Numerical methods for systems of highly oscillatory ordinary differential equations

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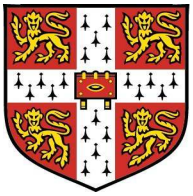

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Abstract

This thesis presents methods for efficient numerical approximation of linear and non-linear systems of highly oscillatory ordinary differential equations.

Phenomena of high oscillation is considered a major computational problem occurring in Fourier analysis, computational harmonic analysis, quantum mechanics, electrodynamics and fluid dynamics. Classical methods based on Gaussian quadrature fail to approximate oscillatory integrals. In this work we introduce numerical methods which share the remarkable feature that the accuracy of approximation improves as the frequency of oscillation increases. Asymptotically, our methods depend on inverse powers of the frequency of oscillation, turning the major computational problem into an advantage.

Evolving ideas from the stationary phase method, we first apply the *asymptotic* method to solve highly oscillatory linear systems of differential equations. The *asymptotic* method provides a background for our next, the *Filon*-type method, which is highly accurate and requires computation of moments. We also introduce two novel methods. The first method, we call it the *FM* method, is a combination of *Magnus* approach and the *Filon*-type method, to solve matrix exponential. The second method, we call it the *WRF* method, a combination of the *Filon*-type method and the *waveform relaxation* methods, for solving highly oscillatory non-linear systems. Finally, completing the theory, we show that the *Filon*-type method can be replaced by a less accurate but moment free *Levin*-type method.

Declaration

I, Marianna Khanamiryan, declare that the thesis entitled "Numerical methods for systems of highly oscillatory ordinary differential equations" and the work presented in the thesis are both my own, and have been generated by me as the result of my own original research and includes nothing which is the outcome of work done in collaboration. I confirm that where I have quoted from the work of others, the source is always given. With the exception of such quotations, this thesis is entirely my own work.

Marianna Khanamiryan

Dedication

For my family, who offered me unconditional love and support throughout the course of this thesis.

Acknowledgements

First of all I would like to express my sincere gratitude to my supervisor, Arieh Iserles. It was Arieh who encouraged me to apply for graduate studies at Cambridge University in the first instance. Arieh's advice on the choice of the research topic and fantastic opportunity to pursue my PhD at the University of Cambridge are invaluable for my career.

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Preface

This thesis presents results of my PhD research in Numerical Analysis of Differential Equations at the Centre for Mathematical Sciences at Cambridge University. The main focus of my PhD was on developing numerical methods efficient for solving linear and non-linear systems of highly oscillatory differential equations.

The key problem of our discussion throughout the thesis is a family of highly oscillatory vector-valued integrals of the form,

$$I[\boldsymbol{f}] = \int_a^b X_\omega \boldsymbol{f} \mathrm{d}t, \qquad X'_\omega = A_\omega X_\omega, \qquad X_\omega(0) = I,$$

where X_ω is a time-dependant highly oscillatory matrix-valued kernel, satisfying matrix linear ordinary differential equation as above and A_ω is a non-singular $d \times d$ matrix with large imaginary eigenvalues, $\sigma(A_\omega) \subset \mathrm{i}\mathbb{R}$. We also assume that $\|{A_\omega}^{-1}\| \ll 1$, $\omega \gg 1$ is a real parameter describing frequency of oscillation and $\boldsymbol{f} \in \mathbb{R}^d$ is a smooth vector-valued function. In current work we present numerical methods for systems of ODEs with a constant matrix A_ω and with a time-dependant matrix $A_\omega(t)$. In our later discussion we also assume non-linearity in a vector-valued function $\boldsymbol{f}$.

The motivation to study family of integrals $I[\boldsymbol{f}]$ appears to be in applications of such integrals in solutions of highly oscillatory linear systems of ODEs,

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

as well as non-linear systems of ODEs,

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

The variation of constants formula provides us with analytic representation of the solution for linear systems of ODEs,

$$\begin{aligned} \boldsymbol{y}(t) &= X_\omega(t)\boldsymbol{y}_0 + \int_0^t X_\omega(t-\tau)\boldsymbol{f}(\tau)\mathrm{d}\tau \\ &= X_\omega(t)\boldsymbol{y}_0 + I[\boldsymbol{f}(t)], \end{aligned}$$

and with implicit representation for non-linear systems of ODEs,

$$\begin{aligned} \boldsymbol{y}(t) &= X_\omega(t)\boldsymbol{y}_0 + \int_0^t X_\omega(t-\tau)\boldsymbol{f}((\tau, \boldsymbol{y}(\tau))\mathrm{d}\tau \\ &= X_\omega(t)\boldsymbol{y}_0 + I[\boldsymbol{f}(t, \boldsymbol{y}(t))]. \end{aligned}$$

We first derive efficient numerical methods for solving family of highly oscillatory vector-valued integrals $I[\boldsymbol{f}]$ and apply the novel methods in solutions to systems of highly oscillatory differential equations.

In essence, the matrix A_ω need not depend on the parameter ω explicitly. Rather, the largest absolute values of the matrix eigenvalues determine the frequency of oscillation in $I[\boldsymbol{f}]$, and the norm of the matrix grows with an increase in frequency. However, for numerical purposes, we have expressed this information in ω, as a way of showing improvement in the accuracy of approximation as ω grows. By this we mean that the larger the eigenvalues of the matrix A_ω, the larger the norm of the matrix, and the better our approximation.

In getting to grips with our underlying task of solving highly oscillatory non-linear systems of ordinary differential equation, we advance gradually, first considering some special cases of the problem.

Before beginning to present our methods, in Chapter 1 we present introduction and background information on classical quadrature

methods, highly oscillatory quadrature rules and exponential integrators, [DR84], [HL03].

In Chapter 2 we briefly describe univariate quadrature methods used to approximate highly oscillatory *Fourier*-type integrals of the form

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

where $f, g \in C^\infty$ are smooth, g is strictly monotone in $[a, b]$, $a \leq x \leq b$ and the frequency is $\omega \gg 1$. We introduce the univariate *asymptotic* and *Filon*-type methods for the scheme of *Fourier*-type integrals. In the same chapter we also provide motivation for our research and provide the link between the our work and the works by A. Iserles and S. Nørsett on the classical quadrature rules for univariate highly oscillatory integrals, [IN05].

In Chapter 3 we present numerical solvers for highly oscillatory linear systems of ODEs with a constant matrix,

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

The analytic solution is given by the formula

$$\boldsymbol{y}(t) = \mathrm{e}^{tA_\omega}\boldsymbol{y_0} + \int_0^t \mathrm{e}^{(t-\tau)A_\omega}\boldsymbol{f}\mathrm{d}\tau = \mathrm{e}^{tA_\omega}\boldsymbol{y_0} + I[\boldsymbol{f}].$$

We assume that A_ω is a non-singular constant matrix with large eigenvalues, $\sigma(A_\omega) \subset \mathrm{i}\mathbb{R}$, $\|{A_\omega}^{-1}\| \ll 1$, $\omega \gg 1$ is a real parameter and $\boldsymbol{f} \in \mathbb{R}^{\mathrm{d}}$ is a smooth vector-valued function. Evolving ideas of the stationary phase approximation [Ste93], we present the *asymptotic* and the *Filon*-type methods to solve linear systems of highly oscillatory ODEs. Expanding the integral $I[\boldsymbol{f}]$ into its asymptotic series we demonstrate the dependence of the error of approximation on the powers of the matrix inverse, having the implication that for both *asymptotic* and the *Filon*-type methods the error depends on the inverse powers of ω. Our methods require explicit availability of more terms in the asymptotic expansion, leading to the assumptions of non singularity of the matrix A_ω and smoothness of the function $\boldsymbol{f}$, [Kha08b].

In Chapter 4 we focus on linear matrix ODEs

$$I[\boldsymbol{f}] = \int_a^b X_\omega(t)\boldsymbol{f}(t)\mathrm{d}t, \qquad X'_\omega = A_\omega X_\omega, \qquad X_\omega(0) = I,$$

where A_ω is a non singular matrix with large imaginary eigenvalues, $det(A_\omega) \neq 0$, $\|{A_\omega}^{-1}\| \ll 1$, $\sigma(A_\omega) \subset \mathrm{i}\mathbb{R}$, $\omega \gg 1$ is a real parameter, $\boldsymbol{f} \in \mathbb{R}^d$ is a smooth vector-valued function. We present *Magnus* methods, modified *Magnus* methods and introduce a novel *FM* method for solving *Lie*-type linear equations, [Kha09a].

With research background provided in previous chapters, in Chapter 5 we solve linear systems with a time dependant matrix,

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

where A_ω is a non-singular matrix with large eigenvalues, $\sigma(A_\omega) \subset \mathrm{i}\mathbb{R}$, $\|A_\omega\| \gg 1$, $\omega \gg 1$ is a real parameter and $\boldsymbol{f} \in \mathbb{R}^{\mathrm{d}}$ is a smooth vector-valued function. We apply the *FM* method for linear systems with a time dependant matrix, [Kha09b].

The special combination of the *Filon*-type methods and iterative *waveform relaxation* methods form a novel *WRF* method, applied for solving highly oscillatory non-linear systems of ODEs. Amazingly, both the *Filon*-type method and the *WRF* method work with end points only, and as such do not require further subdivision of the integration interval. One can obtain an high order of approximation by adding higher order derivatives in $I[\boldsymbol{f}]$. We apply the *FM* method for linear systems with a time dependant matrix and develop the *WRFM* method, a combination of the *WRF* and *FM* methods for non-linear systems. This is a subject of discussion in Chapter 6, [Kha08b], [Kha09b].

In Chapter 7 we present the conclusion to our work and explain why the numerical methods based on Taylor's reasoning fail to approximate highly oscillatory systems versus the remarkable feature of the numerical methods based on the asymptotic expansion, where the the error term decays with inverse powers of frequency. Indeed, we show that oscillatory equations are beneficial.

Our methods are designed for large frequencies, meaning that the numerical solution improves with an increase in frequency.

We mention by passing that the *Filon*-type methods require computation of moments, which may not always be available. In Chapter 8 we provide our current project, [Kha08a], on alternative moment-free *Filon* and *Levin*-type methods. We also provide our plans for future work in applications to PDEs. It is a fascinating fact that oscillations occur in many mathematical models describing not only physical systems but also for example biological systems or even models in human society. We also would like to mention an important application such as medicine, where the quality of computational tomography and medical image analysis improves once better techniques are applied to read oscillating patterns in image processing. The bottom line is that oscillatory equations have a great deal in many interdisciplinary subjects with applications in a very broad sense, but appear to be a major computational problem in those fields.

This dissertation is the result of my own work and is based on a series of articles, [Kha08b], [Kha09b], [Kha08a], [Kha09a].

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Chapter 1

Introduction

1.1 Classical quadrature rules

Numerical integration constitutes a broad family of algorithms for calculating the numerical value of a definite integral, and by extension, the term is also sometimes used to describe the numerical solution of differential equations. The term numerical quadrature, often abbreviated to quadrature, is more or less a synonym for numerical integration, especially as applied to univariate integrals. Multivariate integration is sometimes described as cubature, although the meaning of quadrature is understood for three and higher dimensional integration as well.

The basic problem considered by numerical integration is to compute an approximate solution to a definite integral:

$$\int_a^b f(x)\mathrm{d}x.$$

If $f(x)$ is a smooth function, and the limits of integration are bounded, there are many methods of approximating the integral with arbitrary precision. We will briefly list some of them, [DR84].

For example, in many applications the integrand $f(x)$ may be known only at certain points, such as obtained by sampling. Or sometimes it may be possible to find an anti-derivative symbolically, but it may be easier to compute a numerical approximation rather than to compute the anti-derivative. This may be the case if the anti-derivative is given as an infinite series or product,

or if its evaluation requires a *special function* which is not available. And finally, a formula for the integrand may be known, but it may be difficult or impossible to find an anti-derivative which is an elementary function. The *error function* is a good example,

$$\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z \mathrm{e}^{-t^2} dt.$$

It is a special non-elementary function, which occurs in probability, statistics, materials science, and partial differential equations.

The error function is an entire function. It has no singularities except that at infinity, and its Taylor expansion always converges. The integral of the error function cannot be evaluated in closed form in terms of elementary functions. However, by expanding the integrand e^{-z^2} into its Taylor series and integrating term by term, one obtains the *error function's* Taylor series,

$$\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-1)^n z^{2n+1}}{n!(2n+1)} = \frac{2}{\sqrt{\pi}} \left(z - \frac{z^3}{3} + \frac{z^5}{10} - \frac{z^7}{42} + \frac{z^9}{216} - \cdots \right).$$

Taylor expansion is a valid tool in constructing classical numerical methods of approximation. However in chapters to come we show that numerical methods based on Taylor's reasoning are not suitable in approximation of highly oscillatory integrals. Instead, methods based on the asymptotic expansion prove to be more accurate in numerical approximation of highly oscillatory integrals.

The following section presents a brief review on numerical integrators. We refer our reader to [AS64], [DR84], [Ise09b] and [RR01] and for more information.

The most straightforward numerical integration technique uses the *Newton -Cotes* formulas, [RR01], which approximate a function tabulated at a sequence of regularly spaced intervals by various degree polynomials. Assume that the function is defined on the interval $[a, b]$ is known at equally spaced points $a = x_0, x_1, \ldots, x_n = b$. There are two types of *Newton-Cotes* formulas, the so called closed type uses the function value at all points, and the open type does not use the function values at the endpoints. The closed *Newton–Cotes* formula of degree n is given by the formula

$$\int_a^b w(x) f(x)\, dx \approx \sum_{i=0}^{n} W_i f(x_i),$$

where $w(x)$ is a weight function and W_i are *Cotes* numbers. The latter is defined as follows,

$$W_i = \int_a^b w(x) l_i(x)\ dx.$$

With the help of Lagrangian interpolation,

$$l_i(x) = \frac{p_{n+1}(x)}{(x - x_i)p'_{n+1}(x_i)}, \quad with \quad p_{n+1}(x) = \prod_{j=0}^{n}(x - x_i),$$

we find the weights,

$$\int_a^b w(x)f(x)\ dx = \sum_{i=0}^{n} W_i f(x_i) + \frac{1}{(n+1)!}\int_a^b w(x)p_{n+1}(x)f^{(n+1)}(\xi)\ dx,$$

where the $n+1$ derivative appears as a multiple in the error term. Thus, W_j recovers polynomials of degree n or less. For the open *Newton–Cotes* formula,

$$\int_a^b w(x)f(x)\ dx \approx \sum_{i=1}^{n-1} W_i f(x_i),$$

with $n-1$ weights and exact polynomial recovery rate $n-2$.

If the endpoints are tabulated, then for $w(x) = 1$ and $n = 1$ from the *Newton–Cotes* formula we obtain the *trapezoidal* rule

$$\int_a^b f(x)\ dx \approx (b-a)\frac{f(a)+f(b)}{2}.$$

To calculate this integral more accurately, one first splits the interval of integration [a,b] into n smaller subintervals, and then applies the trapezoidal rule on each of them. This results in the *composite trapezoidal* rule,

$$\int_a^b f(x)\ dx \approx \frac{b-a}{n}\left[\frac{f(a)+f(b)}{2} + \sum_{k=1}^{n-1} f\left(a + k\frac{b-a}{n}\right)\right].$$

A generalization of the trapezoidal rule is *Romberg integration*, which can yield accurate results for many fewer function evaluations. The method

uses acceleration techniques, such as *Richardson extrapolation* to improve the results of a numerical method, from a method of order $\mathcal{O}(h^p)$ it gives us a method of order $\mathcal{O}(h^p)$.

Suppose we want to approximate a quantity Q, and you have available approximations $Q(h)$ for $h > 0$. Typically, this approximation is of a certain order, $Q = Q(h) + \mathcal{O}(h^p)$. But often, more can be said, for some quantity A not depending on h, $Q = Q(h) + Ah^p + \mathcal{O}(h^{p+1})$.

The idea of Richardson extrapolation is to take two different values of h, typically we take $h_1 = h$ and $h_2 = h/2$, and eliminate the A term.

$$Q_R = \frac{h_2^p Q(h_1) - h_1^p Q(h_2)}{h_2^p - h_1^p}$$

Now, the *Romberg integration* method can be defined inductively as follows,

$$\begin{aligned} R(0,0) &= \frac{1}{2}(b-a)(f(a)+f(b)) \\ R(n,0) &= \frac{1}{2}R(n-1,0) + h_n \sum_{k=1}^{2^{n-1}} f(a+(2k-1)h_n) \\ R(n,m) &= R(n,m-1) + \frac{1}{4^m - 1}(R(n,m-1) - R(n-1,m-1)). \end{aligned}$$

In the same way as for the *trapezoidal rule*, *Simpson's rule* can be derived from the *Newton–Cotes*formula for $n = 2$,

$$\int_a^b f(x)\,dx \approx \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right].$$

Simpson's rule is a special case of *Romberg's method*. The theory of this method shows that *Simpson's rule* is exact when the integrand is a polynomial of degree three or lower.

The composite *Simpson's rule* is given by

$$\int_a^b f(x)\,dx \approx \frac{h}{3}\left[f(x_0) + 2\sum_{j=1}^{n/2-1} f(x_{2j}) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + f(x_n)\right],$$

where $x_j = a + jh$ for $j = 0, 1, ..., n$ with $h = (b-a)/n$, in particular, $x_0 = a$ and $x_n = b$. The above formula can also be written as

$$\int_a^b f(x)\,dx \approx \frac{h}{3}\Big[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + \cdots + 4f(x_{n-1}) + f(x_n)\Big].$$

The error committed by the composite *Simpson's* rule is bounded in absolute value by

$$\frac{h^4}{180}(b-a)\max_{\xi\in[a,b]}|f^{(4)}(\xi)|,$$

where $h = (b-a)/n$ is a step size.

This formulation splits the interval [a,b] in subintervals of equal length. In practice, it is often advantageous to use subintervals of different lengths, and concentrate the efforts on the places where the integrand is less well-behaved. This leads to the adaptive Simpson's method.

If the functions are known analytically instead of being tabulated at equally spaced intervals, the best numerical method of integration is called Gaussian quadrature. By picking the abscissas at which to evaluate the function, Gaussian quadrature produces the most accurate approximations possible. An n-point Gaussian quadrature rule is a quadrature rule constructed to yield an exact result for polynomials of degree $2n-1$ or less by a suitable choice of the points x_i and weights w_i for $i = 1, ..., n$. The formula

$$\int_a^b f(x)\ dx \approx \frac{b-a}{2}\sum_{i=1}^{n} w_i f\left(\frac{b-a}{2}x_i + \frac{a+b}{2}\right)$$

is used whenever the integrand is sufficiently smooth, and the gain in the number of nodes is substantial.

Suppose that the integrated function can be written as $f(x) = W(x)g(x)$, where $g(x)$ is approximately polynomial, and $W(x)$ is known, then there are alternative weights such that

$$\int_{-1}^{1} f(x)\,dx = \int_{-1}^{1} W(x)g(x)\,dx \approx \sum_{i=1}^{n} w_i g(x_i).$$

Common weighting functions include Gauss-Chebyshev

$$W(x) = (1 - x^2)^{-1/2}$$

and Gauss-Hermite

$$W(x) = \mathrm{e}^{-x^2}$$

functions.

1.2 Highly oscillatory quadrature

The first known numerical quadrature scheme for oscillatory integrals was developed in 1928 by Louis Napoleon George Filon [IN05]. Filon presented a method for efficiently computing the Fourier integrals,

$$\int_a^b f(x)\sin(\omega x)\mathrm{d}x \quad \text{and} \quad \int_a^b \frac{f(x)}{x}\sin(\omega x)\mathrm{d}x.$$

We will see that often asymptotic expansions lie at the heart of oscillatory quadrature. We aim to find and investigate methods which preserve the asymptotic properties of an asymptotic expansion, whilst allowing for arbitrarily high accuracy for a fixed frequency. Fortunately, methods have been developed with these properties, in particular the *Filon* method and *Levin* collocation method.

As originally constructed, the *Filon* method consists of dividing the interval into $2n$ panels of size h, and applying a modified Simpson's rule on each panel. In other words, f is interpolated at the endpoints and midpoint of each panel by a quadratic. In each panel the integral becomes a polynomial multiplied by the oscillatory kernel $\sin \omega x$, which can be integrated in closed form.

We determine the quadratic for the k^{th} panel as

$$v_k(x) = c_{k,0} + c_{k,1}x + c_{k,2}x^2,$$

by solving the system

$$\begin{aligned} v_k(x_k) &= f(x_k) \\ v_k(x_{k+1}) &= f(x_{k+1}) \\ v_k(x_{k+2}) &= f(x_{k+2}). \end{aligned}$$

We thus sum up the approximation on each subinterval,

$$\int_a^b f(x)\sin(\omega x)\mathrm{d}x \approx \sum_{k=0}^{n-1}\int_{x_{2k}}^{x_{2k+2}} v(x_k)\sin(\omega x)\mathrm{d}x.$$

The infinite integral was then computed using a series transformation, since the moments $\int_a^b x^k \sin(\omega x)\mathrm{d}x$ are known explicitly. These ideas were generalized and developed further by Arieh Iserles and Syvert Nørsett in a number of articles by the authors, [IN05], [IN06], [IN04], [Ise04b], [Ise05], [INO06].

In the original paper by Filon, it is shown that the error of the Filon method is bounded by

$$C\sin\frac{h\omega}{2}\left(1-\frac{1}{16}\sec\frac{h\omega}{4}\right).$$

However, it was noticed in papers by Arieh Iserles and Syvert Nørsett that h need not shrink as ω increases, rather, if anything, it should increase, thus reducing the required number of operations. This is the most important property of the Filon method, its accuracy actually improves as the frequency increases! Indeed, for a fixed step size the error decays like $\mathcal{O}(\omega^{-2})$.

1.3 Exponential integrators

Referring to Hochbruck [Hoc04], we relate our work to the class of works on *exponential integrators* and present a brief review on the methods.

Definition 1.3.1 *[Hoc04] An exponential integrator is a numerical method which involves an exponential function or a related function of the Jacobian or an approximation to it.*

Recently, there has been a great deal of interest in the construction of exponential integrators. These integrators, as their name suggests, use the exponential function (and related functions) of the Jacobian or an approximation to it, inside the numerical method. Various methods have been developed for the differential equation

$$y(t) = f(y(t)) = Ly(t) + N(y(t)) \quad \text{with} \quad y(t_n) = y_n.$$

The first paper to construct what are now known as exponential integrators, was by Certaine, published in 1960.

Before introducing the framework of exponential integrators, we examine several well known extensions of the Euler method. Linearising the initial value problem for $f(y(t))$, gives

$$y'(t) = f(y_{n-1}) + f'(y_{n-1})(y - y_{n-1}).$$

The exact solution to this linearised problem is

$$y_n = y_{n-1} + h\phi_1(hf'(y_{n-1}))f(y_{n-1}),$$

where the function ϕ_1 , is defined as

$$\phi_1(z) = \frac{\mathrm{e}^z - 1}{z}.$$

This method is of order two, for general problems of the form $f(y(t))$, and exact for problems, where

$$f(y) = Ly + N.$$

The method is known as the exponential Euler method. Assume, that we use L as an approximation to the full Jacobian in the method above, then the Exponential Time Differencing (ETD) Euler is, [Nør69]

$$\begin{aligned} y_n &= y_{n-1} + h\phi_1(hL)(Ly_{n-1} + N(y_{n-1})) \\ &= \mathrm{e}^{hL}y_{n-1} + h\phi_1(hL)N(y_{n-1}). \end{aligned}$$

Chapter 2

Fourier-type oscillators

It was shown by A. Iserles and S. Nørsett in [IN05] that the standard numerical approach based on *Gauss–Christoffel* quadrature fails to approximate highly oscillatory integrals since the error of approximation is $\mathcal{O}(1)$ for $\omega \to \infty$. Instead the authors developed the *asymptotic* and the *Filon*-type methods, which share the feature that accuracy improves as ω increases.

