm{d}t\\&=\Big[\sigma_0(t)B_\omega^{-1}(t)\bar{\boldsymbol{X}}_\omega(t)\Big]_a^b-\int_a^b\sigma_1(t)\bar{\boldsymbol{X}}_\omega(t)\mathrm{d}t.\end{aligned}$$

Suppose the identity holds for some $k\in\mathbb{N}$, we prove for $k+1$.

$$\begin{aligned}\int_a^b\sigma_{k+1}(t)\bar{\boldsymbol{X}}_\omega(t)\mathrm{d}t&=\int_a^b\sigma_{k+1}(t)B_\omega^{-1}(t)\bar{\boldsymbol{X}}'_\omega(t)\mathrm{d}t\\&=\Big[\sigma_{k+1}(t)B_\omega^{-1}(t)\bar{\boldsymbol{X}}_\omega(t)\Big]_a^b-\int_a^b\sigma_{k+2}(t)\bar{\boldsymbol{X}}_\omega(t)\mathrm{d}t.\end{aligned}$$

By induction, $\sigma_k = \mathcal{O}(\hat{\boldsymbol{F}}\hat{B}^k)$. Indeed, for $k=0$, $\sigma_0 = \boldsymbol{F} = \mathcal{O}(\hat{\boldsymbol{F}})$. We assume the equality holds for some σ_k, then

$$\begin{aligned}\sigma_{k+1} &= \left[\sigma_k B_\omega^{-1}\right]' = \sigma_k' B_\omega^{-1} + \sigma_k B_\omega^{-1'} \\ &= \mathcal{O}(\hat{\boldsymbol{F}}\hat{B}^k)\mathcal{O}(\hat{B}) + \mathcal{O}(\hat{\boldsymbol{F}}\hat{B}^k)\mathcal{O}(\hat{B}) = \mathcal{O}(\hat{\boldsymbol{F}}\hat{B}^{k+1}).\end{aligned}$$

And finally,

$$\begin{aligned}\int_a^b \sigma_s \bar{\boldsymbol{X}}_\omega \mathrm{d}t &= \left[\sigma_s B_\omega^{-1}\bar{\boldsymbol{X}}_\omega\right]_a^b - \int_a^b \sigma_{s+1}\bar{\boldsymbol{X}}_\omega \mathrm{d}t \\ &= \mathrm{O}(\hat{\boldsymbol{F}}\hat{B}^{s+1}\hat{\boldsymbol{X}}) + \mathrm{O}(\hat{\boldsymbol{F}}\hat{B}^{s+1}\hat{\boldsymbol{X}}) = \mathrm{O}(\hat{\boldsymbol{F}}\hat{B}^{s+1}\hat{\boldsymbol{X}}).\end{aligned}$$

□

Corollary 1 *If*

$$\boldsymbol{f}^{(k)}(a) = \boldsymbol{f}^{(k)}(b) = 0, \quad \textit{for } k = 0, 1, \ldots, s-1,$$

then,

$$I[\boldsymbol{f}] = \mathrm{O}(\hat{\boldsymbol{F}}\hat{B}^{s+1}\hat{\boldsymbol{X}}).$$

Example 2 For practical purposes consider integral

$$I_h[\boldsymbol{f}] = \int_0^h \mathrm{e}^{\Omega(h-\tau)}\boldsymbol{f}(\tau)\mathrm{d}\tau,$$

and recall that Ω is defined in (3). Note that,

$$\begin{aligned}\mathrm{e}^{\Omega(h-\tau)}\,|_{\tau=0} &= \mathrm{e}^{\Omega(h)} = X_\omega(h), \\ \mathrm{e}^{\Omega(h-\tau)}\,|_{\tau=h} &= \boldsymbol{I} = X_\omega(0).\end{aligned}$$

Once we vectorise the system to obtain the *asymptotic* method, $\bar{\boldsymbol{I}}$ stands for a vectorised identity matrix $\boldsymbol{I}$, and $\bar{\boldsymbol{X}}_\omega$ stands for a vectorised matrix e^{Ω}. For $s=2$ the *asymptotic* method using information at the end points only, is

$$\begin{aligned}Q_2^A = &[\boldsymbol{F}(h)B_\omega^{-1}(0) - \boldsymbol{F}'(h)B_\omega^{-2}(0) - \boldsymbol{F}(h)B_\omega^{-1'}(0)B_\omega^{-1}(0)]\bar{\boldsymbol{I}} \\ &-[\boldsymbol{F}(0)B_\omega^{-1}(h) - \boldsymbol{F}'(0)B_\omega^{-2}(h) - \boldsymbol{F}(0)B_\omega^{-1'}(h)B_\omega^{-1}(h)]\bar{\boldsymbol{X}}_\omega(h).\end{aligned}$$

Employing initial-value integrator,

$$\boldsymbol{y}_{n+1} = \mathrm{e}^{\Omega_s}\boldsymbol{y}_n + \int_0^h \mathrm{e}^{\Omega_s(h-\tau)}\boldsymbol{f}(t_n+\tau)\mathrm{d}\tau, \tag{6}$$

where Ω_s stands for a truncated *Magnus* expansion, we can now solve (2) with the *asymptotic* method,

$$\boldsymbol{y}_{n+1} = \mathrm{e}^{\Omega_s}\boldsymbol{y}_n + Q_s^A.$$

Lemma 2 *The asymptotic method Q_s^A, applied to a family of integrals $I[\boldsymbol{f}]$ in (4), is independent of the step-size of numerical integration.*

