On the Use of the Gautschi-Type Exponential Integrator for Wave Equations

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Summary. Wave equations are especially challenging for numerical integrators since the solution is often not smooth and there is no smoothing in time. The largest usable step size of standard integrators, as for example the often used Störmer-Verlet-Leap-Frog-scheme, depends on the space discretisation. The better the approximation in space, the smaller the required step size of the integrator. The presented exponential integrator allows for error bounds independent of the space discretisation but only dependent on constants arising from the original problem. This favourable property is demonstrated with the Sine–Gordon equation.

1 Introduction

Semilinear wave equations appear in many physical relevant applications. They can often be formulated as abstract evolutionary equations on a Hilbert space H:

$$u'' + Au = g(u), \qquad u(0) = u_0, u'(0) = u_0',$$

with an unbounded linear operator A. The primes indicate time derivatives. Spacial discretisation usually leads to an ordinary differential equation on $\mathbb{R}^n$:

$$y'' + A_n y = g_n(y), \qquad y(0) = y_0, y'(0) = y_0',$$

where $A_n = \Omega_n^2$ is a symmetric and positive semi-definite real matrix of large norm. If n refers to the number of freedoms in the space discretisation, the norm of A_n is tending to infinity for finer and finer space discretisations, reflecting the unbounded operator properly, while g_n and its derivatives remain bounded. The large norm of A_n restricts the step size of standard integrators and introduces an oscillatory solution. Choosing a "stiff" integrator for the semi-discretisation does not help for improving the accuracy, since the solution y is often not smooth. Due to these specific difficulties connected with the oscillatory solution, these differential equations are called oscillatory or highly-oscillatory. Oscillatory differential equations are a topic of current interest, see, e.g., [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16]).

To show that an integrator does not suffer from a step-size restriction introduced by the norm of A_n, one needs to prove error bounds independent of this norm or, in more physical terms, of the frequencies, which are the eigenvalues of Ω_n. Error bounds of this type have been proved for the *mollified impulse method*, proposed in [5], and the *Gautschi-type exponential integrator*, proposed an analysed in [11] and shown to be completely independent of the norm of A_n in [7]. These bounds are derived via a finite-energy condition. In this paper, it is shown that these methods provide error bounds in time which are independent of the refinement of the space discretisation. Rather than by writing down all technical details, the result is demonstrated for the Sine–Gordon equation and the Gautschi-type exponential integrator. But the results apply to general semilinear wave equations and more general exponential integrators.

This paper is organised as follows. In Section 2, the Sine–Gordon equation is given with emphasis on its natural properties that are important for understanding the performance of the Gautschi-type exponential integrator. Section 3 discusses how the properties of the abstract equation affect the ordinary differential equations arising from a semi-discretisation in space. The Gautschi-type integrator is introduced in Section 4 together with the main theorem on its error bounds for wave equations. Finally, in Section 5, the findings are numerically illustrated.

2 Sine–Gordon Equation

The Sine–Gordon equation can be written as

$$u_{tt} = -Au - g(u), \qquad u(0) = u_0 \in V = H_0^1(0,1),\, u'(0) = u_0' \in H = L^2(0,1), \tag{1}$$

with $A = -u_{xx}$, $g(u) = \sin(u)$ and $V = \mathcal{D}(A^{\frac{1}{2}})$. The nonlinearity g is often smooth in semilinear wave equations and we assume the bounds $\|g\|_H \leq M_1$, $\|g_u\|_H \leq M_2$ and $\|g_{uu}\|_H \leq M_3$ in the Hilbert-space norm or the operator norms, respectively. For the Sine–Gordon equation, we have $M_1 = M_2 = M_3 = 1$. (The notation of the norms is quite compressed. Note that $\|\cdot\|_H$ designates different norms depending on the argument and that the norms are to be considered from V to H.)

The energy of the wave is given by

$$H(u, u') = \frac{1}{2}\|u'\|_H^2 + \frac{1}{2}\|A^{\frac{1}{2}}u\|_H^2 + G(u),$$

where

$$G(u) = \int_0^1 (f(tu), u)_H \, dt = \int_0^1 \int_{\Omega=[0,1]} \sin(tu(x))u(x)\, dx\, dt$$

Therefore and due to the bounds

$$-\|u\|_H^2 - C \le G(u) \le D + \|A^{\frac{1}{2}}u\|_H^2, \tag{2}$$

where C and D are moderate constants, g is called a gradient operator. For the one-dimensional Sine–Gordon equation, $C = 1/4$ and $D = 1/\pi^2$. The bounds (2) immediately imply that the *finite energy*

$$H_e(u,u') = \frac{1}{2}\|u'\|_H^2 + \frac{1}{2}\|A^{\frac{1}{2}}u\|_H^2 \le \frac{1}{2}K^2$$

is moderately bounded by a constant K whenever $H(u,u')$ is. These properties are intrinsic to wave equations and only these properties will be used in the following discussion.