Our research is very much inspired by early works by A. Iserles and S. Nørsett. Below we present initial ideas from the research done by these authors and explain continuous connection between our work and works on oscillatory quadrature rules by A. Iserles and S. Nørsett, [Ise04b, IN04, IN05]. Bear in mind linear system of ODEs

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

with the exact solution

$$\boldsymbol{y}(t) = \mathrm{e}^{tA_\omega}\boldsymbol{y_0} + \int_0^t \mathrm{e}^{(t-\tau)A_\omega}\boldsymbol{f}(\tau)\mathrm{d}\tau = \mathrm{e}^{tA_\omega}\boldsymbol{y_0} + I[\boldsymbol{f}]. \tag{2.0.1}$$

The following assumptions hold: A_ω is a constant non-singular matrix with large imaginary eigenvalues, $\sigma(A_\omega) \subset \mathrm{i}\mathbb{R}$, $\|A_\omega\| \gg 1$, $\omega \gg 1$ is a real parameter and $\boldsymbol{f} \in \mathbb{R}^{\mathrm{d}}$ is a smooth vector-valued function.

For a 2π-periodic function $f(x)$, integrable on $[-\pi, \pi]$ the well known *Fourier* series is given by

$$\frac{a_0}{2} + \sum_{n=1}^{\infty} [a_n \cos(nx) + b_n \sin(nx)].$$

The *Fourier* coefficients are oscillatory functions described as follows,

$$a_n = \frac{1}{\pi}\int_{-\pi}^{\pi} f(t)\cos(nt)\,dt, \quad n \geq 0$$

and

$$b_n = \frac{1}{\pi}\int_{-\pi}^{\pi} f(t)\sin(nt)\,dt, \quad n \geq 1.$$

Employing *Euler's* formula, $\mathrm{e}^{\mathrm{i}nx} = \cos(nx) + \mathrm{i}\sin(nx)$, we can rewrite the sum in term of exponential function,

$$f(x) = \sum_{n=-\infty}^{\infty} c_n \mathrm{e}^{\mathrm{i}nx}.$$

The *Fourier* coefficients are now determined as

$$c_n = \frac{1}{2\pi}\int_{-\pi}^{\pi} f(x)\mathrm{e}^{-\mathrm{i}nx}\,dx,$$

and $a_n = c_n + c_{-n}$ for $n = 0, 1, 2, \ldots$, while $b_n = i(c_n - c_{-n})$ for $n = 1, 2, \ldots$.

In order to present our readers motivation for our research we now briefly state the two important theorems from [IN05], describing the quadrature methods used to approximate a more general family of *Fourier*-type highly oscillatory integrals of the form,

$$I[f] = \int_a^b f(x)\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x, \tag{2.0.2}$$

where $f, g \in C^\infty$ are smooth, g is strictly monotone in $[a, b], a \leq x \leq b$ and the frequency is $\omega \gg 1$. Later in this chapter we will explain the link between linear systems of ODEs above and *Fourier*-type integrals given in (2.0.2).

2.1 The univariate asymptotic method

Suppose that f and g are differentiable up to a sufficiently high order, and g is free of stationary points on $[a, b]$. In that case we can obtain the *asymptotic* expansion for the *Fourier*-type integral

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

The truncated *asymptotic* expansion appears to be a powerful tool in approximation of the integral $I[f]$ as compared to aforementioned classical methods. The accuracy of approximation will improve as the frequency grows large, $\omega \gg 1$. Once the assumption on differentiability of the functions is satisfied, the *asymptotic* method uses very little information about function values and derivatives at the end points. We can obtain the expansion straight by repeatedly integrating $I[f]$ by parts,

$$\begin{aligned} I[f] &= \int_a^b f(x)\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x = \frac{1}{\mathrm{i}\omega}\int_a^b \frac{f(x)}{g'(x)}\frac{\mathrm{d}}{\mathrm{d}x}\mathrm{e}^{\mathrm{i}\omega g(x)} \\ &= \frac{1}{\mathrm{i}\omega}\left[\frac{f(b)}{g'(b)}\mathrm{e}^{\mathrm{i}\omega g(b)} - \frac{1}{\mathrm{i}\omega}\frac{f(a)}{g'(a)}\mathrm{e}^{\mathrm{i}\omega g(a)}\right] - \frac{1}{\mathrm{i}\omega}\int_a^b \frac{\mathrm{d}}{\mathrm{d}x}\left[\frac{f(x)}{g'(x)}\right]\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x. \end{aligned}$$

The error term shares the property,

$$-\frac{1}{\mathrm{i}\omega}I\left[\frac{\mathrm{d}}{\mathrm{d}x}\left[\frac{f(x)}{g'(x)}\right]\right] = \mathcal{O}(\omega^{-2}).$$

It is now evident that the error term depends on the inverse powers of frequency and itself is an oscillatory function. Hence, one can apply integration by parts further to obtain arbitrary higher order methods of approximation.

Lemma 2.1.1 *[A. Iserles & S. Nørsett][IN05] Let $f, g \in C^\infty$, $g'(x) \neq 0$ on $[a, b]$ and*

$$\begin{aligned} \sigma_0[f](x) &= f(x), \\ \sigma_{k+1}[f](x) &= \frac{d}{dx}\frac{\sigma_k[f](x)}{g'(x)}, \qquad k = 0, 1, ... \end{aligned}$$

Then, for $\omega \gg 1$,

$$I[f] \sim -\sum_{m=1}^{\infty} \frac{1}{(-iw)^m}\left[\frac{\mathrm{e}^{\mathrm{i}\omega g(b)}}{g'(b)}\sigma_{m-1}[f(b) - \frac{\mathrm{e}^{\mathrm{i}\omega g(a)}}{g'(a)}\sigma_{m-1}[f](a)\right].$$

The *asymptotic* method is defined as follows,

$$Q_s^A[f] = -\sum_{m=1}^{s} \frac{1}{(-i\omega)^m}\left[\frac{\mathrm{e}^{\mathrm{i}\omega g(b)}}{g'(b)}\sigma_{m-1}[f](b) - \frac{\mathrm{e}^{\mathrm{i}\omega g(a)}}{g'(a)}\sigma_{m-1}[f](a)\right].$$

Theorem 2.1.2 *[A. Iserles & S. Nørsett] [IN05] For every smooth f and g, such that $g'(x) \neq 0$ on $[a, b]$, it is true that*

$$Q_s^A[f] - I[f] \sim \mathcal{O}(\omega^{-s-1}), \qquad \omega \to \infty.$$

2.2 The univariate Filon-type method

A precursor of a *Filon*-type method was first pioneered in the work of L. N. G. Filon in 1928, modified by E. A. Flinn [Fli60], and developed by A. Iserles and S. Nørsett in [IN05] and later by A. Iserles, S. Nørsett and S. Olver in [INO06]. The method replaces f in (2.0.2) by its Hermite interpolant,

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

which satisfies $v^{(j)}(c_l) = f^{(j)}(c_l)$, at node points $a = c_1 < c_2 < ... < c_\nu = b$, with $\theta_1, \theta_2, ..., \theta_\nu \geq 1$ associated multiplicities, $j = 0, 1, ..., \theta_l - 1, l = 1, 2, ..., \nu$ and $r = \sum_{l=1}^{\nu} \theta_l - 1$ being the order of approximation polynomial.

For the *Filon*-type method, by definition,

$$Q_s^F[f] = I[v] = \int_a^b v(x) \mathrm{e}^{i\omega g(x)} \mathrm{d}x = \sum_{l=1}^{\nu} \sum_{j=0}^{\theta_l - 1} b_{l,j}(\omega) f^{(j)}(c_l),$$

where

$$b_{l,j} = \int_a^b \alpha_{l,j}(x) \mathrm{e}^{\mathrm{i}\omega g(x)} \mathrm{d}x, \qquad j = 0, 1, ..., \theta_l - 1, \qquad l = 1, 2, ..., \nu.$$

Theorem 2.2.1 *[A. Iserles & S. Nørsett][IN05] Suppose that* $s = \min\{\theta_1, \theta_\nu\}$. *For every smooth* f *and* g, $g'(x) \neq 0$ *on* $[a, b]$, *it is true that*

$$I[f] - Q_s^F[f] \sim \mathcal{O}(\omega^{-s-1}), \quad \omega \to \infty.$$

Example 2.2.1 Here we consider the *asymptotic* and the *Filon*-type method with first derivatives for (2.0.2) over the interval $[0, 1]$ for the case $g(x) = x$.

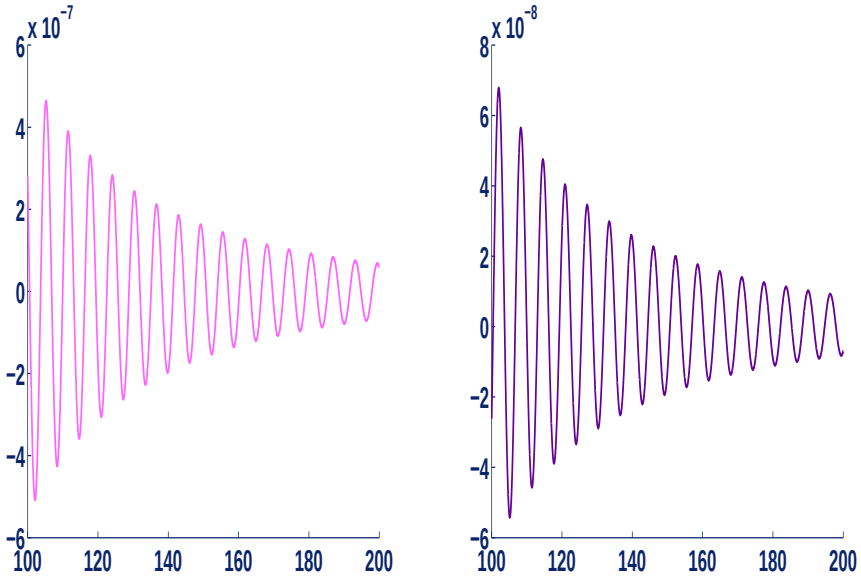

Figure 2.2.1: The global error of the *asymptotic* method Q_2^A (right) and the *Filon*-type method Q_2^F (left) for the (2.0.2), $f(x) = \cos(x)$, $g(x) = x$, $x \in [0, 1]$, $\theta_1 = \theta_2 = 2$ and $100 \leq \omega \leq 200$.

$$
\begin{aligned}
Q_2^A &= \frac{\mathrm{e}^{\mathrm{i}\omega} f(1) - f(0)}{\mathrm{i}\omega} + \frac{\mathrm{e}^{\mathrm{i}\omega} f'(1) - f'(0)}{\omega^2}, \\
Q_2^F &= \left(-\frac{1}{\mathrm{i}\omega} - 6\frac{1+\mathrm{e}^{\mathrm{i}\omega}}{\mathrm{i}\omega^3} + 12\frac{1-\mathrm{e}^{\mathrm{i}\omega}}{\omega^4} \right) f(0) \\
&\quad + \left(-\frac{\mathrm{e}^{\mathrm{i}\omega}}{\mathrm{i}\omega} + 6\frac{1+\mathrm{e}^{\mathrm{i}\omega}}{\mathrm{i}\omega^3} - 12\frac{1-\mathrm{e}^{\mathrm{i}\omega}}{\omega^4} \right) f(1) \\
&\quad + \left(-\frac{1}{\omega^2} - 2\frac{2+\mathrm{e}^{\mathrm{i}\omega}}{\mathrm{i}\omega^3} + 6\frac{1-\mathrm{e}^{\mathrm{i}\omega}}{\omega^4} \right) f'(0) \\
&\quad + \left(\frac{\mathrm{e}^{\mathrm{i}\omega}}{\omega^2} - 2\frac{1+\mathrm{e}^{\mathrm{i}\omega}}{\mathrm{i}\omega^3} + 6\frac{1-\mathrm{e}^{\mathrm{i}\omega}}{\omega^4} \right) f'(1).
\end{aligned}
$$

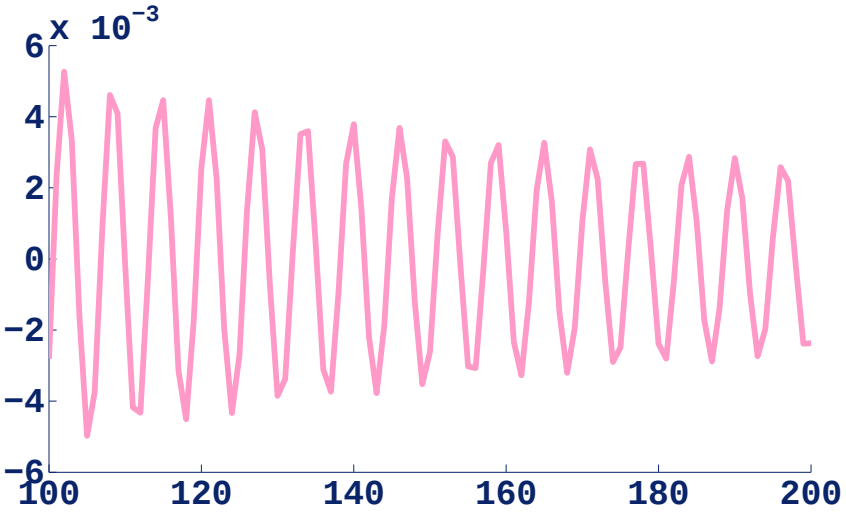

Figure 2.2.2: This plot describes the exact solution for the *Fourier*-type integral (2.0.2) with $f(x) = \cos(x)$, $g(x) = x$, $x \in [0, 1]$ and $100 \leq \omega \leq 200$.

In Figure 2.2.1 we present numerical results on the *asymptotic* and *Filon*-type methods with function values and its first derivatives at the end points only, $c_1 = 0, c_2 = 1$, for the integral

$$I[f] = \int_0^1 \cos(x) \mathrm{e}^{\mathrm{i}\omega x} \mathrm{d}x, \qquad 100 \leq \omega \leq 200.$$

Both methods have the same asymptotic order and use exactly the same information. However as we can see from Figure 2.2.1, the *Filon*-type method yields a greater measure of accuracy than the *asymptotic* method. We would like to emphasize that the *Filon*-type method works for small values of ω as well. With *Gaussian* points it is equivalent to the *Gauss-Christoffel* quadrature for $\omega \to 0$, using the same information.

In [IN05] it was shown by the authors that adding more internal points leads to the decay of the leading error constant, resulting in a marked improvement in the accuracy of approximation. This addition does not affect asymptotic order but rather its contributory end points.

We would like to mention here that these results remain valid for vector-valued functions as well as for vector-valued polynomials. This is particularly important while constructing similar methods for oscillatory ODEs. Having both large and small eigenvalues in the system makes difference in applications. And the beauty of the *Filon*-type method is that it is valid for both large and small eigenvalues, as it is valid for large and small ω. This means that one does not need to split the system and apply different methods to its large and small parts. Instead, the *Filon* method takes care of both parts.

Note that while replacing function f by a polynomial, the *Filon*-type method requires computation of the moments $\int_a^b x^m \mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x, m \geq 0$, which may not always be available. As a consequence, since $I[f]$ may appear to be elements of the vector-valued integral $I[\boldsymbol{f}]$ in oscillatory systems, the latter may also not always be available once $\boldsymbol{f}$ is replaced by a vector-valued polynomial.

We used both MATLAB numerical package and its symbolic toolbox linked to a MAPLE kernel to perform numerical evaluations for this work.

Numerical approximation of highly oscillatory integrals is a an advanced topic of research and involves wide spectrum of different approaches including moment–free approximation. This includes *Levin*-type methods, [Lev82, Lev97], invented by D. Levin and further extended by S. Olver, [Olv07]. The second alternative method we refer to is *numerical steepest descent* method by D. Huybrechs and S. Vandewalle, [HO08, HV06]. There is a very relevant work using exponential integrators for oscillatory equations by V. Grimm and M. Hochbruck, [GH06]. For asymptotic methods for integrals we refer to [dB81, Olv74, Won01].

2.3 Applications to linear systems

The work presented in this thesis entails the extension of the introduced points from [IN05]. Namely, we develop the *asymptotic* and the *Filon*-type methods further with a purpose of approximation of highly oscillatory integrals $I[\boldsymbol{f}]$ with a matrix-valued kernel and a vector-valued function. The results of our approximation are being used to solve linear and non-linear systems of highly oscillatory ODEs. We should mention that all norms hereafter are L^∞ norms.

Having introduced *asymptotic* and *Filon*-type methods for the family of

integrals (2.0.2), we now explain the link between the present work published in [Kha08b] and early results from [IN05]. Take for simplicity a spectral decomposition of the matrix $A_\omega = PDP^{-1}$, having a pure imaginary spectrum $\sigma(A_\omega) = \{i\omega_k\}_{k=1}^d$, $\omega_k \in \mathbb{R}$,

$$A_\omega = P \begin{pmatrix} i\omega_1 & 0 & \dots & 0 \\ 0 & i\omega_2 & \dots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & i\omega_d \end{pmatrix} P^{-1},$$

therefore

$$A_\omega^{-1} = P \begin{pmatrix} \frac{1}{i\omega_1} & 0 & \dots & 0 \\ 0 & \frac{1}{i\omega_2} & \dots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & \frac{1}{i\omega_d} \end{pmatrix} P^{-1},$$

and

$$\mathrm{e}^{A_\omega} = P \begin{pmatrix} \mathrm{e}^{i\omega_1} & 0 & \dots & 0 \\ 0 & \mathrm{e}^{i\omega_2} & \dots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & \mathrm{e}^{i\omega_d} \end{pmatrix} P^{-1}.$$

This suggests that to approximate a highly oscillatory integral $I[\boldsymbol{f}]$ with a matrix-valued kernel and a vector-valued function in (2.0.1), we need to approximate a highly oscillatory integral of the kind (2.0.2) in $I[\boldsymbol{f}]$. Needless to mention the asymptotic order of our approximation to $I[\boldsymbol{f}]$ depends on the inverse powers of the eigenvalues, thus we wish the error will decay as the eigenvalues grow. For smaller eigenvalues the method is comparable with the classical methods, while in the case of zero eigenvalues the method will be equivalent to the polynomial approximation of the integrable function, [Kha08b].

Chapter 3

Highly oscillatory linear systems with constant variables

3.1 The asymptotic method for matrix-valued kernels

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

$$I[\boldsymbol{f}] = \int_a^b X_\omega(t)\boldsymbol{f}(t)dt, \qquad X'_\omega = A_\omega X_\omega, \tag{3.1.1}$$

where the matrix kernel X_ω satisfies a linear differential equation (3.1.1) with a constant non-singular matrix A_ω of large eigenvalues, $\|A_\omega^{-1}\| \ll 1$, $\sigma(A_\omega) \subset \mathrm{i}\mathbb{R}$, ω is a real parameter and $\boldsymbol{f} \in \mathbb{R}^{\mathrm{d}}$ is a smooth vector-valued function: $\boldsymbol{f} \in C^\infty[a, b]$. The fact that the matrix X_ω satisfies linear matrix ODE (3.1.1) allows us to integrate (3.1.1) by parts,

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

We define *asymptotic* method Q_s^A as

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

representing s-partial sum of the asymptotic expansion for $I[\boldsymbol{f}]$, (3.1.1).

At this point of discussion it will be appropriate if we introduce some notation on matrix and function asymptotics from [Olv07]. 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 $AB = \mathcal{O}(\tilde{A}\tilde{B})$, [Kha08b], [Kha09b].

Note that the constant in $AB = \mathcal{O}(\tilde{A}\tilde{B})$ does not depend on the dimension of the matrices, rather on the largest absolute value of a constant in element-wise estimates of the entries of a matrix-product. The reason for this is the following: 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 say that

$$A(x) = \mathcal{O}(\tilde{A}), \quad \text{if} \quad a_{ij}(x) = \mathcal{O}(\tilde{a}_{ij})$$

element-wise as $\omega \to \infty$. In other words,

$$\|a_{ij}\| \leq C_{ij}\|\tilde{a}_{ij}\|,$$

hence, in the estimate $A(x) = \mathcal{O}(\tilde{A})$ the constant depends on the maximum value $C = \max\{C_{ij}\}$. The same rule applies to the product of a two matrices. For $Z = AB$, and $\tilde{Z} = \tilde{A}\tilde{B}$, where $Z(x) = (z_{ij}(x))$ and $\tilde{Z} = (\tilde{z}_{ij})$, $\tilde{z}_{ij} \geq 0$ we have

$$Z = AB = \mathcal{O}(\tilde{A}\tilde{B}) = \mathcal{O}(\tilde{Z}),$$

whereby

$$\|z_{ij}\| \leq \tilde{C}_{ij}\|\tilde{z}_{ij}\|.$$

Thus, the constant in $AB = \mathcal{O}(\tilde{A}\tilde{B})$ depends on the maximum value $\tilde{C} = \max\{\tilde{C}_{ij}\}$ which will provide a uniform estimate for $\forall\|z_{ij}\| \leq \tilde{C}\|\tilde{z}_{ij}\|$ and not on the dimension of the matrices.

Lemma 3.1.1 *[Kha08b] 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 $\boldsymbol{f} : \mathbb{R} \to \mathbb{R}^{\mathrm{d}}$ 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 $\psi = \max\{\|\boldsymbol{f}^{(s)}\|, \|\boldsymbol{f}^{(s+1)}\|\}$,

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

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

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

element wise.

Proof: By induction,

$$Q_s^A[\boldsymbol{f}] = I[\boldsymbol{f}] - (-A_\omega)^{-s}\int_a^b X_\omega(t)\boldsymbol{f}^{(s)}(t)dt = I[\boldsymbol{f}] - (-A_\omega)^{-s}I[\boldsymbol{f}^{(s)}].$$

Indeed, for $s = 0$ the identity $Q_s^A = I[\boldsymbol{f}]$. Suppose that the equality holds for some $s \geq 1$, we now prove it for $s+1$. This follows from

$$I[\boldsymbol{f}^s] = \int_a^b X_\omega(t)\boldsymbol{f}^{(s)}(t)\mathrm{d}t = A_\omega^{-1}\left[X_\omega(b)\boldsymbol{f}^{(s)}(b) - X_\omega(a)\boldsymbol{f}^{(s)}(a)\right] - A_\omega^{-1}\int_a^b X_\omega(t)\boldsymbol{f}^{(s+1)}(t)\mathrm{d}t.$$

For L^∞ norms,

$$\begin{aligned} I[\boldsymbol{f}^{(s)}] \sim \mathcal{O}(\|A_\omega^{-1}\|\|X_\omega\|\|\boldsymbol{f}^{(\boldsymbol{s})}\|) + \mathcal{O}(\|A_\omega^{-1}\|\|X_\omega\|\|\boldsymbol{f}^{(\boldsymbol{s+1})}\|) \\ = \mathcal{O}(\|A_\omega^{-1}\|\|X_\omega\|\psi), \end{aligned}$$

therefore

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

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

$$I[\boldsymbol{f}^{(s)}] = \mathcal{O}(A_\omega^{-1}\hat{X}_\omega\tilde{\boldsymbol{f}}) + \mathcal{O}(A_\omega^{-1}\hat{X}_\omega\tilde{\boldsymbol{f}}) = \mathcal{O}(A_\omega^{-1}\hat{X}_\omega\tilde{\boldsymbol{f}}),$$

yielding the further result

$$Q_s^A[\boldsymbol{f}] - I[\boldsymbol{f}] = \mathcal{O}(A_\omega^{-s-1}\hat{X}_\omega\tilde{\boldsymbol{f}}).$$

□

Corollary 3.1.2 *[Kha08b] If*

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

then in L^∞ norm,

$$I[\boldsymbol{f}] \sim \mathcal{O}(\|A_\omega^{-s-1}\|\|X_\omega\|\psi),$$

and

$$I[\boldsymbol{f}] = \mathcal{O}(A_\omega^{-s-1}\hat{X}_\omega\tilde{\boldsymbol{f}})$$

element-wise.