Proof Let us assume the opposite and introduce a mesh with n node points and a step-size of integration h, $t_n = t_{n-1} + h$. Now the *asymptotic method*, a truncated asymptotic sum, is

$$\begin{aligned} Q_s^A[\boldsymbol{f}] &= Q_s^A[\boldsymbol{f}](t_1) - Q_s^A[\boldsymbol{f}](t_0) + Q_s^A[\boldsymbol{f}](t_2) - Q_s^A[\boldsymbol{f}](t_1) \\ &\quad + Q_s^A[\boldsymbol{f}](t_3) - Q_s^A[\boldsymbol{f}](t_2) + \cdots \\ &\quad + Q_s^A[\boldsymbol{f}](t_{n-1}) - Q_s^A[\boldsymbol{f}](t_{n-2}) + Q_s^A[\boldsymbol{f}](t_n) - Q_s^A[\boldsymbol{f}](t_{n-1}) \\ &= Q_s^A[\boldsymbol{f}](t_n) - Q_s^A[\boldsymbol{f}](t_0). \end{aligned}$$

The summands of the *asymptotic method* Q_s^A, evaluated at node points, appear in pairs with an opposite sign, except the values at the end points. Consequently, no matter how we truncate the interval, we obtain the same representation for the *asymptotic method* Q_s^A evaluated at the end points only. □

4 The Filon-type method

Employing classical *Filon*-type quadrature [17], proven to have high accuracy for increasing ω, we construct an r-degree polynomial interpolation $\boldsymbol{v}$ for the vector-valued function $\boldsymbol{f}$ in (5),

$$\boldsymbol{v}(t) = \sum_{l=1}^{\nu} \sum_{j=0}^{\theta_l - 1} \alpha_{l,j}(t) \boldsymbol{f}^{(j)}(t_l),$$

which agrees with function values and derivatives $\boldsymbol{v}^{(j)}(t_l) = \boldsymbol{f}^{(j)}(t_l)$ at node points $a = t_1 < t_2 < \cdots < t_\nu = b$, with associated $\theta_1, \theta_2, \ldots, \theta_\nu$ multiplicities, $j = 0, 1, \ldots, \theta_l - 1$, and $l = 1, 2, \ldots, \nu$.

By definition, *Filon*-type method is

$$Q_s^F[\boldsymbol{f}] = \int_a^b X_\omega(t) \boldsymbol{v}(t) \mathrm{d}t = \sum_{l=1}^{\nu} \sum_{j=0}^{\theta_l - 1} \beta_{l,j} \boldsymbol{f}^{(j)}(t_l),$$

where $\beta_{l,j} = \int_a^b X_\omega(t) \alpha_{l,j}(t) \mathrm{d}t$.

Theorem 3 *Postulate that*

$$I[\boldsymbol{f}] = \int_a^b X_\omega(t) \boldsymbol{f}(t) \mathrm{d}t, \quad \textit{and} \quad X'_\omega = A_\omega(t) X_\omega.$$

A_ω is an arbitrary non-singular matrix, $\sigma(A_\omega) \subset i\mathbb{R}$, ω is a real parameter and $\boldsymbol{f} \in \mathbb{R}^d$ is a smooth vector-valued function.

If $\boldsymbol{F}_\omega = \mathcal{O}(\hat{\boldsymbol{F}})$, $B_\omega^{-1} = \mathcal{O}(\hat{B})$ *and* $\bar{\boldsymbol{X}}_\omega = \mathrm{O}(\hat{\boldsymbol{X}}_\omega)$, *then*

$$I[\boldsymbol{f}] - Q_s^F[\boldsymbol{f}] = (-1)^s \int_a^b \sigma_s(t)\bar{\boldsymbol{X}}_{\boldsymbol{\omega}}(t)\mathrm{d}t$$
$$= \mathrm{O}(\hat{\boldsymbol{F}}\hat{B}^{s+1}\hat{\boldsymbol{X}}), \quad \text{as } \omega \to \infty.$$

Proof Observing that $I[\boldsymbol{f}-\boldsymbol{v}] = I[\boldsymbol{f}] - Q_s^F[\boldsymbol{f}]$, the proof follows by replacing $\boldsymbol{f}$ in the *asymptotic* method (2) by $\boldsymbol{f}-\boldsymbol{v}$ and the fact that $[\boldsymbol{f}-\boldsymbol{v}]^{(j)}(a) = [\boldsymbol{f}-\boldsymbol{v}]^{(j)}(b) = 0$, for $j = 0, 1, \ldots, s-1$. □

Theorem 4 *Let* $\theta_1, \theta_v \geq s$, $r = \sum_{l=1}^{v}\theta_l - 1$. *Then* r *is the numerical order of the Filon-type method applied to the linear systems* (6),

$$\boldsymbol{y}(t_n) - \boldsymbol{y}_n = \mathcal{O}(h^{r+1}).$$

Proof The proof is equivalent to that in Theorem 3.3, [19].

We present $\boldsymbol{f}$ as a sum of a polynomial approximation and the error of the approximation,

$$\boldsymbol{f} = \boldsymbol{v} + \boldsymbol{p},$$

where $\boldsymbol{v}$ is an r-degree vector-valued polynomial approximation (e.g. Hermite, [16, 31]) to $\boldsymbol{f}$, and $\boldsymbol{p}$ is an approximation error

$$\boldsymbol{p} = \frac{p_r}{r!}\boldsymbol{f}^{(r)}(\xi), \quad p_r = \prod_{l=1}^{v}(t-t_l)^{\theta_l}.$$

For the local error of our numerical solver,

$$I[\boldsymbol{p}] = \int_0^h \mathrm{e}^{\Omega}\boldsymbol{p}(t_n+\tau)\mathrm{d}\tau = \int_0^h \mathrm{e}^{\Omega}\frac{p_r(\tau)}{r!}\boldsymbol{f}^{(r)}(\xi)\mathrm{d}\tau,$$

where $p_r(\tau) = \mathcal{O}(\tau^r)$.

