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ON THE METHOD OF NEUMANN SERIES FOR HIGHLY OSCILLATORY EQUATIONS *

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Abstract.

The main purpose of this paper is to describe and analyse techniques for the numerical solution of highily oscillatory ordinary differential equations by exploying a Neumann expansion. Once the variables in the differential system are changed with respect to a rapidly rotating frame of reference, the Neumann method becomes very effective indeed. However, this effectiveness rests upon suitable quadrature of highly oscillatory multivariate integrals, and we devote part of this paper to describe how to accomplish this to high accuracy with a modest computational effort.

1 Introduction

The purpose of this paper is to design and analyse effective discretization methods for highly oscillatory ordinary differential equations, with an emphasis on equations obtained once highly oscillatory initial-value partial differential equations are semidiscretized. It is based on combining two ideas: a transformation of variables with respect to a fast-rotating frame of reference and Neumann series.

Suppose that the solution of the linear system

$$\boldsymbol{y}' = A(t)\boldsymbol{y}, \quad t \geq 0, \qquad \boldsymbol{y}(0) = \boldsymbol{y}_0 \in \mathbb{R}^N, \tag{1.1}$$

oscillates rapidly. To avoid possible instabilities, we assume further that the spectrum of $A(t)$ is pure imaginary. Let $\boldsymbol{y}_n \approx \boldsymbol{y}(t_n)$, $n \geq 0$, and $h = t_{n+1} - t_n$. The first step recommended in [9] is to change the variables locally,

$$\boldsymbol{y}(t) = \mathrm{e}^{(t-t_n)\tilde{A}}\boldsymbol{x}(t - t_n), \qquad t \geq t_n, \tag{1.2}$$

where $\tilde{A} = A(t_n + \frac{1}{2}h)$, and solve for $\boldsymbol{x}$. In other words, we precondition the solution of (1.1) locally by the known solution of a linear system with constant coefficients and solve

$$\boldsymbol{x}' = B(t)\boldsymbol{x}, \quad t \geq 0, \qquad \boldsymbol{x}(0) = \boldsymbol{y}_n, \tag{1.3}$$

where

$$B(t) = \mathrm{e}^{-t\tilde{A}}[A(t_n + t) - \tilde{A}]\mathrm{e}^{t\tilde{A}}.$$

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The transformation (1.2) has been recently generalized in [6]: we choose a matrix $\tilde{A}$ with purely-imaginary spectrum so that $\|A(t)-\tilde{A}\|$ is small and proceed as in (1.2). Note that $\tilde{A}$ need not be a value of A at a point. Even more far reaching generalization, which we do not pursue further in this paper, is $A(t) = \tilde{A}(t-t_n) + C(t-t_n)$, where $\|C\|$ is small and the matrix function $\tilde{A}$ resides in a *solvable* Lie algebra. In other words, the solution of $\Phi' = \tilde{A}(t_n+t)\Phi$, $\Phi(0) = I$, can be evaluated exactly (and, hopefully, cheaply). In that case we replace (1.2) by $\boldsymbol{y}(t_n+t) = \Phi(t)\boldsymbol{x}(t)$, $t \geq 0$, and $B(t)$ by $\Phi^{-1}(t)C(t)\Phi(t)$.

On the face of it, we have replaced one linear system by another. Worse, (1.3) is likely to be more complicated and the computation of B is clearly more expensive than that of A. Having said this, the system (1.3) enjoys one crucial advantage over (1.1): the entries of the matrix B are themselves rapidly oscillating functions. This is not very helpful when (1.3) is solved by a classical numerical method, e.g. Runge–Kutta or multistep. Suppose, however, that we solve the transformed equation by a time-stepping method that requires repeated evaluation of integrals of B, its products and commutators. Precisely since B oscillates, its integrals are scaled by the fastest oscillation mode. An example, thoroughly analysed in [9], is the Magnus expansion. Letting $\boldsymbol{x}(t) = \mathrm{e}^{\Omega(t)}\boldsymbol{y}_n$, we can expand

$$\begin{aligned}\Omega(t) \quad = \quad & \int_0^t B(x)\mathrm{d}x - \tfrac{1}{2}\int_0^t\int_0^{x_1}[B(x_2),B(x_1)]\mathrm{d}x_2\mathrm{d}x_1 \\ & + \tfrac{1}{4}\int_0^t\int_0^{x_1}\int_0^{x_2}[[B(x_3),B(x_2)],B(x_1)]\mathrm{d}x_3\mathrm{d}x_2\mathrm{d}x_1 \\ & + \tfrac{1}{12}\int_0^t\int_0^{x_1}\int_0^{x_3}[B(x_3),[B(x_2),B(x_1)]]\mathrm{d}x_3\mathrm{d}x_2\mathrm{d}x_1 + \cdots.\end{aligned}$$

A general algorithm, allowing recursive generation of Magnus terms, has been presented in [13], but for our purposes the above expansion suffices. If the highest frequency in B is $\omega \gg 1$ then each consecutive integration roughly divides the amplitude by ω, therefore the series converges very rapidly indeed. We refer the reader to [6, 9, 10] for numerical results, which confirm the viability of this approach.

Having approximated $\Omega(h)$ by the matrix $\tilde{\Omega}$, a procedure that requires the truncation of the Magnus series and a replacement of integrals by quadrature, we let

$$\boldsymbol{y}_{n+1} = \mathrm{e}^{h\tilde{A}}\mathrm{e}^{\tilde{\Omega}}\boldsymbol{y}_n \tag{1.4}$$

and continue with time stepping for as long as necessary. We mention an important feature of the method (1.4), namely that, provided that $A(t)$ evolves in some Lie algebra $\mathfrak{g}$, hence the exact solution of (1.1) resides in the corresponding Lie group $\mathcal{G}$, it is true that $\boldsymbol{y}_n \in \mathcal{G}$, $n \geq 0$. This is, therefore, an example of a *Lie-group method* [12]. However, this important attribute of this method plays lesser role in this paper.

