Noname manuscript No.
(will be inserted by the editor)

Symmetric and arbitrarily high-order time-stepping methods for solving nonlinear Klein–Gordon equations

Changying Liu · Arieh Iserles · Xinyuan Wu

Received: date / Accepted: date

Abstract The Klein–Gordon equation with nonlinear potential features in a large number of applications, yet its computation represents a major challenge. The main theme of this paper is the construction of symmetric and arbitrarily high-order time-stepping numerical methods for the nonlinear Klein–Gordon equation and the analysis of their stability and convergence. To this end, subject to periodic boundary conditions, we construct an abstract ordinary differential equation in a suitable function space. Subsequently, we introduce an operator-variation-of-constants formula to derive a symmetric and arbitrarily high-order time-integration formula for the nonlinear abstract ODE. Stability and convergence are proved once the spatial differential operator is approximated by an appropriate positive semi-definite matrix, subject to sufficient temporal and spatial smoothness. Numerical results demonstrate the advantage and efficiency of our new methods in comparison with the existing numerical approaches.

Keywords Nonlinear Klein–Gordon equation · Abstract ordinary differential equation · Hermite interpolation · Operator-variation-of-constants formula ·

The research is supported in part by the Natural Science Foundation of China under Grant 11271186, by NSFC and RS International Exchanges Project under Grant 11411130115, by the Specialized Research Foundation for the Doctoral Program of Higher Education under Grant 20130091110041, by the 985 Project at Nanjing University under Grant 9112020301, and by the Priority Academic Program Development of Jiangsu Higher Education Institutions.

Changying Liu
Department of Mathematics, Nanjing University; State Key Laboratory for Novel Software Technology at Nanjing University, Nanjing 210093, P.R.China
E-mail: chyliu88@gmail.com

Arieh Iserles
Department of Applied Mathematics and Theoretical Physics, University of Cambridge, United Kingdom
E-mail: A.Iserles@damtp.cam.ac.uk

Xinyuan Wu
Department of Mathematics, Nanjing University; State Key Laboratory for Novel Software Technology at Nanjing University, Nanjing 210093, P.R.China
E-mail: xywu@nju.edu.cn

Brikhoff–Hermite quadrature formula · Waveform relaxation algorithm · Symmetric finite difference · Fourier spectral collocation

Mathematics Subject Classification (2010) 35C15 · 65M06 · 65M12 · 65M15 · 65M20 · 65M70

1 Introduction

The nonlinear wave equation plays a prominent role in a wide range of applications in engineering and science, inclusive of nonlinear optics, solid state physics and quantum field theory [14]. In particular, the *Klein–Gordon equation,* a relativistic counterpart of the Schrödinger equation, is used to model diverse nonlinear phenomena, such as the propagation of dislocations in crystals and the behaviour of elementary particles and of Josephson junctions (see [15, Chap. 2] for details).

Its computation presents numerous enduring challenges which motivate us to derive and analyse symmetric and arbitrarily high-order numerical methods for the nonlinear Klein–Gordon equation.

In this paper we restrict ourselves to the one-dimensional case, noting that all our ideas, algorithms and analysis extend easily to the solution of a nonlinear Klein–Gordon equations in a moderate number of space dimensions.

We consider the following nonlinear Klein–Gordon equation,

$$\begin{aligned} &u_{tt} - a^2 \Delta u = f(u), \qquad t_0 < t \leq T, \quad x \in \mathbf{\Omega}, \\ &u(x,t_0) = \varphi_1(x), \quad u_t(x,t_0) = \varphi_2(x), \;\; x \in \bar{\mathbf{\Omega}}, \end{aligned} \tag{1}$$

where $u(x,t)$ represents the wave displacement at position x and time t, and the nonlinear function $f(u)$ is the negative derivative of a potential energy $V(u) \geq 0$. For simplicity, we assume that the initial value problem (1) is accompanied by the periodic boundary condition on the domain $\mathbf{\Omega} = (-\pi,\pi)$,

$$u(x,t) = u(x+2\pi,t), \qquad x \in (-\pi,\pi], \tag{2}$$

where 2π is the fundamental period with respect to x. In the literature, there are various choices of the potential $f(u)$: the best known is the sine-Gordon equation

$$u_{tt} - a^2 \Delta u + \sin(u) = 0,$$

but also polynomials f feature in many applications. An important structural feature of (1–2) is that $u(\cdot,t) \in H^1(\mathbf{\Omega})$ and $u_t(\cdot,t) \in L^2(\mathbf{\Omega})$ imply energy conservation,

$$E(t) = \frac{1}{2}\int_{\mathbf{\Omega}} \left[u_t^2 + a^2|\nabla u|^2 + 2V(u)\right]\mathrm{d}x \equiv E(t_0). \tag{3}$$

This is an crucial e.g. in soliton theory and ideally should be preserved by a numerical discretization.

Historically, the Klein–Gordon equation has received a great deal of attention, focussing on both its numerical and analytical aspects. On the analytical front, the initial value problem (1) was investigated e.g. by [7,18,26,32,41]). In particular, for the defocusing case, $V(u) \geq 0, u \in \mathbb{R}$, the global existence of solutions was established in [7], and for the focusing case, $V(u) \leq 0, u \in \mathbb{R}$, possible finite time blow-up was investigated. In numerical analysis, various solution procedures have been proposed and studied inclusive of classical finite difference methods such as explicit, semi-implicit, compact finite difference and symplectic conservative discretisations [1,4,16,33,38]. Other effective integrators, such as the finite element method and the spectral method were also studied in [11,12,20,44]. Although various numerical methods for the nonlinear Klein–Gordon equation have been derived and investigated in the literature, their accuracy is limited and little attention has been paid to the special structure produced by spatial discretisations.

Motivated by recent interest in exponential integrators for semilinear parabolic problems [13,23–25,30], and based on the operator spectrum theory (see, e.g. [6]) we first formulate the nonlinear Klein–Gordon equation (1–2) as an abstract second-order ordinary differential equation. Subsequently, the operator-variation-of-constants formula (also known as the *Duhamel Principle*) for the abstract equation is introduced: this is an implicit expression of the solution of the nonlinear Klein–Gordon equation (1–2). Similarly to the powerful approach to dealing with the semiclassical Schrödinger equation in [3], this work foregoes the standard steps of first semidiscretising and then dealing with the semidiscretisation. Using the derived operator-variation-of-constants formula, we interpolate the nonlinear integrators by two-point Hermite interpolation, this leads to a class of symmetric and arbitrarily high-order time integration formulæ. The semidiscretisation is deferred to the very last moment, and this enables us to take a subtle but powerful advantage of dealing with the undiscretised operator Δ and incorporate the special structure produced by spatial discretisations into the new integrator.

The main purpose of this paper is to present symmetric and arbitrarily high-order time-stepping methods for the nonlinear Klein–Gordon equation (1–2) and analyse their stability and convergence. Its outline is as follows. We commence in Section2 by representing (1–2)as an abstract ordinary differential system on the Hilbert space $L^2(\mathbf{\Omega})$. In Section 3, keeping the eventual discretisation in mind, we apply a two-point Hermite interpolation to the operator-variation-of-constants formula and develop our time integration formula of arbitrarily high order in an infinite-dimensional function space. Moreover, some properties of the operator functions and the Birkhoff–Hermite quadrature formula can ensure that our time integration formula is independent of integrals and is symmetric. The analysis of its stability and convergence for the fully discrete scheme are studied in Section 4 and Section 5, respectively. Section 6 is concerned with the semidiscretisation. The choice of spatial discretisation at this stage does allow us some flexibility. After the discretisation, a class of numerical schemes is presented. However, since these schemes are implicit, iteration cannot be avoided in practical computations. Therefore, we introduce a waveform relaxation algorithm and prove its convergence in Section 7. In Section 8, we display preliminary numerical results which demonstrate the advantages and efficiency of our new algorithms in comparison with existing numerical methods. The last section is devoted to brief conclusions and pointers for future research.

2 The formulation of abstract ordinary differential equations

We use operator theory (see, e.g. [6]) first to formulate (1–2) as an abstract second-order ordinary differential equation in the infinity-dimensional function space $L^2(\mathbf{\Omega})$ and then to present implicitly its solution as an operator-variation-of-constants formula. To this end, some bounded operator functions are defined in advance and those are essential in introducing the formula.

We commence by defining the functions

$$\phi_j(x) := \sum_{k=0}^{\infty} \frac{(-1)^k x^k}{(2k+j)!}, \qquad j \in \mathbb{Z}_+ \qquad \text{for} \quad \forall x \geq 0. \tag{4}$$

It is easy to see that the functions ϕ_j are bounded for all $x \geq 0$. For instance,

$$\phi_0(x) = \cos(\sqrt{x}), \quad \phi_1(x) = \operatorname{sinc}(\sqrt{x}),$$

and it is obvious that $|\phi_j(x)| \leq 1$ for $j = 0, 1$ and $\forall x \geq 0$. We now consider the linear differential operator $\mathcal{A}$ defined by

$$(\mathcal{A}v)(x) = -a^2 v_{xx}(x)$$

in order to gain an abstract formulation for the problem (1–2). While $\mathcal{A}$ is a linear, unbounded positive semi-definite operator, whose domain is

$$D(\mathcal{A}) := \left\{ v \in H^1(\mathbf{\Omega}) : v(x) = v(x + 2\pi) \right\}.$$

The operator $\mathcal{A}$ has a complete system of orthogonal eigenfunctions $\left\{ e^{ikx} : k \in \mathbb{Z} \right\}$ in the Hilbert space $L^2(\mathbf{\Omega})$, and the corresponding eigenvalues are a^2k^2, $k \in \mathbb{Z}$. Because of the isomorphism between L^2 and l^2, the operator $\mathcal{A}$ induces a corresponding operator on l^2 (see, e.g. [6,25]). Consequently, the functions (4) induce the operator

$$\phi_j(t\mathcal{A}): \; L^2(\mathbf{\Omega}) \to L^2(\mathbf{\Omega})$$

for $j \in \mathbb{Z}_+$ and $t_0 \leq t \leq T$:

$$\phi_j(t\mathcal{A})v(x) = \sum_{k=-\infty}^{\infty} \hat{v}_k \phi_j(ta^2k^2) e^{ikx} \quad \text{for} \quad v(x) = \sum_{k=-\infty}^{\infty} \hat{v}_k e^{ikx}. \tag{5}$$