Since integral is a linear operator, the statement $\boldsymbol{f} = \boldsymbol{v} + \boldsymbol{p}$ implies $I[\boldsymbol{f}] = I[\boldsymbol{v}] + I[\boldsymbol{p}]$, hence

$$I[\boldsymbol{p}] = I[\boldsymbol{f}] - I[\boldsymbol{v}] = I[\boldsymbol{f}] - Q_s^F[\boldsymbol{f}] = \mathcal{O}(h^{r+1}), \tag{7}$$

which proves the order of the *Filon*-type method. □

For the *Filon*-type method Q_s^F,

$$Q_s^F[\boldsymbol{f}] = \int_a^b \mathrm{e}^{\Omega_s}(t)\boldsymbol{v}(t)\mathrm{d}t = \sum_{l=1}^{v}\sum_{j=0}^{\theta_l-1}\beta_{l,j}\boldsymbol{f}^{(j)}(t_l),$$

where $\beta_{l,j} = \int_a^b \mathrm{e}^{\Omega_s}(t)\alpha_{l,j}(t)\mathrm{d}t$, and

$$I[\boldsymbol{f}] = \int_0^h \mathrm{e}^{\Omega_s} f(t_n+\tau)\mathrm{d}\tau.$$

Example 3 We consider an *Airy*-type second order linear ODE $y''(t) = -\omega t y(t) - \cos(t)$, with a real parameter $\omega \gg 1$ and $t \geq 0$. The equation can be rewritten in a vector form,

$$\boldsymbol{y}'(t) = A_\omega(t)\boldsymbol{y}(t) + \boldsymbol{f}(t),$$

where

$$A_\omega = \begin{pmatrix} 0 & 1 \\ -\omega t & 0 \end{pmatrix} \quad \text{and} \quad \boldsymbol{f}(t) = \begin{bmatrix} 0 \\ -\cos(t) \end{bmatrix}.$$

Note, that matrix A_ω has pure imaginary spectrum and belongs to a *Lie* algebra g, and the fundamental matrix of this system belongs to a matricial *Lie* group $\mathcal{G}$. Once we employ a time-step integrator for this system,

$$\boldsymbol{y}_{n+1} = \mathrm{e}^{\Omega_s(h)}\boldsymbol{y}_n + \int_0^h \mathrm{e}^{\Omega_s(h-\tau)}\boldsymbol{f}(\tau)\mathrm{d}\tau,$$

we can now solve this system with the *Filon*-type method Q_s^F. Here, Ω_s stands for the truncated Magnus expansion with nested integral commutators of the matrix A_ω.

The following scheme describes numerical approximation of systems of highly oscillatory ODEs (6), solved with the *Filon*-type method Q_s^F,

$$\boldsymbol{y}_{n+1} = \mathrm{e}^{\Omega_s}\boldsymbol{y}_n + Q_s^F[f].$$

In Figs. 1 and 2 we present numerical results for the *Filon*-type method Q_2^F employing end-points only and multiplicities all 2. We consider a second order ODE $y''(t) = -t\omega y(t) - \cos(t)$, with $0 \leq t \leq 1000$, $[0, 1]^\intercal$ initial condition and step-size $h = \frac{1}{4}$ and $h = \frac{1}{100}$, see Example 3. Figure 1 illustrates that for a fixed step-size $h = \frac{1}{4}$ and growing values of $\omega = 10$, $\omega = 10^2$ and $\omega = 10^3$ the approximation improves as the frequency of oscillation grows, the error decays from 10^{-5}, 10^{-6} to 10^{-7} respectively.

In Fig. 2 we consider a fixed step-size $h = \frac{1}{100}$ and large values of $\omega = 10^4$, $\omega = 10^5$ and $\omega = 10^6$. For a fixed step-size the accuracy of approximation improves with an increase in frequency, the error improves from 10^{-12}, 10^{-13} to 10^{-14} respectively. For the reference we have computed nested integral commutators exactly.

5 The WRF method

In Sects. 3 and 4 we have developed powerful tools for solving highly oscillatory linear systems of ODEs. It is natural to ask yourself if one can extend those methods for solving non-linear systems with similar assumption,

$$\boldsymbol{y}'(t) = A_\omega(t)\boldsymbol{y}(t) + \boldsymbol{f}(t, \boldsymbol{y}(t)), \qquad \boldsymbol{y}(0) = \boldsymbol{y}_0 \in \mathbb{R}^d, \quad t \geq 0, \tag{8}$$

where the matrix A_ω is time dependant and has large imaginary eigenvalues, $\sigma(A_\omega) \subset i\mathbb{R}$, $\|A_\omega\| \gg 1$, $\|A_\omega^{-1}\| \ll 1$, $\boldsymbol{f} : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$ is a smooth vector-valued function and $\omega \gg 1$ is a real parameter.