This approach is very effective when the dimension d is small, since the evaluation of the two exponentials in (1.4) is then quite cheap. This is not the case,

however, when we consider problems of high dimension, a case in point being a semidiscretization of highly oscillatory PDEs. In principle, the exponentials can be approximated by rational approximations [3], Krylov subspace methods [8] or special methods that are designed to respect Lie-group structure [5, 16]. Yet, even in that case the computation is bound to be fairly expensive.

The two exponentials in (1.4) are not, however, of equal standing. For most large problems the matrix $\tilde{A}$ is likely to possess structure, rendering the computation of its exponential considerably cheaper, while $\tilde{\Omega}$ is typically devoid of any helpful structure. An illustration is provided by the semidiscretization of the *linear Schrödinger equation*

$$\mathrm{i}\frac{\mathrm{d}u}{\mathrm{d}t} = \nabla^2 u + \lambda(t,\boldsymbol{x}), \qquad t \ge 0, \quad \boldsymbol{x} \in \Theta,$$

where $u = u(\boldsymbol{x}, t)$, $\boldsymbol{x} \in \Theta$ and Θ is a suitable two-dimensional (say) domain. Appropriate initial and boundary conditions are specified on $\{t = 0,\ \boldsymbol{x} \in \Theta\}$ and $\{t \ge 0,\ \boldsymbol{x} \in \partial\Theta\}$ respectively. Once the Laplacian is replaced by the standard five-point approximation on a square grid, we obtain the ODE system

$$\mathrm{i}\boldsymbol{u}' = \frac{1}{(\Delta x)^2} S\boldsymbol{u} + \Lambda(t)\boldsymbol{u}, \tag{1.5}$$

where $\boldsymbol{u} = \boldsymbol{u}(t)$ is made up of approximations to u at the grid points, in natural ordering, while the matrix Λ is diagonal. If the boundary conditions are Dirichlet then the "discrete Laplacian" S itself is a block-TST (Toeplitz, symmetric, tridiagonal) matrix, whose sub-matrices are themselves TST. In the case of periodic boundary conditions the matrix S is block-circulant, made out of circulant submatrices. In either case we can evaluate its exponential cheaply using the *fast Fourier transform (FFT).* We rewrite (1.5) in the form

$$\mathrm{i}\boldsymbol{u}' = A(t)\boldsymbol{u} + \tilde{\Lambda}(t)\boldsymbol{u},$$

where

$$A(t) = (\Delta x)^{-2} S + \tilde{\lambda} I \qquad \text{and} \qquad \tilde{\Lambda}(t) = \Lambda(t) - \tilde{\lambda}(t) I,$$

with $\tilde{\lambda}(t) = (\mathrm{vol}\,\Theta)^{-1} \int_\Theta \lambda(t,\boldsymbol{x})\mathrm{d}\boldsymbol{x}$. Since A differs from $(\Delta x)^{-2}S$ by a multiple of the identity matrix, also its exponential can be computed cheaply by FFT, while the procedure ensures that the "remainder" $\tilde{\Lambda}$ is small. (Note that we have adopted here the procedure pioneered in [6]: the matrix $\tilde{A} = A(t_n + \frac{1}{2}h)$ samples a "dominant part" of the vector field $(\Delta x)^{-2}S + \Lambda$.

The first exponential is therefore relatively easy to evaluate but, unfortunately, the matrix $\tilde{\Omega}$, a linear combination of commutators of $\tilde{A}$, does not seem to exhibit any helpful structure. The computation of its exponential is thus exceedingly expensive, and this renders the modified Magnus approach of [9] unrealistic for a problem of this size. This is a serious shortcoming of modified Magnus, since the linear Schrödinger equation is but one example of the many important highly-oscillatory PDEs which are ubiquitous in applications [14].

We are thus on the horns of a dilemma. We are minded to avoid using Magnus expansions in a PDE setting, but nonetheless wish to retain the crucial feature

of these expansions, namely that they can be derived by forming a linear combination of integrals of highly oscillation matrices. Fortunately, there exists an alternative to Magnus that shares the above feature: a *Neumann expansion.* Given the formal equation

$$Y' = \mathcal{A}(t)Y, \quad t \geq 0, \qquad Y(0) = Y_0,$$

where $\mathcal{A}$ might be, for example, a matrix, a differential operator or an integral operator, its solution is given by the series

$$Y(t) = (I - \mathcal{K})^{-1} Y_0 = \sum_{m=0}^{\infty} \mathcal{K}^m Y_0, \tag{1.6}$$

where

$$\mathcal{K}^0 X = X(t), \qquad \mathcal{K}^{m+1} X = \int_0^t \mathcal{A}(x) \mathcal{K}^m X(x) \mathrm{d}x, \quad m \geq 0$$

[2]. The expansion converges, provided that $\|\mathcal{K}\| < 1$ and this can be always ensured for sufficiently small $t > 0$. Note that the Neumann expansion is known in physics as *Dyson series* and in matrix analysis as the method of successive approximations or *Peano series* [7].

The use of Neumann expansions for the solution of the linear ODE (1.1) has been originally advocated in [1]. In the context of the modified system (1.3) this procedure was introduced in [6]. Thus, instead of using a truncated Magnus expansion, we might truncate (1.6), whence

$$\begin{aligned} \boldsymbol{x}_{n+1} \quad = \quad & \boldsymbol{y}_n + \int_0^h B(x) \mathrm{d}x \, \boldsymbol{y}_n \\ & + \int_0^h \int_0^{x_1} B(x_1) B(x_2) \mathrm{d}x_2 \mathrm{d}x_1 \, \boldsymbol{y}_n \\ & + \cdots + \int_0^h \int_0^{x_1} \cdots \int_0^{x_{r-1}} B(x_1) B(x_2) \cdots B(x_r) \mathrm{d}x_r \cdots \mathrm{d}x_2 \mathrm{d}x_1 \, \boldsymbol{y}_n. \end{aligned} \tag{1.7}$$

Since the formation of $\boldsymbol{x}_{n+1}$ from $\boldsymbol{y}_n$ requires just integration, the method shares the most salient feature of modified Magnus expansion: high oscillation of B rapidly attenuates the amplitude of integrals. Of course, a truncated Neumann expansion no longer respects Lie-group structure. This might be sometimes a significant limitation, e.g. often it is crucial to discretize Schrödinger equations while preserving unitarity. Having said this, the basic step underlying a Neumann expansion in this paper is the transformation (1.2), which always preserves Lie-group structure. Departures from a Lie group might occur only in the function $\boldsymbol{x}$, in other words in the correction term. This is likely to result in far less severe loss of Lie-group structure than is the case with, say, classical Runge–Kutta and multistep methods.