We next show that the above operators are bounded. To this end, we first derive the norm of the function in $L^2(\mathbf{\Omega})$, which in the frequency space becomes

$$\|v\|^2 = 2\pi \sum_{k=-\infty}^{\infty} |\hat{v}_k|^2,$$

[40]. It now follows from the definition of operator norm that

$$\|\phi_j(t\mathcal{A})\|_*^2 = \sup_{\|v\| \neq 0} \frac{\|\phi_j(t\mathcal{A})v\|^2}{\|v\|^2} \leq \sup_{t_0 \leq t \leq T} |\phi_j(ta^2k^2)|^2 \leq \gamma_j^2, \tag{6}$$

where $\|\cdot\|_*$ is the Sobolev norm $\|\cdot\|_{L^2(\mathbf{\Omega}) \leftarrow L^2(\mathbf{\Omega})}$, γ_j are the bounds of the functions $|\phi_j(x)|$ for $j = 0, 1, 2, \ldots$ and $x \geq 0$. For example,

$$\|\phi_0(t\mathcal{A})\|_*^2 \leq 1 \qquad \text{and} \qquad \|\phi_1(t\mathcal{A})\|_*^2 \leq 1.$$

We now define $u(t)$ as the function that maps x to $u(x,t)$, $u(t) := [x \mapsto u(x,t)]$, and formulate the system (1–2) as an abstract second-order ordinary differential equation on the infinity-dimensional function space $L^2(\mathbf{\Omega})$,

$$\begin{cases} u''(t) + \mathcal{A}u(t) = f\big(u(t)\big), \qquad t_0 < t \leq T, \\ u(t_0) = \varphi_1(x), \qquad u'(t_0) = \varphi_2(x). \end{cases} \tag{7}$$

Following the above discussion, we are now in a position to present an integral formula for the nonlinear Klein–Gordon equation (1–2). The solution of the abstract ordinary differential equations (7) can be characterized by the following operator-variation-of-constants formula.

Theorem 1 *The solution of* (7) *and its derivative satisfy the following operator-variation-of-constants formula*

$$\begin{cases} u(t) = \phi_0\big((t-t_0)^2\mathcal{A}\big)u(t_0) + (t-t_0)\phi_1\big((t-t_0)^2\mathcal{A}\big)u'(t_0) \\ \qquad\quad + \displaystyle\int_{t_0}^{t}(t-\zeta)\phi_1\big((t-\zeta)^2\mathcal{A}\big)f\big(u(\zeta)\big)\mathrm{d}\zeta, \\ u'(t) = -(t-t_0)\mathcal{A}\phi_1\big((t-t_0)^2\mathcal{A}\big)u(t_0) + \phi_0\big((t-t_0)^2\mathcal{A}\big)u'(t_0) \\ \qquad\quad + \displaystyle\int_{t_0}^{t}\phi_0\big((t-\zeta)^2\mathcal{A}\big)f\big(u(\zeta)\big)\mathrm{d}\zeta, \end{cases} \tag{8}$$

for $t_0 \leq t \leq T$, where $\phi_0\big((t-t_0)^2\mathcal{A}\big)$ and $\phi_1\big((t-t_0)^2\mathcal{A}\big)$ are bounded operators.

Proof Applying the *Duhamel Principle* to equations (1) or (7) yields

$$\begin{bmatrix} u(t) \\ u'(t) \end{bmatrix} = \exp\left((t-t_0)\begin{bmatrix} 0 & I \\ -\mathcal{A} & 0 \end{bmatrix}\right)\begin{bmatrix} u(t_0) \\ u'(t_0) \end{bmatrix} + \int_{t_0}^{t}\exp\left((t-\zeta)\begin{bmatrix} 0 & I \\ -\mathcal{A} & 0 \end{bmatrix}\right)\begin{bmatrix} 0 \\ f\big(u(\zeta)\big) \end{bmatrix}\mathrm{d}\zeta,$$

whereby (8) follows by expanding the exponential operator. □

Remark 1 For the nonlinear Klein–Gordon equations, the nonlinear integral equation (8) reflects the variations of the solution with time t and is helpful in deriving and analysing novel numerical integration methods for the nonlinear Klein–Gordon equations. However, for $f(u) = 0$ (1) becomes identical to the homogenous wave equation

$$\begin{cases} u_{tt} - a^2\Delta u = 0, \; t_0 < t \leq T, \qquad x \in \mathbf{\Omega}, \\ u(x,t_0) = \varphi_1(x), \qquad u_t(x,t_0) = \varphi_2(x). \end{cases}$$

The formula (8) can integrate exactly the homogeneous linear wave equation and gives its closed-form solution.

3 A symmetric, arbitrarily high–order time integration formula

In this section, keeping the eventual discretisation in mind and applying a two-point Hermite interpolation to the formula (10), we develop a class of arbitrarily high order and symmetric time integration formulæ in the infinite-dimensional Hilbert space $L^2(\mathbf{\Omega})$. We commence with few useful preliminaries.

Lemma 1 *The bounded functions* (4) *satisfy*

$$\begin{aligned}&\int_0^1 (1-z)\phi_1\big((1-z)^2\mathcal{A}\big)z^j\mathrm{d}z = j!\phi_{j+2}(\mathcal{A}), \qquad j\in\mathbb{Z}_+,\\ &\int_0^1 \phi_0\big((1-z)^2\mathcal{A}\big)z^j\mathrm{d}z = j!\phi_{j+1}(\mathcal{A}), \qquad j\in\mathbb{Z}_+.\end{aligned} \tag{9}$$

Proof The proof of the Lemma 1 can be found in [48]. □

Corollary 1 *For every* $m,n\in\mathbb{Z}_+$ *the operators* (5) *obey*

$$\int_0^1 (1-z)^{m+1}\phi_1\big((1-z)^2\mathcal{A}\big)z^n\mathrm{d}z = \sum_{i=0}^m C_m^i(-1)^{m-i}(m+n-i)!\phi_{m+n-i+2}(\mathcal{A}),$$
$$\int_0^1 (1-z)^{m}\phi_0\big((1-z)^2\mathcal{A}\big)z^n\mathrm{d}z = \sum_{i=0}^m C_m^i(-1)^{m-i}(m+n-i)!\phi_{m+n-i+1}(\mathcal{A}),$$

where $C_m^i=\binom{m}{i}$ *is the binomial symbol.*

Proof The two sets of identities can be derived easily from Lemma 1. □

Following from Theorem 1, the solution of (7) and of its derivative at a time point $t_{n+1}=t_n+\Delta t$, $n\in\mathbb{Z}_+$, are

$$\begin{cases} u(t_{n+1}) =\phi_0\big(\mathcal{V}\big)u(t_n)+\Delta t\phi_1\big(\mathcal{V}\big)u'(t_n)+\Delta t^2\displaystyle\int_0^1(1-z)\phi_1\big((1-z)^2\mathcal{V}\big)\tilde{f}(z)\mathrm{d}z,\\ u'(t_{n+1}) =-\Delta t\mathcal{A}\phi_1\big(\mathcal{V}\big)u(t_n)+\phi_0\big(\mathcal{V}\big)u'(t_n)+\Delta t\displaystyle\int_0^1\phi_0\big((1-z)^2\mathcal{V}\big)\tilde{f}(z)\mathrm{d}z,\end{cases} \tag{10}$$

where $\mathcal{V}=\Delta t^2\mathcal{A}$ and $\tilde{f}(z)=f\big(u(t_n+z\Delta t)\big)$.

Before presenting our time integration formula, we first focus our attention on efficient integrators for approximating the nonlinear integrals

$$\begin{aligned}I_1 &:= \int_0^1 (1-z)\phi_1\big((1-z)^2\mathcal{V}\big)\tilde{f}(z)\mathrm{d}z,\\ I_2 &:= \int_0^1 \phi_0\big((1-z)^2\mathcal{V}\big)\tilde{f}(z)\mathrm{d}z.\end{aligned} \tag{11}$$

Typically the function $f(u)$ is nonlinear, and only its values at the endpoints can be used in the construction of efficient numerical approximations. We thus interpolate $\tilde{f}(z)$ by a two-point Hermite interpolation $p_r(z)$ of degree $2r+1$ [19,39].

Lemma 2 *Suppose that* $\tilde{f}\in C^{2r+2}\big([0,1]\big)$. *Then there exists a Hermite interpolating polynomial* $p_r(z)$ *of degree* $2r+1$

$$p_r(z)=\sum_{j=0}^r\Big[\beta_j(z)\tilde{f}^{(j)}(0)+(-1)^j\beta_j(1-z)\tilde{f}^{(j)}(1)\Big] \tag{12}$$

with

$$\beta_j(z)=\frac{z^j}{j!}(1-z)^{r+1}\sum_{s=0}^{r-j}C_{r+s}^s z^s \tag{13}$$

satisfying the interpolation conditions

$$p_r^{(j)}(0) = \tilde{f}^{(j)}(0), \quad p_r^{(j)}(1) = \tilde{f}^{(j)}(1), \qquad j = 0, 1, 2, \ldots, r.$$

Moreover, the error on $[0,1]$ *is given by*

$$R_r = \tilde{f}(z) - p_r(z) = (-1)^{r+1} z^{r+1} (1-z)^{r+1} \frac{\tilde{f}^{(2r+2)}(\xi)}{(2r+2)!}, \quad \xi \in (0,1). \tag{14}$$

Replacing $\tilde{f}(z)$ in (11) by the Hermite interpolation $p_r(z)$ where $\tilde{f}(z) = f\big(u(t_n + z\Delta t)\big)$ and $\tilde{f}^{(j)}(z) = \Delta t^j f_t^{(j)}\big(u(t_n + z\Delta t)\big)$, we obtain

$$\begin{aligned} \tilde{I}_1^r &= \sum_{j=0}^{r} \Delta t^j \Big[I_1[\beta_j(z)] f_t^{(j)}\big(u(t_n)\big) + (-1)^j I_1[\beta_j(1-z)] f_t^{(j)}\big(u(t_{n+1})\big) \Big], \\ \tilde{I}_2^r &= \sum_{j=0}^{r} \Delta t^j \Big[I_2[\beta_j(z)] f_t^{(j)}\big(u(t_n)\big) + (-1)^j I_2[\beta_j(1-z)] f_t^{(j)}\big(u(t_{n+1})\big) \Big]. \end{aligned} \tag{15}$$

Here $f_t^{(j)}\big(u(t)\big)$ denotes the jth derivative of $f\big(u(t)\big)$ with respect to t.