3 Discretisation

Two different discretisations, namely pseudo-spectral and finite-difference, are considered for the (abstract) Sine–Gordon equation (1). The two of them lead to an ordinary differential equation

$$y'' + A_n y = g_n(y), \qquad y(0) = y_0, y'(0) = y_0', \tag{3}$$

in $(\mathbb{R}^n, \|\cdot\|_\Delta)$, where $\|\cdot\|_\Delta$ is just an appropriately scaled Euclidean norm. The important point is that equation (3) inherits the properties of the abstract wave equation. The norm of A_n tends to infinity if n tends to infinity, reflecting the unbounded operator A. The remaining properties are summarised in the following proposition.

Proposition 1. *The initial values of (3) satisfy the finite-energy condition*

$$\frac{1}{2}\|y'(0)\|_\Delta^2 + \frac{1}{2}\|A_n^{\frac{1}{2}}y(0)\|_\Delta^2 \le \frac{1}{2}K^2,$$

with the same constant K as in the abstract formulation and the bounds $\|g_n\|_\Delta \le \|g\|_H \le M_1$, $\|g_{n,y}\|_\Delta \le \|g_u\|_H \le M_2$ and $\|g_{n,yy}\|_\Delta \le \|g_{uu}\|_H \le M_3$ hold.

Details on the discretisations and the proof of Proposition 1 are given in the following two subsections.

3.1 Pseudo-Spectral Discretisation

The eigenfunctions and eigenvalues of the operator A,

$$e_k = \sqrt{2}\sin \pi k x, \qquad \lambda_k = \pi^2 k^2,$$

form an orthonormal basis of H. Choosing $V_h = \{e_1, \cdots, e_n\}$ gives an n-dimensional subspace of H. With the projection P_n on this subspace, one is left with a system of ordinary differential equations in the space $I\!R^n$ with the norm $\|\cdot\|_\Delta = \|\cdot\|_2$, where $\|\cdot\|_2$ is the Euclidean norm. The system of ordinary differential equation reads

$$y'' = -A_n y + g_n(y), \qquad y(t_0) = y_0, \quad y'(t_0) = y_0',$$

with $A_n = \operatorname{diag}(\lambda_1, \ldots, \lambda_n)$,

$$y_0 = \begin{bmatrix} (u_0, e_1) \\ \vdots \\ (u_0, e_n) \end{bmatrix}, \qquad y_0' = \begin{bmatrix} (u_0', e_1) \\ \vdots \\ (u_0', e_n) \end{bmatrix} \quad \text{and} \quad g_n(y) = F_n \sin(F_n^{-1} y),$$

where $F_n = \frac{\sqrt{2}}{n+1} \left(\sin \frac{kj\pi}{n+1} \right)_{k,j=1}^{n}$ is the matrix belonging to the Discrete Sine Transform (DST) and the evaluation of sin at a vector is to be understood pointwise.

The statements in the proposition above are easily verified. Namely,

$$\frac{1}{2}\|y_0'\|_\Delta^2 + \frac{1}{2}\|A_n^{\frac{1}{2}} y_0\|_\Delta^2 = \frac{1}{2}\|P_n u_0'\|_H^2 + \frac{1}{2}\|P_n A^{\frac{1}{2}} u_0\|_H^2 \le \frac{1}{2}\|u_0'\|_H^2 + \frac{1}{2}\|A^{\frac{1}{2}} u_0\|_H^2 \le \frac{1}{2} K^2$$

By differentiation, $\|g_n\|_\Delta \le \|g\|_H$, $\|g_{n,y}\|_\Delta \le \|g_u\|_H$ and $\|g_{n,yy}\|_\Delta \le \|g_{uu}\|_H$ follow.

3.2 Finite-Difference Approximation

For a finite-difference discretisation in space, a regular grid $x_i = ih$ for $i = 0, \ldots, n$ with $h = \frac{1}{n+1}$ is chosen. By setting $y_i(t) := u(x_i, t)$ for $i = 1, \ldots, n$ and approximating the second derivative by a symmetric finite-difference of order 2, one arrives at

$$y'' = -A_n y + g_n(y), \quad y(0) = y_0 = (u_0(x_1, 0), \ldots, u_0(x_n, 0))^T, \quad y'(0) = R_n u'(0),$$

where $A_n = \frac{-1}{h^2} \operatorname{tridiag}(1, -2, 1) \in I\!R^{n,n}$, $y \in I\!R^n$ and $R_n : L^2(0,1) \to I\!R^n$, with

$$R_n u = \left(\frac{1}{h} \int_{x_1 - \frac{h}{2}}^{x_1 + \frac{h}{2}} u(x)\, dx, \ldots, \frac{1}{h} \int_{x_n - \frac{h}{2}}^{x_n + \frac{h}{2}} u(x)\, dx \right)^T.$$