The purpose of this paper is to address two issues that are crucial in the implementation of the modified Neumann method (1.7). Firstly, in Section 2, we compute the size of $\|\mathcal{K}\|$ and explore how it is attenuated by rapid oscillation. Subsequently, in Section 3 we describe how to evaluate (1.7) numerically by quadrature.

2 The norm of $\mathcal{K}$

We wish to explore $\|\mathcal{K}\|$, where $\|\cdot\|$ is the Euclidean norm and

$$\mathcal{K}\boldsymbol{z} = \int_0^h B(x)z(x)\mathrm{d}x$$

for every suitable vector function $\boldsymbol{z}$. Moreover,

$$B(t) = \mathrm{e}^{-t\tilde{A}}C(t)\mathrm{e}^{t\tilde{A}},$$

where $\sigma(\tilde{A}) \subset \mathrm{i}\mathbb{R}$, $\tilde{A} = A(t_n + \frac{1}{2}h)$ and $C(t) = A(t_n + t) - \tilde{A} = O(t)$.

Given a function $f(t)$ (scalar, vector or matrix) and $1 \le p \le \infty$, we denote by $\|f\|_p$ the $\mathrm{L}_p[0,h]$ norm of f. A naive estimate is

$$\|\mathcal{K}\boldsymbol{z}\| = \left\| \int_0^h B(x)\boldsymbol{z}\mathrm{d}x \right\| \le \|\boldsymbol{z}\|_\infty \int_0^h \|B(x)\|\mathrm{d}x.$$

Since $A(t_n + t) = \tilde{A} + (t - \frac{1}{2}h)\tilde{F} + O(h^2)$, where $\tilde{F} = A'(t_n + \frac{1}{2}h)$, we readily deduce that

$$\|\mathcal{K}\| \le \tfrac{1}{4}\|\mathrm{e}^{-t\tilde{A}}\tilde{F}\mathrm{e}^{t\tilde{A}}\|_\infty h^2 + O(h^3). \tag{2.1}$$

Therefore $\|\mathcal{K}\|$ scales with h^2, rather than with h in standard applications of Neumann expansions to, say, Fredholm equations of the second kind.

The estimate (2.1) owes the h^2 factor to the fact that C vanishes at the midpoint. Although we know that the integral should attenuate because the integrand oscillates rapidly, this is not reflected in this crude estimate. More powerful estimates are available for the *nonautonomous harmonic oscillator*

$$y'' + g(t)y = 0, \tag{2.2}$$

where $g(t) \gg 1$ for large $t > 0$, converted to a vector form. Indeed, this was the model equation in [9], that demonstrated the power of modified Magnus expansion.

Letting $\omega = \sqrt{g(t_n + \frac{1}{2}h)}$ and $v(t) = g(t_n + t) - g(t_n + \frac{1}{2}h)$, we have explicitly

$$B(t) = v(t)\begin{bmatrix} (2\omega)^{-1}\sin 2\omega t & \omega^{-2}\sin^2\omega t \\ -\cos^2\omega t & -(2\omega)^{-1}\sin 2\omega t \end{bmatrix}.$$

Therefore

$$\|B(t)\| = \cos^2\omega t + \frac{\sin^2\omega t}{\omega^2}$$

and, after straightforward algebra,

$$\int_0^h \|B(x)\|\mathrm{d}x = \frac{h}{2}\left(1 + \frac{1}{\omega^2}\right) + \frac{\sin 2\omega h}{2\omega}\left(1 - \frac{1}{\omega^2}\right) := q(h,\omega).$$

Therefore

$$\|\mathcal{K}\| \le q(h,\omega)\|v\|_\infty = \frac{h}{2}\|v\|_\infty + O(\omega^{-1}).$$

Although this estimate scales with h, rather than with h^2 like (2.1), it is arguably more useful because of the absence of the term $\|e^{-tA}\tilde{F}\mathrm{e}^{tA}\|$. Having said this, the bound (2.1) can also be improved a great deal for the present choice of B. We commence by noting that

$$B(t) = v(t) \begin{bmatrix} \omega^{-1}\sin\omega t \\ -\cos\omega t \end{bmatrix} \begin{bmatrix} \cos\omega t & \omega^{-1}\sin\omega t \end{bmatrix}. \tag{2.3}$$

For every $m \geq 0$ we let

$$\mathcal{N}_m = \int_0^h \int_0^{x_1} \cdots \int_0^{x_{m-1}} B(x_1)B(x_2)\cdots B(x_m)\mathrm{d}x_m \cdots \mathrm{d}x_2\mathrm{d}x_1,$$

therefore $\mathcal{K}^m = \mathcal{N}_m$, $m \geq 0$, and $\boldsymbol{x}(h) = \sum_{m=0}^{\infty} \mathcal{N}_m \boldsymbol{y}_n$.