Using the Brikhoff–Hermite quadrature formula (cf. [17,29,37]), we elucidate the coefficients $I_1[\beta_j(z)], I_2[\beta_j(z)], I_1[\beta_j(1-z)]$ and $I_2[\beta_j(1-z)]$: defined below:

$$\begin{aligned} I_1[\beta_j(z)] &:= \int_0^1 (1-z)\phi_1\big((1-z)^2\mathcal{V}\big)\beta_j(z)\mathrm{d}z \\ &= \sum_{s=0}^{r-j}\sum_{i=0}^{r+1} (-1)^{r-i+1} C_{r+s}^s C_{r+1}^i \frac{(r+s+j-i+1)!}{j!} \phi_{r+s+j-i+3}\big(\mathcal{V}\big), \end{aligned} \tag{16}$$

$$\begin{aligned} I_2[\beta_j(z)] &:= \int_0^1 \phi_0\big((1-z)^2\mathcal{V}\big)\beta_j(z)\mathrm{d}z \\ &= \sum_{s=0}^{r-j}\sum_{i=0}^{r+1} (-1)^{r-i+1} C_{r+s}^s C_{r+1}^i \frac{(r+s+j-i+1)!}{j!} \phi_{r+s+j-i+2}\big(\mathcal{V}\big), \end{aligned} \tag{17}$$

$$\begin{aligned} I_1[\beta_j(1-z)] &:= \int_0^1 (1-z)\phi_1\big((1-z)^2\mathcal{V}\big)\beta_j(1-z)\mathrm{d}z \\ &= \sum_{s=0}^{r-j}\sum_{i=0}^{r+j} (-1)^{s+j-i} C_{r+s}^s C_{s+j}^i \frac{(r+s+j-i+1)!}{j!} \phi_{r+s+j-i+3}\big(\mathcal{V}\big), \end{aligned} \tag{18}$$

$$\begin{aligned} I_2[\beta_j(1-z)] &:= \int_0^1 \phi_0\big((1-z)^2\mathcal{V}\big)\beta_j(1-z)\mathrm{d}z \\ &= \sum_{s=0}^{r-j}\sum_{i=0}^{r+j} (-1)^{s+j-i} C_{r+s}^s C_{s+j}^i \frac{(r+s+j-i+1)!}{j!} \phi_{r+s+j-i+2}\big(\mathcal{V}\big). \end{aligned} \tag{19}$$

Boundedness follows at once,

$$\begin{aligned} &\|I_1[\beta_j(z)]\|_* \le \max_{0\le z\le 1} |\beta_j(z)| \le 1 \text{ and } \|I_1[\beta_j(1-z)]\|_* \le \max_{0\le z\le 1} |\beta_j(1-z)| \le 1, \\ &\|I_2[\beta_j(z)]\|_* \le \max_{0\le z\le 1} |\beta_j(z)| \le 1 \text{ and } \|I_2[\beta_j(1-z)]\|_* \le \max_{0\le z\le 1} |\beta_j(1-z)| \le 1. \end{aligned}$$

Let $u^n \approx u(t_n)$ and $\mu^n \approx u'(t_n)$. Using above analysis and the formula (10), we present the following time integration formula for the abstract ODEs (7).

Definition 1 *Our time integrator for the abstract ODEs* (7) *is defined by*

$$
\begin{cases}
u^{n+1} = \phi_0(\mathcal{V})u^n + \Delta t\phi_1[\mathcal{V})\mu^n + \sum_{j=0}^{r} \Delta t^{j+2}\Big(I_1[\beta_j(z)]f_t^{(j)}(u^n) \\
\qquad + (-1)^j I_1[\beta_j(1-z)]f_t^{(j)}(u^{n+1})\Big], \\
\mu^{n+1} = -\Delta t\mathcal{A}\phi_1[\mathcal{V})u^n + \phi_0(\mathcal{V})\mu^n + \sum_{j=0}^{r} \Delta t^{jm1}\Big(I_2[\beta_j(z)]f_t^{(j)}(u^n) \\
\qquad + (-1)^j I_2[\beta_j(1-z)]f_t^{(j)}(u^{n+1})\Big],
\end{cases}
\tag{20}
$$

where $I_1[\beta_j(z)], I_2[\beta_j(z)], I_1[\beta_j(1-z)]$ *and* $I_2[\beta_j(1-z)]$ *have been defined by (16–19), respectively.*

Theorem 2 *Suppose that* $f\big(u(\cdot,t)\big) \in C^{2r+2}([t_0,T])$ *and* $f_t^{(2r+2)}\big(u(x,\cdot)\big) \in L^2(\mathbf{\Omega})$. *Subject to local assumptions on* $u^n = u(t_n)$, $\mu^n = u'(t_n)$, *local error bounds of the time integration formula* (20) *are*

$$
\|u(t_{n+1}) - u^{n+1}\| \leq C_1\Delta t^{2r+4} \quad \text{and} \quad \|u'(t_{n+1}) - \mu^{n+1}\| \leq C_2\Delta t^{2r+3}, \tag{21}
$$

where the constants C_1 *and* C_2 *are*

$$
C_1 = \frac{(r+2)!(r+1)!}{(2r+2)!(2r+4)!} \max_{t_0 \leq t \leq T} \|f_t^{(2r+2)}\big(u(t)\big)\|
$$

and

$$
C_2 = \frac{\big[(r+1)!\big]^2}{(2r+2)!(2r+3)!} \max_{t_0 \leq t \leq T} \|f_t^{(2r+2)}\big(u(t)\big)\|.
$$

Proof It follows from (10) and (20) that

$$
u(t_{n+1}) - u^{n+1} = \Delta t^2 \int_0^1 (1-z)\phi_1\big((1-z)^2\mathcal{V}\big)\Big(f\big(u(t_n + z\Delta t)\big) - p_r(z)\Big)\mathrm{d}z, \tag{22}
$$

and

$$
u'(t_{n+1}) - \mu^{n+1} = \Delta t \int_0^1 \phi_0\big((1-z)^2\mathcal{V}\big)\Big(f\big(u(t_n + z\Delta t)\big) - p_r(z)\Big)\mathrm{d}z. \tag{23}
$$

Noting that $\tilde{f}^{(j)}(z) = \Delta t^j f_t^{(j)}\big(u(t_n + z\Delta t)\big)$, and using Lemma 2, we have

$$
f\big(u(t_n + z\Delta t)\big) - p_r(z) = \Delta t^{2r+2} z^{r+1}(1-z)^{r+1} \frac{f_t^{(2r+2)}\big(u(t_n + \xi^n\Delta t)\big)}{(2r+2)!}. \tag{24}
$$

Finally, inserting (24) into (22) and (23) yields

$$
\begin{aligned}
\|u(t_{n+1}) - u^{n+1}\| &\leq \Delta t^{2r+4} \frac{\|f_t^{(2r+2)}\big(u(t_n + \xi^n\Delta t)\big)\|}{(2r+2)!} \int_0^1 (1-z)^{r+2} z^{r+1}\mathrm{d}z \\
&\leq C_1\Delta t^{2r+4},
\end{aligned}
$$

and

$$\begin{aligned}\|u'(t_{n+1}) - \mu^{n+1}\| &\leq \Delta t^{2r+3} \frac{\|f_t^{(2r+2)}\big(u(t_n + \xi^n \Delta t)\big)\|}{(2r+2)!} \int_0^1 (1-z)^{r+1} z^{r+1} \mathrm{d}z \\ &\leq C_2 \Delta t^{2r+3},\end{aligned}$$

completing the proof. □

The Klein–Gordon equation (1) is time symmetric and a most welcome feature of (20) is that it preserves time symmetry. As a first step, let us introduce some useful properties of the operator-valued functions ϕ_0, ϕ_1 and the coefficients defined by (16–19) in the following two lemmas.

Lemma 3 *The bounded operators $\phi_0(\mathcal{A})$ and $\phi_1(\mathcal{A})$ defined by (5) satisfy*

$$\phi_0^2(\mathcal{A}) + \mathcal{A}\phi_1^2(\mathcal{A}) = I, \tag{25}$$

where $\mathcal{A}$ is an arbitrary positive semi-definite operator or matrix.

Lemma 4 *The coefficients $I_1[\beta_j(z)], I_2[\beta_j(z)], I_1[\beta_j(1-z)]$ and $I_2[\beta_j(1-z)]$ from (20) satisfy*

$$\begin{aligned}\phi_0(\mathcal{V})I_1[\beta_j(z)] - \phi_1(\mathcal{V})I_2[\beta_j(z)] &= -I_1[\beta_j(1-z)], \\ \mathcal{V}\phi_1(\mathcal{V})I_1[\beta_j(z)] + \phi_0(\mathcal{V})I_2[\beta_j(z)] &= I_0[\beta_j(1-z)],\end{aligned} \tag{26}$$

where $\beta_j(z)$ $j = 0, 1, \ldots, r$ are defined by (13) and $\mathcal{V} = \Delta t^2 \mathcal{A}$ and $\mathcal{A}$ an arbitrary positive semi-definite operator or matrix.

