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On error bounds for the Gautschi-type exponential integrator applied to oscillatory second-order differential equations

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Summary. This paper studies a numerical method for second-order oscillatory differential equations in which high-frequency oscillations are generated by a linear time- and/or solution-dependent part. For constant linear part, it is known that the method allows second-order error bounds independent of the product of the step-size with the frequencies and is therefore a long-time-step method. Most real-world problems are not of that kind and it is important to study more general equations. The analysis in this paper shows that one obtains second-order error bounds even in the case of a time- and/or solution-dependent linear part if the matrix is evaluated at averaged positions.

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1 Introduction

This paper deals with differential equations of type

$$(1) \qquad y'' = -A(t, y)y + g(t, y), \qquad y(t_0) = y_0, \qquad y'(t_0) = y'_0,$$

where $A(t, y)$ is a symmetric and positive semi-definite real matrix of an arbitrarily large norm. The large norm of $A(t, y)$ introduces an oscillatory solution and therefore differential equations of this type are called oscillatory or highly-oscillatory.

Oscillatory differential equations are currently a subject of high interest (e.g. [1–3,6,7,10,12–14]). For a survey in connection with the results presented here, one can refer to [7], chap. XIII.

Oscillatory differential equations arise in many different applications. For example in spatial discretisation of partial differential equations (as semilinear wave equations) and in N-body problems from classical molecular dynamics. There, $A(t, y)$ represents the Jacobian of the fast forces generated by atoms in close proximity. In both applications $A(t, y)$ is a real symmetric matrix of large dimension but sparse and $g(t, y)$ is often costly to evaluate. Further the solution satisfies a finite-energy condition which bounds the amplitudes of the high oscillations.

In the applications mentioned above scientists are more interested in long-time solutions than in short-time calculations. But the nature of oscillatory solutions is such that for accurate numerical solutions, one needs to implement standard methods with step-size h smaller than the square-root of the inverse of $\|A\|$. If $g(t, y)$ is costly to evaluate, this leads to a long simulation time for the desired result.

So the aim in this paper is to use step-sizes which are not restricted by the frequencies of A (i.e. square roots of eigenvalues of A). Methods which allow such time-steps are called long-time-step methods in [3]. To prove this property, one has to prove error bounds independent of $\|A\|$. This was already known to García-Archilla, Sanz-Serna and Skeel (cf. [3]), who proposed and analysed a method for oscillatory differential equations, which they called *mollified impulse method*. Their analysis is for the case of a differential equation of type (1) with a constant matrix.

Hochbruck and Lubich (cf. [10]) proposed and analysed a Gautschi-type method for oscillatory differential equations with constant matrix. In the case of solution dependent matrix $A(y)$, they proposed to use a similar method with the matrix evaluated at averaged positions (cf. [8]), but they did not examine whether this additional work is necessary. Aside from small changes this method is studied here in detail.

Most real world problems are not of the kind where the differential equation can be transformed to (1) with constant matrix A. But it is well known that many systems exist which have a nearly harmonic behaviour and can be transformed to (1). It is therefore important to know methods that allow larger time-steps for these more general systems.

The analysis in this paper and numerical experiments show that the Gautschi-type method with the matrix evaluated at averaged positions is a long-time step method for systems of type (1), and that averaging is necessary to obtain non-smooth second-order error bounds. The analysis gives new insight into the development of numerical methods for more general equations with highly-oscillatory solutions.

This paper is organised as follows: In Section 2 the numerical method is presented. Section 3 describes the main result, some conclusions and an outline of proof. Since the proof works with the variation-of-constants formula

instead of Taylor series expansion, the proof is presented again in more detail in section 4. The method considered in this paper requires the computation of the product $\psi(A)v$ of an analytic function ψ of a matrix A with a vector v in every time step. The known results for how this can be done efficiently are briefly reviewed in Section 5, along with another note on implementation. Lastly in section 6 a numerical experiment is presented.

2 The integration scheme

Using the variation-of-constants formula for (1) at time t_n gives

$$y(t_n + h) = \cos h\Omega_n y(t_n) + h \operatorname{sinc} h\Omega_n y'(t_n) + \int_0^h \Omega_n^{-1} \sin(h - s)\Omega_n g(t_n + s, y(t_n + s))\, ds, \tag{2}$$

with $\Omega_n = \Omega(t_n, y(t_n)) := \sqrt{A(t_n, y(t_n))}$. Here, all signs following an analytic function up to and including the next matrix belong to the argument of the analytic function. This way, a lot of brackets can be omitted. Note that $\operatorname{sinc}(x)$ designates the function $\sin(x)$ divided by x.

Approximating the integrand by $\Omega_n^{-1} \sin(h - s)g(t_n, y(t_n))$ and adding the formula (2) evaluated at $-h$ to (2) delivers

$$y(t_n + h) - 2\cos h\Omega_n y(t_n) + y(t_n - h) \approx h^2 \operatorname{sinc}^2 \tfrac{h}{2}\Omega_n \; g(t_n, y(t_n)). \tag{3}$$

This suggests the numerical integration scheme

$$y_{n+1} - 2\cos h\Omega_n y_n + y_{n-1} = h^2 \operatorname{sinc}^2 \tfrac{h}{2}\Omega_n \; g_n, \tag{4}$$

with $\Omega_n = \Omega(t_n, y_n)$ and $g_n = g(t_n, y(t_n))$, for approximations y_n to the solution $y(t_n)$ at time $t_n = t_0 + nh$. However, like in [3] and [10], it turns out to be favourable to take a modified argument in Ω and g. Numerical experiments and the theory in this paper suggest to use

$$g_n = g(t_n, \phi(h\Omega_n)y_n) \quad \text{and} \quad \Omega_n = \Omega(t_n, \phi(h\Omega(t_n, y_n))y_n),$$

where the *filter function* $\phi(x)$ is a suitably chosen real function depending smoothly on x^2, whose purpose is to filter out resonant frequencies. Further assumptions on ϕ are

$$\phi(0) = 1, \qquad \phi(k\pi) = 0, \qquad k = 1, 2, 3, \dots,$$

and

$$|\phi(x)| \le 1, \qquad |\phi'(x)| \le 1, \qquad x \ge 0.$$

The bound 1 is not necessary. It suffices that ϕ, ϕ' are bounded by a small constant. The choice

$$\phi(x) = \operatorname{sinc} x \, (1 + \tfrac{1}{3} \sin^2 \tfrac{1}{2} x) \tag{5}$$

was found to give particularly good accuracy in the case of a constant matrix A in [10]. A simpler choice is

$$\phi(x) = \operatorname{sinc} x, \tag{6}$$

proposed in [3].