The restriction R_n is necessary since $u'(0)$ is not necessarily continuous. The properties of this discretisation, stated in Proposition 1, are readily justified. A_n is a symmetric positive definite Matrix and $\Omega_n := A_n^{\frac{1}{2}}$ is defined. With $\|y\|_\Delta^2 = h\|y\|_2^2$, often called discrete Sobolev norm, we have

$$\frac{1}{2}\|y'(0)\|_\Delta^2 + \frac{1}{2}\|\Omega_n y(0)\|_\Delta^2 \le \frac{1}{2}\|u'(0)\|_H^2 + \frac{1}{2}\|A^{\frac{1}{2}} u\|_H^2 \le \frac{1}{2} K^2,$$

since

$$
\begin{aligned}
\|y'(0)\|_\Delta^2 &= h\sum_{i=1}^n \left(\frac{1}{h}\int_{x_i-\frac{h}{2}}^{x_i+\frac{h}{2}} u'(x,0)\,dx\right)^2 \le \frac{1}{h}\sum_{i=1}^n \left(\int_{x_i-\frac{h}{2}}^{x_i+\frac{h}{2}} |u'(x,0)|\,dx\right)^2 \\
&\overset{\text{CSU}}{\le} \frac{1}{h}\sum_{i=1}^n h\int_{x_i-\frac{h}{2}}^{x_i+\frac{h}{2}} |u'(x,0)|^2\,dx = \int_{x_1-\frac{h}{2}}^{x_n+\frac{h}{2}} |u'(x,0)|^2\,dx \le \|u'(0)\|_H^2
\end{aligned}
$$

and (with $y_{0,0} = y_{0,n+1} := 0$)

$$
\begin{aligned}
\|\Omega_n y(0)\|_\Delta^2 = h(A_n y_0, y_0) &= -h\sum_{i=1}^n \frac{y_{0,i+1} - 2y_{0,i} + y_{0,i-1}}{h^2}\cdot y_{0,i} \\
&= h\sum_{i=1}^n \frac{y_{0,i+1} - y_{0,i}}{h}\cdot\frac{y_{0,i+1} - y_{0,i}}{h} = \frac{1}{h}\sum_{i=0}^n \left(\int_{x_i}^{x_{i+1}} u_x(x,0)\,dx\right)^2 \\
&\le \sum_{i=0}^n \int_{x_i}^{x_{i+1}} |u_x(x,0)|^2\,dx = \|u_x(0)\|_H^2 = \|A^{\frac{1}{2}}u(0)\|_H^2.
\end{aligned}
$$

The statements $\|g_n\|_\Delta \le \|g\|_H$, $\|g_{n,y}\| \le \|g_u\|_H$ and $\|g_{n,yy}\|_\Delta \le \|g_{uu}\|_H$ follow by differentiation.

4 The Gautschi-type Exponential Integrator

In [11], Hochbruck and Lubich consider the Gautschi-type method for the solution of systems of oscillatory second-order differential equations like (3). The Gautschi-type method, which is based on the requirement that it solves exactly linear problems with constant inhomogeneity g, is given by

$$
y_{m+1} - 2\cos(\tau\Omega)\; y_m + y_{m-1} = \tau^2 \operatorname{sinc}^2\left(\frac{\tau\Omega}{2}\right) g(\phi(\tau\Omega)y_m),
$$

with the *filter function* ϕ whose purpose is to filter out resonant frequencies at integer multiples of π.

Combining the error bound for the Gautschi-type method, which is proved in [11], with the result in [7] and slight modifications of the proof give the following theorem.

Theorem 1. *If the solution of the abstract wave equation (1) satisfies the finite-energy condition at the starting values*

$$
\frac{1}{2}\|u'(0)\|_H^2 + \frac{1}{2}\|A^{\frac{1}{2}}u(0)\|_H^2 \le \frac{1}{2}K^2,
$$

then the error of the Gautschi-type method, by application on the semi-discretised systems, for $0 \le t_m = mh \le T$ *is bounded by*

$$
\|y(t_m) - y_m\|_\Delta \le \tau^2 C,
$$

where C *only depends on* T, K, $\|g\|_H, \|g_u\|_H, \|g_{uu}\|_H$ *and* ϕ.

This is an extraordinary error bound. The error of the discretisation in time is independent of the chosen discretisation in space. The bound only depends on constants that stem from the original formulation of the wave equation.