Proof It follows from the definitions of $I_1[\beta_j(z)]$ and $I_2[\beta_j(z)]$ that

$$\begin{aligned}&\phi_0(\mathcal{V})I_1[\beta_j(z)] - \phi_1(\mathcal{V})I_2[\beta_j(z)] \\ =&\int_0^1 \Big((1-z)\phi_0(\mathcal{V})\phi_1\big((1-z)^2\mathcal{V}\big) - \phi_1(\mathcal{V})\phi_0\big((1-z)^2\mathcal{V}\big)\Big)\beta_j(z)\mathrm{d}z \\ =&\int_0^1 \big(z\phi_0(\mathcal{V})\phi_1(z^2\mathcal{V}) - \phi_1(\mathcal{V})\phi_0(z^2\mathcal{V})\big)\beta_j(1-z)\mathrm{d}z \\ =&-\int_0^1 (1-z)\phi_1\big((1-z)^2\mathcal{V}\big)\beta_j(1-z)\mathrm{d}z = -I_1[\beta_j(1-z)].\end{aligned}$$

The second formula of (26) can be proved in a similar way and we skip the details. □

We are now in a position to prove time symmetry of (20).

Theorem 3 *The time integration formula (20) is symmetric with respect to the time variable.*

Proof Exchanging $u^{n+1} \leftrightarrow u^n, \mu^{n+1} \leftrightarrow \mu^n$ and replacing Δt by $-\Delta t$ in formula (20) yield

$$\begin{aligned} u^n =& \phi_0(\mathcal{V}) u^{n+1} - \Delta t \phi_1(\mathcal{V}) \mu^{n+1} \\ &+ \sum_{j=0}^{r} \Delta t^{j+2} \left\{ (-1)^j I_1[\beta_j(z)] f_t^{(j)}(u^{n+1}) + I_1[\beta_j(1-z)] f_t^{(j)}(u^n) \right\}, \end{aligned} \tag{27}$$

$$\begin{aligned} \mu^n =& \Delta t \mathcal{A} \phi_1\{\mathcal{V}) u^{n+1} + \phi_0(\mathcal{V}) \mu^{n+1} \\ &- \sum_{j=0}^{r} \Delta t^{j+1} \Big((-1)^j I_2[\beta_j(z)] f_t^{(j)}(u^{n+1}) + I_2[\beta_j(1-z)] f_t^{(j)}(u^n) \Big\}. \end{aligned} \tag{28}$$

Combining $\phi_0(\mathcal{V}) \times (27) + \Delta t \phi_1(\mathcal{V}) \times (28)$, we have

$$\begin{aligned} u^{n+1} =& \phi_0(\mathcal{V}) u^n + \Delta t \phi_1(\mathcal{V}) \mu^n \\ &- \sum_{j=0}^{r} \Delta t^{j+2} \Big\{ (-1)^j \big(\phi_0(\mathcal{V}) I_1[\beta_j(z)] - \phi_1(\mathcal{V}) I_2[\beta_j(z)] \big) f_t^{(j)}(u^{n+1}) \\ &+ \big(\phi_0(\mathcal{V}) I_1[\beta_j(1-z)] - \phi_1(\mathcal{V}) I_2[\beta_j(1-z)] \big) f_t^{(j)}(u^n) \Big\}. \end{aligned} \tag{29}$$

Similarly, $-\Delta t \mathcal{A} \phi_1(\mathcal{V}) \times (27) + \phi_0(\mathcal{V}) \times (28)$ results in

$$\begin{aligned} \mu^{n+1} =& -\Delta t \mathcal{A} \phi_1(\mathcal{V}) u^n + \phi_0(\mathcal{V}) \mu^n \\ &+ \sum_{j=0}^{r} \Delta t^{j+1} \Big\{ (-1)^j \big(\mathcal{V} \phi_1(\mathcal{V}) I_1[\beta_j(z)] + \phi_0(\mathcal{V}) I_2[\beta_j(z)] \big) f_t^{(j)}(u^{n+1}) \\ &+ \big(\mathcal{V} \phi_1(\mathcal{V}) I_1[\beta_j(1-z)] + \phi_0(\mathcal{V}) I_2[\beta_j(1-z)] \big) f_t^{(j)}(u^n) \Big\}. \end{aligned} \tag{30}$$

Applying Lemma 4 to (29) and (30) yields the statement of the theorem. □

4 Stability of the fully discrete scheme

In this section we show the stability of our methods, once the differential operator $\mathcal{A}$ is replaced by a suitable matrix A. Throughout this section $\|\cdot\|$ presents both the vector 2-norm and the matrix 2-norm (the spectral norm).

Suppose that the perturbed problem of (7) is

$$\begin{cases} v''(t) + \mathcal{A} v(t) = f\big(v(t)\big), & t \in [t_0, T], \\ v(t_0) = \varphi_1(x) + \tilde{\varphi}_1(x), & v'(t_0) = \varphi_2(x) + \tilde{\varphi}_2(x), \end{cases} \tag{31}$$

where $\tilde{\varphi}_1$ and $\tilde{\varphi}_2$ are perturbation functions. Letting $\eta(t) = v(t) - u(t)$ and subtracting (7) from (31), we obtain

$$\begin{cases} \eta''(t) + \mathcal{A} \eta(t) = f\big(v(t)\big) - f\big(u(t)\big), & t \in [t_0, T], \\ \eta(t_0) = \tilde{\varphi}_1(x), \quad \eta'(t_0) = \tilde{\varphi}_2(x). \end{cases} \tag{32}$$

In general, we prefer to approximate operator $\mathcal{A}$ by a symmetric and positive semi-definite differential matrix A, since this assists in structure preservation. In that case there exist an orthogonal matrix P and a diagonal matrix Λ with non-negative diagonal such that

$$A = P^\top \Lambda P.$$

We let $D = P^\top \Lambda^{\frac{1}{2}} P$, hence $A = D^2$. The bounded operators $\phi_j(t^2\mathcal{A})$ are replaced by the matrix functions $\phi_j(t^2 A)$. Similarly, we also have

$$\|\phi_j(t^2A)\| = \sqrt{\lambda_{\max}\Big(\phi_j^2(t^2A)\Big)} \le \gamma_j, \qquad j \in \mathbb{Z}_+. \tag{33}$$

In what follows, we will analyse the stability for the time-stepping method (20). We assume that

$$\eta^n \approx \eta(t_n), \quad \zeta^n \approx \eta'(t_n) \qquad \text{and} \qquad v^n \approx v(t_n), \quad w^n \approx v'(t_n).$$

Applying our method to (32), we obtain

$$\begin{cases} \eta^{n+1} = \phi_0(V)\eta^n + \Delta t\phi_1(V)\zeta^n + \displaystyle\sum_{j=0}^{r} \Delta t^{j+2} \Big\{ I_1[\beta_j(z)]\big[f_t^{(j)}(v^n) \\ \qquad - f_t^{(j)}(u^n)\big] + (-1)^j I_1[\beta_j(1-z)]\big[f_t^{(j)}(v^{n+1}) - f_t^{(j)}(u^{n+1})\big]\Big\}, \\ \zeta^{n+1} = -\Delta t A\phi_1(V)\eta^n + \phi_0(V)\zeta^n + \displaystyle\sum_{j=0}^{r} \Delta t^{j+1} \Big\{ I_2[\beta_j(z)]\big[f_t^{(j)}(v^n) \\ \qquad - f_t^{(j)}(u^n)\big] + (-1)^j I_2[\beta_j(1-z)]\big[f_t^{(j)}(v^{n+1}) - f_t^{(j)}(u^{n+1})\big]\Big\}, \end{cases} \tag{34}$$

where $V = \Delta t^2 A$, $I_1[\beta_j(z)], I_2[\beta_j(z)], I_1[\beta_j(1-z)]$ and $I_2[\beta_j(1-z)]$ are defined by (16–19), respectively. Likewise, we have

$$\|I_1[\beta_j(z)]\| \le \max_{0\le z\le 1} |\beta_j(z)| \le 1 \quad \text{and} \quad \|I_1[\beta_j(1-z)]\| \le \max_{0\le z\le 1} |\beta_j(1-z)| \le 1,$$
$$\|I_2[\beta_j(z)]\| \le \max_{0\le z\le 1} |\beta_j(z)| \le 1 \quad \text{and} \quad \|I_2[\beta_j(1-z)]\| \le \max_{0\le z\le 1} |\beta_j(1-z)| \le 1.$$

We rewrite the schemes (34) in a matrix-vector form,

$$\begin{aligned} \begin{bmatrix} D\eta^{n+1} \\ \zeta^{n+1} \end{bmatrix} =& \Omega \begin{bmatrix} D\eta^n \\ \zeta^n \end{bmatrix} + \sum_{j=0}^{r} \Delta t^{j+1} \int_0^1 \Omega_j(z)\mathrm{d}z \begin{bmatrix} 0 \\ f_t^{(j)}(v^n) - f_t^{(j)}(u^n) \end{bmatrix} \\ &+ \sum_{j=0}^{r} (-1)^j \Delta t^{j+1} \int_0^1 \Omega_j(1-z)\mathrm{d}z \begin{bmatrix} 0 \\ f_t^{(j)}(v^{n+1}) - f_t^{(j)}(u^{n+1}) \end{bmatrix}, \end{aligned} \tag{35}$$

where

$$\Omega = \begin{bmatrix} \phi_0(V) & \Delta t D\phi_1(V) \\ -\Delta t D\phi_1(V) & \phi_0(V) \end{bmatrix} \tag{36}$$

and

$$\Omega_j(z) = \beta_j(z) \begin{bmatrix} \phi_0((1-z)^2V) & \Delta t(1-z)D\phi_1((1-z)^2V) \\ -\Delta t(1-z)D\phi_1((1-z)^2V) & \phi_0((1-z)^2V) \end{bmatrix}. \tag{37}$$

Before embarking on stability analysis, we first investigate the spectral norm of matrices Ω and $\Omega_j(z)$ for $j = 0, 1, \ldots, r$.