Proof: Follows immediately from Lemma (3.1.1). □

Corollary 3.1.3 *[Kha08b] If $X_\omega = \mathcal{O}(\mathbf{1})$ and $\boldsymbol{f} = \mathcal{O}(\mathbf{1})$, then*

$$Q_s^A[\boldsymbol{f}] - I[\boldsymbol{f}] = \mathcal{O}(A_\omega^{-s-1}\mathbf{1}).$$

Proof: The statement follows from the notation on matrix asymptotics and Lemma(3.1.1). □

The point of departure in construction of our numerical solvers for the systems of ordinary differential equations is the initial-value integrator

$$\boldsymbol{y}_{n+1} = \mathrm{e}^{hA_\omega}\boldsymbol{y}_n + \int_0^h \mathrm{e}^{(h-\tau)A_\omega}\boldsymbol{f}(t_n+\tau)\mathrm{d}\tau. \tag{3.1.2}$$

Example 3.1.1 Let

$$I_h[\boldsymbol{f}] = \int_0^h \mathrm{e}^{A_\omega(h-t)}\boldsymbol{f}(t)\mathrm{d}t.$$

The *asymptotic* method for $s = 2$ with end points only is

$$Q_2^A[\boldsymbol{f}] = -A_\omega^{-1}\left(\boldsymbol{f}(h) - \mathrm{e}^{A_\omega h}\boldsymbol{f}(0)\right) - A_\omega^{-2}\left(\boldsymbol{f}'(h) - \mathrm{e}^{A_\omega h}\boldsymbol{f}'(0)\right).$$

In the sequel we provide some applications of the *asymptotic* method to solve highly oscillatory linear systems. Figures 3.1.1 and 3.1.2 capture how the accuracy of the method increases with ω, as long as the step size h is fixed and the characteristic frequency $h\omega \gg 1$. The method remains accurate for magnitudes of $\omega = 10^4$ and $h\omega = 10^3$. This allows us to work with larger step-sizes, taking into account that it is the ω that reduces the error small rather than step-size.

Our method may be compared with the fourth order Runge–Kutta method presented in Figure 3.1.3 for the same equation and same step size, and MATLAB ode15s and ode113 solvers in Figure 3.2.5. For a fixed step-size $h = \frac{1}{10}$ the error of the fourth order Runge–Kutta method increases with ω. Due to stability of the Runge–Kutta method the error remains bounded as in the right Figure 3.1.2. However the method is accurate only for small values of t around the origin, whilst on a large time scale the approximation has nothing to do with exact solution for increasing ω.

3.2 The Filon-type method for matrix-valued kernels

In this section we extend the *Filon*-type method [IN05] to solve systems of ordinary differential equations. We interpolate a vector-valued function $\boldsymbol{f}$ in (3.1.1) by a r-degree vector-valued polynomial $\boldsymbol{v}$

$$\boldsymbol{v}(t) = \sum_{l=1}^{\nu}\sum_{j=0}^{\theta_l-1}\alpha_{l,j}(t)\boldsymbol{f}^{(j)}(t_l), \tag{3.2.1}$$

such that $\boldsymbol{v}^{(j)}(t_l) = \boldsymbol{f}^{(j)}(t_l)$ at node points $a = t_1 < t_2 < ... < t_\nu = b$, $\theta_1, \theta_2, ..., \theta_\nu \geq 1$ being the associated multiplicities, $j = 0, 1, ..., \theta_l - 1$ and $l = 1, 2, ..., \nu$, [Kha08b].

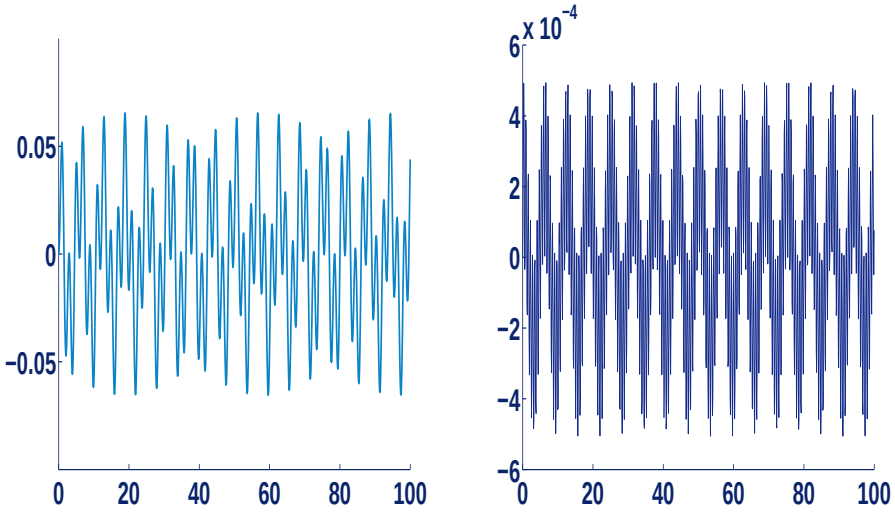

Figure 3.1.1: Global error of the *asymptotic* method Q_2^A with end points only for the equation $y''(t) = -\omega y(t) - \cos(t)$, $0 \leq t \leq 100$, with $[1,0]^\intercal$ initial conditions and step-size $h = \frac{1}{10}$ for $\omega = 10$ (left figure), $\omega = 10^2$ (right figure).

We define the *Filon*-type method as follows,

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

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

Theorem 3.2.1 *[Kha08b] Let*

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

where A_ω is a constant non-singular matrix of a pure imaginary spectrum, $\sigma(A_\omega) \subset \mathrm{i}\mathbb{R}$, $\|A_\omega^{-1}\| \ll 1$, $\theta_1, \theta_\nu \geq s$ and $\boldsymbol{f} : \mathbb{R} \to \mathbb{R}^{\mathrm{d}}$ is a smooth vector-valued

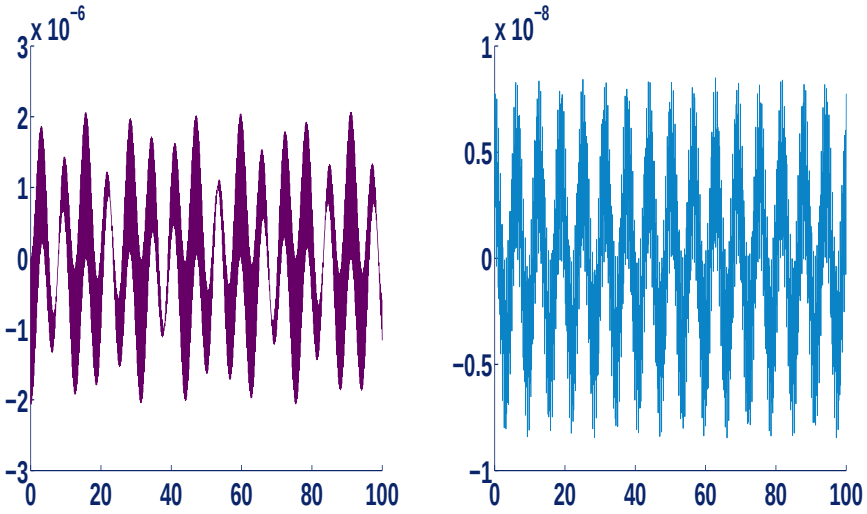

Figure 3.1.2: Global error of the *asymptotic* method Q_2^A with end points only for the equation $y''(t) = -\omega y(t) - \cos(t)$, $0 \leq t \leq 100$, with $[1, 0]^\intercal$ initial conditions and step-size $h = \frac{1}{10}$ for $\omega = 10^3$ (left figure), $\omega = 10^4$ (right figure).

function. Then, for $\psi = \max\{\|\boldsymbol{f}^{(s)}\|, \|\boldsymbol{f}^{(s+1)}\|\}$,

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

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

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

Proof: The proof is equivalent to that for the classical *Filon*-type method. As a consequence of Corollary (3.1.2), replacing $\boldsymbol{f}$ in the asymptotic method with $\boldsymbol{f} - \boldsymbol{v}$, implies that $[\boldsymbol{f} - \boldsymbol{v}]^{(j)}(a) = [\boldsymbol{f} - \boldsymbol{v}]^{(j)}(b) = 0$, for $j = 0, 1, ..., s-1$. □

Corollary 3.2.2 *[Kha08b] If* $X_\omega = \mathcal{O}(\mathbf{1})$ *and* $\boldsymbol{f} = \mathcal{O}(\mathbf{1})$, *then*

$$Q_s^F[\boldsymbol{f}] - I[\boldsymbol{f}] = \mathcal{O}(A_\omega^{-s-1}\mathbf{1}).$$

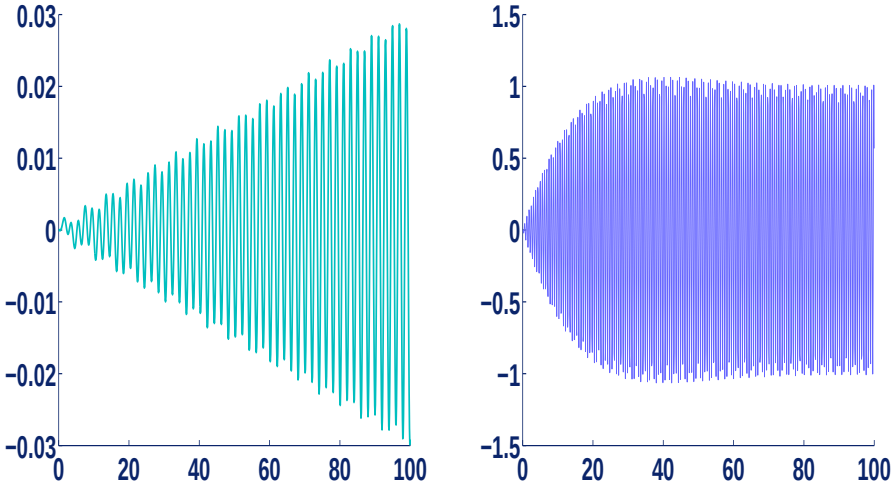

Figure 3.1.3: Global error of the fourth order Runge–Kutta method for the equation $y''(t) = -\omega y(t) - \cos(t)$, $0 \leq t \leq 100$, with $[1, 0]^\intercal$ initial conditions, step–size $h = \frac{1}{10}$, for $\omega = 10$ (left) and $\omega = 10^2$ (right).

PROOF: The statement follows from the notation on matrix asymptotics and Corollary (3.1.3). □

Employing the initial-value integrator (5.1.3), we present the *Filon*-type method for the systems of highly oscillatory ODEs,

$$\begin{aligned} \boldsymbol{y}_{n+1} &= \mathrm{e}^{hA_\omega}\boldsymbol{y}_n + \int_0^h \mathrm{e}^{(h-\tau)A_\omega}\boldsymbol{v}(t_n+\tau)\mathrm{d}\tau \\ &= \mathrm{e}^{hA_\omega}\boldsymbol{y}_n + Q_s^F[\boldsymbol{f}]. \end{aligned} \tag{3.2.2}$$

Here $Q_s^F = I[\boldsymbol{v}]$ stands for an approximation to $I[\boldsymbol{f}]$.

Example 3.2.1 Take the same integral $I_h[\boldsymbol{f}]$ as in the Example (3.1.1). For

$s = 2$, $t_1 = 0, t_2 = h$ and $\boldsymbol{f} = [f_1, f_2]^\intercal$ we derive the *Filon*-type method,

$$\begin{aligned} Q_s^F[\boldsymbol{f}] = I_h[\boldsymbol{v}] &= \int_0^h \mathrm{e}^{A_\omega(h-t)}\boldsymbol{v}(t)\mathrm{d}t \\ &= \left[\int_0^h \mathrm{e}^{A_\omega(h-t)}v_1(t)\mathrm{d}t\right]\boldsymbol{f}(0) + \left[\int_0^h \mathrm{e}^{A_\omega(h-t)}v_2(t)\mathrm{d}t\right]\boldsymbol{f}(h) \\ &+ \left[\int_0^h \mathrm{e}^{A_\omega(h-t)}v_3(t)\mathrm{d}t\right]\boldsymbol{f}'(0) + \left[\int_0^h \mathrm{e}^{A_\omega(h-t)}v_4(t)\mathrm{d}t\right]\boldsymbol{f}'(h). \end{aligned}$$

We note by passing that the computational cost is relatively cheap. The algorithm requires only some linear algebra once we have precomputed moments in $I_h[\boldsymbol{v}]$.

Theorem 3.2.3 *[Kha08b] Let $\theta_1, \theta_\nu \geq s$, $r = \sum_{l=1}^{\nu}\theta_l - 1$. Then r is the numerical order of the Filon-type method applied to the linear system,*

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

Proof: Suppose that $\boldsymbol{f} = \boldsymbol{v} + \boldsymbol{p}$, where $\boldsymbol{v}$ is an r-degree vector-valued polynomial approximation (e.g. Hermite, 3.2.1) to $\boldsymbol{f}$, with an approximation error

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

We can now derive the local error of our numerical solver,

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

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

Recall that

$$I[\boldsymbol{p}] = I[\boldsymbol{f}] - I[\boldsymbol{v}] = I[\boldsymbol{f}] - Q_s^F[\boldsymbol{f}] = \mathcal{O}(h^{r+1}), \tag{3.2.3}$$

which proves the order of the method. □

Theorem 3.2.4 *[Kha08b] The numerical solution (3.2.2) is convergent.*

PROOF: Presenting matrix A_ω in its Jordan normal form $J = P^{-1}A_\omega P$, we let

$$C_\omega = \{\|P\|\|P^{-1}\| : P^{-1}A_\omega P = J\},$$

and consider the following bounds for matrix exponential,

$$\|\mathrm{e}^{tA_\omega}\| = \|P\mathrm{e}^{tJ}P^{-1}\| \le C_\omega\|\mathrm{e}^{tJ}\|.$$

We would like to remind our reader that $\sigma(A_\omega) \subset \mathrm{i}\mathbb{R}$, which means that the norm of the matrix exponential is always bounded, $\mathrm{e}^{tJ} = \mathcal{O}(\mathbf{1})$. In other words, for a fixed value of parameter ω, the convergence of the numerical scheme to the exact solution follows from the estimate of the residual term,

$$\|I[\boldsymbol{p}]\| \le \frac{C_\omega h}{r!}\|p_r(\tau)\|\|\boldsymbol{f}^{(r)}\|,$$

as step-size h tends to zero.

□

Note that the method requires information only about the function values and its derivatives at the end points. Figures 3.2.1 and 3.2.2 offer some numerical examples, where a step size h is fixed and ω increases. The examples demonstrate a gain in accuracy with the increase of ω. Comparison will note that the *Filon*-type method performs better than the *asymptotic* method, although both methods are of the same asymptotic order. It is evident now that for a larger step-size $h = \frac{1}{4}$ than that assumed with the asymptotic method ($h = \frac{1}{10}$) the accuracy of approximation improves as $h\omega \gg 1$.

We can compare our solutions with MATLAB solvers, presented in Figure 3.2.5. To achieve better results with MATLAB we set it to AbsTol=ReTol= 10^{-8}. Accuracy decreases for the solver ode15s while remaining the same for ode113. Both methods work with variable step size, but taking an average for $\omega = 100$ it is $h \approx \frac{1}{186}$ for ode15s and $h \approx \frac{1}{60}$ for ode113, reducing to the exceptionally small values for $\omega = 10^4$ of $h \approx 5 \times 10^{-4}$ in ode15s and $h \approx 10^{-3}$ in ode113, which is in no way comparable with $h = \frac{1}{4}$ of the *Filon*-type method. The logarithmic error in Figure 3.2.4 describes both numerical and asymptotic analysis of the method for increasing ω.

These considerations leave us at a point where the connections between [IN05] and the present work are evident. It follows from the spectral decomposition of the matrix A_ω that the factor $\mathrm{e}^{\mathrm{i}\lambda_k}f$ appears in the fundamental

matrix in the solutions of both linear and non linear systems of highly oscillatory ODEs, and provides valid reasons to extend described methods for the given setting.

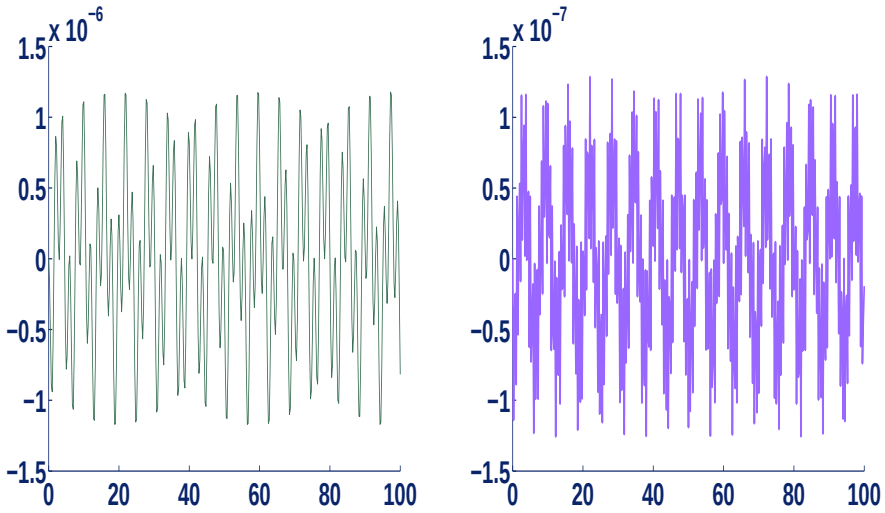

Figure 3.2.1: Global error of the *Filon*-type method Q_2^F with end points only and multiplicities all 2, for the equation $y''(t) = -\omega y(t) - \cos(t)$, $0 \leq t \leq 100$, with $[1, 0]^\intercal$ initial conditions and step-size $h = \frac{1}{4}$ for $\omega = 10$ (left figure) and $\omega = 10^2$ (right figure)

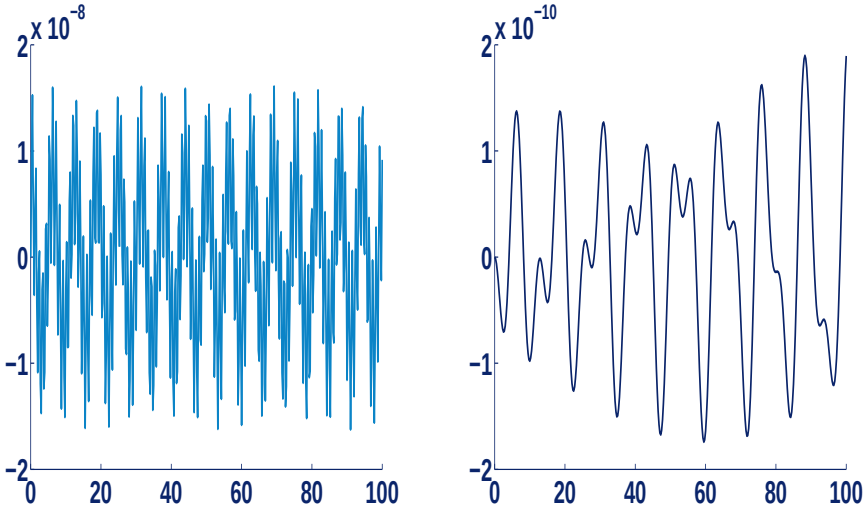

Figure 3.2.2: Global error of the *Filon*-type method Q_2^F with end points only and multiplicities all 2, for the equation $y''(t) = -\omega y(t) - \cos(t)$, $0 \leq t \leq 100$, with $[1, 0]^\intercal$ initial conditions and step-size $h = \frac{1}{4}$ for $\omega = 10^3$ (left figure) and $\omega = 10^4$ (right figure).

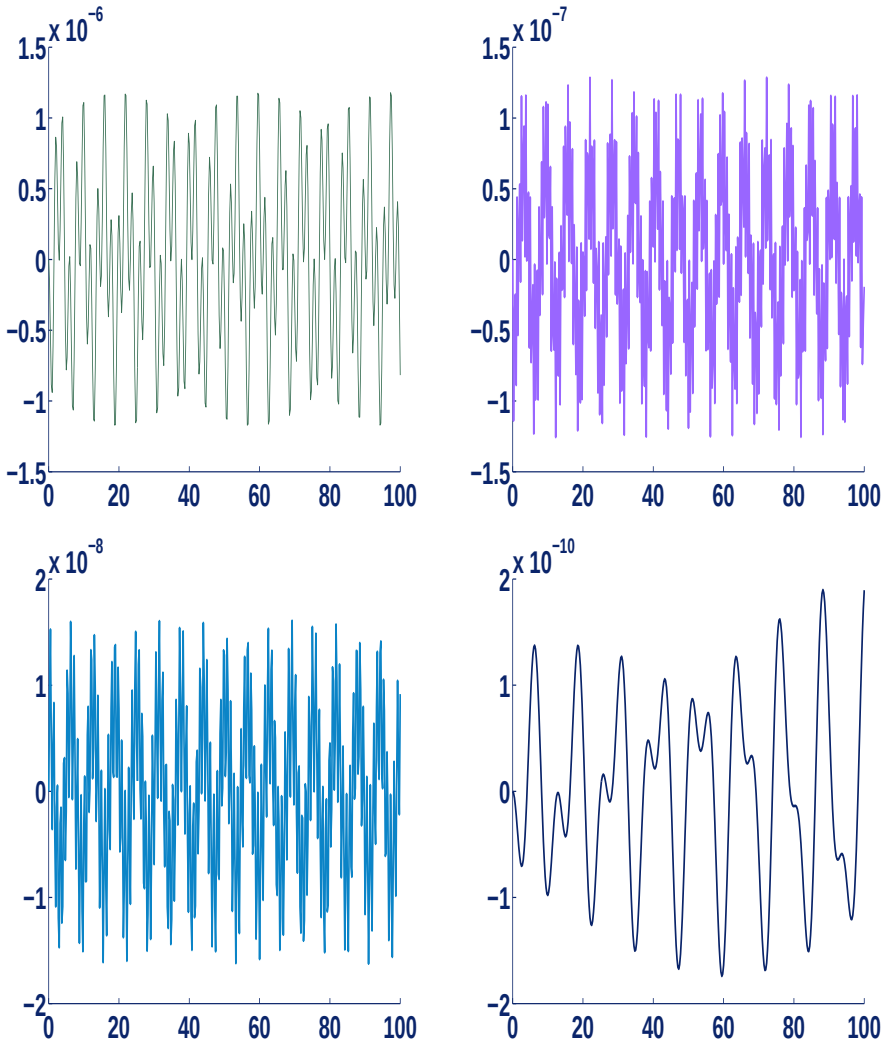

Figure 3.2.3: Global error of the *Filon*-type method Q_2^F with end points only and multiplicities all 2, for the equation $y''(t) = -\omega y(t) - \cos(t)$, $0 \leq t \leq 100$, with $[1, 0]^\intercal$ initial conditions and step-size $h = \frac{1}{4}$ for $\omega = 10$ (top figure, left) and $\omega = 10^2$ (top figure, right), $\omega = 10^3$ (left, bottom figure) and $\omega = 10^4$ (right, bottom figure).