Because of (2.3) we have

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

and, by induction,

$$\begin{aligned} \mathcal{N}_m &= \frac{1}{\omega^{m-1}} \int_0^h \int_0^{x_1} \cdots \int_0^{x_{m-1}} \prod_{l=1}^{m} v(x_l) \prod_{l=1}^{m-1} \sin\omega(x_{l+1}-x_l) \\ &\quad \times \begin{bmatrix} \omega^{-1}\sin\omega x_1 \\ -\cos\omega x_1 \end{bmatrix} \begin{bmatrix} \cos\omega x_m & \omega^{-1}\sin\omega x_m \end{bmatrix} \mathrm{d}x_m \cdots \mathrm{d}x_2\mathrm{d}x_1. \end{aligned}$$

We observe that

$$\begin{aligned} & \left\| \begin{bmatrix} \omega^{-1}\sin\omega x \\ -\cos\omega x \end{bmatrix} \begin{bmatrix} \cos\omega y & \omega^{-1}\sin\omega y \end{bmatrix} \right\| \\ = \;& \cos^2\omega x \cos^2\omega y + \frac{\sin 2\omega x \cos^2\omega y + \cos^2\omega x \sin^2\omega y}{\omega^2} + \frac{\sin^2\omega x \sin^2\omega y}{\omega^4} \\ \leq \;& \left(1 + \frac{1}{\omega^2}\right)^2. \end{aligned}$$

Therefore, using the Cauchy–Schwartz inequality,

$$\|\mathcal{N}_m\| \leq \frac{1+\omega^{-2}}{\omega^{m-1}} \theta_m^{1/2} \|v\|_2^m,$$

where

$$\theta_m = \int_0^h \int_0^{x_1} \cdots \int_0^{x_{m-1}} \prod_{l=1}^{m-1} \sin^2\omega(x_l - x_{l+1})\mathrm{d}x_m \cdots \mathrm{d}x_2\mathrm{d}x_1.$$

Herewith the first few θ_ms,

$$\theta_1 = h,$$

$$\begin{aligned}
\theta_2 &= \frac{h^2}{4} - \frac{\sin^2 \omega h}{4\omega^2} \\
\theta_3 &= \frac{h^3}{24} - \frac{h(1+\frac{1}{4}\cos 2\omega h)}{8\omega^2} + \frac{5\sin 2\omega h}{64\omega^3}, \\
\theta_4 &= \frac{h^4}{192} - \frac{h^2(3-\frac{1}{4}\cos 2\omega h)}{64\omega^2} + \frac{13h\sin 2\omega h}{512\omega^3} + \frac{3\sin^2 \omega h}{32\omega^4}, \\
\theta_5 &= \frac{h^5}{1920} - \frac{h^3(1+\frac{1}{32}\cos 2\omega h)}{96\omega^2} + \frac{h^2 \sin 2\omega h}{256\omega^3} + \frac{h(5+\frac{71}{32}\cos 2\omega h)}{128\omega^4} \\
&\quad - \frac{231\sin 2\omega h}{8192\omega^5}.
\end{aligned}$$

LEMMA 2.1. *For every $m \geq 1$ it is true that*

$$\theta_m = \frac{h^m}{2^{m-1}m!} + O(\omega^{-2}). \tag{2.4}$$

PROOF. We commence by noting that

$$\theta_m = \frac{1}{2^{m-1}} \int_0^h \int_0^{x_1} \cdots \int_0^{m-1} \prod_{l=1}^{m-1} [1 - \cos 2\omega(x_{l+1} - x_l)] \mathrm{d}x_m \cdots \mathrm{d}x_2 \mathrm{d}x_1.$$

We prove by induction on $r = 0, 1, \ldots, m-1$ that

$$\begin{aligned}
\theta_m &= \frac{1}{2^{m-1}r!} \int_0^h \cdots \int_0^{x_{m-r-1}} x_{m-r}^r \prod_{l=1}^{m-r-1} [1 - \cos 2\omega(x_{l+1} - x_l)] \mathrm{d}x_{m-r} \cdots \mathrm{d}x_1 \\
&\quad + O(\omega^{-2}). \qquad (2.5)
\end{aligned}$$

This is certainly true for $r = 0$. Moreover, integrating twice by parts,

$$\begin{aligned}
&\int_0^t x^r [1 - \cos 2\omega(x-t)] \mathrm{d}x \\
&= \frac{t^{r+1}}{r+1} - \int_0^t x^r \cos 2\omega(x-t) \mathrm{d}x = \frac{t^{r+1}}{r+1} + \frac{r}{2\omega} \int_0^t x^{r-1} \sin 2\omega(x-t) \mathrm{d}x \\
&= \frac{t^{r+1}}{r+1} - \frac{r}{4\omega^2}[t^{r-1} - 0^{r-1}\cos 2\omega t] + \frac{(r-1)r}{4\omega^2} \int_0^t x^{r-2} \cos 2\omega(x-t) \mathrm{d}x.
\end{aligned}$$

We let $t = x_{m-r-1}$ and substitute in (2.5), thereby advancing induction from r to $r+1$. Letting $r = m$ confirms (2.4). □

We deduce that

$$\|\mathcal{N}_m\| \leq \frac{1}{\omega^{m-1}} \frac{\|v\|_2^m h^{m/2}}{2^{(m-1)/2}\sqrt{m!}} + O(\omega^{-m-1}).$$

Note that $\|v\|_2$ above is itself quite small: expanding into Taylor series about $\frac{1}{2}h$, we have

$$\|v\|_2^2 = \int_0^h [g(t_n + x) - g(t_n + \tfrac{1}{2}h)]^2 \mathrm{d}x = \tfrac{1}{12}[g'(t_n + \tfrac{1}{2}h)]^2 h^3 + O(h^4).$$

We conclude that $\|\mathcal{N}_m\|$ decays very rapidly indeed with m:

$$\|\mathcal{N}_m\| \le \frac{\sqrt{2}\omega}{\sqrt{m!}}\left[\frac{|g'(t_n+\frac{1}{2}h)|h^2}{\sqrt{12}\omega}\right]^m + O\left(\frac{1}{\omega^{m+1}}, \frac{h^{2m+1/2}}{\omega^{m-1}}\right), \quad m \ge 1. \tag{2.6}$$

This indicates that just few terms are required in the Neumann expansion. Moreover, the larger the frequency ω, the more rapid the convergence.