Lemma 5 *Assume that A is a symmetric and positive semi-definite matrix and that $V = \Delta t^2 A$. Then the spectral norms of matrices Ω and $\Omega_j(z)$ satisfy*

$$\|\Omega\| = 1 \quad \textit{and} \quad \|\Omega_j(z)\| = |\beta_j(z)| \leq 1, \qquad z \in [0,1], \quad j = 0, 1, \ldots, r. \tag{38}$$

Proof According to Lemma 3 and formulæ (36) and (37), it is trivial that

$$\Omega^\top \Omega = I_{2M\times 2M} \quad \text{and} \quad \Omega_j^\top(z)\Omega_j(z) = \beta_j^2(z) I_{2M\times 2M}. \tag{39}$$

Therefore

$$\|\Omega\| = 1 \quad \text{and} \quad \|\Omega_j(z)\| = |\beta_j(z)| \leq 1, \qquad z \in [0,1], \quad j = 0, 1, \ldots, r,$$

and the lemma follows. □

4.1 Linear stability analysis

In this subsection we focus our attention on analysing the stability of our methods for $f(u) = u$. In this case

$$f_t^{(2k)}\big(u(t)\big) = (I - \mathcal{A})^k u(t) \quad f_t^{(2k+1)}\big(u(t)\big) = (I - \mathcal{A})^k u'(t), \qquad k \in \mathbb{Z}_+. \tag{40}$$

Lemma 6 *Assume that A is a symmetric matrix. Then*

$$\|(I - A)^k\| \leq \big(1 + \rho(A)\big)^k, \qquad k \in \mathbb{Z}_+,$$

where $\rho(A)$ is the spectral radius of A.

Proof An immediate consequence of the definition of the spectral norm:

$$\|(I - A)^k\| = \sqrt{\lambda_{\max}\big((I - A)^{2k}\big)} \leq (1 + \max_{1\leq j\leq M} |\lambda_j|)^k = \big(1 + \rho(A)\big)^k,$$

where λ_j are the eigenvalues of A. □

Theorem 4 *Let the operator $\mathcal{A}$ be approximated by a symmetric and positive semi-definite differential matrix A and suppose that the sufficiently small time stepsize Δt satisfies $\Delta t^2\big(1 + \rho(A)\big) \leq 1$ with $\Delta t \leq [4(r+1)]^{-1}$. Then*

$$\|\eta^n\| \leq \exp\big(2(4r+5)T\big)\Big(\|\tilde{\varphi}_1\| + \sqrt{\|D\tilde{\varphi}_1\|^2 + \|\tilde{\varphi}_2\|^2}\Big),$$
$$\|\zeta^n\| \leq \exp\big(2(4r+5)T\big)\Big(\|\tilde{\varphi}_1\| + \sqrt{\|D\tilde{\varphi}_1\|^2 + \|\tilde{\varphi}_2\|^2}\Big),$$

where $\tilde{\varphi}_l = \big(\tilde{\varphi}_l(x_0), \tilde{\varphi}_l(x_1), \ldots, \tilde{\varphi}_l(x_{M-1})\big)^\top$, while $\tilde{\varphi}_l(x_i)$ are the values of the perturbation functions $\tilde{\varphi}_l$, $l = 1, 2$, at the grid points $\{x_i\}_{i=0}^{M-1}$.

Proof It follows from the first formula in (34) and from (35) that

$$\begin{aligned}\|\eta^{n+1}\| \le \|\eta^n\| + \Delta t\|\zeta^n\| + \sum_{j=0}^{r} \Delta t^{j+2}\big(\|f_t^{(j)}(v^n) - f_t^{(j)}(u^n)\| \\ + \|f_t^{(j)}(v^{n+1}) - f_t^{(j)}(u^{n+1})\|\big),\end{aligned}$$

and

$$\begin{aligned}\sqrt{\|D\eta^{n+1}\|^2 + \|\zeta^{n+1}\|^2} \le \sqrt{\|D\eta^n\|^2 + \|\zeta^n\|^2} + \sum_{j=0}^{r} \Delta t^{j+1}\big(\|f_t^{(j)}(v^n) - f_t^{(j)}(u^n)\| \\ + \|f_t^{(j)}(v^{n+1}) - f_t^{(j)}(u^{n+1})\|\big).\end{aligned}$$

Summing up the above and using (40), we obtain

$$\begin{aligned}&\|\eta^{n+1}\| + \sqrt{\|D\eta^{n+1}\|^2 + \|\zeta^{n+1}\|^2} \le \|\eta^n\| + \sqrt{\|D\eta^n\|^2 + \|\zeta^n\|^2} + \Delta t\|\zeta^n\| \\ &+ \Delta t(1+\Delta t)\sum_{j=0}^{r} \Delta t^j \|(I-A)^{[\frac{j}{2}]}\|\big(\|\eta^n\| + \|\zeta^n\| + \|\eta^{n+1}\| + \|\zeta^{n+1}\|\big).\end{aligned} \tag{41}$$

Applying Lemma 6 to inequality (41), we have

$$\begin{aligned}&\|\eta^{n+1}\| + \sqrt{\|D\eta^{n+1}\|^2 + \|\zeta^{n+1}\|^2} \le \|\eta^n\| + \sqrt{\|D\eta^n\|^2 + \|\zeta^n\|^2} + \Delta t\|\zeta^n\| \\ &\quad + \Delta t(1+\Delta t)\sum_{j=0}^{r} \Delta t^j \big(1+\rho(A)\big)^{[\frac{j}{2}]}\big(\|\eta^n\| + \|\zeta^n\| + \|\eta^{n+1}\| + \|\zeta^{n+1}\|\big).\end{aligned}$$

Since the stepsize satisfies $\Delta t^2\big(1+\rho(A)\big) \le 1$,

$$\begin{aligned}&\|\eta^{n+1}\| + \sqrt{\|D\eta^{n+1}\|^2 + \|\zeta^{n+1}\|^2} \\ &\le \left[1 + \frac{\Delta t(4r+5)}{1-2\Delta t(r+1)}\right]\left(\|\eta^n\| + \sqrt{\|D\eta^n\|^2 + \|\zeta^n\|^2}\right).\end{aligned}$$

Moreover, $\Delta t \le [4(r+1)]^{-1}$, consequently

$$\begin{aligned}&\|\eta^{n+1}\| + \sqrt{\|D\eta^{n+1}\|^2 + \|\zeta^{n+1}\|^2} \\ &\le \Big[1 + 2(4r+5)\Delta t\Big]\left(\|\eta^n\| + \sqrt{\|D\eta^n\|^2 + \|\zeta^n\|^2}\right).\end{aligned}$$

An inductive argument yields

$$\begin{aligned}&\|\eta^{n+1}\| + \sqrt{\|D\eta^{n+1}\|^2 + \|\zeta^{n+1}\|^2} \\ &\le \exp\big(2(4r+5)T\big)\left(\|\tilde\varphi_1\| + \sqrt{\|D\tilde\varphi_1\|^2 + \|\tilde\varphi_2\|^2}\right)\end{aligned}$$

and the proof is complete. □

4.2 Nonlinear stability analysis

Following the method of proof for the linear case, we now analyse the stability of our methods for nonlinear problems. Our main assumptions are as follows.

Assumption 1 *Both* (7) *and* (31) *possess sufficiently smooth solutions and* $f : D(\mathcal{A}) \to \mathbb{R}$ *is sufficiently Fréchet differentiable in a strip along the exact solution.*

It is known from [47, Chap. 3] that

$$f_t^{(k)}\big(u(t)\big) = \sum_{\tilde{t}\in \mathrm{SENT}^f_{k+2}} \alpha(\tilde{t})\mathcal{F}(\tilde{t})\big(u(t), u'(t)\big), \tag{42}$$

where $\mathrm{SENT}^f = \{\tau_2\} \cup \big\{\tilde{t} = [\tilde{t}_1, \ldots, \tilde{t}_m]_2 : \tilde{t}_i \in \mathrm{SENT}\big\}$ and SENT is the set of special extended Nyström trees is defined in [47], $\alpha(\tilde{t})$ is the number of possible monotonic labellings of an extended Nyström tree $\tilde{t}$, and $\mathcal{F}(\tilde{t})\big(u, u'\big)$ is the corresponding elementary differential.

Assumption 2 $\mathrm{d}^k f(u)/\mathrm{d}u^k : D(\mathcal{A}) \to \mathbb{R}$ *for* $k = 0, 1, 2, \ldots, r$ *are locally Lipschitz continuous in a strip along the exact solution* u*. Thus, there exist real numbers* $L(R, \rho(A)^{\lfloor \frac{k}{2} \rfloor})$ *such that*

$$\begin{aligned}&\|\mathcal{F}(\tilde{t})\big(v(t), v'(t)\big) - \mathcal{F}(\tilde{t})\big(w(t), w'(t)\big)\|\\ \le& L(R, \rho(A)^{\lfloor \frac{k}{2} \rfloor})\Big(\|v(t) - w(t)\| + \|v'(t) - w'(t)\|\Big), \ \forall \tilde{t} \in \mathrm{SENT}^f_{k+2},\end{aligned}$$

for all $t \in [t_0, T]$ *and* $\max\Big(\|v - u(t)\|, \|w - u(t)\|, \|v' - u'(t)\|, \|w' - u'(t)\|\Big) \le R.$

We next enunciate the statement on nonlinear stability.