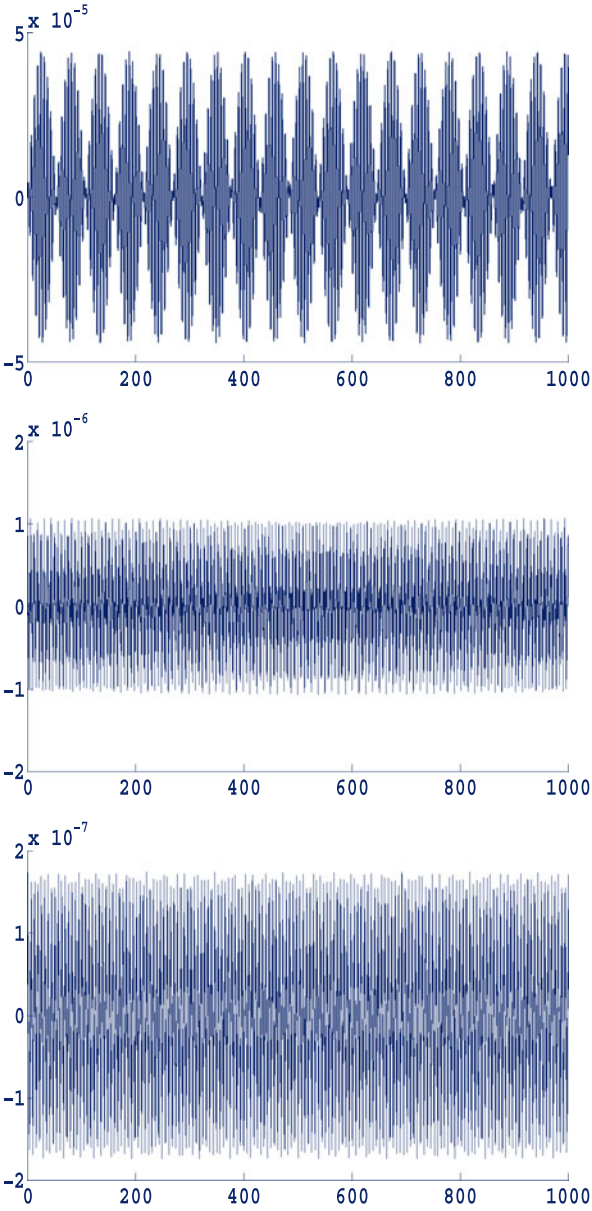

Fig. 1 Global error of the *Filon*-type method Q_2^F with end points only and multiplicities all 2, for the equation $y''(t) = -\omega t y(t) - \cos(t)$, $0 \le t \le 1000$, with $[0, 1]^\intercal$ initial condition, step-size $h = \frac{1}{4}$ for $\omega = 10$ (*first figure from the top*), $\omega = 10^2$ (*second figure from the top*), $\omega = 10^3$ (*third figure from the top*)

In this section we present iterative techniques, namely, waveform relaxation algorithms, for solving non-linear ordinary differential equations with associated initial conditions,

$$\frac{\mathrm{d}}{\mathrm{d}t} z(t) = f(t, z), \qquad z(0) = z_0, \quad t \in [0, T],$$

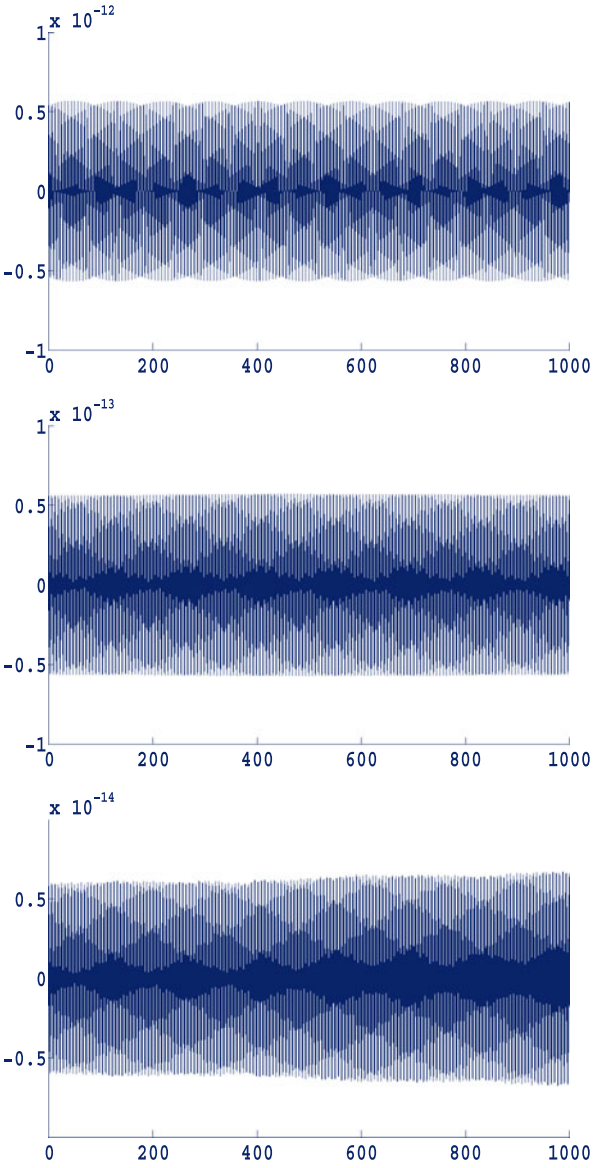

Fig. 2 Global error of the *Filon*-type method Q_2^F with end points only and multiplicities all 2, for the equation $y''(t) = -\omega t\, y(t) - \cos(t)$, $0 \le t \le 100$, with $[0, 1]^\intercal$ initial condition, step-size $h = \frac{1}{100}$ for $\omega = 10^4$ (*first figure from the top*), $\omega = 10^5$ (*second figure from the top*), $\omega = 10^6$ (*third figure from the top*)

where $T \ge 0$, $f : [0, T] \times \mathbb{R}^n \to \mathbb{R}^n$, $\boldsymbol{z}_0 = [z_{1,0}, z_{2,0}, \ldots, z_{n,0}] \in \mathbb{R}^n$ is the vector of initial values, and $\boldsymbol{z}(t) = [z_1(t), z_2(t), \ldots, z_n(t)] \in \mathbb{R}^n$ is the solution vector.

Let us define waveform relaxation operator $\mathcal{F}$, mapping "old" iterate into a new one, [32],

$$\boldsymbol{z}^{[\nu]} = \mathcal{F}(\boldsymbol{z}^{[\nu-1]}).$$

A "one-step" iteration method can be written as,

$$\frac{\mathrm{d}}{\mathrm{d}t}z^{[\nu]} = \mathcal{F}(z^{[\nu-1]}, z^{[\nu]}), \qquad z^{[\nu]}(0) = z_0,$$

where $\mathcal{F}(u, v)$ is defined so, that $\mathcal{F}(t, v, v) = f(t, v)$. The well known Picard iteration, as well as Jacobi and Gauss-Seidel schemes can be written in the formulae,

$$\begin{aligned}
\mathcal{F}_i(t, u, v) &= f_i(t, u_1, u_2, \ldots, u_i, \ldots, u_n) \quad \text{(Picard)},\\
\mathcal{F}_i(t, u, v) &= f_i(t, u_1, u_2, \ldots, u_{i-1}, v_i, u_{i+1}, \ldots, u_n) \quad \text{(Jacobi)},\\
\mathcal{F}_i(t, u, v) &= f_i(t, v_1, v_2, \ldots, v_{i-1}, v_i, u_{i+1}, \ldots, u_n) \quad \text{(Gauss-Seidel)}.
\end{aligned}$$

The convergence of sequences $\{z^{[\nu]}\}_{\nu=0}^{\infty}$ is analysed in the context of *Banach* spaces, namely, completed, normed, linear spaces. We consider continuous vector-valued functions defined on $[0, T]$, i.e. $C([0, T]; \mathbb{R}^n)$, with maximum of the norm,

$$\|z\|_T = \max_{t\in[0,T]} \|z(t)\|,$$

and a vector norm $\|\cdot\|$ in $\mathbb{R}^n$.