A second starting value for the recursion (4) is obtained by

$$y_1 = \cos h\Omega_0 y_0 + h \operatorname{sinc} h\Omega_0 y_0' + \frac{1}{2} h^2 \operatorname{sinc}^2 \tfrac{h}{2} \Omega_0 \; g_0. \tag{7}$$

Analogously, the following approximation scheme for the velocities can be derived

$$y_{n+1}' - y_{n-1}' = -2\Omega_n \sin h\Omega_n y_n + 2h \operatorname{sinc} h\Omega_n g_n. \tag{8}$$

3 Finite-time error analysis

The theorem stated in this section makes no smoothness assumptions about the highly oscillatory solution. It is only required that the exact solution y of (1) satisfies the **finite-energy condition**

$$H(t, y, y') = \frac{1}{2} \|y'\|^2 + \frac{1}{2} y^T A(t, y) y \le \frac{1}{2} K^2, \tag{9}$$

where $A(t, y)$ is symmetric and positive semi-definite.

The following theorem shows second-order convergence of y_n in the Euclidean norm. The Euclidean norm and induced norms are denoted by $\|\cdot\|$.

Theorem 1 *In equation* (1)*, let A be a symmetric and positive semi-definite $N \times N$ matrix. Assume the solution satisfies the finite-energy condition* (9) *for $t_0 \le t \le t_0 + T$. Then there is a h_0 such that for all $0 < h < h_0$ by application of the scheme* (4)*,* (8) *with filter function ϕ on system* (1)*, and for all $0 \le nh \le T$, it holds that*

$$\|y(t_n) - y_n\| \le h^2 \, C \, \ell(n, N),$$
$$\|y'(t_n) - y_n'\| \le h \, C \, \ell(n, N).$$

Here, C and h_0 depend on $\|y(t_0)\|$, T, K, $\|g\|$, $\|g_y\|$, $\|g_{yy}\|$, $\|g_t\|$, $\|g_{tt}\|$, $\|g_{ty}\|$, $\|A_y\|$, $\|A_{yy}\|$, $\|A_t\|$, $\|A_{tt}\|$, $\|A_{ty}\|$ and ϕ. The term $\ell(n, N) = \min\{\log(n+1) \log(N+1), \sqrt{N}\}$ is slowly growing.

The most important thing to note here is that neither h_0 nor C depend on the norm of A. In fact $\|A\|$ can be arbitrarily large without any effect on the

error bounds, as long as the finite-energy condition holds. It is exactly this property of the bounds that ensures the Gautschi-type exponential integrator is a long-time-step method for systems of type (1).

Since the proof presented below is quite long, the main ideas are summarised now. First of all, since no smoothness assumptions are used other than the inherent finite-energy condition, the variation-of-constants formula has to be used as a replacement for the Taylor series expansion to examine the local defects of the scheme. After that, the main idea is to trace the proof back to the known proof of the error bounds in the case of constant matrix A. To do this, perturbation results of the form

$$\|\phi(\Omega) - \phi(\tilde{\Omega})\| \leq C_\phi \|A - \tilde{A}\|, \tag{10}$$

for symmetric positive semi-definite matrices A, $\tilde{A}$ and $\Omega := \sqrt{A}$, $\tilde{\Omega} := \sqrt{\tilde{A}}$ have to be used. Such perturbation results hold for all even analytic functions with a constant depending on $\sqrt{N}$ (cf. [4]). Special filter functions allow a perturbation result without dependence on $\sqrt{N}$ (cf. lemma 6). It is interesting to note that all filter functions proposed so far are of this kind. Strictly speaking, the term $\ell(n, N)$ has to be replaced by $\sqrt{N}$ in the above theorem if an arbitrary analytic filter function is to be used. By using the variation-of-constants formula and the perturbation result, a recursion for the errors is derived. To bound the accumulated local errors, the results from the case for the constant matrix are used. At this point the analysis shows clearly that the simpler scheme using $\Omega_n = \sqrt{A(t_n, y_n)}$ instead of the averaged version $\Omega_n = \sqrt{A(t_n, \phi(h\Omega(y_n))y_n)}$ does not lead to second-order error bounds due to resonances at integer multiples of π. Finally, a discrete Gronwall inequality is used to finish the proof.

The resonances appearing in the analysis are not 'theoretical artifacts'. They can be observed numerically (cf. [4]). Therefore the given analysis describes the performance of the Gautschi-type exponential integrator closely.

4 Proof of the error bounds

The proof of theorem 1 is split up into a few lemmata. For simplicity the proof is given only for the case of solution dependent A and without g since the proof of the general case with g follows the proof given in [10]. A complete proof can be found in [4].

Substituting the exact solution values $y(t_n)$ of (1) for y_n in the numerical scheme gives a correct equation despite the small defect d_n due to the approximation. The defects d_n are defined by:

$$y(t_n + h) - 2\cos h\Omega(\bar{y}_h(t_n))y(t_n) + y(t_n - h) = d_n,$$

with $\bar{y}_h(t_n) := \phi(h\Omega(y(t_n)))y(t_n)$.

Lemma 1 *The local defects d_n are given by*

$$d_n = h^3 L_n \Omega y(t_n) + h^4 l_n,$$

with $\Omega := \Omega(y(t_0))$,

$$\|L_n\| \leq C, \qquad \textit{and} \qquad \|l_n\| \leq C.$$

Here, C depends on $\|y(t_0)\|$, T, K, $\|A_y\|$, $\|A_{yy}\|$ and ϕ.