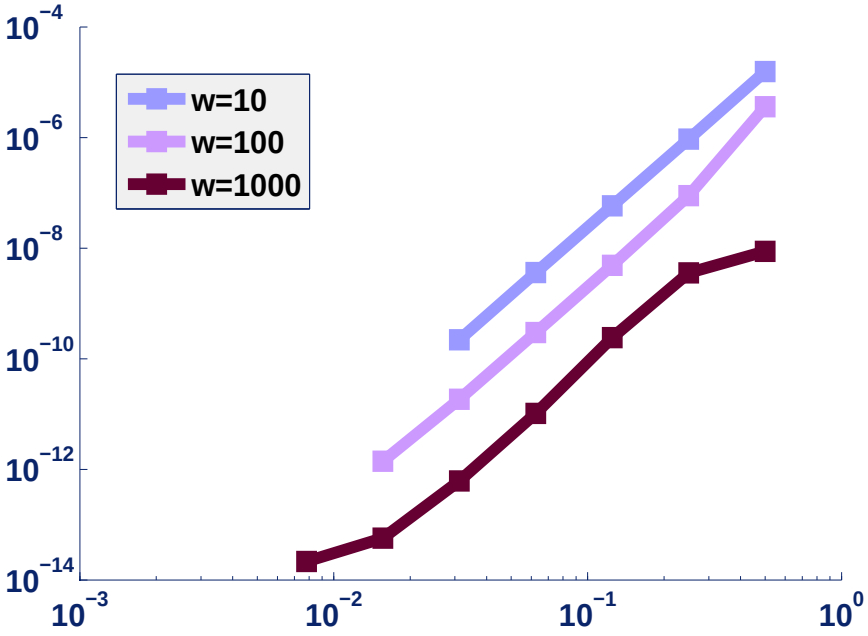

Figure 3.2.4: Logarithmic error (y-axis) and the step-size (x-axis) of the *Filon*-type method Q_2^F, with endpoints only and multiplicities all 2, for the equation $y''(t) = -\omega y(t) - \cos(t)$, with initial values in $[1, 0]^\intercal$.

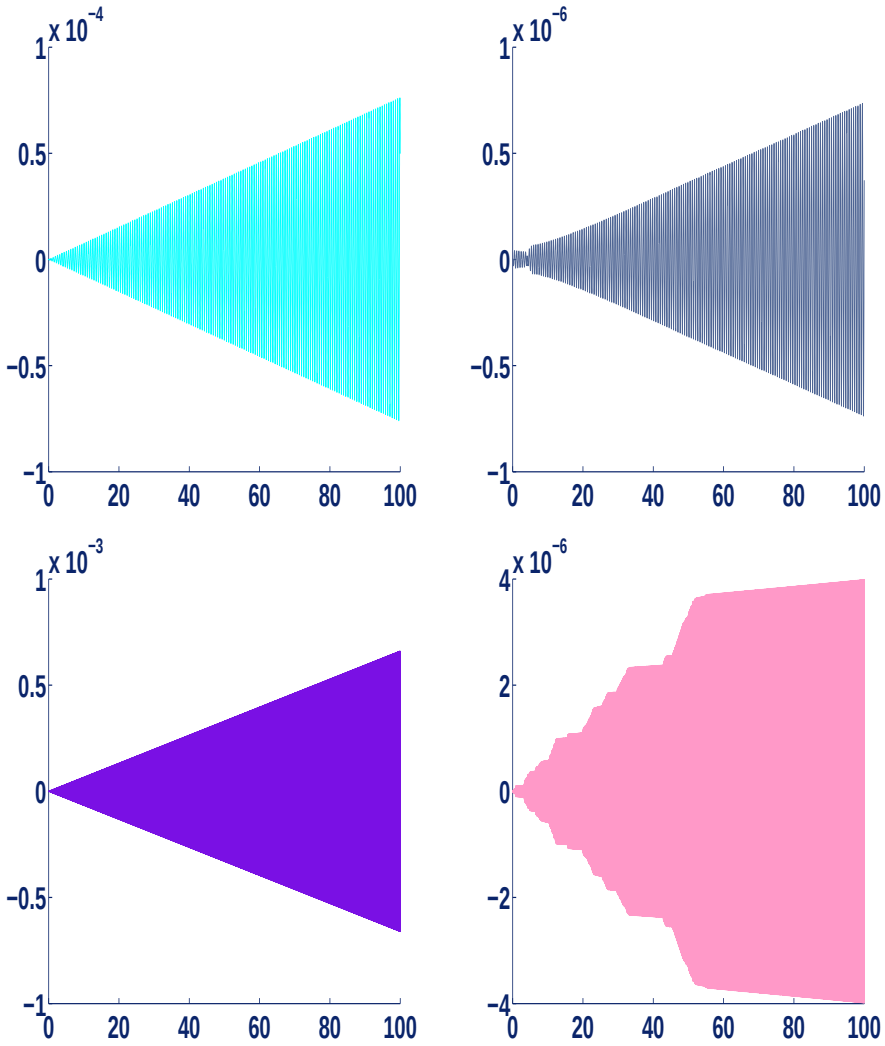

Figure 3.2.5: Global error of MATLAB ode15s routine (top figure, left) and ode113 routine (top figure, right) set to RelTol= $1e-08$, AbsTol= $1e-08$, for the equation $y''(t) = -\omega y(t) - \cos(t)$, $0 \leq t \leq 100$, with $[1,0]^\intercal$ initial conditions and $\omega = 10^2$; the same solvers with the same properties and $\omega = 10^4$ (two figures in the bottom respectively).

Chapter 4

The FM methods

4.1 The matrix linear ODEs

In this chapter we present a new method from [Kha09a] for solving *Lie*-type equations $X'_\omega = A_\omega(t)X_\omega$, $X_\omega(0) = I$. The solution to the equations of this type have the following representation $X_\omega = \exp(\Omega)$. Here ω stands for an infinite *Magnus* series of integral commutators. We assume that the matrix A_ω has large imaginary spectrum and ω is a real parameter describing the frequency of oscillation. The novel method, called the *FM* method, combines the *Magnus* method, which is based on iterative techniques to approximate Ω, and the *Filon*-type method, an efficient quadrature rule for solving oscillatory integrals. We show that the *FM* method has superior performance compared to the classical *Magnus* method when applied to oscillatory differential equations.

We proceed with the matrix ordinary differential equation

$$X'_\omega = A_\omega X_\omega, \qquad X_\omega(0) = I, \qquad X_\omega = \mathrm{e}^{\Omega}, \tag{4.1.1}$$

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

$$\begin{aligned}\Omega(t) = &\int_0^t A_\omega(t)dt \\ &+\frac{1}{2}\int_0^t [A_\omega(\tau), \int_0^\tau A_\omega(\xi)d\xi]d\tau \\ &+\frac{1}{4}\int_0^t [A_\omega(\tau), \int_0^\tau [A_\omega(\xi), \int_0^\xi A_\omega(\zeta)d\zeta]d\xi]d\tau \\ &+\frac{1}{12}\int_0^t [[A_\omega(\tau), \int_0^\tau A_\omega(\xi)d\xi], \int_0^\tau A_\omega(\zeta)d\zeta]d\tau \\ &+\cdots .\end{aligned}$$

We make the following assumptions: $A_\omega(t)$ is a smooth matrix-valued function, the spectrum $\sigma(A_\omega)$ of the matrix A_ω has large imaginary eigenvalues and that $\omega \gg 1$ is a real parameter describing frequency of oscillation.

It has been shown by *Hausdorff*, [Hau06], that the solution of the linear matrix equation in (4.1.1) is a matrix exponential $X_\omega(t) = \mathrm{e}^{\Omega(t)}$, where $\Omega(t)$ satisfies the following non-linear differential equation,

$$\Omega' = \sum_{j=0}^{\infty} \frac{B_j}{j!}\mathrm{ad}_\omega^j(A_\omega) = \mathrm{dexp}_\Omega^{-1}(A_\omega(t)), \quad \Omega_0 = 0, \tag{4.1.2}$$

as long as $\|\Omega(t)\| < \pi$, to insure that the operator $\mathrm{dexp}_\Omega^{-1}(t)$ is invertible. Here B_j are Bernoulli numbers and the adjoint operator is defined as

$$\begin{aligned}\mathrm{ad}_\Omega^0(A_\omega) &= A_\omega \\ \mathrm{ad}_\Omega(A_\omega) &= [\Omega, A_\omega] = \Omega A_\omega - A_\omega\Omega \\ \mathrm{ad}_\Omega^{j+1}(A_\omega) &= [\Omega, \mathrm{ad}_\Omega^j A_\omega].\end{aligned}$$

Later it was observed by *W. Magnus*, [Mag54], that solving equation (4.1.2) with Picard iteration it is possible to obtain an infinite recursive series for Ω and then the truncated expansion can be used in approximation of Ω.

Magnus methods preserve peculiar geometric properties of the solution, ensuring that if X_ω is in matricial Lie group G and A_ω is in associated Lie algebra g of G, then the numerical solution after discretization stays on the manifold. Moreover, *Magnus* methods preserve time-symmetric properties of

the solution after discretization, for any $a > b$, $X_\omega(a,b)^{-1} = X_\omega(b,a)$ yields $\Omega(a,b) = -\Omega(b,a)$. These properties appear to be valuable in applications.

Employing the *Magnus* method to solve highly oscillatory differential equations we develop it in combination with appropriate quadrature rules, such as *Filon*-type methods, proved to be more efficient for oscillatory equations than for example classical *Gaussian* quadrature.

Below we remind our reader the *Filon*-type method and the *asymptotic* method, applied to approximate highly oscillatory integrals of the form

$$I[f] = \int_a^b f(x)\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x. \tag{4.1.3}$$

The *asymptotic* method provides theoretical background for the *Filon*-type method. Suppose $f, g \in C^\infty$ are smooth, g is strictly monotone in $[a,b], a \leq x \leq b$ and the frequency is $\omega \gg 1$.

We interpolate function f in (4.1.3) at chosen node points. For instance, take Hermite interpolation

$$\tilde{v}(x) = \sum_{l=1}^{\nu}\sum_{j=0}^{\theta_l-1} \alpha_{l,j}(x) f^{(j)}(c_l), \tag{4.1.4}$$

which satisfies $\tilde{v}^{(j)}(c_l) = f^{(j)}(c_l)$, at node points $a = c_1 < c_2 < ... < c_\nu = b$, with $\theta_1, \theta_2, ..., \theta_\nu \geq 1$ associated multiplicities, $j = 0, 1, ..., \theta_l - 1, l = 1, 2, ..., \nu$ and $r = \sum_{l=1}^{\nu} \theta_l - 1$ being the order of approximation polynomial. Then, for the *Filon*-type method, by definition,

$$Q_s^F[f] = I[\tilde{v}] = \int_a^b \tilde{v}(x)\mathrm{e}^{i\omega g(x)}\mathrm{d}x = \sum_{l=1}^{\nu}\sum_{j=0}^{\theta_l-1} b_{l,j}(w) f^{(j)}(c_l),$$

where

$$b_{l,j} = \int_0^1 \alpha_{l,j}(x)\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x, \qquad j = 0, 1, ..., \theta_l - 1, \qquad l = 1, 2, ..., \nu.$$

The *Filon*-type method has the same asymptotic order as the *asymptotic* method. For formal proof of the asymptotic order of the *Filon*-type method for univariate integrals, we refer the reader to [IN05] and for matrix and

vector-valued functions we refer to [Kha08b]. The following theorem from [Kha08b] is on the numerical order of the *Filon*-type method. It was also shown in [Kha08b] that the numerical solution obtained after discretization of the integral with *Filon*-type method is convergent.

Theorem 4.1.1 *[MK][Kha08b] Let* $s = \min\{\theta_1, \theta_\nu\}$. *Then the numerical order of the Filon-type method is equal to* $r = \sum_{l=1}^{\nu} \theta_l - 1$.

Adding more internal interpolation points leads to the decay of the leading error constant, resulting in a marked improvement in the accuracy of approximation. However, interpolating function f at internal points does not contribute to the higher asymptotic order of the *Filon*-type method.

4.2 The Magnus method

In this section we focus on *Magnus* methods for approximation of a matrix-valued function X_ω in (4.1.1). There is a large list of publications available on the *Lie*-group methods, here we refer to some of them: [BCR00], [CG93], [Ise09a], [Ise02a], [MK98], [OM97], [Zan96].

Currently, the most general theorem on the existence and convergence of the *Magnus* series is proved for a bounded linear operator $A(t)$ in a Hilbert space, [Cas07]. The following theorem gives us sufficient condition for convergence of the *Magnus* series, extending Theorem 3 from [MN08], where the same results are stated for real matrices.

Theorem 4.2.1 *(F. Casas, [Cas07]) Consider the differential equation* $X' = A(t)X$ *defined in a Hilbert space* $\mathcal{H}$ *with* $X(0) = I$, *and let* $A(t)$ *be a bounded linear operator on* $\mathcal{H}$. *Then, the Magnus series* $\Omega(t)$ *in (4.1.2) converges in the interval* $t \in [0, T)$ *such that*

$$\int_0^T \|A(\tau)\| \mathrm{d}\tau < \pi$$

and the sum $\Omega(t)$ *satisfies* $\exp\ \Omega(t) = X(t)$.

For recent results on the error bounds for the Magnus method for Schrödinger equation the author refers to work by M. Hochbruck and C. Lubich available

in [HL03]. The authors in [HL03] considered Schrödinger equation with a time-dependant Hamiltonian

$$\mathrm{i}\frac{\mathrm{d}\psi}{\mathrm{d}t} = H(t)\psi, \quad \psi(t_0) = \psi_0.$$

Here $H(t)$ is a finite dimensional Hermitian operator and as a result of discretization of an unbounded operator, typically a sum of discretized negative Laplacian and a time-dependent potential, $H(t)$ my have an arbitrary large norm. In the paper authors provide asymptotically sharp error bounds for Magnus integrators in the framework applied to time-dependent Schrödinger equation where there is no restrictions on smallness nor bounds on $h\|H(t)\|$, h stands for a step-size of a numerical integrator.

Given the representation for $\Omega(t)$ in (4.1.2), the numerical task on evaluating the commutator brackets is fairly simple, [BCR00], [Ise09a], [Ise02a]. For example, choosing symmetric grid $c_1, c_2, ..., c_\nu$, suppose taking Gaussian points with respect to $\frac{1}{2}$, consider set $\{A_1, A_2, ..., A_\nu\}$, with $A_k = hA(t_0 + c_k h), k = 1, 2, ..., \nu$. Linear combinations of this basis form an adjoint basis $\{B_1, B_2, ..., B_\nu\}$, with

$$A_k = \sum_{l=1}^{\nu} (c_k - \frac{1}{2})^{l-1} B_l, \quad k = 1, 2, ..., \nu.$$

In this basis the six-order method, with Gaussian points $c_1 = \frac{1}{2} - \frac{\sqrt{15}}{10}, c_2 = \frac{1}{2}, c_3 = \frac{1}{2} + \frac{\sqrt{15}}{10}$, $A_k = hA(t_0 + c_k h)$, is

$$\begin{aligned}\Omega(t_0 + h) \approx B_1 + \frac{1}{12}B_3 - \frac{1}{12}[B_1, B_2] + \frac{1}{240}[B_2, B_3] \\ + \frac{1}{360}[B_1, [B_1, B_3]] - \frac{1}{240}[B_2, [B_1, B_2]] + \frac{1}{720}[B_1[B_1, [B_1, B_2]]],\end{aligned}$$

where

$$B_1 = A_2, \quad B_2 = \frac{\sqrt{15}}{3}(A_3 - A_1), \quad B_3 = \frac{10}{3}(A_3 - 2A_2 + A_1).$$

This can be reduced further and written in a more compact manner [Ise02a], [Ise09a],

$$\Omega(t_0 + h) \approx B_1 + \frac{1}{12}B_3 + P_1 + P_2 + P_3,$$

where

$$P_1 = [B_2, \frac{1}{12}B_1 + \frac{1}{240}B_3],$$
$$P_2 = [B_1, [B_1, \frac{1}{360}B_3 - \frac{1}{60}P_1]],$$
$$P_3 = \frac{1}{20}[B_2, P_1].$$

A more profound approach taking Taylor expansion of $A(t)$ around the point $t_{1/2} = t_0 + \frac{h}{2}$ was introduced in [BCR00],

$$A(t) = \sum_{i=0}^{\infty} a_i (t - t_{1/2})^i, \quad \text{with} \quad a_i = \frac{1}{i!} \frac{\mathrm{d}^n A(t)}{\mathrm{d}t^i}|_{t=t_{1/2}}.$$

This can be substituted in the univariate integrals of the form

$$B^{(i)} = \frac{1}{h^{i+1}} \int_{-h/2}^{h/2} t^i A\left(t + \frac{h}{2}\right) \mathrm{d}t, \quad i = 0, 1, 2, ...$$

to obtain a new basis

$$B^{(0)} = a_0 + \frac{1}{12}h^2 a_2 + \frac{1}{80}h^4 a_4 + + \frac{1}{448}h^6 a_6 ...$$
$$B^{(1)} = \frac{1}{12}h a_1 + \frac{1}{80}h^3 a_3 + \frac{1}{448}h^5 a_5 + ...$$
$$B^{(2)} = \frac{1}{12}a_0 + \frac{1}{80}h^2 a_2 + \frac{1}{448}h^4 a_4 + \frac{1}{2304}h^6 a_6 + ...$$

In these terms a second order method will look as follows, [BCR00], $\mathrm{e}^{\Omega} = \mathrm{e}^{hB^{(0)}} + \mathcal{O}(h^3)$. Whereas for a six-order method, [BCR00], $\Omega = \sum_{i=1}^{4} \tilde{\Omega}_i + \mathcal{O}(h^7)$, one needs to evaluate only four commutators, [BCR00],

$$\tilde{\Omega}_1 = hB^{(0)}$$
$$\tilde{\Omega}_2 = h^2[B^{(1)}, \frac{3}{2}B^{(0)} - 6B^{(2)}]$$
$$\tilde{\Omega}_3 + \tilde{\Omega}_4 = h^2[B^{(0)}, [B^{(0)}, \frac{1}{2}hB^{(2)} - \frac{1}{60}\tilde{\Omega}_2]] + \frac{3}{5}h[B^{(1)}, \tilde{\Omega}_2].$$

Numerical behaviour of the fourth and six order classical *Magnus* method is illustrated in Figures 4.2.1, 4.2.2 and 4.2.3, and 4.2.4, 4.2.5 and 4.2.6,

respectively. The method is applied to solve Airy equation $y''(t) = -ty(t)$ with $[1, 0]^\intercal$ initial conditions, $t \in [0, 1000]$, for varies step-sizes, $h = \frac{1}{4}$, $h = \frac{1}{10}$ and $h = \frac{1}{25}$. Comparison shows that for a bigger interval steps h both fourth and six order methods give similar results, as illustrated in Figures 4.2.1, 4.2.2, 4.2.3 and 4.2.6. However, for smaller steps six order *Magnus* method has a more rapid improvement in approximation compared to a fourth order method, Figures 4.2.3 and 4.2.6.

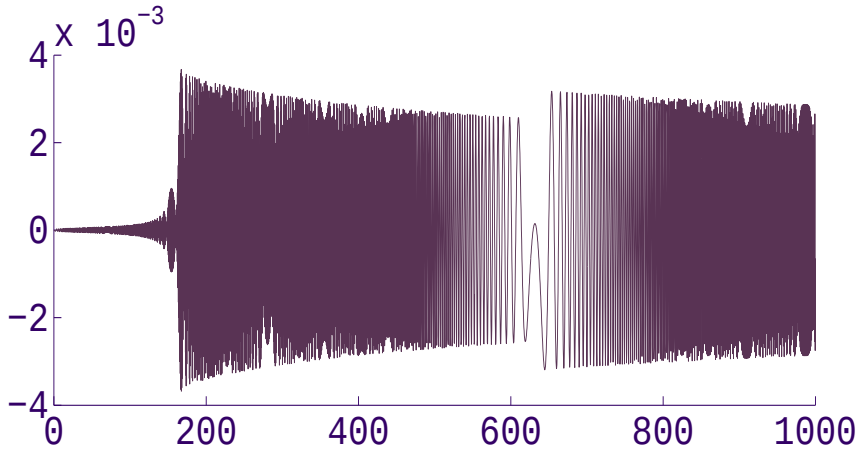

Figure 4.2.1: Global error of the fourth order *Magnus* method for the Airy equation $y''(t) = -ty(t)$ with $[1, 0]^\intercal$ initial conditions, $0 \leq t \leq 1000$ and step-size $h = \frac{1}{4}$.

In current work we present an alternative method to solve equations of the kind (4.1.1), [Kha09a]. We apply the *Filon* quadrature to evaluate integral commutators for Ω and then solve the matrix exponential X_ω with the *Magnus* method or the *modified Magnus* method. The combination of the *Filon*-type methods and the *Magnus* methods forms the *FM* method, presented in the next section. Application of the *FM* method to solve systems of highly oscillatory ordinary differential equation can be found in [Kha09b], [Kha09a].

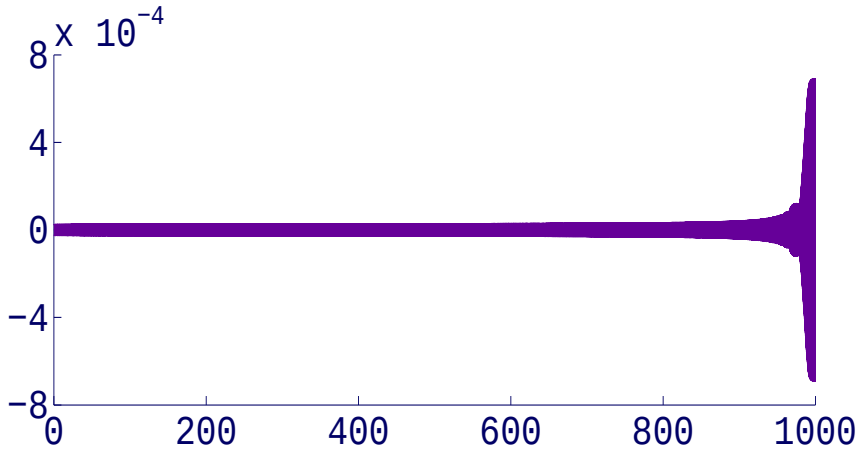

Figure 4.2.2: Global error of the fourth order *Magnus* method for the Airy equation $y''(t) = -ty(t)$ with $[1, 0]^\intercal$ initial conditions, $0 \leq t \leq 1000$ and step-size $h = \frac{1}{10}$.

4.3 The modified Magnus method

In this section we continue our discussion on the solution of the matrix differential equation

$$X'_\omega = A_\omega(t)X_\omega, \quad X_\omega(0) = I, \quad X_\omega = \exp(\Omega). \tag{4.3.1}$$

It was shown in [Ise02c] that one can achieve better accuracy in approximation of the fundamental matrix X_ω, if one solves (4.3.1) at each time step locally for a constant matrix A_ω.