Waveform relaxation methods have been studied by a number of authors, we list here some of them, [1, 7, 10, 11, 18–21, 23, 24, 26–28, 32, 33].

Definition 4 [12] Let $(\mathcal{X}, \|\cdot\|_{\mathcal{X}})$ be a normed linear space and the associated norm. An operator $\mathcal{U} : \mathcal{X} \to \mathcal{X}$ is called a contraction if there exists a γ, with $0 \le \gamma < 1$, such that for all $x, y \in \mathcal{X}$ it is true that

$$\|\mathcal{U}(x) - \mathcal{U}(y)\| \le \gamma \|x - y\|_{\mathcal{X}}.$$

Theorem 5 (Banach Fixed Point Theorem, [12]) *Let $\mathcal{X}$ be a Banach space and $\mathcal{U}$ a contraction. Then there is a unique $x^\star \in \mathcal{X}$, such that $\mathcal{U}(x^\star) = x^\star$. Moreover, if $x^{[0]}$ is any point in $\mathcal{X}$, and we define the sequence $\{x^{[\nu]}\}_{\nu=0}^{\infty}$ by $x^{[1]} = \mathcal{U}(x^{[1]})$, then $x^{[\nu]} \to x^\star$ as $\nu \to \infty$.*

Classical theory states that fixed point iterative methods are convergent. These include Picard iteration, Jacobi and Gauss-Seidel waveform relaxation methods, as well as Newton's method and Runge-Kutta method.

To prove convergence of the waveform relaxation schemes applied to (8), we introduce an exponentially scaled norm,

$$\|z\|_b = \max_{t\in[0,T]} \mathrm{e}^{-bt} \|z(t)\|,$$

for some $b > 0$, so that for sufficiently large b and any element $z(t)$ of the space it is true that $\|z(t)\|_\infty \le \|z(t)\|_b$, for all $t \in [0, T]$. It was proved in [32] that the iteration is contraction for the derivatives of the iterate:

$$\left\| \frac{\mathrm{d}}{\mathrm{d}t}z^{[n+1]} - \frac{\mathrm{d}}{\mathrm{d}t}z^{[k+1]} \right\|_b \le \gamma \left\| \frac{\mathrm{d}}{\mathrm{d}t}z^{[n]} - \frac{d}{dt}z^{[k]} \right\|_b, \quad \gamma \le 1.$$

Theorem 6 [32] *Suppose $f(t,z)$ is continuous on $D=[0,T]\times R^d$, and satisfies a Lipschitz condition, that is, $\|f(t,y)-f(t,z)\|\le L\|y-z\|$, for all $(t,y),(t,z)\in D$ and for some positive constant L. Then, the Jacobi and Gauss-Seidel waveform relaxation converge.*

The Lipschitz condition on $\boldsymbol{f}(t,\boldsymbol{y}(t))$ induces a Lipschitz condition on $\mathcal{F}(t,u,v)$, namely, there exist positive constants l_1 and l_2 such that for all $u_1,u_2,v_1,v_2\in\mathbb{R}^d$, $t\in[0,T]$,

$$\|\mathcal{F}(t,u_1,v_1)-\mathcal{F}(t,u_2,v_2)\|\le l_1\|u_1-u_2\|+l_2\|v_1-v_2\|.$$

Theorem 7 *Suppose that $\boldsymbol{f}(t,\boldsymbol{y}(t))$ is continuous and satisfies Lipschitz conditions on $D=[0,T]\times R^d$, and $\mathcal{F}$ is a waveform relaxation operator*

$$\boldsymbol{y}^{[\nu+1]}=\mathcal{F}(\boldsymbol{y}^{[\nu]}),\qquad \boldsymbol{y}^{[0]}=\boldsymbol{y}_0,$$

applied to a non-linear system (2),

$$\boldsymbol{y}^{[\nu+1]}(t)=X(t)\boldsymbol{y_0}+\int_{t_0}^{t}X(t-\tau)\boldsymbol{f}(\tau,\boldsymbol{y}^{[\nu]}(\tau))\mathrm{d}\tau.$$

Then, the Picard, Jacobi and Gauss-Seidel waveform relaxation methods applied to the system of non-linear ODEs in (1) *converge.*

Proof One step iteration of a continuous function $\boldsymbol{y}$ with a waveform relaxation method returns, $\boldsymbol{y}^{[1]}:=\mathcal{F}(\boldsymbol{y})$,

$$\boldsymbol{y}^{[1]}(t)=X(t)\boldsymbol{y}_0+\int_{t_0}^{t}X(t-\tau)\mathcal{F}(\tau,\boldsymbol{y}(\tau),\boldsymbol{y}^{[1]}(\tau))\mathrm{d}\tau.$$

First we prove that $\mathcal{F}$ is a contraction. We introduce a second continuous function $\boldsymbol{z}$, such that $\boldsymbol{z}(0)=\boldsymbol{y}_0$, and similarly, one-step iteration results in,

$$\boldsymbol{z}^{[1]}(t)=X(t)\boldsymbol{y}_0+\int_{t_0}^{t}X(t-\tau)\mathcal{F}(\tau,\boldsymbol{z}(\tau),\boldsymbol{z}^{[1]}(\tau))\mathrm{d}\tau.$$

Consider the difference,

$$\begin{aligned}\|\boldsymbol{y}^{[1]}(t)-\boldsymbol{z}^{[1]}(t)\|\le\int_0^t\|X(t-\tau)(\mathcal{F}(\tau,\boldsymbol{y}(\tau),\boldsymbol{y}^{[1]}(\tau))\\-\mathcal{F}(\tau,\boldsymbol{z}(\tau),\boldsymbol{z}^{[1]}(\tau)))\|\mathrm{d}\tau.\end{aligned}$$