The equation of the numerical scheme reads:

$$y_{n+1} - 2\cos h\Omega(\bar{y}_n) y_n + y_{n-1} = 0,$$

with $\bar{y}_n = \phi(h\Omega(y_n))y_n$. By subtracting these two equations, the following lemma is deduced. Therein H_n^1 is a linear mapping and H_n^2 is bilinear.

Lemma 2 *The errors $e_n = y(t_n) - y_n$ satisfy the recursion*

$$e_{n+1} - 2\cos h\Omega(\bar{y}_h(t_n))e_n + e_{n-1} = h^2 H_n^1[e_n] + h^2 H_n^2[e_n, e_n] + d_n,$$

with

$$\|H^1\|, \ \|H^2\| \ \leq C.$$

Here, C depends on $\|y(t_0)\|$, T, K, $\|A_y\|$, $\|A_{yy}\|$ and ϕ.

Lemma 3 *With $\Omega := \Omega(y(t_0))$ the errors satisfy the recursion*

$$e_{n+1} - 2\cos h\Omega e_n + e_{n-1} = h^2 H_n^1[e_n] + h^2 H_n^2[e_n, e_n] + d_n,$$

where $\|H_n^1\|, \|H_n^2\| < C$. Here, C depends on the same constants as in lemma 2 above.

Verbatim as in [10] the following lemma can be proved:

Lemma 4 *The errors satisfy*

$$e_{n+1} = -W_{n-1}e_0 + W_n e_1 + h^2 \sum_{j=1}^{n} W_{n-j}(H_n^1[e_n] + H_n^2[e_n, e_n]) + \sum_{j=1}^{n} W_{n-j} d_j,$$

with $W_n = \operatorname{sinc}(n+1)h\Omega$.

Lemma 5

$$\left\| \sum_{j=1}^{n} W_{n-j} d_j \right\| \leq h^2 C,$$

where C depends on $\|y(t_0)\|$, T, K, $\|A_y\|$, $\|A_{yy}\|$ and ϕ.

Proof (of theorem 1) To simplify matters let $e_0 = \mathcal{O}(h^3)$ and $e_1 = \mathcal{O}(h^3)$. For example these bounds hold for unperturbed initial values and the starting value given by (7). On the chosen interval I according to lemma 5 and because of $\|W_{n-1}e_0\| \leq h^2TC$ and $\|W_n e_1\| \leq h^2TC$, the difference inequality below holds:

$$\|e_{n+1}\| \leq h^2C \sum_{j=1}^{n}(n-j+1)(\|e_j\| + \|e_j\|^2) + h^2D.$$

Since $0 \leq nh \leq T$ and because $h(n-j+1) \leq T$, the following inequality is derived:

$$\|e_{n+1}\| \leq hC \sum_{j=1}^{n}(\|e_j\| + \|e_j\|^2) + h^2D, \qquad n = 0, 1, \ldots$$

Then a discrete Gronwall lemma assures the first error bound. One proceeds analogously to prove the second error bound. □

Proof (of lemma 1) With $\bar{y}_h(t_n) = \phi(h\Omega(y(t_n)))y(t_n)$ the exact solution satisfies:

$$\begin{aligned} & y(t_n+h) - 2\cos h\Omega(\bar{y}_h(t_n))y(t_n) + y(t_n-h) \\ &\quad = \int_0^h \Omega(\bar{y}_h(t_n))^{-1}\sin(h-s)\Omega(\bar{y}_h(t_n)) \\ &\qquad \cdot\Big(A(\bar{y}_h(t_n)) - A(y(t_n+s))\Big)y(t_n+s)\,ds \qquad (11) \\ &\qquad + \int_0^h \Omega(\bar{y}_h(t_n))^{-1}\sin(h-s)\Omega(\bar{y}_h(t_n)) \\ &\qquad \cdot\Big(A(\bar{y}_h(t_n)) - A(y(t_n-s))\Big)y(t_n-s)\,ds. \qquad (12) \end{aligned}$$

The last two terms are estimated first. Using $\Omega = \Omega(y(t_0))$, (11) can be split as follows:

$$\begin{aligned} & -h\int_0^1 \Omega^{-1}\sin h(1-s)\Omega \\ & \cdot\Big(A(y(t_n+hs) - A(\bar{y}_h(t_n))\Big)y(t_n+hs)\,ds \qquad (13) \\ & -h\int_0^1 \Big(\Omega(\bar{y}_h(t_n))^{-1}\sin h(1-s)\Omega(\bar{y}_h(t_n)) - \Omega^{-1}\sin h(1-s)\Omega\Big) \\ & \cdot\Big(A(y(t_n+hs) - A(\bar{y}_h(t_n))\Big)y(t_n+hs)\,ds. \qquad (14) \end{aligned}$$

By using lemma 6, the last term (14) can be transformed to:

$$h^5 \int_0^1 (1-s)^3 \int_0^1 u(1-u)\,\mathrm{sinc}\, h(1-u)(1-s)\Omega \cdot\Big(A(\bar{y}_h(t_n)) - A(y(t_0))\Big)\,\mathrm{sinc}\, hu(1-s)\Omega(\bar{y}_h(t_n))\,du \cdot\frac{1}{h}\Big(A(y(t_n+hs) - A(\bar{y}_h(t_n))\Big)y(t_n+hs)\,ds := h^5 r_{n,A}.$$