We commence from a linear oscillator studied in [Ise02c],

$$\boldsymbol{y}' = A_\omega(t)\boldsymbol{y}, \quad \boldsymbol{y}(0) = \boldsymbol{y}_0.$$

We also assume that the spectrum of the matrix $A_\omega(t)$ has large imaginary values. Introducing local change of variables at each mesh point, we write the solution in the form,

$$\boldsymbol{y}(t) = \mathrm{e}^{(t-t_n)A_\omega(t_n+\frac{1}{2}h)}\boldsymbol{x}(t-t_n), \qquad t \geq t_n,$$

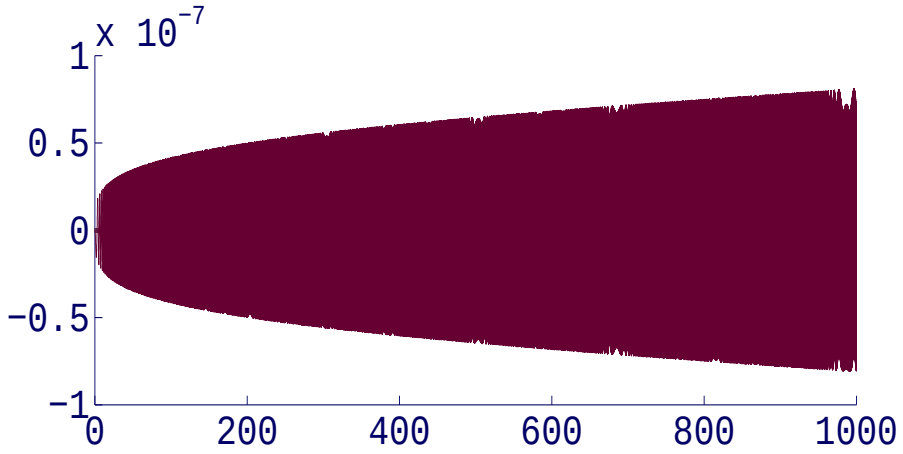

Figure 4.2.3: Global error of the fourth order *Magnus* method for the Airy equation $y''(t) = -ty(t)$ with $[1,0]^\intercal$ initial conditions, $0 \leq t \leq 1000$ and step-size $h = \frac{1}{25}$.

and observe that

$$\boldsymbol{x}' = B(t)\boldsymbol{x}, \qquad \boldsymbol{x}(0) = \boldsymbol{y}_n,$$

with

$$B(t) = \mathrm{e}^{-tA_\omega(t_n+\frac{1}{2}h)}[A_\omega(t_n+t)-A_\omega(t_{n+\frac{1}{2}})]\mathrm{e}^{tA_\omega(t_n+\frac{1}{2}h)}, \quad \text{where} \quad t_{n+\frac{1}{2}} = t_n+\frac{h}{2}.$$

The *modified Magnus* method is defined as a local approximation of the solution vector $\boldsymbol{y}$ by solving

$$\boldsymbol{x}' = B(t)\boldsymbol{x}, \qquad \boldsymbol{x}(0) = \boldsymbol{y}_n,$$

with classical *Magnus* method. This approximation results in the following algorithm,

$$\begin{aligned} \boldsymbol{y}_{n+1} &= \mathrm{e}^{hA_\omega(t_n+h/2)}\boldsymbol{x}_n, \\ \boldsymbol{x}_n &= \mathrm{e}^{\tilde{\Omega}_s}\boldsymbol{y}_n. \end{aligned}$$

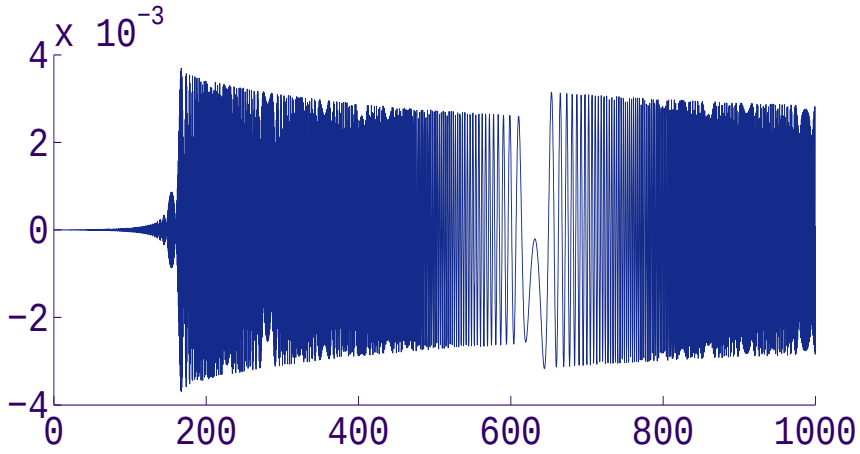

Figure 4.2.4: Global error of the six order *Magnus* method for the Airy equation $y''(t) = -ty(t)$ with $[1,0]^\intercal$ initial conditions, $0 \leq t \leq 1000$ and step-size $h = \frac{1}{4}$.

Performance of the *modified Magnus* method is better than that of the classical *Magnus* method due to a number of reasons. Firstly, the fact that the matrix B is small, $B(t) = \mathcal{O}(t - t_{n+\frac{1}{2}})$, contributes to higher order correction to the solution. Secondly, the order of the *modified Magnus* method increases from $p = 2s$ to $p = 3s + 1$, [Ise02b].

4.4 The FM method

In this section we present a novel *FM* method for solving matrix ODEs, [Kha09a]. The method combines ideas on Filon methods and Lie group methods for solving matrix exponential with nested integral commutators.

Consider the *Airy*-type equation

$$y''(t) + g(t)y(t) = 0, \quad g(t) > 0 \quad \text{for} \quad t > 0, \quad \text{and} \quad \lim_{t\to\infty} g(t) = +\infty.$$

Replacing the second order differential equation by the first order system, we

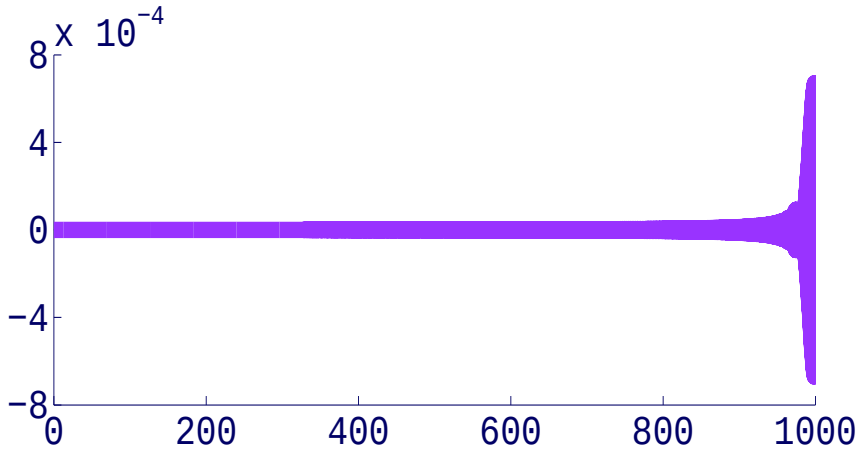

Figure 4.2.5: Global error of the six order *Magnus* method for the Airy equation $y''(t) = -ty(t)$ with $[1,0]^\intercal$ initial conditions, $0 \leq t \leq 1000$ and step-size $h = \frac{1}{10}$.

obtain $\boldsymbol{y}' = A_\omega(t)\boldsymbol{y}$, where

$$A_\omega(t) = \begin{pmatrix} 0 & 1 \\ -g(t) & 0 \end{pmatrix}.$$

Due to a large imaginary spectrum of the matrix A_ω, this *Airy*-type equation is rapidly oscillating. We apply the *modified Magnus* method to solve the system $\boldsymbol{y}' = A_\omega(t)\boldsymbol{y}$,

$$\boldsymbol{y}_{n+1} = \mathrm{e}^{hA_\omega(t_n+h/2)}\mathrm{e}^{\tilde{\Omega}_n}\boldsymbol{y}_n.$$

Here the integral commutators in $\tilde{\Omega}_n$ are computed according to the rules of the *Filon* quadrature. This results in highly accurate numerical method, the *FM* method. Taking into account that the entries of the matrix $B(t)$ are likely to be oscillatory, the advantage of the *Filon*-type method is evident.

In the example below we provide a more detailed evaluation of the *FM* method applied to solve the *Airy*-type equation $\boldsymbol{y}' = A_\omega(t)\boldsymbol{y}$.

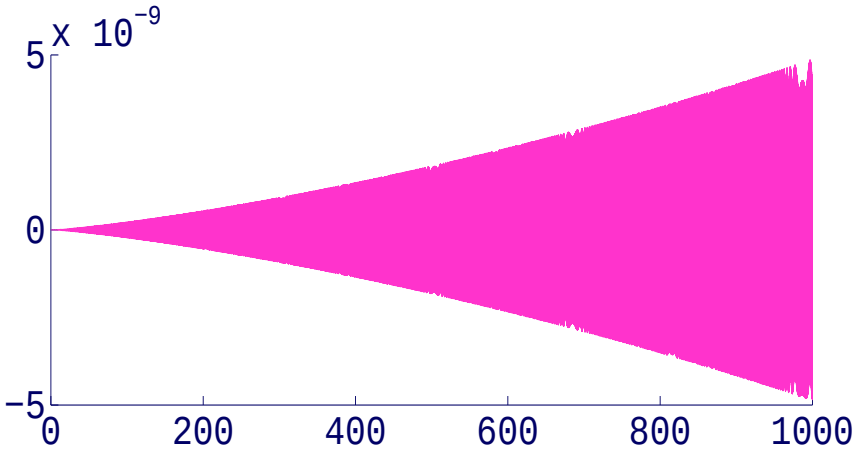

Figure 4.2.6: Global error of the six order *Magnus* method for the Airy equation $y''(t) = -ty(t)$ with $[1,0]^\intercal$ initial conditions, $0 \leq t \leq 1000$ and step-size $h = \frac{1}{25}$.

Example 4.4.1 *Once we have obtained the representation for $\tilde{\Omega}_n$, the commutator brackets are now formed by the matrix $B(t)$. It is possible to reduce cost of evaluation of the matrix $B(t)$ by simplifying it, [Ise04a]. Denote $q = \sqrt{g(t_n + \frac{1}{2}h)}$ and $v(t) = g(t_n + t) - g(t_n + \frac{1}{2}h)$. Then,*

$$\begin{aligned} B(t) &= v(t) \begin{bmatrix} (2q)^{-1} \sin 2qt & q^{-2} \sin^2 qt \\ -\cos^2 qt & -(2q)^{-1} \sin 2qt \end{bmatrix} \\ &= v(t) \begin{bmatrix} q^{-1} \sin qt \\ -\cos qt \end{bmatrix} \begin{bmatrix} \cos qt & q^{-1} \sin qt \end{bmatrix}, \end{aligned}$$

and for the product

$$B(t)B(s) = v(t)v(s) \frac{\sin q(s-t)}{q} \begin{bmatrix} q^{-1} \sin qt \\ -\cos qt \end{bmatrix} \begin{bmatrix} \cos qs & q^{-1} \sin qs \end{bmatrix}.$$

It was shown in [Ise04a] that

$$\|B(t)\| = \cos^2 \omega t + \frac{\sin^2 \omega t}{\omega^2} \quad \text{and} \quad B(t) = \mathcal{O}(t - t_{n+\frac{1}{2}}).$$

We can now estimate integral

$$\int_0^h \|B(t)\|dt = \frac{h}{2}(1+\frac{1}{\omega^2}) + \frac{\sin 2\omega h}{2\omega}(1-\frac{1}{\omega^2}) := q(h,\omega).$$

To meet requirements stated in Theorem 4.2.1 we allow

$$q(h,\omega) \leq \pi.$$

In other words, to satisfy Theorem 4.2.1 we obtain the following condition on the step-size h,

$$h \leq \frac{2\pi\omega^3 - \omega^2 + 1}{\omega(\omega^2+1)}.$$

Given the compact representation of the matrix $B(t)$ with oscillatory entries, we solve $\Omega(t)$ with a *Filon*-type method. We approximate functions in $B(t)$ by a polynomial $\tilde{v}(t)$, for example Hermite polynomial (4.1.4), as in classical *Filon*-type method. Furthermore, in our approximation we use end points only, although the method is general and more nodes of approximation can be required.

In Figure 4.4.1 we present the global error of the fourth order *modified Magnus* method with exact integrals for the Airy equation $y''(t) = -ty(t)$ with $[1,0]^\intercal$ initial conditions, $0 \leq t \leq 2000$ time interval and step-size $h = \frac{1}{5}$. This can be compared with the global error of the *FM* method applied to the same equation with exactly the same conditions and step-size, Figure 4.4.2. In Figures 4.4.3 and 4.4.4 we compare the fourth order classical *Magnus* method with a remarkable performance of the fourth order *FM* method, applied to the *Airy* equation with a large step-size equal to $h = \frac{1}{2}$. While in Figures 4.4.5 and 4.4.6 we show the solution for the *Airy* equation with the fourth order *FM* method with step-sizes $h = \frac{1}{4}$ and $h = \frac{1}{10}$ respectively.

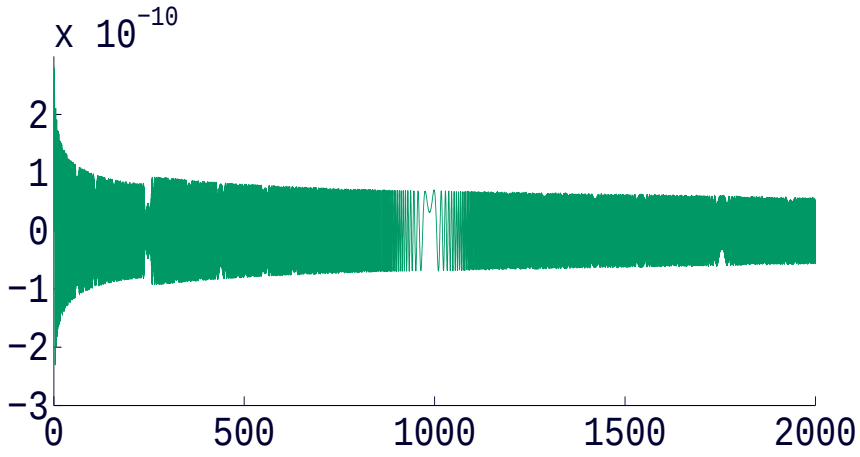

Figure 4.4.1: Global error of the fourth order *Modified Magnus* method with exact evaluation of integral commutators for the Airy equation $y''(t) = -ty(t)$ with $[1, 0]^\intercal$ initial conditions, $0 \leq t \leq 2000$ and step-size $h = \frac{1}{5}$.

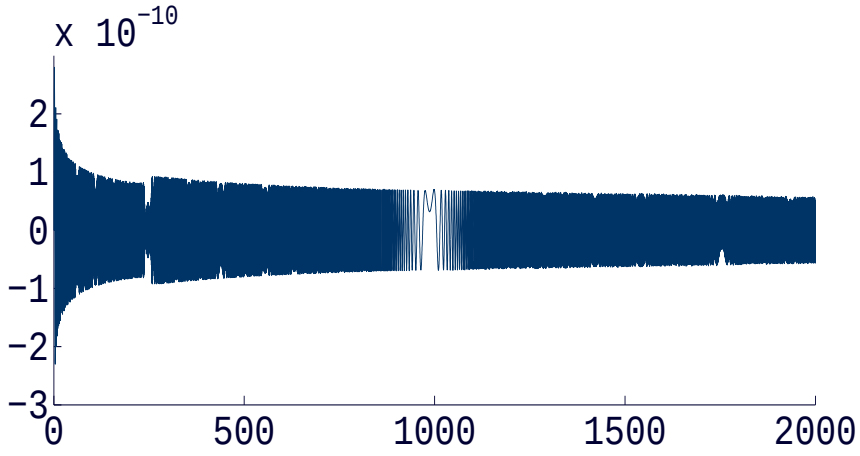

Figure 4.4.2: Global error of the fourth order *FM* method with end points only and multiplicities all 2 for the Airy equation $y''(t) = -ty(t)$ with $[1, 0]^\intercal$ initial conditions, $0 \leq t \leq 2000$ and step-size $h = \frac{1}{5}$.

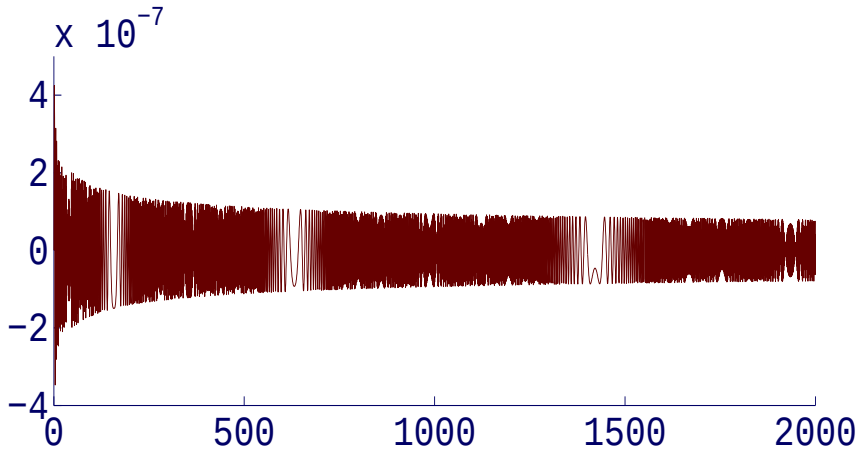

Figure 4.4.3: Global error of the fourth order *FM* method with end points only and multiplicities all 2 for the Airy equation $y''(t) = -ty(t)$ with $[1, 0]^\intercal$ initial conditions, $0 \leq t \leq 2000$ and step-size $h = \frac{1}{2}$.

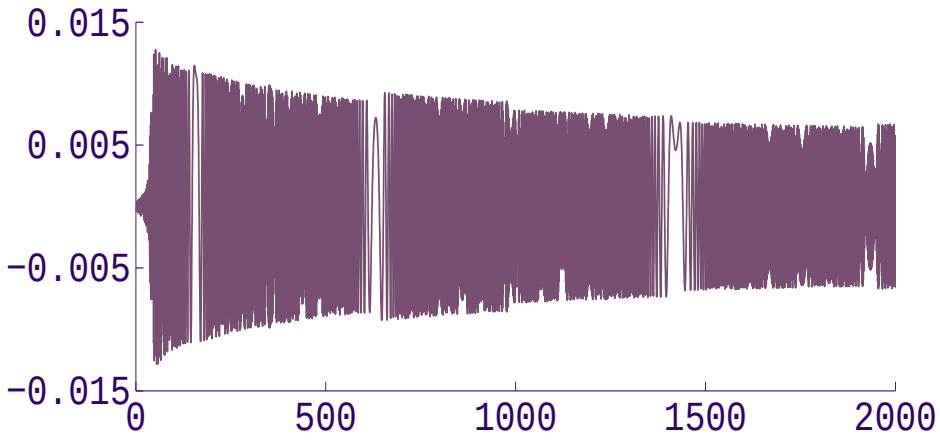

Figure 4.4.4: Global error of the fourth order *Magnus* method for the Airy equation $y''(t) = -ty(t)$ with $[1, 0]^\intercal$ initial conditions, $0 \leq t \leq 2000$ and step-size $h = \frac{1}{2}$.

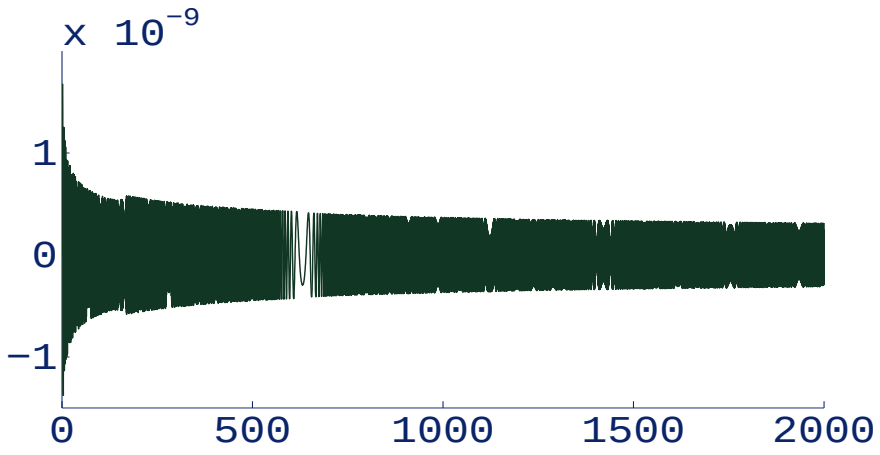

Figure 4.4.5: Global error of the fourth order *FM* method with end points only and multiplicities all 2, for the Airy equation $y''(t) = -ty(t)$ with $[1, 0]^\intercal$ initial conditions, $0 \leq t \leq 2000$ and step-size $h = \frac{1}{4}$.

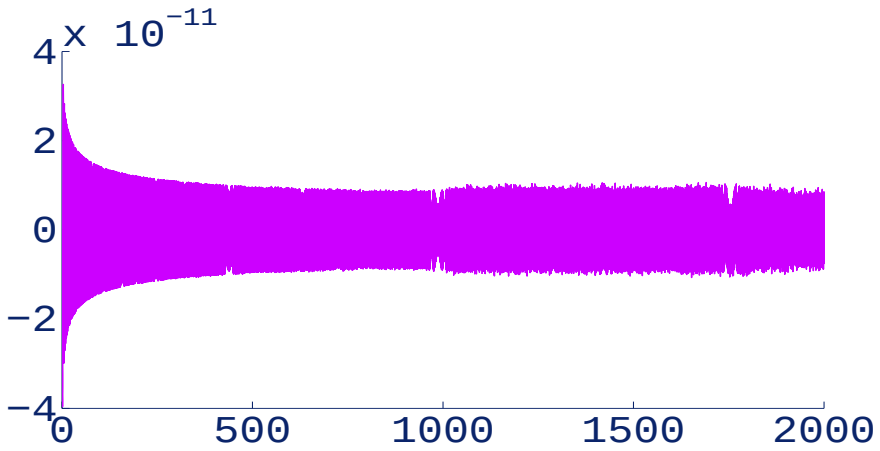

Figure 4.4.6: Global error of the fourth order *FM* method with end points only and multiplicities all 2, for the Airy equation $y''(t) = -ty(t)$ with $[1, 0]^\intercal$ initial conditions, $0 \leq t \leq 2000$ and step-size $h = \frac{1}{10}$.

Chapter 5

Highly oscillatory linear systems with variable coefficients

5.1 The asymptotic method

In this chapter we introduce our reader further applications of the FM methods. In particular, we develop the FM method for solving highly oscillatory systems of ODEs with a time-dependent matrix, [Kha09b], [Kha09a]. We solve the matrix exponential in Lie groups applying Magnus method. For discretizing nested commutators we apply Filon quadrature and develop the FM method.

We commence from a system of ordinary differential equations written in a vector form,

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

where A_ω is a non-singular matrix with large imaginary eigenvalues, $\sigma(A_\omega) \subset \mathrm{i}\mathbb{R}$, $\|A_\omega\| \gg 1$, $\omega \gg 1$ is a real parameter describing frequency of oscillation and $f : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$ is a smooth vector-valued function.

In present chapter we allow matrix A_ω to be time-dependent non-singular matrix as compared to a constant matrix A_ω, discussed previously and presented in [Kha08b]. For more generality one can assume that A_ω can be a function from $[0, \infty)$ to the set of matrices. However, the scope of this

thesis is to provide answers while A_ω is the source of the oscillation occurring in the system and the methods introduced in our work are beneficial for large frequencies of oscillation. While for small frequencies or even in absence of oscillation our discretization methods are of the same order as *Gauss-Christopher* rule with Gaussian point.

The analytic solution of the system is given by the variation of constants formula,

$$\boldsymbol{y}(t) = X_\omega(t)\boldsymbol{y_0} + \int_0^t X_\omega(t-\tau)\boldsymbol{f}(\tau, \boldsymbol{y}(\tau))\mathrm{d}\tau = X_\omega \boldsymbol{y_0} + I[\boldsymbol{f}]. \quad (5.1.1)$$

The fact that A_ω is no longer a constant matrix results in a more complex solution of a fundamental matrix X_ω, satisfying matrix linear ODE,

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

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

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

The challenge is to evaluate highly oscillatory integral $I[\boldsymbol{f}]$ in (5.1.1) efficiently. We already know that ordinary methods based on *Gauss–Christoffel* quadrature fail to approximate highly oscillatory integrals for increasing ω, [IN05]. Hence, we first focus on developing numerical methods to evaluate highly oscillatory integrals with a matrix-valued kernel and next we use our results in numerical approximation to (5.1.1).