There exist positive constants l_1,l_2, such that for all $t\in[0,T]$ it is true that,

$$\begin{aligned}\|\boldsymbol{y}^{[1]}(t)-\boldsymbol{z}^{[1]}(t)\|\le\max_{t\in[0,T]}\|X(t)\|\Big[l_1\int_0^t\|\boldsymbol{y}(\tau)-\boldsymbol{z}(\tau)\|\mathrm{d}\tau\\+l_2\int_0^t\|\boldsymbol{y}^{[1]}(\tau)-\boldsymbol{z}^{[1]}(\tau)\|\mathrm{d}\tau\Big].\end{aligned}$$

We multiply both sides by e^{-bt} and maximise over $[0, T]$,

$$\max_{t\in[0,T]} \mathrm{e}^{-bt}\|\bar{\boldsymbol{y}}(t)-\bar{\boldsymbol{z}}(t)\| \le \max_{t\in[0,T]} \mathrm{e}^{-bt}\|X(t)\|_\infty \times \left[l_1 \int_0^t \mathrm{e}^{b\tau} \max_{s\in[0,T]} \mathrm{e}^{-bs}\|\boldsymbol{y}(s)-\boldsymbol{z}(s)\|\mathrm{d}\tau + l_2 \int_0^t \mathrm{e}^{b\tau} \max_{s\in[0,T]} \mathrm{e}^{-bs}\|\bar{\boldsymbol{y}}(s)-\bar{\boldsymbol{z}}(s)\|\mathrm{d}\tau \right].$$

It is easy to notice that,

$$\max_{t\in[0,T]} \mathrm{e}^{-bt} \int_0^t \mathrm{e}^{b\tau}\mathrm{d}\tau \le 1/b,$$

and since $X(t)$ is continuous, hence it is bounded over the finite interval $[0, T]$. Therefore, using *b-norm* notation we can write,

$$\|\boldsymbol{y}^{[1]}-\boldsymbol{z}^{[1]}\|_b \le c\frac{l_1}{b}\|\boldsymbol{y}-\boldsymbol{z}\|_b + c\frac{l_2}{b}\|\boldsymbol{y}^{[1]}-\boldsymbol{z}^{[1]}\|_b.$$

Thus, for sufficiently large b we have,

$$\|\boldsymbol{y}^{[1]}-\boldsymbol{z}^{[1]}\|_b \le \gamma\|\boldsymbol{y}-\boldsymbol{z}\|_b, \quad \gamma = c\frac{l_1/b}{1/c-l_2/b} < 1,$$

which proves that $\mathcal{F}$ is a contraction mapping. □

From step to step, the error of approximation with a waveform relaxation method decreases, when measured in *b-norm*. Indeed,

$$\|\boldsymbol{y}^{[\nu]}-\boldsymbol{y}\|_b \le \gamma\|\boldsymbol{y}^{[\nu-1]}-\boldsymbol{y}\|_b, \quad \text{for some } 0\le\gamma<1 \text{ and } b>0.$$

Definition 5 [32] A differential system is said to have a strict WR contractivity property on $[0, T]$, if the waveform relaxation algorithm applied to the system contracts in the maximum norm on $[0, T]$,

$$\|z^{[\nu+1]}-z^{[\nu]}\|_T \le \gamma\|z^{[\nu]}-z^{[\nu-1]}\|_T, \quad \gamma<1,\ \nu\ge 1. \tag{9}$$

Theorem 8 *For a non-linear ODEs* (4)*, which satisfy the assumptions of the Banach fixed point Theorem* 5*, there exist a* $T > 0$ *such that the system has the strict WR contractivity property on* $[0, T]$.

Proof Let $\boldsymbol{y} = \boldsymbol{y}^{[\nu]}$ and $\boldsymbol{z} = \boldsymbol{y}^{[\nu-1]}$, then

$$\|\boldsymbol{y}^{[\nu+1]}(t)-\boldsymbol{y}^{[\nu]}(t)\| \le l_1\int_0^t \|\boldsymbol{y}^{[\nu]}(s)-\boldsymbol{y}^{[\nu-1]}(s)\|\mathrm{d}s + l_2\int_0^t \|\boldsymbol{y}^{[\nu+1]}(s)-\boldsymbol{y}^{[\nu]}(s)\|\mathrm{d}s.$$

Maximising over the interval $[0, T]$

$$\|\boldsymbol{y}^{[\nu+1]} - \boldsymbol{y}^{[\nu]}\|_T \le l_1 T \|\boldsymbol{y}^{[\nu]} - \boldsymbol{y}^{[\nu-1]}\|_T + l_2 T \|\boldsymbol{y}^{[\nu+1]} - \boldsymbol{y}^{[\nu]}\|_T$$

for sufficiently small T we get

$$\|\boldsymbol{y}^{[\nu+1]} - \boldsymbol{y}^{[\nu]}\|_T \le \gamma \|\boldsymbol{y}^{[\nu]} - \boldsymbol{y}^{[\nu-1]}\|_T, \quad \text{with } \gamma = \frac{l_1 T}{1 - l_2 T} < 1. \qquad \square$$

In approximation of highly oscillatory non-linear systems of ODEs we use the implicit representation of the solution (2) and the initial value integrator

$$\boldsymbol{y}_{n+1} = \mathrm{e}^{\Omega(h)} \boldsymbol{y}_n + \int_0^h \mathrm{e}^{\Omega(h-\tau)} \boldsymbol{f}(t_n + \tau, \boldsymbol{y}(t_n + \tau)) \mathrm{d}\tau.$$