Since

$$A(\bar{y}_h(t_n)) - A(y(t_0)) = \int_0^1 A_y(y(t_0) + u(\bar{y}_h(t_n) - y(t_0)))\,du\,[\bar{y}_h(t_n) - y(t_0)],$$

the finite-energy condition gives

$$\|A(\bar{y}_h(t_n)) - A(y(t_0))\| \le \|A_y\|\,\|\phi(h\Omega(y(t_n)))y(t_n) - y(t_0)\| \le T K\,\|A_y\|\left(1 + \max_{x\ge 0}\left|\frac{\phi(x)-1}{x}\right|\right),$$

where the second estimate follows from

$$\phi(h\Omega(y(t_n)))y(t_n) - y(t_0) = h\frac{\phi(h\Omega(y(t_n)))y(t_n) - I}{h\Omega(y(t_n))}\Omega(y(t_n))y(t_n) + \int_{t_0}^{t_n} y'(s)\,ds$$

and the finite-energy condition. Furthermore using

$$\frac{1}{h}\Big(A(y(t_n+hs)) - A(\bar{y}_h(t_n))\Big) = \int_0^1 A_y(\bar{y}_h(t_n) + u(y(t_n+hs) - \bar{y}_h(t_n)))\,du \cdot\left[\frac{1}{h}(y(t_n+hs) - \bar{y}_h(t_n))\right]$$

and

$$\frac{1}{h}(y(t_n+hs) - \bar{y}_h(t_n)) = \frac{1}{h}\Big(y(t_n+hs) - y(t_n) + y(t_n) - \phi(h\Omega(y(t_n)))y(t_n)\Big) = s\int_0^1 y'(t_n+hsu)\,du - \frac{\phi(h\Omega(y(t_n))) - I}{h\Omega(y(t_n))}\Omega(y(t_n))y(t_n),$$

it follows at last that for $s \in [0, 1]$:

$$\begin{aligned}\|\frac{1}{h}\Big(A(y(t_n + hs)) - A(\bar{y}_h(t_n))\Big)\| &\le \|A_y\|\Big(s + \max_{x\ge 0}\left|\frac{\phi(x)-1}{x}\right|\Big)K \\ &\le \|A_y\|\Big(1 + \max_{x\ge 0}\left|\frac{\phi(x)-1}{x}\right|\Big)K.\end{aligned}$$

With this, the rough estimate

$$\|r_{n,A}\| \le T\|A_y\|^2\Big(1 + \max_{x\ge 0}\left|\frac{\phi(x)-1}{x}\right|\Big)^2 K^2(\|y(t_0)\| + TK)$$

follows. Since

$$\begin{aligned}h\Omega\, r_{n,A} = \int_0^1 (1-s)^2 \int_0^1 u \sin h(1-u)(1-s)\Omega\Big(A(y(t_n)) - A(y(t_0))\Big) \\ \cdot \operatorname{sinc} hu(1-s)\Omega(\bar{y}_h(t_n))\, du \\ \cdot\frac{1}{h}\Big(A(y(t_n + hs) - A(\bar{y}_h(t_n))\Big)y(t_n + hs)\, ds,\end{aligned}$$

then

$$\|h\Omega\, r_{A,n}\| \le T\|A_y\|^2\Big(1 + \max_{x\ge 0}\left|\frac{\phi(x)-1}{x}\right|\Big)^2 K^2(\|y(t_0)\| + TK).$$

Hence (14) is of order $\mathcal{O}(h^4)$. If an $\mathcal{O}$-term appears here or anywhere in the paper, it is always meant that the bound in the $\mathcal{O}$-term only depends on the constants given in theorem 1 and that $h\Omega$ times the expression is of the same order, too. This is always done as for $r_{n,A}$ above and not presented in the following.

The leading term (13) can be split further to give

$$\begin{aligned}&-h\int_0^1 \Omega^{-1}\sin h(1-s)\Omega \\ &\quad\cdot\Big(A(y(t_n + hs)) - A(\bar{y}_h(t_n))\Big)y(t_n)\, ds \qquad (15)\\ &-h\int_0^1 \Omega^{-1}\sin h(1-s)\Omega\,\Big(A(y(t_n + hs)) - A(\bar{y}_h(t_n))\Big) \\ &\quad\cdot\Big(y(t_n + hs) - y(t_n)\Big)\, ds. \qquad (16)\end{aligned}$$

The second term (16) can be displayed as

$$\begin{aligned}-h^4\int_0^1 (1-s)\operatorname{sinc} h(1-s)\Omega\frac{1}{h}\Big(A(y(t_n + hs)) - A(\bar{y}_h(t_n))\Big) \\ \cdot\frac{1}{h}\Big(y(t_n + hs) - y(t_n)\Big)\, ds := h^4 r_{n,A},\end{aligned}$$

with

$$\|r_{n,A}\| \le \|A_y\| \Big(1 + \max_{x \ge 0} \left| \frac{\phi(x) - 1}{x} \right| \Big) K^2,$$

and is therefore of order $\mathcal{O}(h^4)$. Finally, the term (15) has to be examined. It can be written as

$$\begin{aligned} &-h \int_0^1 \Omega^{-1} \sin h(1-s)\Omega \, A_y(\bar{y}_h(t_n)) \\ &\quad \cdot \Big(y(t_n + hs) - \bar{y}_h(t_n) \Big) \, ds \; y(t_n) \qquad (17) \\ &-h \int_0^1 \Omega^{-1} \sin h(1-s)\Omega \\ &\quad \cdot \int_0^1 (1-u) A_{yy}(\bar{y}_h(t_n) + u(y(t_n + hs) - \bar{y}_h(t_n))) \, du \\ &\quad \cdot [y(t_n + hs) - \bar{y}_h(t_n)]^2 \; y(t_n) \, ds. \qquad (18) \end{aligned}$$

The second term (18) is of order $\mathcal{O}(h^4)$. This can be seen with the same techniques as before.