5 Numerical Example

To illustrate the bound numerically, the Sine–Gordon equation is integrated with initial values

$$u(0) = 0, \quad \text{and} \quad u'(0) = 1_{[\frac{1}{4},\,\frac{3}{4}]}(x),$$

where $1_I(x)$ denotes the indicator function for the interval I. Figure 1 shows the global error after an integration time of 1 versus the chosen step-size for the Gautschi-type method and the Verlet-scheme, which is one of the most used second-order standard integrators. The semi-discretisation is finite-differences with 34 points. The Verlet-scheme fails to integrate the differential equation for larger step-sizes due to its dependence of the space discretisation. The result was the same if a pseudo-spectral discretisation would have been chosen. The Verlet-scheme needs smaller time-steps for finer grids. For 128 grid points, the Verlet-scheme does not give a reasonable solution for the whole interval [0.01, 1] in Figure 1, whereas the graph of the error for the Gautschi-type method hardly changes. This impressively demonstrates the advantage of the presented error bounds.

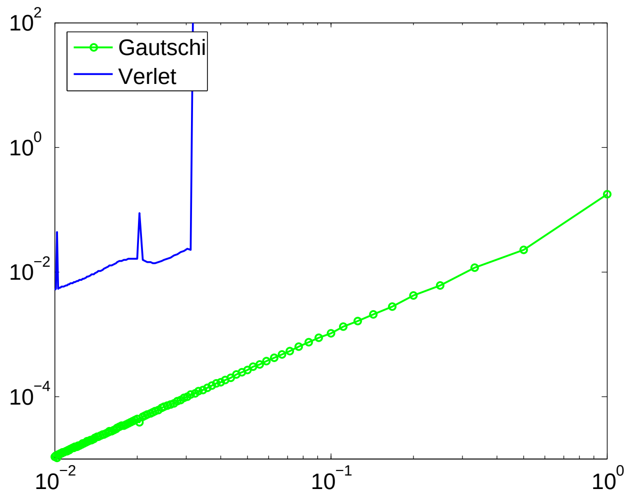

Fig. 1. Global error versus step-size

References

1. Ascher, U. M., Reich, S.: On some difficulties in integrating highly oscillatory Hamiltonian systems. In Proc. Computational Molecular Dynamics, Springer Lecture Notes, 281–296, (1999)
2. Cohen, D.: Conservation properties of numerical integrators for highly oscillatory hamiltonian systems. IMA J. Numer. Anal., **26**, 34–59 (2005)
3. Cohen, D., Hairer, E., Lubich, Ch.: Modulated fourier expansions of highly oscillatory differential equations. Foundations of Comput. Maths., **3**, 327–450 (2003)
4. Cohen, D., Hairer, E., Lubich, Ch.: Numerical energy conservation for multi-frequency oscillatory differential equations. BIT, **45**, 287–305 (2005)
5. García-Archilla, B., Sanz-Serna, J., Skeel, R.: Long-time-step methods for oscillatory differential equations. SIAM J. Sci. Comput., **30**, 930–963 (1998)
6. Grimm, V.: Exponentielle Integratoren als Lange-Zeitschritt-Verfahren für oszillatorische Differentialgleichungen zweiter Ordnung. PhD Thesis, Heinrich-Heine-Universität, Düsseldorf (2002)
7. Grimm, V.: A note on the Gautschi-type method for oscillatory second-order differential equations. Numer. Math., **102**, 61–66 (2005)
8. Grimm, V.: On error bounds for the Gautschi-type exponential integrator applied to oscillatory second-order differential equations. Numer. Math., **100**, 71–89 (2005)
9. Hairer, E., Lubich, Ch.: Long-time energy conservation of numerical methods for oscillatory differential equations. SIAM J. Numer. Anal., **38**, 414–441 (2000)
10. Hairer, E., Lubich, Ch., Wanner, G.: Geometric Numerical Integration. Springer-Verlag (2002)
11. Hochbruck, M., Lubich, Ch. A Gautschi-type method for oscillatory second-order differential equations. Numer. Math., **83**, 403–426 (1999)
12. Iserles, A.: On the global error of discretization methods for highly-oscillatory ordinary differential equations. BIT, **42**, 561–599 (2002)
13. Iserles, A.: Think globally, act locally: solving highly-oscillatory ordinary differential equations. Appld. Num. Anal., **43**, 145–160 (2002)
14. Iserles, A.: On the method of Neumann series for highly oscillatory equations. BIT, **44**, 473–488 (2004)
15. Lorenz, K., Jahnke, T., Lubich, Ch.: Adiabatic integrators for highly oscillatory second order linear differential equations with time-varying eigendecomposition. BIT, **45**, 91–115 (2005)
16. Petzold, L., Jay, L. and Yen, J.: Numerical Solution of Highly Oscillatory Ordinary Differential Equations. Acta Numerica, **6**, 437–484 (1997)