A classical waveform relaxation algorithm applied to (2), is

$$\begin{aligned}
\boldsymbol{y}_{n+1}^{[0]} &= \boldsymbol{y}_n^{[s]}, \\
\boldsymbol{y}_{n+1}^{[1]} &= \mathrm{e}^{\Omega(h)} \boldsymbol{y}_n^{[s]} + \int_0^h \mathrm{e}^{\Omega(h-\tau)} \boldsymbol{f}(t_n + \tau, \boldsymbol{y}_{n+1}^{[0]}) \mathrm{d}\tau, \\
&\vdots \\
\boldsymbol{y}_{n+1}^{[s]} &= \mathrm{e}^{\Omega(h)} \boldsymbol{y}_n^{[s]} + \int_0^h \mathrm{e}^{\Omega(h-\tau)} \boldsymbol{f}(t_n + \tau, \boldsymbol{y}_{n+1}^{[s-1]}(t_n + \tau)) \mathrm{d}\tau.
\end{aligned}$$

Employing the *Filon*-type method, we develop the *WRF* method, iterating system (2) at each step and discretizing integral $I[\boldsymbol{f}]$, with the *Filon* quadrature,

$$I[\boldsymbol{f}] = \int_a^b X_\omega(t) \boldsymbol{f}(t, \boldsymbol{y}(t)) \mathrm{d}t, \quad \text{where } X'_\omega = A_\omega X_\omega \text{ and } \|A_\omega^{-1}\| \ll 1.$$

Formally, the asymptotic expansion for the integral $I[\boldsymbol{f}]$ has the following representation,

$$I[\boldsymbol{f}] \sim \sum_{k=0}^{\infty} (-1)^k \left(\sigma_k(b) B_\omega^{-1}(b) \bar{\boldsymbol{X}}_\omega(b) - \sigma_k(a) B_\omega^{-1}(a) \bar{\boldsymbol{X}}_\omega(a) \right). \tag{10}$$

For the notation on matrix asymptotics we refer to Sect. 3. For non-linear systems, the representation for the matrix $\boldsymbol{F}$ is more complex, it will depend on the entries of the vector-valued function $\boldsymbol{f}(t, \boldsymbol{y}(t))$. It follows from Theorem 2, that if $\boldsymbol{F}_\omega = \mathcal{O}(\hat{\boldsymbol{F}})$, $B_\omega^{-1} = \mathcal{O}(\hat{B})$ and $\bar{\boldsymbol{X}}_\omega = \mathcal{O}(\hat{\boldsymbol{X}}_\omega)$, then

$$\begin{aligned}
I[\boldsymbol{f}] - Q_s^A[\boldsymbol{f}] &= (-1)^s \int_a^b \sigma_s(t) \bar{\boldsymbol{X}}_{\boldsymbol{\omega}}(t) \mathrm{d}t \\
&= \mathrm{O}(\hat{\boldsymbol{F}} \hat{B}^{s+1} \hat{\boldsymbol{X}}), \quad \text{as } \omega \to \infty.
\end{aligned}$$

The error of approximation depends on the inverse powers of the matrix B_ω, consequently on the inverse powers of the matrix A_ω and its eigenvalues, therefore on inverse powers of the frequency of oscillation. Note that the solution $\boldsymbol{y}$ is oscillatory, hence the function $\boldsymbol{f}(t, \boldsymbol{y})$ is also likely to be oscillatory. Therefore, for efficiency, we discretize $I[\boldsymbol{f}]$ according the *Filon* quadrature, choosing a vector-valued polynomial (e.g. Hermite), which agrees with our function values and its derivatives $\boldsymbol{f}^{(m)}$ at the node points.

The *WRF* method iterates $\boldsymbol{y}$ in (2) with a *waveform* method, solving $I[\boldsymbol{f}]$ at each step with *Filon* quadrature,

$$\begin{aligned}
\boldsymbol{y}_{n+1}^{[0]} &= \boldsymbol{y}_n^{[s]}, \\
\boldsymbol{y}_{n+1}^{[1]} &= \mathrm{e}^{A_\omega h}\boldsymbol{y}_n^{[s]} + \int_0^h \mathrm{e}^{(h-\tau)A_\omega}\boldsymbol{f}(t_n+\tau, \boldsymbol{y}_{n+1}^{[0]})\mathrm{d}\tau, \\
&\vdots \\
\boldsymbol{y}_{n+1}^{[s]} &= \mathrm{e}^{A_\omega h}\boldsymbol{y}_n^{[s]} + \int_0^h \mathrm{e}^{A_\omega(h-\tau)}\boldsymbol{v}(t_n+\tau, \boldsymbol{y}_{n+1}^{[s-1]}(t_n+\tau))\mathrm{d}\tau,
\end{aligned}$$

where $\boldsymbol{v}$ is a polynomial approximation to $\boldsymbol{f}$. The method takes the initial value $\boldsymbol{y}_{n+1}^{[0]}$ at a first step of iteration to obtain the first value of $\boldsymbol{y}_{n+1}^{[1]}$. Having values at two endpoints we can now evaluate the derivatives at those points and construct a polynomial, which agrees with function values and derivatives at the end points. *WRF* method employs end points only, otherwise adding internal points would have led to increasingly fine discretization of the interval. Computational cost of the *WRF* method is comparable to that of the *Filon*-type method. Having precomputed the vector-valued moments, all that remains are only some linear algebra operations.

Theorem 9 [19] *Suppose that r is the numerical order of a waveform relaxation method and s is the numerical order of the quadrature discretization applied to a non-linear system of ODEs*

$$\boldsymbol{y}' = A\boldsymbol{y} + \boldsymbol{f}(t, \boldsymbol{y}), \qquad \boldsymbol{y}(t_0) = \boldsymbol{y}_0, \quad t \geq 0,$$

of arbitrary matrix A and $\boldsymbol{f} : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$ satisfying the Lipschitz condition. Then,

$$\boldsymbol{y}(h) - \boldsymbol{y}_h = \mathcal{O}(h^{q+1}),$$

where $q = \min\{r, s\}$.

Corollary 2 [19] *The numerical order of the WRF method is the minimum of the Filon quadrature and the waveform method applied to solve non-linear system* (2).

Thus, once we have chosen the quadrature rule of a given order, we iterate the equation until obtaining the order of the of the quadrature and further iteration is pointless. In the upcoming paper we will have more discussion regarding the *WRF* method.