Since (cf. (10))

$$\begin{aligned} \|\phi(h\Omega) - \phi(h\Omega(y(t_n)))\| &\le h^2 C_\Phi \|A(y(t_n)) - A(y(t_0))\| \\ &\le h^2 C_\Phi \|A_y\| T K, \end{aligned}$$

one can rewrite (17), up to $\mathcal{O}(h^4)$, as

$$\begin{aligned} &-h \int_0^1 \Omega^{-1} \sin h(1-s)\Omega \, A_y(\bar{y}_h(t_n)) \\ &\quad \cdot \Big(y(t_n + hs) - \phi(h\Omega) y(t_n) \Big) \, ds \; y(t_n). \qquad (19) \end{aligned}$$

By using the representation

$$\begin{aligned} &y(t_n + hs) - \phi(h\Omega) y(t_n) \\ &\quad = \big(\cos hs\Omega - \phi(h\Omega) \big) y(t_n) + \Omega^{-1} \sin hs\Omega \, y'(t_n) \\ &\qquad + hs \int_0^1 \Omega^{-1} \sin hs(1-u)\Omega \\ &\qquad \cdot \Big((A(y(t_0)) - A(y(t_n + hsu))) y(t_n + hsu) \Big) \, du \\ &\quad = \mathcal{O}((sh)^2) + \big(\cos hs\Omega - \phi(h\Omega) \big) y(t_n) + \Omega^{-1} \sin hs\Omega \, y'(t_n), \qquad (20) \end{aligned}$$

(19) can be rewritten as

$$\begin{aligned} &-h \int_0^1 \Omega^{-1} \sin h(1-s)\Omega \, A_y(\bar{y}_h(t_n)) \\ &\quad \cdot \Big(\big(\cos hs\Omega - \phi(h\Omega) \big) y(t_n) + \Omega^{-1} \sin hs\Omega \, y'(t_n) \Big) \, ds \; y(t_n), \qquad (21) \end{aligned}$$

aside from a term of order $\mathcal{O}(h^4)$. Because of

$$\begin{aligned}\|A_y(\bar{y}_h(t_n)) - A_y(y(t_n))\| &\le \|A_{yy}\|\,\|\bar{y}_h(t_n) - y(t_n)\| \\ &\le \|A_{yy}\| \max_{x\ge 0}\left|\frac{\phi(x)-1}{x}\right| Kh,\end{aligned}$$

(11) is at long last seen to be

$$\begin{aligned}&\mathcal{O}(h^4) - h\int_0^1 \Omega^{-1}\sin h(1-s)\Omega\, A_y(y(t_n)) \\ &\cdot\Big(\big(\cos hs\Omega - \phi(h\Omega)\big)y(t_n) + \Omega^{-1}\sin hs\Omega\, y'(t_n)\Big)\, ds\, y(t_n).\end{aligned} \tag{22}$$

The same computation with $-h$ instead of h delivers

$$\begin{aligned}(11)+(12) &= \mathcal{O}(h^4) - 2h\int_0^1 \Omega^{-1}\sin h(1-s)\Omega \\ &\quad\cdot A_y(y(t_n))\,\big[\big(\cos hs\Omega - \phi(h\Omega)\big)y(t_n)\big]\, ds\, y(t_n) \\ &= \mathcal{O}(h^4) - 2h^3\int_0^1 (h\Omega)^{-1}\sin h(1-s)\Omega \\ &\quad\cdot A_y(y(t_n))\,\big[y(t_n), \big(\cos hs\Omega - \phi(h\Omega)\big)(h\Omega)^{-1}\,\Omega y(t_n)\big]\, ds.\end{aligned}$$

The boundedness of $\|\Omega y(t_n)\|$ can be seen easily by using the variation-of-constants formula. By using the abbreviation

$$G_A(t)[\cdot] := A_y(y(t))[y(t), \cdot], \tag{23}$$

(11) + (12) can be written, up to harmless $\mathcal{O}(h^4)$-terms, as

$$\begin{aligned}&-2h^3\int_0^1 (h\Omega)^{-1}\sin h(1-s)\Omega \\ &\cdot G_A(t_n)\big(\cos hs\Omega - \phi(h\Omega)\big)(h\Omega)^{-1}\, ds\,\Omega y(t_n)\end{aligned} \tag{24}$$

with

$$G_A'(t) = A_{yy}(y(t_n))[y'(t), y(t)] + A_y(y(t_n))[y'(t)] \tag{25}$$

and therefore

$$\|G_A'(t)\| \le \|A_{yy}\|K(\|y(t_0)\| + KT) + \|A_y\|K.$$

Now the lemma with L_n defined as

$$2\int_0^1 (h\Omega)^{-1}\sin h(1-s)\Omega\ (-G_A(t_n))\,\frac{\cos hs\Omega - \phi(h\Omega)}{h\Omega}\, ds$$

is proved. □

Proof (of lemma 2) By subtracting the numerical and exact solution, it is deduced that

$$e_{n+1} - (2\cos h\Omega(\bar{y}_h(t_n))y(t_n) - 2\cos h\Omega(\bar{y}_n)y_n) + e_{n-1} = d_n. \tag{26}$$

Since the difference below appears several times, a simpler representation of it is deduced at first.

$$\begin{aligned}\bar{y}_h(t_n) - \bar{y}_n &= \phi(h\Omega(y(t_n)))y(t_n) - \phi(h\Omega(y_n))y_n \\ &= (\phi(h\Omega(y(t_n))) - \phi(h\Omega(y_n)))\, y(t_n) + \phi(h\Omega(y_n))e_n.\end{aligned}$$

The estimate presented here works for general ϕ. Most filter functions allow better estimates which do not increase like $\sqrt{N}$. This can be seen by using lemma 6. Defining $\tilde{\phi}(x) = \phi(\sqrt{x})$ it follows that

$$\begin{aligned}\bar{y}_h(t_n) - \bar{y}_n &= \left(\tilde{\phi}(h^2A(y(t_n))) - \tilde{\phi}(h^2A(y_n))\right) y(t_n) + \phi(h\Omega(y_n))e_n \\ &= M_n[e_n], \end{aligned} \tag{27}$$

with

$$\begin{aligned}M_n[\,\cdot\,] := h^2 \int_0^1 \frac{d\tilde{\phi}}{dA}\left(h^2(A(y_n) + u(A(y(t_n)) - A(y_n)))\right) \\ \cdot \left[\int_0^1 A_y(y_n + ve_n)[\,\cdot\,]\,dv\right] du\; y(t_n) + \phi(h\Omega(y_n))[\,\cdot\,]\end{aligned}$$