Theorem 5 *Subject to Assumptions 1 and 2 and to the sufficiently small time stepsize satisfying*

$$\Delta t^2 L(R, \rho(A)) \le 1 \qquad \text{and} \qquad \Delta t \sum_{j=0}^{r} \sum_{\tilde{t}\in \mathrm{SENT}^f_{j+2}} \alpha(\tilde{t}) \le \frac{1}{4},$$

approximating the operator $\mathcal{A}$ *by a symmetric and positive semi-definite matrix* A*, we obtain the following stability results,*

$$\begin{aligned}\|\eta^n\| &\le \exp\Big(2T\big(1 + 4\sum_{j=0}^{r} \sum_{\tilde{t}\in \mathrm{SENT}^f_{j+2}} \alpha(\tilde{t})\big)\Big)\Big(\|\tilde{\varphi}_1\| + \sqrt{\|D\tilde{\varphi}_1\|^2 + \|\tilde{\varphi}_2\|^2}\Big),\\ \|\zeta^n\| &\le \exp\Big(2T\big(1 + 4\sum_{j=0}^{r} \sum_{\tilde{t}\in \mathrm{SENT}^f_{j+2}} \alpha(\tilde{t})\big)\Big)\Big(\|\tilde{\varphi}_1\| + \sqrt{\|D\tilde{\varphi}_1\|^2 + \|\tilde{\varphi}_2\|^2}\Big),\end{aligned}$$

where $\tilde{\varphi}_l = \big(\tilde{\varphi}_l(x_0), \tilde{\varphi}_l(x_1), \ldots, \tilde{\varphi}_l(x_{M-1})\big)^\top$ *and* $\tilde{\varphi}_l(x_i)$ *are the values of the perturbation functions* $\tilde{\varphi}_l$*,* $l = 1, 2$*, at the spatial grid points* $\{x_i\}_{i=0}^{M-1}$.

Proof It follows from the first formula in (34) and from (35) that

$$\begin{aligned}\|\eta^{n+1}\| \leq & \|\eta^n\| + \Delta t\|\zeta^n\| + \sum_{j=0}^{r} \Delta t^{j+2} \big[\|f_t^{(j)}(v^n) - f_t^{(j)}(u^n)\| \\ & + \|f_t^{(j)}(v^{n+1}) - f_t^{(j)}(u^{n+1})\|\big], \\ \sqrt{\|D\eta^{n+1}\|^2 + \|\zeta^{n+1}\|^2} \leq & \sqrt{\|D\eta^n\|^2 + \|\zeta^n\|^2} + \sum_{j=0}^{r} \Delta t^{j+1} \big(\|f_t^{(j)}(v^n) - f_t^{(j)}(u^n)\| \\ & + \|f_t^{(j)}(v^{n+1}) - f_t^{(j)}(u^{n+1})\|\big).\end{aligned} \tag{43}$$

Summing up (43) and inserting (42) into the right-hand side, we obtain

$$\begin{aligned}&\|\eta^{n+1}\| + \sqrt{\|D\eta^{n+1}\|^2 + \|\zeta^{n+1}\|^2} \leq \|\eta^n\| + \Delta t\|\zeta^n\| + \sqrt{\|D\eta^n\|^2 + \|\zeta^n\|^2} \\ &+ \Delta t(1+\Delta t) \sum_{j=0}^{r} \sum_{\tilde{t} \in \mathrm{SENT}_{j+2}^f} \alpha(\tilde{t}) \Delta t^j \Big[\|\mathcal{F}(\tilde{t})(v^n, w^n) - \mathcal{F}(\tilde{t})(u^n, \mu^n)\| \\ &+ \|\mathcal{F}(\tilde{t})(v^{n+1}, w^{n+1}) - \mathcal{F}(\tilde{t})(u^{n+1}, \mu^{n+1})\|\Big].\end{aligned} \tag{44}$$

On the other hand, using Assumption 2 on the right-hand side of (44) yields

$$\begin{aligned}&\|\eta^{n+1}\| + \sqrt{\|D\eta^{n+1}\|^2 + \|\zeta^{n+1}\|^2} \leq \|\eta^n\| + \Delta t\|\zeta^n\| + \sqrt{\|D\eta^n\|^2 + \|\zeta^n\|^2} \\ &+ \Delta t(1+\Delta t) \sum_{j=0}^{r} \sum_{\tilde{t} \in \mathrm{SENT}_{j+2}^f} \alpha(\tilde{t}) \Delta t^j L(R, \rho(A)^{\lfloor \frac{j}{2} \rfloor}) \big(\|\eta^n\| + \|\zeta^n\| + \|\eta^{n+1}\| + \|\zeta^{n+1}\|\big).\end{aligned} \tag{45}$$

The time stepsize Δt satisfies $\Delta t^2 L(R, \rho(A)) \leq 1$, hence inequality (45) leads to

$$\begin{aligned}&\|\eta^{n+1}\| + \sqrt{\|D\eta^{n+1}\|^2 + \|\zeta^{n+1}\|^2} \\ &\leq \left\{1 + \frac{\Delta t\big[1 + 4\sum_{j=0}^{r} \sum_{\tilde{t} \in \mathrm{SENT}_{j+2}^f} \alpha(\tilde{t})\big]}{1 - 2\Delta t \sum_{j=0}^{r} \sum_{\tilde{t} \in \mathrm{SENT}_{j+2}^f} \alpha(\tilde{t})}\right\} \Big(\|\eta^n\| + \sqrt{\|D\eta^n\|^2 + \|\zeta^n\|^2}\Big).\end{aligned}$$

Moreover, $\Delta t \sum_{j=0}^{r} \sum_{\tilde{t} \in \mathrm{SENT}_{j+2}^f} \alpha(\tilde{t}) \leq \frac{1}{4}$, therefore

$$\begin{aligned}&\|\eta^{n+1}\| + \sqrt{\|D\eta^{n+1}\|^2 + \|\zeta^{n+1}\|^2} \\ \leq &\Big[1 + 2\Delta t\big(1 + 4\sum_{j=0}^{r} \sum_{\tilde{t} \in \mathrm{SENT}_{j+2}^f} \alpha(\tilde{t})\big)\Big] \big(\|\eta^n\| + \sqrt{\|D\eta^n\|^2 + \|\zeta^n\|^2}\big).\end{aligned}$$

An inductive argument yields

$$\begin{aligned}&\|\eta^{n+1}\| + \sqrt{\|D\eta^{n+1}\|^2 + \|\zeta^{n+1}\|^2} \\ \leq &\exp\Big(2T\big(1 + 4\sum_{j=0}^{r} \sum_{\tilde{t} \in \mathrm{SENT}_{j+2}^f} \alpha(\tilde{t})\big)\Big) \big(\|\tilde{\varphi}_1\| + \sqrt{\|D\tilde{\varphi}_1\|^2 + \|\tilde{\varphi}_2\|^2}\big),\end{aligned}$$

completing the proof. □

5 Convergence of the fully discrete scheme

As is well known, convergence of the classical methods for linear partial differential equations is governed by the Lax equivalence theorem: convergence equals consistency plus stability [27]. Our methods are obviously consistent, and the stability of the fully discrete scheme for linear problems has been proved in Subsection 4.1. Therefore, the convergence of our method for linear problems can be obtained by applying the Lax equivalence theorem. However, the Lax equivalence theorem need not be valid for nonlinear problems.

In this section, we analyse the convergence of the fully discrete scheme for nonlinear problems. Subject to suitable assumptions on smoothness and spatial discretisation strategies, the original continuous system (1) or (7) can be discretised as the following,

$$\begin{cases} U''(t) + AU(t) = f\big(U(t)\big) + \delta(\Delta x), \qquad t \in [t_0, T], \\ U(t_0) = \varphi_1, \qquad U'(t_0) = \varphi_2, \end{cases} \tag{46}$$

where $U(t) = \big(u(x_0,t), u(x_1,t), \ldots, u(x_{M-1},t)\big)^\top$, A is a positive semi-definite differential matrix and $\varphi_l = \big(\varphi_l(x_0), \varphi_l(x_1), \ldots, \varphi_l(x_{M-1})\big)^\top$, $l = 1, 2$.

Let $\delta(\Delta x)$ be the truncation error produced by approximating the spatial differential operator $\mathcal{A}$ with a positive semi-definite matrix A. For example, once we replace the spatial derivative by the classical forth-order finite difference method (see, e.g. [5,34]), the truncation error $\delta(\Delta x)$ is $\|\delta(\Delta x)\| = O(\Delta x^4)$.

Applying the time integration formula (20) to (46) results in

$$\begin{cases} U(t_{n+1}) = \phi_0(V)U(t_n) + \Delta t\phi_1(V)U'(t_n) + \sum_{j=0}^{r} \Delta t^{j+2}\Big\{ I_1[\beta_j(z)] f_t^{(j)}\big(U(t_n)\big) \\ \qquad + (-1)^j I_1[\beta_j(1-z)] f_t^{(j)}\big(U(t_{n+1})\big)\Big\} + R^n, \\ U'(t_{n+1}) = -\Delta t A\phi_1(V)U(t_n) + \phi_0(V)U'(t_n) + \sum_{j=0}^{r} \Delta t^{j+1}\Big\{ I_0[\beta_j(z)] f_t^{(j)}\big(U(t_n)\big) \\ \qquad + (-1)^j I_0[\beta_j(1-z)] f_t^{(j)}\big(U(t_{n+1})\big)\Big\} + r^n, \end{cases} \tag{47}$$

where $R^n = \big(R_1^n, \ldots, R_M^n\big)^\top$ and $r^n = \big(r_1^n, \ldots, r_M^n\big)^\top$ are truncation errors,

$$\begin{aligned} R_j^n =& (-1)^{r+1}\Delta t^{2r+4} \frac{f_t^{(2r+2)}\big(u(x_j, t_n + \xi^n \Delta t)\big)}{(2r+2)!} \int_0^1 (1-z)^{r+2}\phi_1\big((1-z)^2 V\big) z^{r+1} \mathrm{d}z \\ &+ \Delta t^2 \int_0^1 (1-z)\phi_1\big((1-z)^2 V\big)\delta_j(\Delta x)\mathrm{d}z \end{aligned}$$

and

$$\begin{aligned} r_j^n =& (-1)^{r+1}\Delta t^{2r+3} \frac{f_t^{(2r+2)}\big(u(x_j, t_n + \xi^n \Delta t)\big)}{(2r+2)!} \int_0^1 (1-z)^{r+1}\phi_0\big((1-z)^2 V\big) z^{r+1} \mathrm{d}z \\ &+ \Delta t \int_0^1 \phi_0\big((1-z)^2 V\big)\delta_j(\Delta x)\mathrm{d}z \end{aligned}$$

respectively. Under suitable assumptions of smoothness, the errors R_j^n and r_j^n can be bounded,

$$|R_j^n| \leq \frac{(r+2)!(r+1)!}{(2r+2)!(2r+4)!} \max_{t_0\leq t\leq T} \max_{x\in\bar{\Omega}} |f_t^{(2r+2)}\big(u(x,t)\big)|\Delta t^{2r+4} + \frac{\Delta t^2}{2}|\delta_j(\Delta x)|, \tag{48}$$

and

$$|r_j^n| \leq \frac{\big((r+1)!\big)^2}{(2r+4)!(2r+3)!} \max_{t_0\leq t\leq T} \max_{x\in\bar{\Omega}} |f_t^{(2r+2)}\big(u(x,t)\big)|\Delta t^{2r+3} + \Delta t|\delta_j(\Delta x)|. \tag{49}$$