In one sense (2.6) is too pessimistic. For fixed ω and small $h > 0$ we have

$$\begin{aligned}
\mathcal{N}_1 &\approx \begin{bmatrix} O(h^3) & O(h^4) \\ O(h^3) & O(h^3) \end{bmatrix}, \\
\mathcal{N}_2 &\approx \begin{bmatrix} O(h^6) & O(h^7) \\ O(h^5) & O(h^6) \end{bmatrix}, \\
\mathcal{N}_3 &\approx \begin{bmatrix} O(h^9) & O(h^{10}) \\ O(h^9) & O(h^9) \end{bmatrix}, \\
\mathcal{N}_4 &\approx \begin{bmatrix} O(h^{12}) & O(h^{13}) \\ O(h^{11}) & O(h^{12}) \end{bmatrix}
\end{aligned}$$

and so on. A general rule can be obtained but its proof is too labourous and long for presentation in this paper. Instead, we note the "classical" order (that is, for fixed ω and small $h > 0$) of different truncated Neumann series, as applied to the harmonic oscillator (2.2):

$$\begin{aligned}
\boldsymbol{x}_{n+1} &= \boldsymbol{y}_n && \text{order 2,} \\
\boldsymbol{x}_{n+1} &= (I+\mathcal{N}_1)\boldsymbol{y}_n && \text{order 4,} \\
\boldsymbol{x}_{n+1} &= (I+\mathcal{N}_1+\mathcal{N}_2)\boldsymbol{y}_n && \text{order 8,} \\
\boldsymbol{x}_{n+1} &= (I+\mathcal{N}_1+\mathcal{N}_2+\mathcal{N}_3)\boldsymbol{y}_n && \text{order 10.}
\end{aligned}$$

Of course, it is not just positive powers of h but also negative powers of ω that mop up the error.

3 Quadrature

Practical implementation of Neumann series (1.7) requires the replacement of multivariate integrals by quadrature. Although multivariate quadrature is usually considered a "hard" problem, it is well known that it is possible to implement Magnus expansions with surprisingly effective and cheap quadrature [12]. Moreover, that quadrature can be amended to cater for highly oscillatory integrands [11]. The purpose of this section is to explore similar approach in the context of Neumann series.

Effective Magnus quadrature combines four components:

1. Once the values $B_l = B(c_l h)$, $l = 1, 2, \ldots, \nu$, where $c_1, c_2, \ldots, c_\nu$ are distinct quadrature nodes, have been computed, they are reused in *all* Magnus

integrals:

$$\begin{aligned}\int_0^h B(x)\mathrm{d}x &\approx h\sum_{l=1}^{\nu} b_l B_l,\\ \int_0^h\int_0^{x_1}[B(x_1),B(x_2)]\mathrm{d}x_2\mathrm{d}x_1 &\approx h^2\sum_{k=1}^{\nu}\sum_{l=1}^{\nu} b_{k,l}[B_k,B_l]\end{aligned}$$

etc. It was proved in [13] that there exist weights so that the order of accuracy for all multivariate integrals coincides with the order of the *univariate* Gauss–Christoffel quadrature at the same points. Needless to say, the latter can be determined in a well-known fashion and we deduce that, other things being equal, the best policy is to use Gauss–Legendre nodes.

2. The function values $B_1,\dots,B_\nu$ are replaced by their linear combinations $M_1,M_2,\dots,M_\nu$ such that $M_l \approx h^l B^{(l-1)}(\frac{1}{2}h)$, $l=1,2,\dots,\nu$. This approach, pioneered in [15], has a number of advantages. Firstly, it results in a time symmetric approximation, allowing for roughly half of the terms to be thrown out. Secondly, many terms can be identified as being of order larger than the required order of approximation, hence can be eliminated. Thirdly, it is possible to use the theory of graded Lie algebras to express terms as linear combinations of a relatively small number of commutators. The outcome is a method that requires relatively modest volume of linear algebra per step.

3. The commutators that need be evaluated can be lumped together and computed in a manner that minimizes numerical work [4]. The outcome is, for example, a sixth-order Magnus method that requires just three function evaluations and three commutators per step.

4. In the important case when the entries of B oscillate rapidly, Gauss–Christoffel quadrature need be replaced by Filon quadrature. While the first is ineffective in the presence of high oscillation, the latter delivers accuracy which, actually, improves with higher oscillation. This approach can be extended, similarly to points 1–2 above, to all the integrals present in a truncated Magnus expansion [11].

Magnus quadrature can be extended readily to the setting of Neumann series. Thus, again, $B_l = B(c_l h)$, $l=1,2,\dots,\nu$, and we approximate

$$\mathcal{N}_m \approx h^m \sum_{k_1=1}^{\nu}\sum_{k_2=1}^{\nu}\cdots\sum_{k_m=1}^{\nu} b_{\boldsymbol{k}}^{(m)} B_{k_1}B_{k_2}\cdots B_{k_m}, \tag{3.1}$$

where

$$b_{\boldsymbol{k}}^{(m)} = \int_0^1\int_0^{x_1}\cdots\int_0^{x_{m-1}}\prod_{j=1}^{\nu}\ell_{k_j}(x_j)\mathrm{d}x_m\cdots\mathrm{d}x_2\mathrm{d}x_1.$$

Here ℓ_k is the kth cardinal polynomial of Lagrangian interpolation,

$$\ell_k(x) = \prod_{\substack{j=1\\ j\neq k}}^{\nu} \frac{x-c_j}{c_l-c_j}, \qquad k=1,2,\ldots,k.$$

LEMMA 3.1. *Suppose that the univariate quadrature at the nodes $c_1, c_2, \ldots, c_\nu$ is of order $p \in \{\nu, \nu+1, \ldots, 2\nu\}$, in other words that*

$$\int_0^1 x^{j-1} \prod_{l=1}^{\nu} (x-c_l) \mathrm{d}x = 0, \qquad j=1,2,\ldots,p-\nu.$$

Then the quadrature (3.1) is also of order p for all $m \geq 0$.