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

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

with an arbitrary non-singular matrix A_ω of large eigenvalues, $\|A_\omega^{-1}\| \ll 1$, $\sigma(A_\omega) \subset \mathrm{i}\mathbb{R}$, a real parameter ω and a smooth vector-valued function $\boldsymbol{f} \in \mathbb{R}^{\mathrm{d}}$.

We would like to remind our reader that if the matrix A_ω was constant, then for example the task of obtaining an asymptotic expansion for the integral $I[\boldsymbol{f}]$ was quite simple, [Kha08b]. Applying rules of integration by parts,

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

we obtain the *asymptotic* method Q_s^A, defined as s-partial sum of the asymptotic expansion for $I[\boldsymbol{f}]$,

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

This is not the case when the matrix A_ω is arbitrary, since substitution $X_\omega = A_\omega^{-1}X_\omega'$ in $I[\boldsymbol{f}]$ is no longer useful to apply tools of integration by parts,

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

However, it is possible to overcome this issue and obtain the asymptotic expansion for $I[\boldsymbol{f}]$ given an arbitrary matrix A_ω.

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

Given,

$$I[\boldsymbol{f}] = \int_a^b X_\omega(t)\boldsymbol{f}(t)\mathrm{d}t, \qquad X_\omega' = A_\omega X_\omega, \qquad X_\omega = \mathrm{e}^{\Omega}, \tag{5.1.2}$$

with a matrix valued kernel X_ω depending on a real parameter $\omega \gg 1$ and satisfying matrix linear differential equation (5.1.2). Assume that A_ω is an arbitrary non-singular matrix of pure imaginary spectrum, $\sigma(A_\omega) \subset \mathrm{i}\mathbb{R}$, $\|A_\omega^{-1}\| \ll 1$ and $\boldsymbol{f} \in \mathbb{R}^{\mathrm{d}}$ is a smooth vector-valued function.

We have already mentioned previously in this chapter that the current representation of the integral $I[\boldsymbol{f}]$ in (5.1.2) is not suitable for obtaining its

asymptotic expansion due to a more general choice of the matrix A_ω. Once we substitute $X_\omega = A_\omega^{-1} X'_\omega$ in $I[\boldsymbol{f}]$ in its current occurrence, then

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

Transforming integral (5.1.2) into an equivalent integral with appropriate representation for our purposes helps to obtain the asymptotic expansion to (5.1.2).

We first vectorize matrix X_ω into

$$\boldsymbol{X}_\omega = [\bar{\boldsymbol{x}}_1, \bar{\boldsymbol{x}}_2, ..., \bar{\boldsymbol{x}}_\mathrm{d}].$$

Next step we take the transpose of $\boldsymbol{X}_\omega$, obtaining a corresponding vector $\bar{\boldsymbol{X}}_\omega$,

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

It is easy to verify that the latter satisfies a linear differential equation

$$\bar{\boldsymbol{X}}'_\omega = B_\omega \bar{\boldsymbol{X}}_\omega, \quad \text{with} \quad B_\omega = \bigoplus_{i=1}^{d} A_\omega,$$

where B_ω represents direct d-tuple sum of the original matrix A_ω.

We also scale an identity matrix $\boldsymbol{I}$ by taking its direct product with the vector-valued function $\boldsymbol{f} := \boldsymbol{f}^\intercal = [f_1, f_2, \ldots, f_\mathrm{d}]$, $\boldsymbol{F} = \boldsymbol{f}_{1\times d} \bigotimes I_{d\times d}$. For instance, take

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

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

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

Thus, $\boldsymbol{F} = \bigcup_{i=1}^{\mathrm{d}} F_i$, where each entry matrix is a diagonal matrix with the corresponding element f_i on the diagonal,

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

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 (5.1.2).

Example 5.1.1 *Let*

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

Then

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

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

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

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

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

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

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

respectively. This transformation allows us to approximate $I[\boldsymbol{F}]$ and thus $I[\boldsymbol{f}]$. Applying integration by parts to $I[\boldsymbol{F}]$ we obtain the asymptotic expansion for the integral $I[\boldsymbol{f}]$,

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

Hereafter we remind our reader the notation on matrix functions asymptotics depending on a real parameter ω. For the entirety of our work, all norms are L^∞ norms, for vectors, matrices and functions. The norm of a function is taken over the 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 Theorem 3.1 from [Olv07] and Lemma 2.1 from [Kha08b]. In Theorem 5.1.3 we generalize these results for a matrix-valued kernel X_ω, a vector-valued function $\boldsymbol{f}$ and a time dependant matrix A_ω in $I[\boldsymbol{f}]$, (5.1.2) .

Theorem 5.1.1 *(S. Olver, [Olv07]) Suppose that $\boldsymbol{y}$ satisfies the differential equation,*

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

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

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

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

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

where

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

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

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

Lemma 5.1.2 *(MK, [Kha08b]) 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* $\boldsymbol{f} : \mathbb{R} \to \mathbb{R}^{\mathrm{d}}$ *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 $\psi = \max\{\|\boldsymbol{f}^{(s)}\|, \|\boldsymbol{f}^{(s+1)}\|\}$*,*

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

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

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

element wise.

Theorem 5.1.3 *[Kha09b] Postulate that*

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

where A_ω is an arbitrary non-singular matrix, $\sigma(A_\omega) \subset \mathrm{i}\mathbb{R}$, ω is an oscillatory parameter and $\boldsymbol{f} \in \mathbb{R}^{\mathrm{d}}$ 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

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

Proof: We first prove the identity by induction,

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

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

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

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 5.1.4 *[Kha09b] If*

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

then,

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

Example 5.1.2 *For practical purposes consider integral*

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

Once we vectorize the system to obtain asymptotic method, $\bar{\boldsymbol{I}}$ *stands for a vectorized identity matrix* $\boldsymbol{I}$*, and* $\bar{\boldsymbol{X}}_\omega$ *stands for a vectorized 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,

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

where Ω_s stands for a truncated *Magnus* expansion, we can now solve (5.1.1) with the *asymptotic* method,

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

We solve matrix exponential e^{Ω_s} with the *FM* method described in [Kha09a]. The method combines the ideas of *Lie group* solvers, namely *Magnus* method, with *Filon* quadrature for solving nested integral commutators in Ω.

The following lemma for analysis of highly oscillatory ODEs instead of Taylor method, present a paragraph on it

Lemma 5.1.5 *[Kha09a] The approximation with the asymptotic method* Q_s^A *applied to an integral* $I[\boldsymbol{f}]$*, is independent of the step-size of integration.*

PROOF: For $\forall$ step-size h and $\forall$ number n of node points $t_n = t_{n-1}+h$, the components evaluated at the internal node points of the truncated asymptotic sum Q_s^A appear in pairs with an opposite sign, except the values at the end points

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

As a result, no matter how we truncate the interval we obtain the same representation for the asymptotic method Q_s^A evaluated at the end points. □

5.2 The FM method

Employing classical *Filon*-type quadrature proven to have high accuracy for increasing ω, as in [Kha08a], we construct an r-degree polynomial interpolation $\boldsymbol{v}$ for the vector-valued function $\boldsymbol{f}$ in (5.1.2),

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

which agrees with function values and derivatives $\boldsymbol{v}^{(j)}(t_l) = \boldsymbol{f}^{(j)}(t_l)$ at node points $a = t_1 < t_2 < ... < t_\nu = b$, with associated $\theta_1, \theta_2, ..., \theta_\nu$ multiplicities, $j = 0, 1, ..., \theta_l - 1$, and $l = 1, 2, ..., \nu$, [Kha09b].

By definition, *Filon*-type method is

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

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

Theorem 5.2.1 *[Kha09b] 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 a non-singular matrix, $\sigma(A_\omega) \subset \mathrm{i}\mathbb{R}$, ω is an oscillatory parameter and $\boldsymbol{f} \in \mathbb{R}^{\mathrm{d}}$ 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

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

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 (5.1.3) by $\boldsymbol{f} - \boldsymbol{v}$ and the fact that $[\boldsymbol{f} - \boldsymbol{v}]^{(j)}(a) = [\boldsymbol{f} - \boldsymbol{v}]^{(j)}(b) = 0$, for $j = 0, 1, ..., s-1$. □

Corollary 5.2.2 *[Kha09b] If $X_\omega = \mathcal{O}(\mathbf{1})$ and $\boldsymbol{f} = \mathcal{O}(\mathbf{1})$, then*

$$Q_s^F[\boldsymbol{f}] - I[\boldsymbol{f}] = \mathcal{O}(A_\omega^{-s-1}\mathbf{1}).$$

Theorem 5.2.3 *[Kha09b] Let $\theta_1, \theta_\nu \geq s$, $r = \sum_{l=1}^{\nu} \theta_l - 1$. Then r is the numerical order of the Filon-type method applied to the linear systems,*

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

Numerical experiments with Q_s^{FM} method, a combination of *Filon* quadrature and *Magnus* method, are available in Figures 5.2.1, 5.2.2, 5.2.3, 5.2.4, 5.2.5, 5.2.6 and 5.2.7.

By definition, *FM* method is

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

where $\beta_{l,j} = \int_a^b \mathrm{e}^{\Omega_s}(t)\alpha_{l,j}(t)\mathrm{d}t$. In our case it is numerical discretization of the integral

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

applied to solve

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

We present numerical results for *FM* method Q_2^{FM} with end points only and multiplicities all 2, for the equation $y''(t) = -ty(t) - \cos(t)$, $0 \leq t \leq 100$, with $[1,0]^\intercal$ initial conditions and various step-sizes in Figures 5.2.1-5.2.7. Initially, we show that employing the *FM* method one can afford large step-sizes, such as $h = 1$ and $h = \frac{1}{2}$, Figures 5.2.1. Decreasing step-size up to $h = \frac{1}{4}$ and $h = \frac{1}{10}$ we obtain accuracy up to 10^{-8}, Figure 5.2.2. In Figure 5.2.4 we show that for a fixed large step-size the accuracy of approximation improves with an increase in frequency, $h = \frac{1}{4}, \omega = 10^2$ and 10^3. For a smaller step-sizes we demonstrate high accuracy in approximation for $\omega = 10^4$, Figure 5.2.5 and $\omega = 10^5$, Figure 5.2.6. While in Figure 5.2.7 we show that for $\omega = 10^6$ and $h\omega = 10^4$ the method introduces highly desirable accuracy, the error is 10^{-14}. This can be compared with Figure 5.2.3 for the same step-size size.

5.3 The modified FM method

In our further discussion we develop a modified *FM* method Q_S^{FM} employing ideas from the modified *Magnus* method, [Ise02c], [Kha09a]. By solving the equation for variable constants locally with a constant matrix we introduce local change of variables. Applications of the *modified Magnus* method include systems of highly oscillatory linear systems of ODEs, [Kha09a]

$$\boldsymbol{y'}(t) = A_\omega(t)\boldsymbol{y}(t) + f(t), \quad \boldsymbol{y}(t_0) = \boldsymbol{y}_0,$$

with analytic solution

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

We assume that the spectrum of the matrix $A_\omega(t)$ has large imaginary values. Introducing local change of variables at each mesh point, we write the solution in the form

$$\boldsymbol{y}(t) = \mathrm{e}^{(t-t_n)A(t_n+\frac{1}{2}h)}\boldsymbol{x}(t-t_n), \qquad t \geq t_n.$$

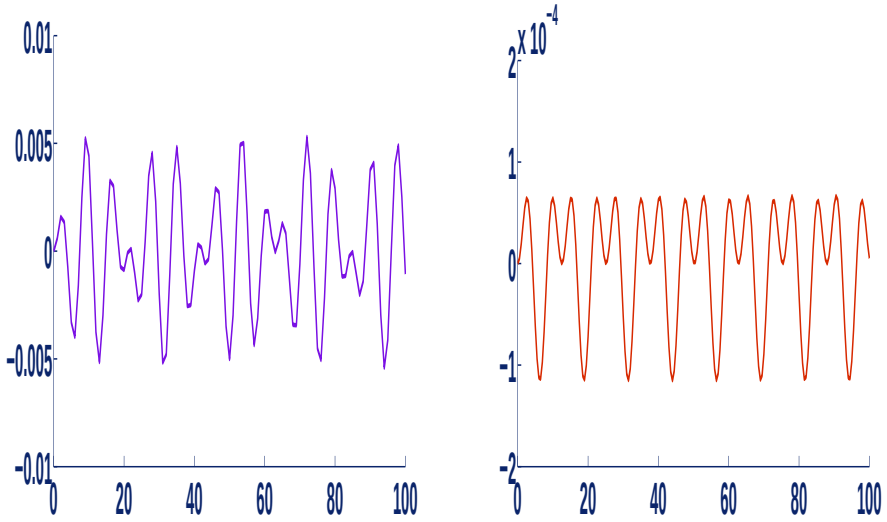

Figure 5.2.1: Global error of the *FM* method Q_2^{FM} with end points only and multiplicities all 2, for the equation $y''(t) = -ty(t) - \cos(t)$, $0 \leq t \leq 100$, with $[1, 0]^\intercal$ initial conditions and step-size $h = 1$ and $h = \frac{1}{2}$ (top two figures from left to right)

We apply modified *Magnus* techniques to the system and solve the system locally with a constant matrix A_ω, while $\boldsymbol{x}(t)$ satisfies a highly oscillatory equation

$$\boldsymbol{x}'(t) = B_\omega(t)X_\omega(t) + \mathrm{e}^{-tA_\omega(t_n)}f(t), \quad t \geq 0,$$

with the same matrix B_ω as for linear matrix ODEs,

$$B_\omega(t) = \mathrm{e}^{-tA_\omega(t_n)}[A_\omega(t) - A_\omega(t_n)]\mathrm{e}^{tA_\omega(t_n)}.$$

It is possible to reduce cost of evaluation of the matrix $B(t)$ by simplifying it, [Ise04a]. Denote $q = \sqrt{g(t_n + \frac{1}{2}h)}$ and $v(t) = g(t_n + t) - g(t_n + \frac{1}{2}h)$. Then,

$$\begin{aligned} B(t) &= v(t) \begin{bmatrix} (2q)^{-1}\sin 2qt & q^{-2}\sin^2 qt \\ -\cos^2 qt & -(2q)^{-1}\sin 2qt \end{bmatrix} \\ &= v(t) \begin{bmatrix} q^{-1}\sin qt \\ -\cos qt \end{bmatrix} \begin{bmatrix} \cos qt & q^{-1}\sin qt \end{bmatrix}, \end{aligned}$$

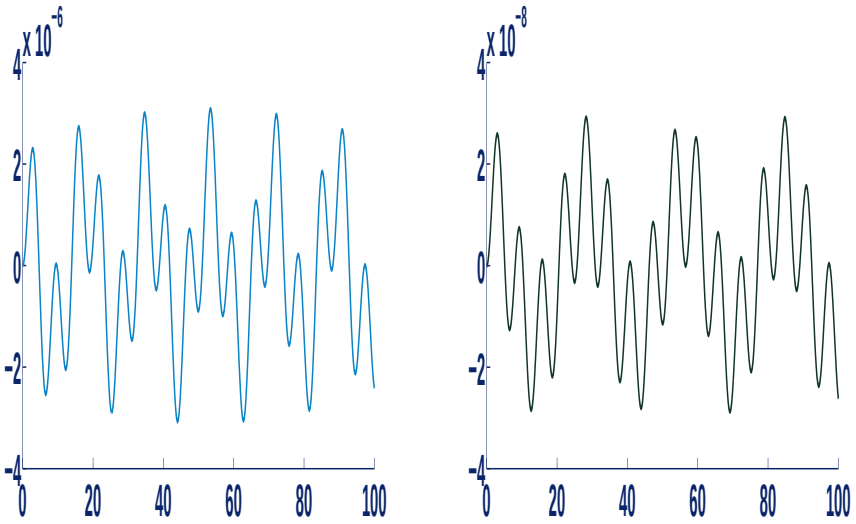

Figure 5.2.2: Global error of the *FM* method Q_2^{FM} with end points only and multiplicities all 2, for the equation $y''(t) = -ty(t) - \cos(t)$, $0 \leq t \leq 100$, with $[1, 0]^\intercal$ initial conditions and step-size $h = \frac{1}{4}$ and $h = \frac{1}{10}$ (from left to right).

and for the product

$$B(t)B(s) = v(t)v(s)\frac{\sin q(s-t)}{q}\begin{bmatrix} q^{-1}\sin qt \\ -\cos qt \end{bmatrix}\begin{bmatrix} \cos qs & q^{-1}\sin qs \end{bmatrix}.$$

It was shown in [Ise04a] that

$$\|B(t)\| = \cos^2 \omega t + \frac{\sin^2 \omega t}{\omega^2} \quad \text{and} \quad B(t) = \mathcal{O}(t - t_{n+\frac{1}{2}}).$$

This approximation results in the following algorithm,

$$\begin{aligned} \boldsymbol{y}_{n+1} &= \mathrm{e}^{hA(t_n+h/2)}\boldsymbol{x}_n \\ \boldsymbol{x}_n &= \mathrm{e}^{\tilde{\Omega}_n}\boldsymbol{y}_n. \end{aligned}$$

Given the compact representation of the matrix $B(t)$ with oscillatory entries, we solve $\Omega(t)$ with a *Filon*-type method, approximating function

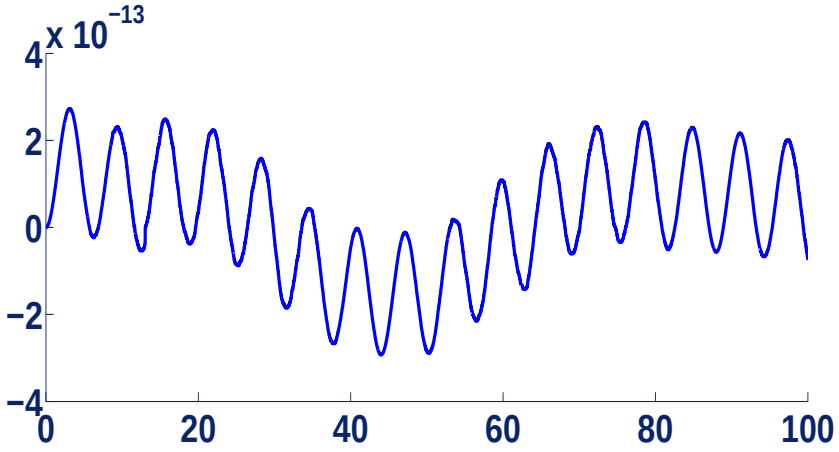

Figure 5.2.3: Global error of the *FM* method Q_2^{FM} with end points only and multiplicities all 2, for the equation $y''(t) = -ty(t) - \cos(t)$, $0 \leq t \leq 100$, with $[1, 0]^\intercal$ initial conditions and step-size $h = \frac{1}{100}$.

$v(t)$ by a polynomial $\tilde{v}(t)$, for example Hermite polynomial, as in classical *Filon*-type method. Furthermore, in our approximation we use end points only, although the method is general and more nodes of approximation can be required.

As a result we can now solve (5.1.2) we *Modified Magnus* method in combination with *Filon* quadrature, which we call the modified *FM method*, and this proves to be more accurate approximation than solving if we solved the commutators with *Gaussian* quadrature. Performance of the *modified Magnus* method improves as compared to classical *Magnus* method due to a number of reasons. The fact due to the fact that the matrix B is small, $B(t) = \mathcal{O}(t - t_{n+\frac{1}{2}})$, contributes to higher order correction to the solution, [Ise02b], [Kha09a]. The order of the *modified Magnus* method increase from $p = 2s$ to $p = 3s + 1$.

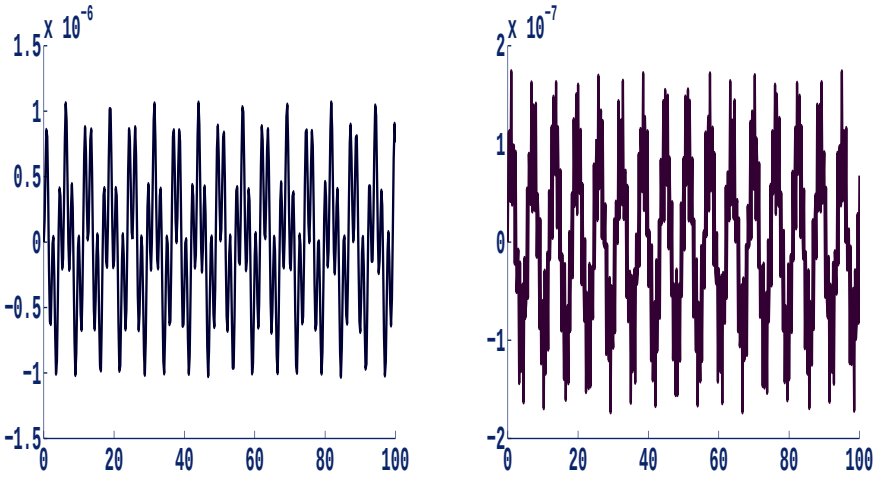

Figure 5.2.4: Global error of the Q_2^{FM} *FM* method with end points only and multiplicities all 2, for the equation $y''(t) = -\omega t y(t) - \cos(t)$, $0 \leq t \leq 100$, with $[1, 0]^\intercal$ initial conditions and step-size $h = \frac{1}{4}$ and $\omega = 10^2$ $\omega = 10^3$ (from left to right).

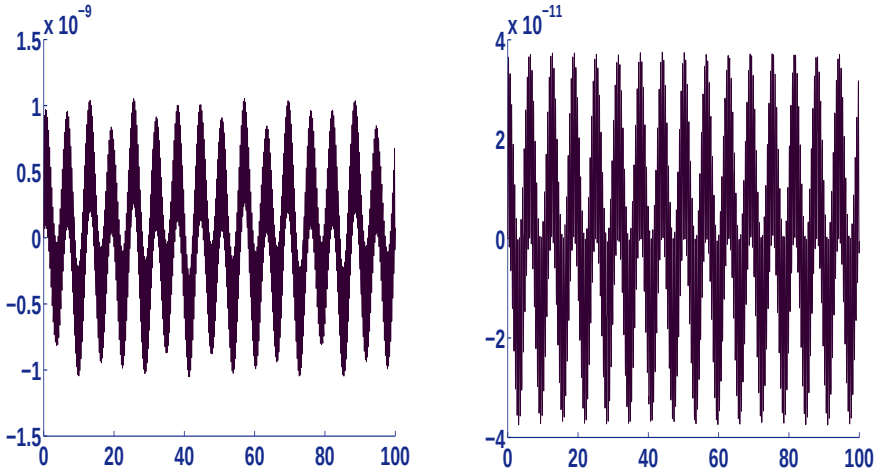

Figure 5.2.5: Global error of the Q_2^{FM} *FM* method with end points only and multiplicities all 2, for the equation $y''(t) = -\omega t y(t) - \cos(t)$, $0 \leq t \leq 100$, with $[1, 0]^\intercal$ initial conditions, $\omega = 10^4$, step-sizes $h = \frac{1}{10}$ and $h = \frac{1}{25}$ (from left to right),

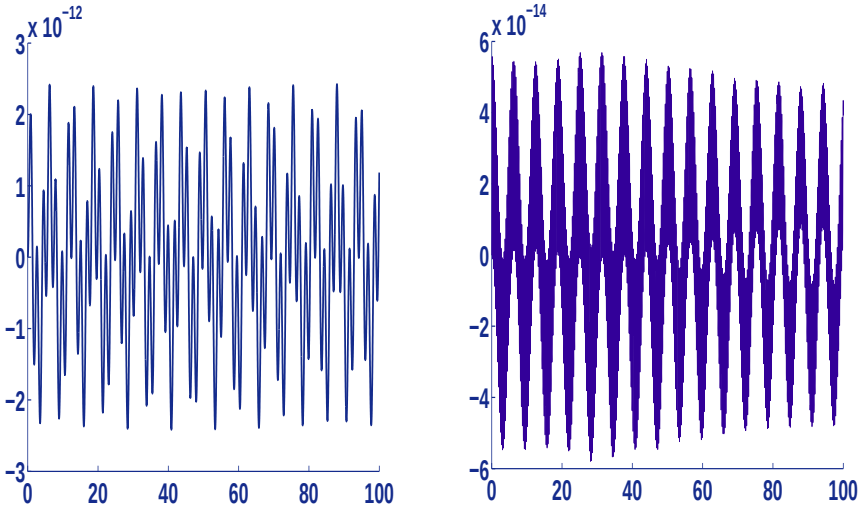

Figure 5.2.6: Global error of the Q_2^{FM} *FM* method with end points only and multiplicities all 2, for the equation $y''(t) = -\omega t y(t) - \cos(t)$, $0 \leq t \leq 100$, with $[1, 0]^\intercal$ initial conditions and step-size $h = \frac{1}{100}$ with $\omega = 25 \times 10^2$ and $\omega = 10^5$ (from left to right.)