Acknowledgement The author wishes to thank her supervisor A. Iserles, D. Levin, O. Nevanlinna, S. Olver and Cambridge Overseas Trusts, University of Cambridge.

References

1. Bellen, A., Zennaro, M.: The use of Runge-Kutta formulae in waveform relaxation methods. Appl. Numer. Math. **11**(1–3), 95–114 (1993)
2. Blanes, S., Moan, P.C.: Fourth- and sixth-order commutator-free Magnus integrators for linear and non-linear dynamical systems. Appl. Numer. Math. **56**(12), 1519–1537 (2006)
3. Blanes, S., Casas, F., Ros, J.: Improved high order integrators based on the Magnus expansion. BIT Numer. Math. **40**(3), 434–450 (2000)
4. Blanes, S., Casas, F., Ros, J.: High order optimized geometric integrators for linear differential equations. BIT Numer. Math. **42**(2), 262–284 (2002)
5. Blanes, S., Casas, F., Oteo, J.A., Ros, J.: The Magnus expansion and some of its applications. Phys. Rep. **470**(5–6), 151–238 (2009)
6. Boyce, W.E., DiPrima, R.C.: Elementary Differential Equations and Boundary Value Problems. Wiley, New York (1965)
7. Burrage, K.: Parallel and Sequential Methods for Ordinary Differential Equations. Numerical Mathematics and Scientific Computation. Clarendon, Oxford University Press, New York (1995)
8. Casas, F.: Sufficient conditions for the convergence of the Magnus expansion. J. Phys. A **40**(50), 15001–15017 (2007)
9. Casas, F., Iserles, A.: Explicit Magnus expansions for nonlinear equations. J. Phys. A **39**(19), 5445–5461 (2006)
10. Condon, M., Deaño, A., Iserles, A., Maczyński, K., Xu, T.: On numerical methods for highly oscillatory problems in circuit simulation. Compel **28**(6), 1607–1618 (2009)
11. Gander, M.J., Vandewalle, S.: Analysis of the parareal time-parallel time-integration method. SIAM J. Sci. Comput. **29**(2), 556–578 (2007) (electronic)
12. Granas, A., Dugundji, J.: Fixed Point Theory. Springer, New York (2003)
13. Hochbruck, M., Lubich, C.: On Magnus integrators for time-dependent Schrödinger equations. SIAM J. Numer. Anal. **41**(3), 945–963 (2003)
14. Hochbruck, M., Ostermann, A.: Exponential integrators. Acta Numer. **19**, 209–286 (2010)
15. Iserles, A.: On the global error of discretization methods for highly-oscillatory ordinary differential equations. BIT Numer. Math. **42**(3), 561–599 (2002)
16. Iserles, A.: A First Course in the Numerical Analysis of Differential Equations, 2nd edn. Cambridge Texts in Applied Mathematics. Cambridge University Press, Cambridge (2009)
17. Iserles, A., Nørsett, S.P.: Efficient quadrature of highly oscillatory integrals using derivatives. Proc. R. Soc., Math. Phys. Eng. Sci. **461**(2057), 1383–1399 (2005)
18. Jackiewicz, Z., Owren, B., Welfert, B.: Pseudospectra of waveform relaxation operators. Comput. Math. Appl. **36**(8), 67–85 (1998)
19. Khanamiryan, M.: Quadrature methods for highly oscillatory linear and nonlinear systems of ordinary differential equations. I. BIT Numer. Math. **48**(4), 743–761 (2008)
20. Lelarasmee, E.: The waveform relaxation method for time domain analysis of large scale integrated circuits: theory and applications. Ph.D. thesis, EECS Department, University of California, Berkeley (1982)
21. Lubich, C., Ostermann, A.: Multigrid dynamic iteration for parabolic equations. BIT Numer. Math. **27**(2), 216–234 (1987)
22. Magnus, W.: On the exponential solution of differential equations for a linear operator. Commun. Pure Appl. Math. **7**, 649–673 (1954)
23. Miekkala, U., Nevanlinna, O.: Convergence of dynamic iteration methods for initial value problem. SIAM J. Sci. Stat. Comput. **8**(4), 459–482 (1987)
24. Miekkala, U., Nevanlinna, O.: Iterative solution of systems of linear differential equations. Acta Numer. **5**, 259–307 (1996)
25. Moan, P.C., Niesen, J.: Convergence of the Magnus series. Found. Comput. Math. **8**(3), 291–301 (2008)
26. Nevanlinna, O.: A note on Picard-Lindelöf iteration. In: Numerical Methods for Ordinary Differential Equations, L'Aquila, 1987. Lecture Notes in Math., vol. 1386, pp. 97–102. Springer, Berlin (1989). doi:10.1007/BFb0089233

27. Nevanlinna, O.: Remarks on Picard-Lindelöf iteration. I. BIT Numer. Math. **29**(2), 328–346 (1989)
28. Nevanlinna, O.: Remarks on Picard-Lindelöf iteration. II. BIT Numer. Math. **29**(3), 535–562 (1989)
29. Olver, S.: Numerical approximation of vector-valued highly oscillatory integrals. BIT Numer. Math. **47**(3), 637–655 (2007)
30. Oteo, J.A., Ros, J.: The Magnus expansion for classical Hamiltonian systems. J. Phys. A **24**(24), 5751–5762 (1991). http://stacks.iop.org/0305-4470/24/5751
31. Ralston, A., Rabinowitz, P.: A First Course in Numerical Analysis, 2nd edn. Dover, New York (2001)
32. Vandewalle, S.: Parallel Multigrid Waveform Relaxation for Parabolic Problems. Teubner Skripten zur Numerik [Teubner Scripts on Numerical Mathematics]. Teubner, Stuttgart (1993)
33. White, J., Odeh, F., Sangiovanni-Vincentelli, A.L., Ruehli, A.: Waveform relaxation: theory and practice. Tech. Rep. UCB/ERL M85/65, EECS Department, University of California, Berkeley (1985)