and

$$\|M_n\| \le T^2 C_\Phi \|A_y\|(\|y(t_0)\| + TK) + \max_{x\ge 0}|\phi(x)|.$$

Further it holds that

$$\begin{aligned}&\cos h\Omega(\bar{y}_n)y_n - \cos h\Omega(\bar{y}_h(t_n))y(t_n) \\ &\quad = (\cos h\Omega(\bar{y}_n) - \cos h\Omega(\bar{y}_h(t_n)))y_n + \cos h\Omega(\bar{y}_h(t_n))(y_n - y(t_n)) \\ &\quad = (\cos h\Omega(\bar{y}_n) - \cos h\Omega(\bar{y}_h(t_n)))(y(t_n) + y_n - y(t_n)) - \cos h\Omega(\bar{y}_h(t_n))e_n \\ &\quad = (\cos h\Omega(\bar{y}_n) - \cos h\Omega(\bar{y}_h(t_n)))y(t_n) \\ &\quad -(\cos h\Omega(\bar{y}_n) - \cos h\Omega(\bar{y}_h(t_n)))e_n - \cos h\Omega(\bar{y}_h(t_n))e_n\end{aligned} \tag{28}$$

and

$$\begin{aligned}
&\cos h\Omega(\bar{y}_n) - \cos h\Omega(\bar{y}_h(t_n)) \\
&\quad = h^2 \int_0^1 (1-s)\,\operatorname{sinc} h(1-s)\Omega(\bar{y}_h(t_n)) \\
&\qquad \cdot \big(A(\bar{y}_h(t_n)) - A(\bar{y}_n)\big)\,\cos hs\Omega(\bar{y}_n))\,ds \\
&\quad = h^2 \int_0^1 (1-s)\,\operatorname{sinc} h(1-s)\Omega(\bar{y}_h(t_n))\,\cdot \\
&\qquad \cdot \int_0^1 A_y(\bar{y}_n + u(\bar{y}_h(t_n) - \bar{y}_n))[\bar{y}_h(t_n) - \bar{y}_n]\,du \\
&\qquad \cdot \cos hs\Omega(\bar{y}_n))\,ds. \qquad (29)
\end{aligned}$$

The expression

$$\begin{aligned}
G_n^{A,1}[\,\cdot\,] &:= \int_0^1 (1-s)\,\operatorname{sinc} h(1-s)\Omega(\bar{y}_h(t_n)) \\
&\cdot \int_0^1 A_y(\bar{y}_n + u(\bar{y}_h(t_n) - \bar{y}_n))[\,\cdot\,]\,du\ \cos hs\Omega(\bar{y}_n))\,ds\ y(t_n) \qquad (30)
\end{aligned}$$

can be bounded by

$$\|G_n^{A,1}\| \le \frac{1}{2}\|A_y\|(\|y(t_0)\| + KT),$$

and the expression

$$\begin{aligned}
G_n^{A,2}[\,\cdot\,,\,\cdot\,] &:= -\int_0^1 (1-s)\,\operatorname{sinc} h(1-s)\Omega(\bar{y}_h(t_n))\,\cdot \\
&\cdot \int_0^1 A_y(\bar{y}_n + u(\bar{y}_h(t_n) - \bar{y}_n))[\,\cdot\,]\,du\ \cos hs\Omega(\bar{y}_n))\,ds\,[\,\cdot\,], \qquad (31)
\end{aligned}$$

can be bounded by

$$\|G_n^{A,2}\| \le \frac{1}{2}\|A_y\|.$$

After defining

$$\begin{aligned}
\tilde{H}_n^1[\,\cdot\,] &:= G_n^{A,1}\,[M_n[\,\cdot\,]\,] \\
\tilde{H}_n^2[\,\cdot\,,\,\cdot\,] &:= G_n^{A,2}\,[M_n[\,\cdot\,],\,\cdot\,],
\end{aligned}$$

it is deduced that

$$\begin{aligned}
&-(2\cos h\Omega(\bar{y}_h(t_n))y(t_n) - 2\cos h\Omega(\bar{y}_n)y_n) \\
&\quad = -2\cos h\Omega(\bar{y}_h(t_n))e_n + 2h^2\,\tilde{H}_n^1[e_n] + 2h^2\,\tilde{H}_n^2[e_n, e_n]. \qquad (32)
\end{aligned}$$

The finite difference equation can now be written as

$$\begin{aligned} e_{n+1} - 2\cos h\Omega(y(t_n))e_n + e_{n-1} &= h^2\left(-2\tilde{H}_n^1[e_n] - 2\tilde{H}_n^2[e_n, e_n]\right) + d_n \\ &=: h^2 H_n^1[e_n] + h^2 H_n^2[e_n, e_n] + d_n. \end{aligned}$$

□

Proof (of lemma 3) The new recursion is deduced from the fact that

$$\begin{aligned} 2(\cos h\Omega(\bar{y}_h(t_n)) - \cos h\Omega) &= 2h^2 \int_0^1 (1-s)\,\mathrm{sinc}\, h(1-s)\Omega \\ &\quad \cdot \int_0^1 A_y(\bar{y}_h(t_n) + u(y(t_0) - \bar{y}_h(t_n))\,du \\ &\quad \cdot [y(t_0) - \phi(h\Omega(y(t_n)))y(t_n)]\,\cos hs\Omega(\bar{y}_n(t_n))\,ds \\ &=: h^2 F_n \end{aligned}$$

with

$$\|F_n\| \le 2\,T\,K\,\|A_y\| \left(1 + \max_{x\ge 0}\left|\frac{\phi(x)-1}{x}\right|\right).$$