PROOF. Identical to the proof for Magnus quadrature in [13]. □

For example, we obtain order 4 by choosing the Gauss–Legendre nodes

$$c_1 = \tfrac{1}{2} - \tfrac{\sqrt{3}}{6}, \qquad c_2 = \tfrac{1}{2} + \tfrac{\sqrt{3}}{6},$$

whence

$$\begin{aligned}
\mathcal{N}_1 &\approx \tfrac{1}{2}h(B_1+B_2),\\
\mathcal{N}_2 &\approx h^2[\tfrac{1}{8}B_1^2 + (\tfrac{1}{8}-\tfrac{\sqrt{3}}{12})B_1B_2 + (\tfrac{1}{8}+\tfrac{\sqrt{3}}{12})B_2B_1 + \tfrac{1}{8}B_2^2],\\
\mathcal{N}_3 &= h^3[\tfrac{1}{48}B_1^3 + (\tfrac{1}{30}-\tfrac{\sqrt{3}}{48})B_1^2B_2 - \tfrac{1}{240}B_1B_2B_1 + (\tfrac{1}{30}+\tfrac{\sqrt{3}}{48})B_2B_1^2\\
&\quad + (\tfrac{1}{30}-\tfrac{\sqrt{3}}{48})B_1B_2^2 - \tfrac{1}{240}B_2B_1B_2 + (\tfrac{1}{30}+\tfrac{\sqrt{3}}{48})B_2^1B_1 + \tfrac{1}{48}B_2^2].
\end{aligned}$$

Next, we take a leaf off [15] and replace $B_1, B_2, \ldots, B_\nu$ by $M_1, M_2, \ldots, M_\nu$, where

$$\sum_{l=1}^{\nu} (c_k - \tfrac{1}{2})^{l-1} M_l = hB_k, \qquad k=1,2,\ldots,\nu.$$

Therefore, in place of (3.1) we have

$$\mathcal{N}_m \approx \sum_{k_1=1}^{\nu} \sum_{k_2=1}^{\nu} \cdots \sum_{k_m=1}^{\nu} \tilde{b}_{\boldsymbol{k}}^{(m)} M_{k_1} M_{k_2} \cdots M_{k_m},$$

where

$$\tilde{b}_{\boldsymbol{k}}^{(m)} = \int_0^1 \int_0^{x_1} \cdots \int_0^{x_{m-1}} \prod_{j=1}^{m} (x_j - \tfrac{1}{2})^{k_j-1} \mathrm{d}x_m \cdots \mathrm{d}x_2 \mathrm{d}x_1.$$

However, by construction

$$M_{k_1} M_{k_2} \cdots M_{k_m} = O(h^{|\boldsymbol{k}|}),$$

where $|\boldsymbol{k}| = \boldsymbol{k}^\top \boldsymbol{1}$. Therefore, once we have decided on order p, we can dispose of all terms with $|\boldsymbol{k}| > p$ and use the quadrature

$$\mathcal{N}_m \approx \sum_{|\boldsymbol{k}|\leq p} \tilde{b}_{\boldsymbol{k}}^{(m)} M_{k_1} M_{k_2} \cdots M_{k_m}. \tag{3.2}$$

Revisiting the case $\nu = 2$ with Gauss–Legendre points, we have

$$M_1 = \tfrac{1}{2}(B_1 + B_2), \qquad M_2 = \sqrt{3}(B_2 - B_1)$$

and

$$\begin{aligned}
\mathcal{N}_1 &\approx M_1, \\
\mathcal{N}_2 &\approx \tfrac{1}{2}M_1^2 + \tfrac{1}{12}[M_2, M_1], \\
\mathcal{N}_3 &\approx \tfrac{1}{6}M_1^3 + \tfrac{1}{24}[M_2, M_1^2], \\
\mathcal{N}_4 &\approx \tfrac{1}{24}M_1^4.
\end{aligned}$$

Note that just few terms are required and that the weights of both M_1^2 and $M_1M_2M_1$ are zero. This results in the fourth-order Neumann method

$$\boldsymbol{x}_{n+1} = \{M_1 + \tfrac{1}{2}M_1^2 + \tfrac{1}{6}M_1^3 + \tfrac{1}{24}M_1^4 + \tfrac{1}{12}[M_2, M_1] + \tfrac{1}{24}[M_2, M_1^2]\}\boldsymbol{y}_n. \tag{3.3}$$

Unfortunately, (3.3) is not equal to the task in hand, since the main feature of the matrix $B(t)$, hence also of the M_ls, is that their entries oscillate rapidly. Indeed, the very reason of the transformation (1.2) was to induce high oscillation in the matrix. However, Gauss–Legendre and other Gauss–Christoffel quadrature formulae are useless in the presence of high oscillation [11]. In many instances a suitable alternative is to use *Filon quadrature,* that has been analysed extensively in [11]. An important case is the harmonic oscillator $y'' + g(t)y = 0$, but in the sequel, in Section 4, we mention the less trivial case of the wave equation with a forcing term.

The univariate form of the Filon quadrature is

$$\int_0^1 f(x)\mathrm{e}^{\mathrm{i}\omega x}\mathrm{d}x \approx \sum_{l=1}^{\nu} b_l(\omega) f(c_l h), \tag{3.4}$$

where $c_1 < c_2 < \cdots < c_\nu$ are, again, quadrature nodes and

$$b_l(\omega) = \int_0^1 \ell_k(x)\mathrm{e}^{\mathrm{i}\omega x}\mathrm{d}x, \qquad l = 1, 2, \ldots, \nu.$$

Provided that $c_1 = 0$, $c_\nu = 1$, it was proved in [11] that the error for $\omega \gg 1$ is $O(\omega^{-2})$, while for small $\omega > 0$ the method is of the same order as the Gauss–Christoffel quadrature with the same nodes.