Disregarding the small terms R^n and r^n in (47) and letting $u_j^n \approx u(x_j,t_n)$, $\mu_j^n \approx u_t(x_j,t_n)$, we obtain the fully discrete scheme

$$\begin{cases} u^{n+1} = \phi_0(V)u^n + \Delta t\phi_1(V)\mu^n + \displaystyle\sum_{j=0}^{r} \Delta t^{j+2}\Big\{I_1[\beta_j(z)]f_t^{(j)}(u^n) \\ \qquad + (-1)^j I_1[\beta_j(1-z)]f_t^{(j)}(u^{n+1})\Big\}, \\ \mu^{n+1} = -\Delta tA\phi_1(V)u^n + \phi_0(V)\mu^n + \displaystyle\sum_{j=0}^{r} \Delta t^{j+1}\Big\{I_0[\beta_j(z)]f_t^{(j)}(u^n) \\ \qquad + (-1)^j I_0[\beta_j(1-z)]f_t^{(j)}(u^{n+1})\Big\}. \end{cases} \tag{50}$$

We consider from first principles the convergence of the fully discrete scheme (50) for nonlinear problems. To this end, we let $e_j^n = u(x_j,t_n) - u_j^n$ and $\omega_j^n = u_t(x_j,t_n) - \mu_j^n$ for $j = 1,2,\ldots,M$—in other words, $e^n = U(t_n) - u^n$ and $\omega^n = U'(t_n) - \mu^n$. Subtracting (50) from (47) and inserting exact initial conditions, we obtain a recurrence for the errors,

$$\begin{cases} e^{n+1} = \phi_0(V)e^n + \Delta t\phi_1(V)\omega^n + \displaystyle\sum_{j=0}^{r} \Delta t^{j+2}\Big\{I_1[\beta_j(z)]\big[f_t^{(j)}(U(t_n)) \\ \qquad - f_t^{(j)}(u^n)\big] + (-1)^j I_1[\beta_j(1-z)]\big[f_t^{(j)}(U(t_{n+1})) - f_t^{(j)}(u^{n+1})\big]\Big\} + R^n, \\ \omega^{n+1} = -\Delta tA\phi_1(V)e^n + \phi_0(V)\omega^n + \displaystyle\sum_{j=0}^{r} \Delta t^{j+1}\Big\{I_0[\beta_j(z)]\big[f_t^{(j)}(U(t_n)) \\ \qquad - f_t^{(j)}(u^n)\big] + (-1)^j I_0[\beta_j(1-z)]\big[f_t^{(j)}(U(t_{n+1})) - f_t^{(j)}(u^{n+1})\big]\Big\} + r^n, \end{cases} \tag{51}$$

with the initial conditions $e^0 = 0$, $\omega^0 = 0$.

In order to analyse convergence we use the Gronwall inequality.

Lemma 7 *(see, e.g. [42]) Let λ be positive, a_k, b_k, $k \in \mathbb{Z}_+$, be nonnegative and assume further that*

$$a_k \leq (1+\lambda\Delta t)a_{k-1} + \Delta t b_k, \qquad k \in \mathbb{Z}_+.$$

Then

$$a_k \leq \exp(\lambda k\Delta t)\Big(a_0 + \Delta t\sum_{m=1}^{k} b_m\Big), \qquad k \in \mathbb{N}.$$

Theorem 6 *Subject to Assumptions 1 and 2, and supposing that $u(x,t)$ satisfies suitable smoothness assumptions, if the time stepsize Δt satisfies*

$$\Delta t^2 L\big(R,\rho(A)\big) \le 1 \qquad \text{and} \qquad \Delta t \sum_{j=0}^{r} \sum_{\tilde{t}\in \mathrm{SENT}_{j+2}^{f}} \alpha(\tilde{t}) \le \frac{1}{4},$$

then there exists a constant C such that

$$\|e^n\| \le CT \exp\Big(2T\big(1+4\sum_{j=0}^{r}\sum_{\tilde{t}\in \mathrm{SENT}_{j+2}^{f}} \alpha(\tilde{t})\Big)\big(\Delta t^{2r+2} + \|\delta(\Delta x)\|\big),$$

$$\|\omega^n\| \le CT \exp\Big(2T\big(1+4\sum_{j=0}^{r}\sum_{\tilde{t}\in \mathrm{SENT}_{j+2}^{f}} \alpha(\tilde{t})\Big)\big(\Delta t^{2r+2} + \|\delta(\Delta x)\|\big).$$

Proof We rewrite the system (51) in a compact form,

$$\begin{aligned}\begin{bmatrix} De^{n+1} \\ \omega^{n+1}\end{bmatrix} &= \Omega \begin{bmatrix} De^{n} \\ \omega^{n}\end{bmatrix} + \sum_{j=0}^{r} \Delta t^{j+1}\int_0^1 \Omega_j(z)\mathrm{d}z \begin{bmatrix} 0 \\ f_t^{(j)}\big(U(t_n)\big) - f_t^{(j)}(u^n)\end{bmatrix} \\ &+ \sum_{j=0}^{r}(-1)^j \Delta t^{j+1}\int_0^1 \Omega_j(1-z)\mathrm{d}z \begin{bmatrix} 0 \\ f_t^{(j)}\big(U(t_{n+1})\big) - f_t^{(j)}(u^{n+1})\end{bmatrix} + \begin{bmatrix} DR^{n} \\ r^{n}\end{bmatrix},\end{aligned} \tag{52}$$

where Ω and $\Omega(z)$ were defined in (36) and (37), respectively.

Taking the l_2 norm on both sides of the first formula in (51) and (52) and summing up the outcome, we obtain

$$\begin{aligned}&\|e^{n+1}\| + \sqrt{\|De^{n+1}\|^2 + \|\omega^{n+1}\|^2} \le \|e^n\| + \Delta t\|\omega^n\| + \sqrt{\|De^{n}\|^2 + \|\omega^{n}\|^2} \\ &+ \Delta t(1+\Delta t)\sum_{j=0}^{r}\Delta t^j\Big[\|f_t^{(j)}\big(U(t_n)\big) - f_t^{(j)}(u^n)\| + \|f_t^{(j)}\big(U(t_{n+1})\big) \\ &- f_t^{(j)}(u^{n+1})\|\Big] + \|R^n\| + \sqrt{\|DR^n\|^2 + \|r^n\|^2}.\end{aligned} \tag{53}$$

On the other hand, inserting (42) into the right-hand side of (53) and employing Assumption 2 leads to

$$\begin{aligned}&\|e^{n+1}\| + \sqrt{\|De^{n+1}\|^2 + \|\omega^{n+1}\|^2} \le \|e^n\| + \Delta t\|\omega^n\| + \sqrt{\|De^{n}\|^2 + \|\omega^{n}\|^2} \\ &+ \Delta t(1+\Delta t)\sum_{j=0}^{r}\sum_{\tilde{t}\in \mathrm{SENT}_{j+2}^{f}} \alpha(\tilde{t})\Delta t^j L\big(R,\rho(A)^{\lfloor \frac{j}{2}\rfloor}\big)\Big(\|e^n\| + \|\omega^n\| + \|e^{n+1}\| \\ &+ \|\omega^{n+1}\|\Big) + \|R^n\| + \sqrt{\|DR^n\|^2 + \|r^n\|^2}.\end{aligned} \tag{54}$$

Since $\Delta t^2 L\big(R,\rho(A)\big) \le 1$, inequality (54) results in

$$\begin{aligned}&\|e^{n+1}\| + \sqrt{\|De^{n+1}\|^2 + \|\omega^{n+1}\|^2} \\ &\le \left\{1 + \frac{\Delta t\big[1 + 4\sum_{j=0}^{r}\sum_{\tilde{t}\in \mathrm{SENT}_{j+2}^{f}} \alpha(\tilde{t})\big]}{1 - 2\Delta t\sum_{j=0}^{r}\sum_{\tilde{t}\in \mathrm{SENT}_{j+2}^{f}} \alpha(\tilde{t})}\right\}\big(\|e^n\| + \sqrt{\|De^{n}\|^2 + \|\omega^{n}\|^2}\big) \\ &+ \frac{1}{1 - 2\Delta t\sum_{j=0}^{r}\sum_{\tilde{t}\in \mathrm{SENT}_{j+2}^{f}} \alpha(\tilde{t})}\big(\|R^n\| + \sqrt{\|DR^n\|^2 + \|r^n\|^2}\big).\end{aligned}$$