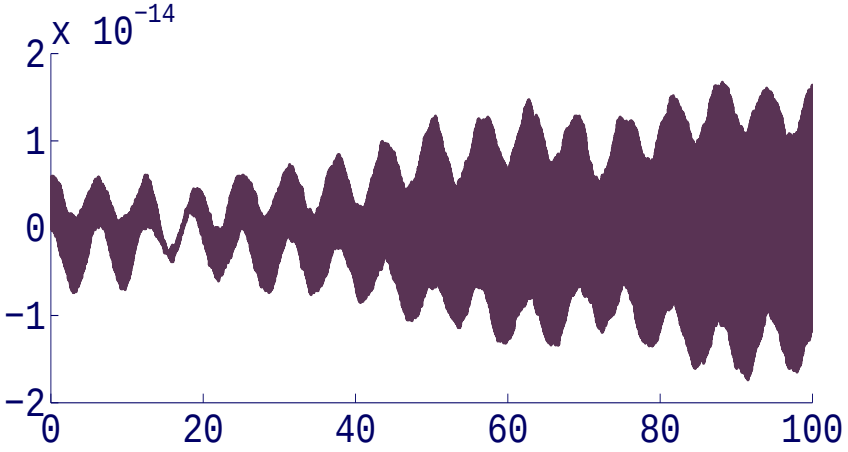

Figure 5.2.7: Global error of the Q_2^{FM} *FM* method with end points only and multiplicities all 2, for the equation $y''(t) = -\omega t y(t) - \cos(t)$, $0 \leq t \leq 100$, with $[1, 0]^\intercal$ initial conditions, step-size $h = \frac{1}{100}$ and $\omega = 10^6$.

Chapter 6

Highly oscillatory non-linear systems

6.1 Waveform relaxation methods

In this chapter we present iteration techniques, namely, *waveform relaxation* algorithms for solving non-linear ordinary differential equations with associated initial conditions:

$$\frac{d}{dt}\boldsymbol{z}(t) = \boldsymbol{f}(t, \boldsymbol{z}), \qquad \boldsymbol{z}(0) = \boldsymbol{z}_0, \qquad t \in [0, T], \tag{6.1.1}$$

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

$$\begin{aligned}
\frac{d}{dt}z_1(t) &= f_1(t, z_1, z_2, ..., z_n), & z_1(0) &= z_{1,0} \\
\frac{d}{dt}z_2(t) &= f_2(t, z_1, z_2, ..., z_n), & z_2(0) &= z_{2,0} \\
&\vdots & &\vdots \\
\frac{d}{dt}z_n(t) &= f_n(t, z_1, z_2, ..., z_n), & z_n(0) &= z_{n,0}.
\end{aligned}$$

A simple example of *waveform relaxation* scheme, which maps the previous iterate $\boldsymbol{z}^{(\nu-1)}$ into new iterate $\boldsymbol{z}^{(\nu)}$ is,

$$\begin{aligned}
\frac{d}{dt}z_1^{(\nu)}(t) &= f_1(t, z_1^{(\nu)}, z_2^{(\nu-1)}, z_3^{(\nu-1)}, ..., z_n^{(\nu-1)}), & z_1^{(\nu)}(0) &= z_{1,0} \\
\frac{d}{dt}z_2^{(\nu)}(t) &= f_2(t, z_1^{(\nu)}, z_2^{(\nu)}, z_3^{(\nu-1)}, ..., z_n^{(\nu-1)}), & z_2^{(\nu)}(0) &= z_{2,0} \\
&\vdots & &\vdots \\
\frac{d}{dt}z_n^{(\nu)}(t) &= f_n(t, z_1^{(\nu)}, z_2^{(\nu)}, z_3^{(\nu)}, ..., z_n^{(\nu)}), & z_n^{(\nu)}(0) &= z_{n,0}.
\end{aligned}$$

The above relaxation scheme is called *Gauss-Seidel* waveform relaxation, similarly to *Gauss-Seidel* iterative method to solve linear and non-linear systems of algebraic equations. The iterative methods simplify the problem of solving large systems of differential equations of n variables to a sequence of differential equations of a single variable. Another example of iteration scheme is the *Jacobi* waveform relaxation method,

$$\begin{aligned}
\frac{d}{dt}z_1^{(\nu)}(t) &= f_1(t, z_1^{(\nu)}, z_2^{(\nu-1)}, z_3^{(\nu-1)}, ..., z_n^{(\nu-1)}), & z_1^{(\nu)}(0) &= z_{1,0} \\
\frac{d}{dt}z_2^{(\nu)}(t) &= f_2(t, z_1^{(\nu-1)}, z_2^{(\nu)}, z_3^{(\nu-1)}, ..., z_n^{(\nu-1)}), & z_2^{(\nu)}(0) &= z_{2,0} \\
&\vdots & &\vdots \\
\frac{d}{dt}z_n^{(\nu)}(t) &= f_n(t, z_1^{(\nu-1)}, z_2^{(\nu-1)}, z_3^{(\nu-1)}, ..., z_n^{(\nu)}), & z_n^{(\nu)}(0) &= z_{n,0}.
\end{aligned}$$

In both cases the iterations scheme picks up initial conditions as an initial approximation $\boldsymbol{z}^{(0)}(t)$

$$z_i^{(0)}(t) = z_{i,0}, \qquad t \in [0, T], \qquad i = 1, ..., n,$$

which is defined along the whole interval of integration. Easy to notice that unlike *Jacobi* algorithm, the *Gauss–Seidel* method is sequential, i.e. one have to solve equations one after another, while the *Jacobi* scheme can be solved in parallel, simultaneously.

Let us define *waveform relaxation* operator $\mathcal{F}$ as

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

Then a one-step iteration method can be written as

$$\frac{d}{dt}\boldsymbol{z}^{(\nu)}(t) = \mathcal{F}(t, \boldsymbol{z}^{(\nu-1)}, \boldsymbol{z}^{(\nu)}), \qquad \boldsymbol{z}^{(\nu)}(0) = \boldsymbol{z}_0,$$

where $\mathcal{F}(u, v)$ is defined so, that $\mathcal{F}(t, v, v) = \boldsymbol{f}(t, v)$.

The well known *Picard* iteration, as well as *Jacobi* and *Gauss–Seidel* schemes can be written in the formulae,

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

Convergence analysis of *waveform relaxation* methods is presented [Van93], [Nev89a], [Nev89b] and [MN87]. The convergence of sequences $\{\boldsymbol{z}^{(\nu)}\}_{\nu=0}^{\infty}$ is analysed in the context of *Banach* spaces.

We consider continuous vector-valued functions defined on $[0, T]$, i.e. $C([0, T]; \mathbb{R}^n)$, with maximum of the norm, defined as:

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

with vector norm $\|\cdot\|$ in R^n.

Definition 6.1.1 *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*

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

It is shown in [Van93] that the *waveform relaxation* is a contraction mapping.

Theorem 6.1.1 *[Van93] 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 $\nu \to \infty$.*

In order to prove some convergence results we introduce an exponentially scaled norm,

$$\|\boldsymbol{z}\|_b = \max_{t\in[0,T]} \mathrm{e}^{-bt}\|\boldsymbol{z}(t)\|, \tag{6.1.2}$$

for some $b > 0$, so that for sufficiently large b and any element $\boldsymbol{z}(t)$ of the space it is true that $\|\boldsymbol{z}(t)\|_\infty \leq \|\boldsymbol{z}(t)\|_b$, for all $t \in [0, T]$.

It was also proved in [Van93] that the iteration is contraction for the derivatives of the iterate,

$$\|\frac{d}{dt}z^{(n)} - \frac{d}{dt}z^{(k)}\|_b \leq \gamma\|\frac{d}{dt}z^{(n+1)} - \frac{d}{dt}z^{(k+1)}\|_b, \qquad \gamma \leq 1.$$

In her current work the author considers an important class of *waveform relaxation* methods, $\frac{d}{dt}v = \mathcal{F}(t, u, v)$, such as Picard, Jacobi and Gauss-Seidel iterations, which are representatives of the more general class of *waveform iteration* methods. 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 $u_1, u_2, v_1, v_2 \in \mathbb{R}^d, t \in [0, T]$,

$$\|\mathcal{F}(t, u_1, v_1) - \mathcal{F}(t, u_2, v_2)\| \leq l_1\|u_1 - u_2\| + l_2\|v_1 - v_2\|. \tag{6.1.3}$$

In the sequel we proof convergence of *Jacobi, Picard* and *Gauss–Seidel waveform relaxation* methods applied to systems of non-linear ODEs. We commence from a system of ordinary differential equations written in a vector form,

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

The following assumptions are hold: $A(t)$ is a $d \times d$ time-dependant matrix and $\boldsymbol{f} : \mathbb{R} \times \mathbb{R}^{\mathrm{d}} \to \mathbb{R}^{\mathrm{d}}$ is a smooth vector-valued function. The analytic solution is presented by the variation of constants formula,

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

The fact that $A(t)$ is not a constant matrix results in a complex solution of a fundamental matrix $X(t)$, satisfying matrix linear ODE,

$$X'(t) = A(t)X(t), \qquad X(t) = \mathrm{e}^{\Omega},$$

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

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

We mention here that the following theorem is valid also for a constant matrix A, representing only a special case.

Theorem 6.1.2 *[Kha09b] Suppose that $\boldsymbol{f}(t, \boldsymbol{y}(t))$ is continuous and satisfies Lipschitz conditions on $D = [0, T] \times \mathbb{R}^d$, and $\mathcal{F}$ is the waveform relaxation operator*

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

defined as

$$\boldsymbol{y}^{(\nu+1)}(t) = X(t)\boldsymbol{y_0} + \int_{t_0}^t X(t-\tau)\mathcal{F}(\tau, \boldsymbol{y}^{(\nu)}(\tau))d\tau.$$

Then the Jacobi, Picard and Gauss-Seidel waveform relaxation methods applied to a non-linear system of ODEs,

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

converge.

Proof: First we prove that $\mathcal{F}$ is a contraction. Consider $\forall \boldsymbol{y}, \boldsymbol{z} \in \mathcal{X}$. Then one-step *waveform relaxation* iteration can we written as

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

and

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

We then take the difference

$$\|\boldsymbol{y}^{(1)}(t) - \boldsymbol{z}^{(1)}(t)\| \\ \leq \int_0^t \|X(t-\tau)(\mathcal{F}(\tau, \boldsymbol{y}(\tau), \boldsymbol{y}^{(1)}(\tau)) - \mathcal{F}(\tau, \boldsymbol{z}(\tau), \boldsymbol{z}^{(1)}(\tau)))\| d\tau.$$

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

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

We multiply both sides by e^{-bt} and maximize over $[0, T]$. It is easy to notice that

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

and soon as $X(t)$ is continuous, hence it is bounded over the finite interval $[0, T]$, i.e. $\exists c > 0$ st $\|X(t)\|_\infty \leq c$. Using *b-norm* notation we can write,

$$\|\boldsymbol{y}^{(1)} - \boldsymbol{z}^{(1)}\|_b \leq c\frac{l_1}{b}\|\boldsymbol{y} - \boldsymbol{z}\|_b + c\frac{l_2}{b}\|\boldsymbol{y}^{(1)} - \boldsymbol{z}^{(1)}\|_b, \tag{6.1.4}$$

and for sufficiently large b we will have

$$\|\boldsymbol{y}^{(1)} - \boldsymbol{z}^{(1)}\|_b \leq \gamma\|\boldsymbol{y} - \boldsymbol{z}\|_b, \qquad \gamma = c\frac{l_1/b}{1/c - l_2/b} < 1, \tag{6.1.5}$$

which proves that $\mathcal{F}$ is a contraction mapping. Convergence follows from Theorem 3.2. □

Remark 6.1.1 *It is shown in [Van93] that from step to step of iteration the error of approximation decreases, when measured in the b-norm. Indeed, i.e. if $\boldsymbol{y}(t)$ is the exact solution and $\boldsymbol{y}^{(\nu-1)}$ is the iterate, then*

$$\|\boldsymbol{y}^{(\nu)} - \boldsymbol{y}\|_b \leq \gamma\|\boldsymbol{y}^{(\nu-1)} - \boldsymbol{y}\|_b, \qquad \textit{for} \qquad 0 \leq \gamma < 1 \qquad \textit{and} \qquad b > 0.$$

Definition 6.1.2 *[Van93] A differential system is said to have the strict WR contractivity property on* $[0,T]$*, if the waveform relaxation algorithm applied to the system contracts in the maximum norm on* $[0,T]$*, i.e.,*

$$\|\boldsymbol{z}^{(\nu+1)} - \boldsymbol{z}^{(\nu)}\|_T \leq \gamma \|\boldsymbol{z}^{(\nu)} - \boldsymbol{z}^{(\nu-1)}\|_T, \qquad \gamma < 1, \qquad \nu \geq 1. \tag{6.1.6}$$

Theorem 6.1.3 *[Van93] For any non-linear system* $\boldsymbol{y}' = \boldsymbol{f}(t, \boldsymbol{y})$*, which satisfies the assumptions of the convergence theorem, there exists 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

$$\begin{aligned}\|\boldsymbol{y}^{(\nu+1)}(t) - \boldsymbol{y}^{(\nu)}(t)\| \\ \leq l_1 \int_0^t \|\boldsymbol{y}^{(\nu)}(s) - \boldsymbol{y}^{(\nu-1)}(s)\| ds + l_2 \int_0^t \|\boldsymbol{y}^{(\nu+1)}(s) - \boldsymbol{y}^{(\nu)}(s)\| ds\end{aligned}$$

Maximizing the norm over the interval $[0,T]$

$$\|\boldsymbol{y}^{(\nu+1)} - \boldsymbol{y}^{(\nu)}\|_T \leq l_1 T \|\boldsymbol{y}^{(\nu)} - \boldsymbol{y}^{(\nu-1)}\|_T + l_2 T \|\boldsymbol{y}^{(\nu+1)} - \boldsymbol{y}^{(\nu)}\|_T$$

for sufficiently small T we get

$$\|\boldsymbol{y}^{(\nu+1)} - \boldsymbol{y}^{(\nu)}\|_T \leq \gamma \|\boldsymbol{y}^{(\nu)} - \boldsymbol{y}^{(\nu-1)}\|_T, \qquad \text{with} \qquad \gamma = \frac{l_1 T}{1 - l_2 T} < 1.$$

□

6.2 WRF method

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

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

Our method further develops some of the implications of the *Filon* quadrature and *waveform relaxation* methods in this setting.

Waveform relaxation (*WR*) methods, a family of iterative techniques designed for analysing dynamical systems, have been studied by a number of authors and we mention here some of them, [AC91], [AHvdD07], [GS98], [GV07], [JOW98], [JV97], [LO87], [MN87], [Nev89a], [Nev89b], [Van93], [WOSVR85].

Assuming that $\boldsymbol{f} : \mathbb{R} \times \mathbb{R}^{\mathrm{d}} \to \mathbb{R}^{\mathrm{d}}$ satisfies the Lipschitz condition, the classical *waveform Picard* algorithm states

$$\boldsymbol{y}^{[s]}(t) = X(t)\boldsymbol{y}_0 + \int_0^t X(t-\tau)\boldsymbol{f}(\tau, \boldsymbol{y}^{[s-1]}(\tau))\mathrm{d}\tau.$$

It is desirable to apply *Filon* quadrature with its nice properties for large ω to non-linear dynamical systems to solve integral

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

Formally, the asymptotic expansion for the integral $I[\boldsymbol{f}]$ as above looks as follows,

$$I[\boldsymbol{f}] \sim \sum_{m=1}^{\infty} (-1)^{m-1} A^{-m} \big[X_w(b)\boldsymbol{f}^{(m-1)}(b, \boldsymbol{y}(b)) - X_w(a)\boldsymbol{f}^{(m-1)}(a, \boldsymbol{y}(a))\big],$$

where the function values and its derivatives at the end point $\boldsymbol{f}^{(m)}(b, \boldsymbol{y}(b))$ are not available any more for $m = 0, 1, 2, \ldots$. To overcome this issue we introduce *waveform methods*. Note that if the solution $\boldsymbol{y}$ is oscillatory, then the function $\boldsymbol{f}(t, \boldsymbol{y})$ is also likely to be oscillatory, causing *waveform relaxation* methods, if used by itself, to be inefficient. Thus, for efficiency, we discretize $I[\boldsymbol{f}]$ according to the rules of 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. Our *WRF* method iterates $\boldsymbol{y}$ 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 $\boldsymbol{f}$ as before. The method takes the initial value constant $\boldsymbol{y}_{n+1}^{[0]}$ 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. In order to obtain any desirably high order method higher order derivatives of the function $\boldsymbol{f}$ are required. In that respect we recommend to differentiate the equation for the system $\boldsymbol{y}' = A\boldsymbol{y} + \boldsymbol{f}(t, \boldsymbol{y})$ itself to obtain higher order derivatives of the solution vector $\boldsymbol{y}$, and use the results in construction of approximation polynomial. The more derivatives at the end points are used in the polynomial approximation the more terms are cancelled in the asymptotic expansion to $I[\boldsymbol{f}]$, leading to higher order methods and hence better accuracy.

We highlight here that the *WRF* method employs end points only, otherwise adding internal points would have led to increasingly fine discretization of the interval. The reason for this is that approximation at internal points themselves requires further partition of the subinterval and this iteration is endless. From the point of view of the function asymptotics, the fundamental point here is that the performance of the *Filon* quadrature is determined by the values at the end points of the integration interval only, making addition of internal points less valuable, Theorem 2.2.1, Theorem 3.2.1.

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 6.2.1 *[Kha08b] 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*

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

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

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

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

PROOF: Let $\boldsymbol{y}(h)$ be an exact solution, $\boldsymbol{y}_h^{[r]}$ its numerical solution by a *waveform* method, and $\boldsymbol{y}_h$ the final numerical solution after discretization. Then, estimating in L^∞-norm,

$$\begin{aligned}\|\boldsymbol{y}(h) - \boldsymbol{y}_h\| &\leq \|\boldsymbol{y}(h) - \boldsymbol{y}_h^{[r]}\| + \|\boldsymbol{y}_h^{[r]} - \boldsymbol{y}_h\| \\ &= \mathcal{O}(h^{r+1}) + \mathcal{O}(h^{s+1}) = \mathcal{O}(h^{q+1}). \end{aligned} \tag{6.2.1}$$

where $q = \min\{r, s\}$. □

Corollary 6.2.2 *[Kha09b] The numerical order of the WRF method is the minimum over both the Filon quadrature and the waveform method applied to solve non-linear systems* $\boldsymbol{y}' = A\boldsymbol{y} + \boldsymbol{f}$.

PROOF: It follows immediately from Theorem (6.2.1). □

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.

Theorem 6.2.3 *[Kha09b] WRF method is convergent.*

PROOF: Follows from (6.2.1) as $h \to 0$. □

In the Table 6.2.1 we demonstrate the accuracy of the *WRF* method for increasing ω in just four iterations. Due to non-linearity, the accuracy improves slightly slower, since we have chosen to iterate oscillatory equations. On the other hand, taking into account rapid oscillation of the solution for large ω, applying only four iteration combined with *Filon* quadrature is a very little exercise to achieve up to ten digits accuracy as it is described the Table 6.2.1. Figure 6.2.1 demonstrates the logarithmic error of the *WRF* method for different values of ω. *Waveform* methods do not contribute to function asymptotics making it harder to parallel the two methods, namely *Filon*-type method and *WRF* method, as it is shown in Figures 6.2.1 and 3.2.4. We have seen that the *Filon*-type methods have the same asymptotic order as the *asymptotic* method, where the error depends on the inverse powers of ω. In the case of asymptotic behaviour of *WRF* method the bottom line is that one iterates the asymptotic expansion, but the advantage of applying the right quadrature rule means that for increasing ω the error amazingly

remains very close to that for smaller ω. *Waveform* methods do not preserve the nice asymptotic features of the *Filon* quadrature, but the latter even in the presence of iteration captures up to 10^{-12} accuracy as ω increases.

Finally, for methods introduced in current work there wasn't any restrictions on the phase of the solution, whilst for discretization of $I[\boldsymbol{f}]$ with *Filon* quadrature some special functions can be considered as the most obvious choice.

The analysis of the *asymptotic*, *Filon*-type and *WRF* methods for a time-dependant matrix using Magnus expansions as well as some alternative choices of the quadrature methods can be found in [Kha08b, Kha09b].

Table 6.2.1: Approximation error of the *WRF* method for the non-linear ODE $y'' = -\omega y - 3y^3$, compared with the results of MATLAB ode45 solver set to RelTol= 10^{-12}, AbsTol= 10^{-16}.

h	$\omega = 10$	h	$\omega = 100$	h	$\omega = 1000$
2.50_{-01}	1.04_{-03}	1.00_{-01}	-8.32_{-04}	4.00_{-02}	-8.90_{-04}
1.00_{-01}	2.25_{-05}	5.00_{-02}	-5.33_{-05}	2.00_{-02}	-5.16_{-05}
5.00_{-02}	1.40_{-06}	2.50_{-02}	-3.35_{-06}	1.00_{-02}	-3.22_{-06}
4.00_{-02}	5.74_{-07}	1.00_{-02}	-8.59_{-08}	3.33_{-02}	-3.98_{-08}
1.25_{-02}	4.83_{-09}	5.00_{-03}	-5.36_{-09}	1.25_{-03}	-6.63_{-10}

6.3 WRFM method

Extending the *WRF* method for non-linear systems with a time dependant matrix, we now make use of the *Filon–Magnus* method, which we call the *FM* method. These ideas nicely combine together, forming an new *WRFM* method.