The discussion in the remainder of this section is restricted to the harmonic oscillator. We commence from $\mathcal{N}_1$, writing it in the form

$$\begin{aligned}
\mathcal{N}_1 \;=\; & \frac{h}{2}\begin{bmatrix} 0 & \omega^{-2} \\ -1 & 0 \end{bmatrix}\int_0^1 v(hx)\mathrm{d}x - \frac{h}{2}\begin{bmatrix} 0 & \omega^{-2} \\ 1 & 0 \end{bmatrix}\int_0^1 v(hx)\cos 2\omega hx\mathrm{d}x \\
& + \frac{h}{2\omega}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\int_0^1 v(hx)\sin 2\omega hx\mathrm{d}x
\end{aligned}$$

To ensure both $O(\omega^{-2})$ decay for $\omega \gg 1$ and order four for small $\omega > 0$, we choose the Lobatto nodes

$$c_1 = 0, \qquad c_2 = \tfrac{1}{2}, \qquad c_3 = 1.$$

Let $v_l = v(c_l h)$, $l = 1, 2, 3$, and note that, by construction, $v_2 = 0$. Then

$$\begin{aligned}
\int_0^1 v(hx)\mathrm{d}x &\approx \tfrac{1}{6}(v_1 + v_3),\\
\int_0^1 v(hx)\cos\eta x\mathrm{d}x &\approx \left[\frac{3+\cos\eta}{\eta^2} - \frac{4\sin\eta}{\eta^3}\right]v_1 + \left[\frac{\sin\eta}{\eta} + \frac{1+3\cos\eta}{\eta^2} - \frac{4\sin\eta}{\eta^3}\right]v_3,\\
\int_0^1 v(hx)\sin\eta x\mathrm{d}x &\approx \left[\frac{1}{\eta} + \frac{\sin\eta}{\eta^2} - \frac{4(1-\cos\eta)}{\eta^3}\right]v_1\\
&\quad + \left[-\frac{\cos\eta}{\eta} + \frac{3\sin\eta}{\eta^2} - \frac{4(1-\cos\eta)}{\eta^3}\right]v_3.
\end{aligned}$$

where $\eta = 2h\omega$.

Bearing in mind the discussion from Section 2, there is no need to evaluate $\mathcal{N}_m$ for $m \geq 2$ to attain order 4. We mention in passing that, were we to desire higher order, we would have needed "oscillation-proof" multivariate quadrature, but this can be accomplished similarly to the formulae for Filon quadrature of modified Magnus in [11].

4 An application: The wave equation with a forcing term

Consider the equation

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} - g(x,t)u, \qquad t \geq 0, \quad 0 \leq x \leq 1, \tag{4.1}$$

accompanied by the initial condition $u(x,0) = \phi(x)$, $\partial u(x,0)/\partial t = \psi(x)$, $0 \leq x \leq 1$, and a periodic boundary condition $u(1,t) = u(0,t)$, $t \geq 0$. We assume that $g(x,t) \geq 0$ throughout its range but our main interest is in large g.

Letting $\Delta x = 1/(M+1)$, where M is a given integer, we let $u_m(t)$ be our approximation to $u(m\Delta x, t)$, $m = 0, 1, \ldots, M$. Discretising space derivatives with standard central finite differences, we obtain the ODE system

$$u_m'' - \frac{1}{(\Delta x)^2}(u_{m-1} - 2u_m + u_{m+1}) + g_m(t)u_m = 0, \quad m = 1, \ldots, M, \tag{4.2}$$

in tandem with the initial condition $u_m(0) = \phi(m\Delta x)$, $u_m'(0) = \psi(m\Delta x)$, and the periodic boundary condition $u_0(t) = u_M(t)$. We rewrite (4.2) in a vector form,

$$\boldsymbol{y}' = \begin{bmatrix} O & I \\ -(\Delta x)^{-2}T - G(t) & O \end{bmatrix}\boldsymbol{y}, \quad t \geq 0, \qquad \boldsymbol{y}(0) = \begin{bmatrix} \boldsymbol{u}(0) \\ \boldsymbol{u}'(0) \end{bmatrix}, \tag{4.3}$$

where

$$T = \begin{bmatrix} 2 & -1 & 0 & \cdots & 0 & -1 \\ -1 & 2 & -1 & \ddots & & 0 \\ 0 & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & & \ddots & -1 & 2 & -1 \\ -1 & 0 & \cdots & 0 & -1 & 2 \end{bmatrix}$$

is a positive-semidefinite circulant matrix, while

$$G(t) = \begin{bmatrix} g_1(t) & 0 & \cdots & 0 \\ 0 & g_2(t) & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & g_M(t) \end{bmatrix}, \qquad g_m(t) = g(m\Delta x, t).$$

To time-step from t_n to $t_{n+1} = t_n + \Delta t$, we let

$$\tilde{g} = \int_0^1 g(x, t_n + \tfrac{1}{2}\Delta t)\mathrm{d}x > 0$$

(if computation of the integral is difficult, we can use simple quadrature) and

$$\tilde{A} = \begin{bmatrix} O & I \\ -(\Delta x)^{-2}T - \tilde{g}I & O \end{bmatrix}.$$

Since $(\Delta x)^{-2}T + \tilde{g}I$ is positive definite, it readily follows that the spectrum of $\tilde{A}$ resides in $\mathrm{i}\mathbb{R}$. More specifically,

$$\frac{1}{(\Delta x)^2}T + \tilde{g}I = QDQ^*,$$

where $Q_{k,l} = \exp(\frac{2\mathrm{i}\pi kl}{M})$ and $D_{k,k} = \tilde{g} + 2[1 - \cos(\frac{2\pi k}{M})]/(\Delta x)^2$, $D_{k,l} = 0$ for $k \neq l$. Note that, because of the specific form of Q, the products $Q\boldsymbol{v}$ and $Q^*\boldsymbol{v}$ can be computed by FFT in $O(M \log_2 M)$ operations for any vector $\boldsymbol{v} \in \mathbb{C}^M$. Moreover,

$$\mathrm{e}^{t\tilde{A}} = Q \begin{bmatrix} \cos(tD^{1/2}) & D^{-1/2}\sin(tD^{1/2}) \\ -D^{1/2}\sin(tD^{1/2}) & \cos(tD^{1/2}) \end{bmatrix} Q^*$$

where the four $M \times M$ blocks are diagonal, e.g.

$$\cos(tD^{1/2}) = \begin{bmatrix} \cos(t\sqrt{D_{1,1}}) & 0 & \cdots & 0 \\ 0 & \cos(t\sqrt{D_{2,2}}) & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \cos(t\sqrt{D_{M,M}}) \end{bmatrix}.$$

We note in passing that the matrix $\mathrm{e}^{t\tilde{A}}$ evolves in the symplectic group $\mathrm{Sp}(M)$, although we will not make further use of this fact.