□

Proof (of lemma 5) By using lemma 1, one can show that

$$\sum_{j=1}^{n} W_{n-j} d_j = h^3 \sum_{j=1}^{n} W_{n-j} L_j \Omega y(t_j) + h^4 \sum_{j=1}^{n} W_{n-j} l_j$$

holds. Because of $\|W_n\| \le n+1$, it is directly deduced that

$$\left\| h^4 \sum_{j=1}^{n} W_{n-j} l_j \right\| \le h^2\, T^2 C.$$

To bound the first sum, one proceeds analogously to [10]. By using the variation-of-constants formula, the first sum can be transformed to

$$h^3 \sum_{j=1}^{n} W_{n-j} L_j \Omega y(t_j) = h^2(a_n + b_n)$$

with

$$\begin{aligned} a_n := 2h \sum_{j=1}^{n} W_{n-j} &\int_0^1 \frac{\sin h(1-s)\Omega}{h\Omega} \\ &\cdot(-G_A(t_j))\,\frac{\cos hs\Omega - \phi(h\Omega)}{h\Omega}\,ds \\ &\cdot\Big(\cos(t_j - t_0)\Omega\,\Omega y(t_0) + \sin(t_j - t_0)\Omega\, y'(t_0)\Big) \end{aligned}$$

and

$$b_n := 2h \sum_{j=1}^{n} W_{n-j} \int_0^1 \frac{\sin h(1-s)\Omega}{h\Omega} \cdot(-G_A(t_j)) \frac{\cos hs\Omega - \phi(h\Omega)}{h\Omega}\, ds \cdot \int_{t_0}^{t_j} \sin(t_j - s)\Omega \Big((A(y(t_0)) - A(y(s)))y(s) + g(y(s)) \Big)\, ds.$$

Partial summation is used to bound a_n and b_n. One proceeds as in [10] to finish the proof. Without a filter function in A, the term

$$\frac{\cos hs\Omega - I}{h\Omega} \tag{33}$$

instead of

$$\frac{\cos hs\Omega - \phi(h\Omega)}{h\Omega}$$

would appear. Applying partial summation with (33) as in [10] shows that a_n and b_n cannot be bounded due to resonances at integer multiples of π. □

The lemma below can be proved by applying the variation-of-constants formula to a second-order matrix differential equation (cf. [4]).

Lemma 6 *Let A, $\tilde{A}$ be real symmetric and positive semi-definite $N \times N$ matrices, $\Omega = \sqrt{A}$ and $\tilde{\Omega} = \sqrt{\tilde{A}}$. Then the representations below hold for $h > 0$:*

$$\frac{\sin h\Omega}{h\Omega} - \frac{\sin h\tilde{\Omega}}{h\tilde{\Omega}} = h^2 \int_0^1 (1-s)\big(h(1-s)\tilde{\Omega}\big)^{-1} \sin h(1-s)\tilde{\Omega} \cdot(\tilde{A} - A)\, s\, \big(hs\Omega\big)^{-1} \sin hs\Omega\, ds \tag{34}$$

and therefore the estimate

$$\left\| \frac{\sin h\Omega}{h\Omega} - \frac{\sin h\tilde{\Omega}}{h\tilde{\Omega}} \right\| \le \frac{h^2}{6} \left\| \tilde{A} - A \right\|,$$

holds, as does the representation

$$\cos h\Omega - \cos h\tilde{\Omega} = h^2 \int_0^1 (1-s)\big(h(1-s)\tilde{\Omega}\big)^{-1} \sin h(1-s)\tilde{\Omega}\, (\tilde{A} - A)\, \cos hs\Omega\, ds \tag{35}$$

and therefore the estimate

$$\left\| \cos h\Omega - \cos h\tilde{\Omega} \right\| \le \frac{h^2}{2} \left\| \tilde{A} - A \right\|.$$

5 Notes on implementation

To apply method (4), terms of the type

$$\varphi(h\Omega)v,$$

with a function $\varphi(x)$, smoothly dependent on x^2, and a vector v have to be computed. Since $\Omega = \sqrt{A}$ is not known in most cases, the function $\psi(x) := \varphi(\sqrt{x})$ is used to compute $\varphi(h\Omega)v$ as

$$\psi(h^2A)v.$$

These terms are approximated by Krylov-techniques as described in [11]. In comparison to other alternatives, this method appears to be the most favourable in the present context (cf. [9]).

The Krylov subspace approximation is of the form

$$\psi(h^2A)v \approx V_m \psi(h^2T_m)e_1\|v\|,$$

where $V_m = [v_1, \ldots, v_m]$ is the matrix containing the orthonormal Lanczos basis of the mth Krylov subspace with respect to A and v, and $T_m = V_m^T A V_m$ is a symmetric tridiagonal matrix. Further e_1 is the first m-dimensional unit vector. Since the iteration number m is typically very small compared with the dimension of the matrix A, $\psi(h^2T_m)e_1$ can be computed quite cheaply by diagonalizing $T_m = Q_m^T D_m Q_m$, with diagonal matrix D_m:

$$\psi(h^2A)v \approx V_m \psi(h^2T_m)e_1\|v\| = V_m Q_m^T \psi(h^2D_m) Q_m e_1\|v\|.$$

Now the method reads

$$y_{n+1} - 2\psi_1(h^2A_n)y_n + y_{n-1} = h^2\, \psi_2(h^2A_n)\; g(\psi_3(h^2A_n)y_n)$$

with

$$\psi_1(x) := \cos(\sqrt{x}), \quad \psi_2(x) := \operatorname{sinc}^2(\tfrac{1}{2}\sqrt{x}), \quad \psi_3(x) := \phi(\sqrt{x}).$$

Or, after a small computation

$$y_{n+1} - 2y_n + y_{n-1} = h^2\, \psi_2(h^2A_n)\; \left(g(\psi_3(h^2A_n)y_n) - A_n y_n\right).$$

The costs to compute $\psi_1(h^2A_n)$ in the first variant are negligible since a Krylov-space with respect to A_n and vector y_n is computed anyway to evaluate the filter function ψ_3.