Consider non-linear system

$$\boldsymbol{y} = A_\omega(t)\boldsymbol{y} + \boldsymbol{f}(t, \boldsymbol{y}), \quad \boldsymbol{y}(t_0) = \boldsymbol{y}_0,$$

where A_ω has large imaginary eigenvalues and $\boldsymbol{f} : \mathbb{R} \times \mathbb{R}^{\mathrm{d}} \to \mathbb{R}^{\mathrm{d}}$ The analytic

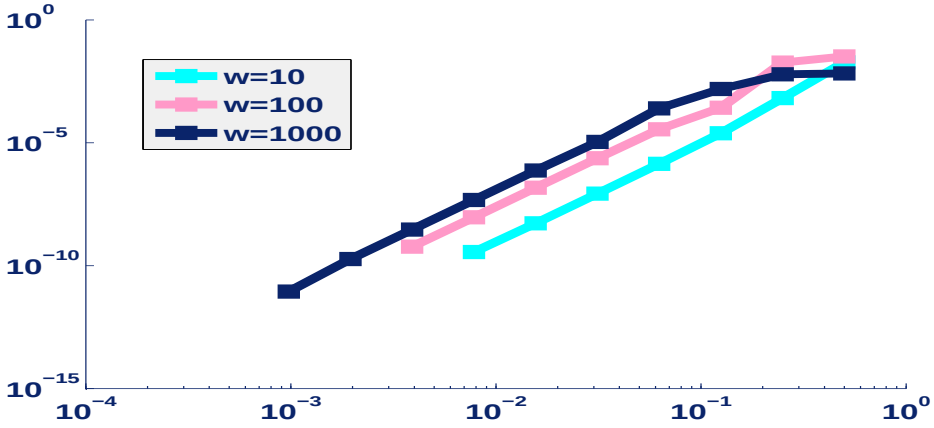

Figure 6.2.1: Logarithmic error (y-axis) and the step-size (x-axis) of the WRF method for the equation $y'' = -\omega y - 3y^3$, initial values in $[1, 1]^\intercal$, with endpoints only and multiplicities all 2.

solution is given by

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

Our *WRFM* method iterates $\boldsymbol{y}$ with a *waveform* method, solving $I[\boldsymbol{f}]$ at each step with *FM* method,

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

where $\boldsymbol{v}$ is a polynomial approximation to $\boldsymbol{f}$ as before.

Modified WRFM method

Further applications of the *Modified Magnus* method include systems of highly oscillatory non linear equations

$$\boldsymbol{y} = A_\omega(t)\boldsymbol{y} + \boldsymbol{f}(t,\boldsymbol{y}), \quad \boldsymbol{y}(t_0) = \boldsymbol{y}_0,$$

with analytic solution

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

We apply modified *Magnus* techniques to the system of non linear ODEs by introducing the following change of variables

$$\boldsymbol{y}(t) = \mathrm{e}^{(t-t_n)A_\omega(t_n+\frac{h}{2})}\boldsymbol{x}(t-t_n), \quad t \geq t_0,$$

and solving the system locally with a constant matrix A_ω, while $\boldsymbol{x}(t)$ satisfies a non linear highly oscillatory equation

$$\boldsymbol{x}'(t) = B_\omega(t)\tilde{X}_\omega(t) + \mathrm{e}^{-tA_\omega(t_n+\frac{h}{2})}\boldsymbol{f}(t,\mathrm{e}^{tA_\omega(t_n+\frac{h}{2})}\boldsymbol{x}(t)), \quad t \geq 0,$$

with exactly the same matrix B_ω as for linear equations,

$$B_\omega(t) = \mathrm{e}^{-tA_\omega(t_n+\frac{h}{2})}[A_\omega(t_n+t) - A_\omega(t_n+h/2)]\mathrm{e}^{tA_\omega(t_n+\frac{h}{2})}.$$

The analytic solution to the new system is of the form,

$$\boldsymbol{x}(t) = \tilde{X}_\omega(t)\boldsymbol{y}_0 + \int_0^t \tilde{X}_\omega(t-\tau)\mathrm{e}^{-\tau A_\omega(t_n+\frac{h}{2})}\boldsymbol{f}(\tau,\mathrm{e}^{\tau A_\omega(t_n+\frac{h}{2})}\boldsymbol{x}(\tau))d\tau, \quad (6.3.1)$$

where

$$\tilde{X}'_\omega(t) = B_\omega(t)\tilde{X}_\omega(t), \quad \text{and} \quad \tilde{X}_\omega(0) = I.$$

The *Magnus* expansion provides us with a solution for the matrix-kernel $\tilde{X}(t)$,

$$\tilde{X}(t) = \mathrm{e}^{\Omega(t)},$$

with

$$\begin{aligned}\Omega(t) = &\int_0^t B_\omega(t)dt \\ &+\frac{1}{2}\int_0^t [B_\omega(\tau), \int_0^\tau B_\omega(\xi)d\xi]d\tau \\ &+\frac{1}{4}\int_0^t [B_\omega(\tau), \int_0^\tau [B_\omega(\xi), \int_0^\xi B_\omega(\zeta)d\zeta]d\xi]d\tau \\ &+\frac{1}{12}\int_0^t [[B_\omega(\tau), \int_0^\tau B_\omega(\xi)d\xi], \int_0^\tau B_\omega(\zeta)d\zeta]d\tau \\ &+\cdots .\end{aligned}$$

The *modified WRFM* method is defined as a local approximation of the solution vector $\boldsymbol{y}$ by solving

$$\boldsymbol{x}'(t) = B_\omega(t)\tilde{X}_\omega(t) + \mathrm{e}^{-tA_\omega(t_n+\frac{h}{2})}\boldsymbol{f}(t, \mathrm{e}^{tA_\omega(t_n+\frac{h}{2})}\boldsymbol{x}(t)), \quad \boldsymbol{x}(0) = \boldsymbol{y}_n,$$

with classical *Magnus* method for linear part of the system and *WRF* method, [Kha08b], for non-linear part. This approximation results in the following algorithm,

$$\begin{aligned}\boldsymbol{x}_{n+1}^{[0]} &= \boldsymbol{y}_n, \\ \boldsymbol{x}_{n+1}^{[1]} &= \mathrm{e}^{\Omega_s}\boldsymbol{y}_n + \int_0^h \mathrm{e}^{\Omega_s(h-\tau)}\mathrm{e}^{-\tau A(t_n+\frac{h}{2})}\boldsymbol{f}(\tau, \mathrm{e}^{\tau A(t_n+\frac{h}{2})}\boldsymbol{x}_{n+1}^{[0]}(\tau))d\tau, \\ &\vdots \\ \boldsymbol{x}_{n+1}^{[s]} &= \mathrm{e}^{\Omega_s}\boldsymbol{y}_n + \int_0^h \mathrm{e}^{\Omega_s(h-\tau)}\mathrm{e}^{-\tau A(t_n+\frac{h}{2})}\boldsymbol{f}(\tau, \mathrm{e}^{\tau A(t_n+\frac{h}{2})}\boldsymbol{x}_{n+1}^{[s-1]}(\tau))d\tau, \\ \boldsymbol{y}_{n+1} &= \mathrm{e}^{hA_\omega(t_n+h/2)}\boldsymbol{x}_{n+1}^{[s]}.\end{aligned}$$

Here Ω_s stand for a truncated *Magnus* expansion $\Omega(t)$.

To prove the convergence results one can use the exponentially scaled norm introduced above 6.1.2. We noticed that for large values of $\|A_\omega\|$ one can replace *b-norm* notation with *A-norm* notation,

$$\|\boldsymbol{z}\|_{\|A_\omega\|} = \max_{t\in[0,T]} \mathrm{e}^{-A_\omega t}\|\boldsymbol{z}(t)\|. \tag{6.3.2}$$

This notation is particularly interesting in the scope of current work, since we consider matrices with large eigenvalues and hence large norm.

Lemma 6.3.1 *[Kha09b] Suppose that $\boldsymbol{f}(t,\boldsymbol{y}(t))$ is continuous and satisfies Lipschitz conditions on $D=[0,T]\times R^d$. Then Jacobi, Picard and Gauss-Seidel waveform relaxation methods applied to the modified system 6.3.1,*

$$\begin{aligned}
\boldsymbol{x}^{[0]}(t) &= \boldsymbol{y}_0,\\
\boldsymbol{x}^{[1]}(t) &= \mathrm{e}^{\Omega_s(t)}\boldsymbol{y}_0 + \int_0^t \mathrm{e}^{\Omega_s(t-\tau)}\mathrm{e}^{-\tau A_\omega(t_n+h/2)}\mathcal{F}(\tau,\mathrm{e}^{\tau A_\omega(t_n+h/2)}\boldsymbol{x}^{[0]}(\tau))d\tau,\\
&\vdots\\
\boldsymbol{x}^{[s]}(t) &= \mathrm{e}^{\Omega_s(t)}\boldsymbol{y}_0 + \int_0^t \mathrm{e}^{\Omega_s(t-\tau)}\mathrm{e}^{-\tau A_\omega(t_n+h/2)}\mathcal{F}(\tau,\mathrm{e}^{\tau A_\omega(t_n+h/2)}\boldsymbol{x}^{[s-1]}(\tau))d\tau,
\end{aligned}$$

are convergent and the system has strict WR contractivity on $[0,T]$.

Proof: The proof in *b-norm* follows from Theorem 6.1.2 and Theorem 6.1.3. The proof in *A-norm* follows from Theorem 6.1.2 and Theorem 6.1.3 by replacing *b-norm* notation with *A-norm* notation,

$$\|\boldsymbol{x}(t)-\boldsymbol{x}^{[1]}(t)\|_\infty \le \gamma_{\|A\|_\omega}\|\boldsymbol{x}(t)-\boldsymbol{x}^{[1]}(t)\|_{\|A\|_\omega}, \qquad \gamma = c\frac{l_1/\|A\|_\omega}{1/c-l_2/\|A\|_\omega} < 1.$$

□

Chapter 7

Conclusions

7.1 Asymptotic expansion versus Taylor expansion for highly oscillatory ODEs

Numerical analysis of DEs is based on the Taylor theorem. This includes fundamental concepts of time-stepping, truncation error, order etc., which underlie the construction and analysis of discretization algorithms. Suppose f has $n+1$ continuous derivatives on an open interval containing a. Then 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 Euler's method, the truncation error can be examined using Taylor's theorem

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

7.1 Asymptotic expansion versus Taylor expansion for highly oscillatory ODEs

The magnitude of the errors arising from for example the Euler method can be demonstrated by comparison with a Taylor expansion of y.

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

But the Taylor theorem is the wrong tool for high oscillations. Each time we differentiate, the amplitude is roughly scaled by frequency. This means that, in methods based on Taylor reasoning, we are compelled to choose a ridiculously small step size.

To the contrary to Taylor's expansion, the *asymptotic expansion* is a more powerful tool in analysis of highly oscillatory ODEs, since the *asymptotic expansion* depends and the error term are expressed in terms of inverse powers of the frequency of oscillation. For instance, for an extrinsic linear oscillator

$$\boldsymbol{y}' = A\boldsymbol{y} + \boldsymbol{\alpha}\sin(\omega t), \quad \text{when} \quad \omega \ggg \|A\|.$$

Note that the *asymptotic expansion* for this equation is available at any given time point, and for the numerical purposes the truncated *asymptotic expansion* can be evaluated for any large time-value t,

$$\begin{aligned}\boldsymbol{y}(t) \sim \mathrm{e}^{At}\boldsymbol{y}_0 + \sum_{n=0}^{\infty} \frac{1}{\omega^{2n+1}}(\mathrm{e}^{At} - I\cos(\omega t))A^{2n}\boldsymbol{\alpha} \\ - \sum_{n=0}^{\infty} \frac{1}{\omega^{2n+2}} A^{2n+1}\boldsymbol{\alpha}\sin(\omega t).\end{aligned}$$

In this work we developed numerical tools based on *asymptotic expansion* for solving systems of highly oscillatory ODEs, where the accuracy of approximation improves with large frequencies of oscillation. We addressed the issues of numerical approximation of systems of ODEs with large frequencies of oscillation, which was an open problem. For small frequencies our methods are comparable with classical methods, but they have a remarkable advantage once applied for equations with large frequencies. This is demonstrated in examples in comparison with classical methods as well as state of the art solvers in Matlab and Maple. Our algorithms for *Filon-type* methods and *FM*-methods as well as parallel computing for non-linear systems are implemented in Matlab, except the symbolic calculation in the *asymptotic* method implemented using Maple symbolic package. Efficiency of the methods was

tested and compared with Matlab built-in routines. The efficiency of our algorithms is superior for large frequencies, when Matlab solvers take hours to overcome computation with variable but incredibly small step-size, while we get the answer within a couple of seconds, roughly by a press of a button. And this is simple to explain. Not only we built our methods with a relatively large step-size, but we also use very little information about function, working with end-points only. Moreover, our methods do not require explicit availability of the derivatives as it was mentioned before. For instance for an interval $[0, 1]$ one can choose to substitute sequence $\frac{1}{\omega}$ around zero and $1 - \frac{1}{\omega}$ for values around point one.

Chapter 8

Future work

8.1 Moment-free approximation

In my current work I am developing moment-free numerical methods, such as moment-free Filon method and Levin-type method for solving highly oscillatory systems of ODEs, [Kha08a].

We presented the *asymptotic* method based on integration by parts, as well as *Filon-type* method approximating f by some polynomial, for example Hermite,

$$\tilde{f}(x) = \sum_{l=1}^{\nu} \sum_{j=0}^{\theta_l} \alpha_{l,j}(x) f^{(j)}(c_l),$$

which satisfies $\tilde{f}^{(j)}(c_l) = f^{(j)}(c_l)$, at node points $0 = c_1 < c_2 < ... < c_\nu = 1$, with $\theta_1, \theta_2, ..., \theta_\nu$ associated multiplicities, and $j = 0, 1, ..., \theta_l, l = 1, 2, ..., \nu$.

However, while replacing function $f(x)$ by a polynomial $\tilde{f}(x)$, the method requires computation of moments $\int_{-\infty}^{\infty} x^m \mathrm{e}^{\mathrm{i}\omega g(x)} dx, m \geq 0$,

$$Q_s^F[f] = I[\tilde{f}] = \sum_{k=0}^{n} c_k I[x^k],$$

which are not always available.

Instead, in current project we consider function $F(x)$, such that

$$\frac{d}{dx}\big[F(x)\mathrm{e}^{\mathrm{i}\omega g(x)}\big] = f(x)\mathrm{e}^{\mathrm{i}\omega g(x)},$$

and obviously $I[f] = [F(x)\mathrm{e}^{\mathrm{i}\omega g(x)}]_a^b$. The idea is to approximate integral by $Q^L[f] = [v(x)\mathrm{e}^{\mathrm{i}\omega g(x)}]_a^b$, where $v(x)$ is some function (e.g. collocation polynomial) approximating $F(x)$, [Lev97], [Olv07] . We now obtain that

$$F'\mathrm{e}^{\mathrm{i}\omega g(x)} + \mathrm{i}\omega g'(x)F(x)\mathrm{e}^{\mathrm{i}\omega g(x)} = f(x)\mathrm{e}^{\mathrm{i}\omega g(x)}$$
$$\mathcal{L}[F](x) = F'(x) + \mathrm{i}\omega g'(x)F(x),$$

so that $\mathcal{L}[F](x) = f(x)$, with operator L defined as $\mathcal{L}[F] = F' + iwg'F$.

Theorem 8.1.1 *[Olv06] Suppose that $g'(x) \neq 0$ for $x \in [a,b]$. Let $\{\psi_k\}_0^n$ be a basis of functions independent of w, s is some positive integer and x_{k0}^{ν} is a set of node points $a = x_0 < x_1 < ...x_\nu = b$ with $\{m_k\}_0^\nu, m_o, m_\nu \geq s$ set of multiplicities associated with the node points. Suppose that $v = \sum_{k=0}^n c_k\psi_k$, where $n = \sum_{k=0}^\nu m_k - 1$, is the solution to the system of collocation equations*

$$\mathcal{L}[v](x_k) = f(x_k)$$
$$\frac{d\mathcal{L}[v]}{dx}(x_k) = f'(x_k)$$
$$\vdots$$
$$\frac{d^{m_k-1}\mathcal{L}[v]}{dx^{m_k-1}}(x_k) = f^{m_k-1}(x_k)$$

for every integer $0 \leq k \leq n$ and $\mathcal{L}[v] = v' + \mathrm{i}\omega g'v$. Define

$$\mathbf{g}_k = [(g'\psi_k)(x_0), ..., (g'\psi_k)^{(m_0-1)}(x_0), ..., (g'\psi_k)(x_\nu), ..., (g'\psi_k)^{(m_\nu-1)}(x_\nu)]^\intercal.$$

If the vectors $\{\mathbf{g_0}, ..., \mathbf{g_n}\}$ are linearly independent, then for sufficiently large ω the system has a unique solution and

$$I[f] - Q^L[f] \sim \mathcal{O}(\omega^{-s-1}),$$

where

$$Q^L[f] \equiv [v(x)\mathrm{e}^{\mathrm{i}\omega g(x)}]_a^b = v(b)\mathrm{e}^{\mathrm{i}\omega g(b)} - v(a)\mathrm{e}^{\mathrm{i}\omega g(a)}.$$

In our work in progress, [Kha08a] we extend these ideas and apply the *Levin-type* method is applied for the vector-valued functions with a matrix-valued kernel,

$$I[f] = \int_a^b X_\omega \boldsymbol{f} dx.$$

The theory is available for the family of vector-valued integrals

$$I[f] = \int_a^b \boldsymbol{f}(x)^\intercal \boldsymbol{y}(x) dx.$$

where $\boldsymbol{f}$ is a vector-valued function and $\boldsymbol{y}$ is a highly oscillatory vector-valued function satisfying differential equation

$$\boldsymbol{y}'(x) = A(x)\boldsymbol{y}(x).$$

Theorem 8.1.2 *[Olv07] Suppose that $\boldsymbol{y}$ satisfies the differential equation*

$$\boldsymbol{y}' = A\boldsymbol{y},$$

on $[a,b]$, for some matrix-valued function A such that $A^{-1} = \mathcal{O}(\hat{A})$ for $w \to \infty$. Let

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

where

$$\boldsymbol{\sigma}_0^\intercal \equiv \boldsymbol{f}^\intercal, \qquad \boldsymbol{\sigma}_{k+1}^\intercal = (\boldsymbol{\sigma}_k^\intercal A^{-1})', \qquad k = 0, 1, ...$$

For $\boldsymbol{f} = \mathcal{O}(\tilde{\boldsymbol{f}})$ and $\boldsymbol{y}(x) = O(\tilde{\boldsymbol{y}})$ it is true that

$$Q_s^A[\boldsymbol{f}] - I[\boldsymbol{f}] = (-1)^{s+1} \int_a^b \boldsymbol{\sigma}_s^\intercal \boldsymbol{y} dx = O\left(\tilde{\boldsymbol{f}}^\intercal \hat{A}^{s+1} \tilde{\boldsymbol{y}}\right), \qquad w \to \infty.$$

More precisely

$$\mathcal{L}[\boldsymbol{F}] = \boldsymbol{f}, \qquad \text{for} \qquad \mathcal{L}[\boldsymbol{F}] = \boldsymbol{F}' + A^{\intercal}\boldsymbol{F}.$$

To compute $\boldsymbol{F}$ exactly in general is not possible, but it is possible to approximate it using collocation methods [17], where the Levin-method for the vector-valued functions is defined as follows. Let $\boldsymbol{v}(x) = \sum_{k=1}^{n} c_k \boldsymbol{\psi}_k(x)$ for some set of basis functions $\{\boldsymbol{\psi}_k\}$, st $\boldsymbol{\psi}_k : R \to R^d, n = d\sum m_k$, the total number of equations in the system. For a sequence of nodes $x_1, ..., x_\nu$ and and multiplicities $m_1, ..., m_\nu$ the coefficients of $\boldsymbol{v}$ are determined by solving the system

$$\mathcal{L}[\boldsymbol{v}](x_k) = \boldsymbol{f}(x_k), ..., \mathcal{L}[\boldsymbol{v}]^{(m_k-1)}(x_k) = \boldsymbol{f}^{(m_k-1)}(x_k),$$

and the Levin-type method will defined as

$$\mathcal{Q}^L[f] = \boldsymbol{v}(b)^{\intercal}\boldsymbol{y}(b) - \boldsymbol{v}(a)^{\intercal}\boldsymbol{y}(a).$$

The method can be applied to solve linear and non-linear systems once we apply matrix transformation to obtain asymptotic expansion for the family of integrals with a matrix-valued kernel as described in Chapter 5.

8.2 Applications to PDEs

The results of our research are particularly interesting in application to partial differential equations. Discretization of oscillatory PDEs results in systems of rapidly oscillatory ODEs. Hence, having obtained efficient solvers for highly oscillatory systems of ODEs, we expect to apply them to solve oscillatory PDEs, at the very core of quantum mechanics, molecular dynamics and electrodynamics, e.g. *Schroedinger* equation with large potentials, the *Helmholtz* equation and *Maxwell* equations. This might well involve the combination of our ideas with other approaches, e.g. homogenization, Wigner measures, the eikonal expansions and geometric optics. These expectations have strong theoretical support, since the methods introduced in our papers are by construction independent of matrix dimension and valid for large and small eigenvalues, and hence for all frequencies. The methods seem promising also for the *Fermi-Pasta-Ulam* problem and for other *Hamiltonian* ODEs with highly oscillatory solutions.

The phenomena of high oscillation observed in certain dynamical systems may have different explanations to its occurrence. Sometimes oscillations occur due a nature of the system itself, the way it is designed due to its inner properties. This is what we call *intrinsic* oscillation, when the oscillation is a global feature of the dynamical system itself. For example, if the system has a dominating imaginary spectrum, then it is the nature of the system to be oscillatory, and hence we deal with *intrinsic* high oscillation. On the other hand, it happens that for numerous reasons there is an oscillatory element embedded into a non oscillatory system. When such an oscillatory forcing term is added to a non oscillatory system, making the solution to oscillate rapidly, we deal with an *extrinsic* high oscillation. For instance, in substantially larger time scales, when the frequency of the input signal is negligible, the *extrinsic* oscillation originates in the forcing term.

A simple example of an *extrinsic* oscillator is

$$\boldsymbol{y}' = A\boldsymbol{y} + \boldsymbol{\alpha} sin(\omega t), \quad \text{when} \quad \omega \ggg \|A\|.$$

Note that the asymptotic expansion for this equation is available at any given time point,

$$\begin{aligned}\boldsymbol{y}(t) \sim \mathrm{e}^{At}\boldsymbol{y}_0 + \sum_{n=0}^{\infty} \frac{1}{\omega^{2n+1}}(\mathrm{e}^{At} - I\cos(\omega t))A^{2n}\boldsymbol{\alpha} \\ - \sum_{n=0}^{\infty} \frac{1}{\omega^{2n+2}} A^{2n+1}\boldsymbol{\alpha}\sin(\omega t).\end{aligned}$$

In our work we are mainly concerned about numerical methods designed for solving dynamical systems with *intrinsic* high oscillation. There are many famous examples of such systems. For instance, take the *Airy* equation,

$$y'' \pm k^2 t y = 0,$$

where the imaginary part of the spectrum insures that the solution is oscillatory. Similarly, a particularly interesting example of *intrinsic* high oscillation is the non-linear *Emden-Fowler* equation,

$$y'' + ty^3 = 0.$$

For applications in mechanics the *Hamiltonian* system is a classical example,

$$H(p,q) = \frac{1}{2}(q_1^2 + q_2^2) + \frac{1}{2}\sin(p_1 - p_2) + 3p_2^4.$$

The *Hamiltonian* is considered to be the closest approach of classical mechanics to the *Schroedinger* equation in quantum mechanics,

$$\imath\hbar\frac{\partial}{\partial t}\Psi(\boldsymbol{r},t) = -\frac{\hbar^2}{2m}\nabla^2\Psi(\boldsymbol{r},t) + V(\boldsymbol{r})\Psi(\boldsymbol{r},t).$$

In chaos theory, the apparent paradox of the results of the *Fermi-Pasta-Ulam* experiment with the hypothesis that essentially any non linearity would lead to a system exhibiting ergodic behaviour has become known as the *Fermi-Pasta-Ulam* problem,

$$y_j'' = (y_{j+1} - 2y_j + y_{j-1}) \times [1 + \frac{1}{2}(y_{j+1} - y_{j-1})].$$

Instead, such physical systems exhibited almost exactly periodic behaviour versus expected ergodic behaviour. At last, the mathematical model describing wave propagation on the surface of shallow water. The equation is known as the *Korteweg-de Vries* equation,

$$\partial_t\phi + \partial_x^3\phi + 6\,\phi\,\partial_x\phi = 0.$$

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