We next change variables in line with (1.3). Thus, letting $C = \cos(tD^{1/2})$ and $S = \sin(tD^{1/2})$, we have

$$\begin{aligned} B(t) &= \mathrm{e}^{-t\tilde{A}} \begin{bmatrix} O & O \\ \tilde{g} - G(t) & O \end{bmatrix} \mathrm{e}^{t\tilde{A}} \\ &= Q \begin{bmatrix} C & -D^{-1/2}S \\ D^{1/2}S & C \end{bmatrix} Q^* \begin{bmatrix} O & O \\ \tilde{G} & O \end{bmatrix} Q \begin{bmatrix} C & D^{-1/2}S \\ -D^{1/2}S & C \end{bmatrix} Q^*, \end{aligned}$$

where $\tilde{G} = \tilde{g}I - G(t)$. In practice, we need to form products of the form $B(t)\boldsymbol{v}$, where $\boldsymbol{v} = [\boldsymbol{v}_1^\top, \boldsymbol{v}_2^\top]^\top \in \mathbb{C}^{2M}$. This requires six FFTs and several multiplications by *diagonal* matrices:

1. Form $\boldsymbol{w}_1 = Q^*\boldsymbol{v}_1$ and $\boldsymbol{w}_2 = Q^*\boldsymbol{v}_2$ at the cost of two FFTs;
2. Let $\boldsymbol{z} = Q[C\boldsymbol{w}_1 + D^{-1/2}S\boldsymbol{w}_2]$: this takes a single FFT;
3. Form $\boldsymbol{s} = Q^*\tilde{G}\boldsymbol{z}$ with a single FFT;
4. Using FFT twice, evaluate $\boldsymbol{\beta}_1 = -QD^{-1/2}S\boldsymbol{s}$ and $\boldsymbol{\beta}_2 = QC\boldsymbol{s}$.

Now $\boldsymbol{\beta} = [\boldsymbol{\beta}_1^\top, \boldsymbol{\beta}_2^\top]^\top = B(t)\boldsymbol{v}$.

Given that we are unlikely to aim for a method of order greater than four in a PDE setting, we need to compute just $\mathcal{N}_1\boldsymbol{y}_n = \int_0^h \boldsymbol{\beta}(x)\mathrm{d}x$ (where now $\boldsymbol{v} = \boldsymbol{y}_n$). Sometimes the entries of $\tilde{G}$ are simple and lend themselves to exact integration. Otherwise, we need to resort to quadrature, while bearing in mind that the integrand oscillates rapidly. Let $\tilde{\boldsymbol{\beta}}_k = Q^*\boldsymbol{\beta}_k$ and $P(t) = Q^*\tilde{G}(t)Q$. Then, letting $\lambda_k = \sqrt{D_{k,k}}$, $k = 1, 2, \ldots, M$, we have, after long yet elementary calculation,

$$\begin{aligned} \tilde{\beta}_{1,k}(t) &= -\frac{1}{2\lambda_k} \sum_{j=1}^{M} P_{k,j}(t) \left\{ [\sin t(\lambda_k - \lambda_j) + \sin t(\lambda_k + \lambda_j)] w_{1,j} \right. \\ &\qquad \left. + [\cos t(\lambda_k - \lambda_j) - \cos t(\lambda_k + \lambda_j)] \frac{w_{2,j}}{\lambda_j} \right\}. \end{aligned}$$

We approximate

$$\int_0^h \tilde{\beta}_{1,k}(x)\mathrm{d}x \approx -\frac{h}{2\lambda_k} \sum_{j=1}^{M} \sum_{l=1}^{3} \left[\gamma_{k,j,l}^{(1)} P_{k,j}(c_l h) w_{1,j} + \gamma_{k,j,l}^{(2)} P_{k,j}(c_l h) \frac{w_{2,j}}{\lambda_j} \right],$$

where $c_1 = 0$, $c_2 = \frac{1}{2}$, $c_3 = 1$,

$$\begin{aligned} \gamma_{k,j,l}^{(1)} &= b_l^{(1)}(h(\lambda_k - \lambda_j)) + b_l^{(1)}(h(\lambda_k + \lambda_j)), \\ \gamma_{k,j,l}^{(2)} &= b_l^{(2)}(h(\lambda_k - \lambda_j)) - b_l^{(2)}(h(\lambda_k + \lambda_j)), \end{aligned}$$

and the Filon–Lobatto weights are

$$\begin{aligned} b_1^{(1)}(\omega) &= \frac{1}{\omega} + \frac{\sin\omega}{\omega^2} - \frac{4(1-\cos\omega)}{\omega^3}, \\ b_2^{(1)}(\omega) &= -\frac{4\sin\omega}{\omega^2} + \frac{8(1-\cos\omega)}{\omega^3}, \\ b_3^{(1)}(\omega) &= -\frac{\cos\omega}{\omega} + \frac{3\sin\omega}{\omega^2} - \frac{4(1-\cos\omega)}{\omega^3} \end{aligned}$$

and

$$\begin{aligned} b_1^{(2)}(\omega) &= \frac{3+\cos\omega}{\omega^2} - \frac{4\sin\omega}{\omega^3}, \\ b_2^{(2)}(\omega) &= -\frac{4(1+\cos\omega)}{\omega^2} + \frac{8\sin\omega}{\omega^3}, \\ b_3^{(2)}(\omega) &= \frac{\sin\omega}{\omega} + \frac{1+3\cos\omega}{\omega^2} - \frac{4\sin\omega}{\omega^3}. \end{aligned}$$

Similar treatment applies to $\tilde{\beta}_{2,k}$.

Implementation of the above Filon–Lobatto quadrature means that we must form the matrix P, at the cost of $O(M^2)$ operations. Yet, this is not prohibitively expensive.

The above algorithm might well be improved. Our intention in this section is emphatically *not* to present a polished, complete algorithm for the solution of the wave equation (4.1). The goal is considerably more modest, to demonstrate that a combination of the change of variables (1.2), Neumann series and Filon-type integration is possible also in a PDE context and that it leads to efficient algorithms.

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