In some applications the differential equations have to be transformed to an equation of type (1). For example in molecular dynamics a splitting

$$y'' = f_1(y) + f_2(y),$$

is often known where the first part f_1 produces high frequencies, the second not. Then one could use the Jacobian of the first equation, i.e with $A(y) = -\partial f_1/\partial y$ and $g(y) = f_1(y) + f_2(y) - A(y)y$ the system is transformed to type (1). It is known that $A(y)$ has a few negative eigenvalues of small absolute value besides the large positive eigenvalues. To deal with these, one has to look at the original derivation of the method. For a symmetric matrix A one can find a matrix Ω with $\Omega^2 = A$. This matrix is not uniquely determined in the presence of negative eigenvalues, but that does not matter. With any matrix satisfying $\Omega^2 = A$ scheme (4) remains valid. No change of the derivation is necessary. This can be added to our method without difficulties. If the diagonalisation of A delivers negative eigenvalues, the use of complex values can be avoided. For example, one could use the relation

$$\cos(\sqrt{\lambda}) = \cos(i\sqrt{-\lambda}) = \cosh(\sqrt{-\lambda})$$

for negative λ when computing $\psi_1(h^2 D_n)$. This is the only addition to the method. Analogously, the other analytic functions are computed.

Remark The last considerations show that the method can be applied for differential equations of type (1) with an arbitrary symmetric matrix. But it is important to note that the application of this method with matrices A containing negative eigenvalues of large absolute value makes no sense. It is only mentioned to avoid shifting the matrix A in the algorithm by a constant factor for matrices with some negative eigenvalues of small absolute value in addition to the large positive ones.

6 Numerical experiment

The simplified model of a protein, as described in [5], is used to test the Gautschi-type exponential integrator. The model is sufficiently small to allow fast computation. It contains most of the terms common in molecular dynamics and is therefore a suitable test problem.

The test simulates a chain of 100 mass points with forces similar to the one appearing in classical molecular dynamics simulations. The potential energies used are

$$U^{\text{bond}} = \sum_{\text{bonds}} \frac{1}{2} K_B (r_{ij} - r_0)^2$$

$$U^{\text{angle}} = \sum_{\text{angles}} \frac{1}{2} K_\theta (\theta - \theta_0)^2$$

$$U^{\text{Lennard-Jones}} = \sum_{\text{pairs } (i,j)} \left(\frac{A}{r_{ij}^{12}} - \frac{B}{r_{ij}^{6}} \right)$$

$$U^{\text{electrostatic}} = \sum_{\text{pairs } (i,j)} \frac{q_i q_j e^2}{r_{ij}},$$

with data $m = 14u$, $r_0 = 1.52\text{Å}$, $K_B = 255\,\text{kcal mol}^{-1}\,\text{Å}^{-2}$, $K_\theta = 45\,\text{kcal mol}^{-1}\,\text{rad}^{-2}$, $\theta_0 = 110\,\text{Grad}$, $A = 6.8 \cdot 10^3\,\text{kJ mol}^{-1}\text{Å}^{12}$ and $B = 1705\,\text{kJ mol}^{-1}\text{Å}^6$. r_{ij} describes the distance between mass point i and j.

The potentials can be split in potential energies leading to fast forces and slow forces. Here the used splitting is

$$\begin{aligned}
U^{\text{fast}} &= U^{\text{fast, bond}} + U^{\text{fast, nonbond}} \\
U^{\text{fast, bond}} &= U^{\text{angle}} + U^{\text{bond}} \\
U^{\text{fast, nonbond}} &= U^{\text{fast, elect}} + U^{\text{fast, Lennard-Jones}} \\
U^{\text{fast,elect}} &= U^{\text{electrostatic}} sw(r_{ij}) \\
U^{\text{fast, Lennard-Jones}} &= U^{\text{Lennard-Jones}} sw(r_{ij}) \\
U^{\text{slow}} &= (1 - sw(r_{ij}))U^{\text{electrostatic}} + (1 - sw(r_{ij}))U^{\text{Lennard-Jones}}
\end{aligned}$$

with the help of a function sw, which drops smoothly from 1 to 0 in a prescribed interval.

After a transformation near an equilibrium point, with the fast forces introduced by the fast potential energies, the method is applied as described in section 5. The numerically computed eigenvalues of $A(y)$ range from -10 to 500. In Figure 1 the Verlet-scheme, most popular in molecular dynamics,

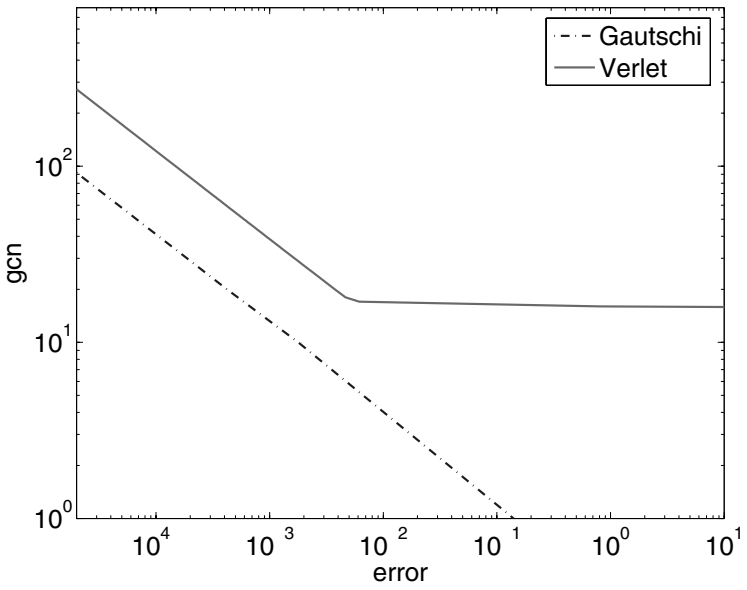

Fig. 1. Error

is compared to the Gautschi-type method. The work is plotted versus the global error for a very short interval of time, where the work is measured as function evaluations of g, which is the computationally expensive part in realistic molecular dynamics simulations. The Gautschi-type method can be used with more than ten times the step-size of the Verlet scheme giving still sufficient accuracy. This leads to a remarkable speed-up in large molecular dynamics simulations.

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