Once the time stepsize Δt also satisfies $\Delta t \sum_{j=0}^{r} \sum_{\tilde{t}\in \mathrm{SENT}_{j+2}^{f}} \alpha(\tilde{t}) \leq \frac{1}{4}$, we obtain

$$\begin{aligned} \|e^{n+1}\| + \sqrt{\|De^{n+1}\|^2 + \|\omega^{n+1}\|^2} &\leq 1 + 2\Delta t\big[1 + 4\sum_{j=0}^{r} \sum_{\tilde{t}\in \mathrm{SENT}_{j+2}^{f}} \alpha(\tilde{t})\big] \\ \big(\|e^{n}\| + \sqrt{\|De^{n}\|^2 + \|\omega^{n}\|^2}\big) &+ 2\big(\|R^n\| + \sqrt{\|DR^n\|^2 + \|r^n\|^2}\big). \end{aligned} \tag{55}$$

Note that truncation errors R_j^n and r_j^n satisfy (48) and (49), respectively. Thus, there exists a constant C such that

$$\|R^n\| + \sqrt{\|DR^n\|^2 + \|r^n\|^2} \leq C\Delta t\Big(\Delta t^{2r+2} + \|\delta(\Delta x)\|\Big).$$

Applying the Gronwall inequality (Lemma 7) to (55) results in

$$\begin{aligned} \|e^{n}\| + \sqrt{\|De^{n}\|^2 + \|\omega^{n}\|^2} &\leq \exp\Big(2n\Delta t\big(1 + 4\sum_{j=0}^{r} \sum_{\tilde{t}\in \mathrm{SENT}_{j+2}^{f}} \alpha(\tilde{t})\Big) \\ &\times \Big[\|e^{0}\| + \sqrt{\|De^{0}\|^2 + \|\omega^{0}\|^2} + Cn\Delta t\big(\Delta t^{2r+2} + \|\delta(\Delta x)\|\big)\Big]. \end{aligned}$$

and the theorem follows. □

6 Spatial discretisation

The symmetric and arbitrarily high order time-stepping formulæ (20) have been presented in operatorial terms in the infinite-dimensional Hilbert space $L^2(\boldsymbol{\Omega})$. To render them into proper numerical algorithms, we must replace the differential operator $\mathcal{A}$ with an suitable differential matrix A. Recalling our stability and convergence analysis, we approximate the differential operator $\mathcal{A}$ by a positive semi-definite matrix A. Fortunately, there exists a great body of research investigating the replacement of spatial derivatives of nonlinear system (1) with periodic boundary conditions (2), and it is easy to find positive semi-definite differentiation matrices in this setting.

In this section, we mainly consider the following spatial discretisations.

1. *Symmetric finite difference (SFD)* (see, e.g. [5])

Finite difference methods are obtained when approximating a function by local polynomial interpolation. Its derivatives are then approximated by differentiating this local polynomial, where 'local' refers to the use of nearby grid points to approximate the function or its derivative at a given point. In general, a finite difference approximation is of moderate order. As an example, we approximate the operator $\mathcal{A}$ by the differential matrix

$$A_{\mathrm{sfd}} = \frac{a^2}{12\Delta x^2} \begin{bmatrix} 30 & -16 & 1 & & & 1 & -16 \\ -16 & 30 & -16 & 1 & & & 1 \\ 1 & -16 & 30 & -16 & 1 & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & 1 & -16 & 30 & -16 & 1 \\ 1 & & & 1 & -16 & 30 & -16 \\ -16 & 1 & & & 1 & -16 & 30 \end{bmatrix}_{M\times M}.$$

The approximation is of order four and the circulant A_{sfd} is clearly positive semi-definite.

2. *Fourier spectral collocation (FSC)* (see, e.g. [22, 40])

Spectral methods are global in character and the computation at any given point depends not only on the information at neighbouring points, but on the entire domain. While the topic of spectral methods is very wide, we focus our attention on spectral collocation. One way of introducing it is as a limit of 'wrapped around' symmetric finite differences of increasing order [22]. Alternatively, the solution is interpolated on an equidistant grid by trigonometric polynomials. The entries of the second-derivative Fourier differentiation matrix $A_{\text{fsc}} = (a_{kj})_{M\times M}$ are given by

$$a_{kj} = \begin{cases} \dfrac{(-1)^{k+j}}{2} a^2 \sin^{-2}\Big(\dfrac{(k-j)\pi}{M}\Big), & k \neq j, \\ a^2\big(\dfrac{M^2}{12} + \dfrac{1}{6}\big), & k = j. \end{cases} \tag{56}$$

The main appeal of spectral methods is that they exhibit spectral convergence to $\mathcal{A}$: the error decays for C^∞ functions faster than $O(M^{-\alpha})$ $\forall \alpha > 0$ for sufficiently large M. Moreover, the differential matrix A_{fsc} is positive semi-definite.

Fig. 1 displays spectral radii for the differential matrices A_{sfd} and A_{fsc}. On the left we show the spectral radius of A_{sfd} and A_{fsc} as a function of M. On the right, letting $\Delta t = \frac{2\pi}{M}, M = 10i$ for $i = 1, 2, \ldots, 40$, we plot $\Delta t^2 \rho(A)$—it is compelling that this quantity is constant, i.e. that $\rho(A) = O(\Delta t^{-2})$.

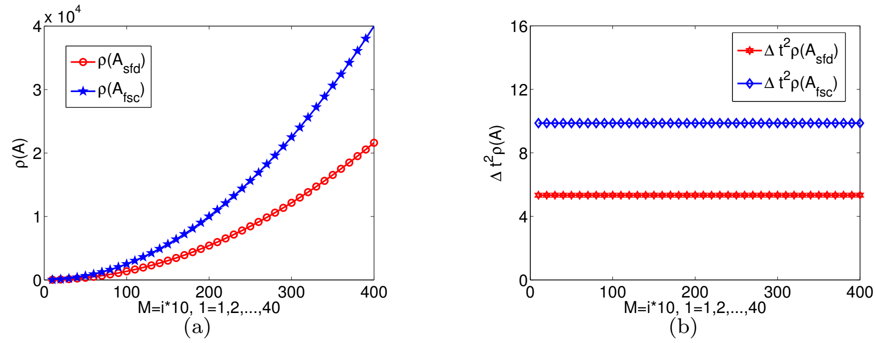


Fig. 1 Plots of of $\rho(A)$ and $\Delta t^2 \rho(A)$ for the differential matrices A_{sfd} and A_{fsc} for $M = 10i, i = 1, 2, \ldots, 40$.

We have already noted that energy conservation (3) is an important property of nonlinear Klein–Gordon equations (1–2). Approximating the operator $\mathcal{A}$ by a positive semi-definite differential matrix A, there is a discrete energy conservation law,

$$\tilde{E}(t) = \frac{\Delta x}{2}\|u'(t)\| + \frac{\Delta x}{2}\|Du(t)\|^2 + \Delta x \sum_{j=1}^{M} V\big(u_j(t)\big) \equiv \tilde{E}(t_0), \tag{57}$$

where the norm $\|\cdot\|$ is the standard vector 2-norm and $\Delta x = 2\pi/M$ is the spatial grid size. This can be regarded as an approximate energy (a semi-discrete energy) of the original continuous system. Therefore, in our numerical experiments we will also test the effectiveness of our methods to preserve (57).

7 Waveform relaxation and its convergence

In previous sections we have derived and analysed a fully discrete scheme for (1–2) and presented its properties. However, the scheme (50) is implicit and must be solved by iteration. In this section we introduce a *waveform relaxation method* as a suitable iterative scheme. Cf. [28,31,35,45,46] for waveform relaxation in different contexts.

Based on the notation in (42), we first rewrite the fully discrete scheme (50),

$$\left\{\begin{aligned} u^{n+1} =& \phi_0(V)u^n + \Delta t\phi_1(V)\mu^n + \sum_{j=0}^{r}\sum_{\tilde{t}\in\mathrm{SENT}^f_{j+2}} \alpha(\tilde{t})\Delta t^{j+2} \\ &\times \Big[I_1[\beta_j(z)]\mathcal{F}(\tilde{t})(u^n,\mu^n) + (-1)^j I_1[\beta_j(1-z)]\mathcal{F}(\tilde{t})(u^{n+1},\mu^{n+1})\Big], \\ \mu^{n+1} =& -\Delta t A\phi_1(V)u^n + \phi_0(V)\mu^n + \sum_{j=0}^{r}\sum_{\tilde{t}\in\mathrm{SENT}^f_{j+2}} \alpha(\tilde{t})\Delta t^{j+1} \\ &\times \Big[I_1[\beta_j(z)]\mathcal{F}(\tilde{t})(u^n,\mu^n) + (-1)^j I_1[\beta_j(1-z)]\mathcal{F}(\tilde{t})(u^{n+1},\mu^{n+1})\Big], \end{aligned}\right.$$

where $I_1[\beta_j(z)], I_2[\beta_j(z)], I_1[\beta_j(1-z)]$, and $I_2[\beta_j(1-z)]$ have been defined in (16–19). We launch waveform relaxation by setting

$$\left\{\begin{aligned} u^{n+1}_{[0]} &= \phi_0(V)u^n + \Delta t\phi_1(V)\mu^n, \\ \mu^{n+1}_{[0]} &= -\Delta t A\phi_1(V)u^n + \phi_0(V)\mu^n, \end{aligned}\right. \tag{58}$$

and subsequently iterate

$$\left\{\begin{aligned} u^{n+1}_{[m+1]} =& u^{n+1}_{[0]} + \sum_{j=0}^{r}\sum_{\tilde{t}\in\mathrm{SENT}^f_{j+2}} \alpha(\tilde{t})\Delta t^{j+2}\left\{I_1[\beta_j(z)]\mathcal{F}(\tilde{t})(u^n,\mu^n\right. \\ &\left. + (-1)^j I_1[\beta_j(1-z)]\mathcal{F}(\tilde{t})(u^{n+1}_{[m]},\mu^{n+1}_{[m]})\right\}, \\ \mu^{n+1}_{[m+1]} =& \mu^{n+1}_{[0]} + \sum_{j=0}^{r}\sum_{\tilde{t}\in\mathrm{SENT}^f_{j+2}} \alpha(\tilde{t})\Delta t^{j+1}\left\{I_1[\beta_j(z)]\mathcal{F}(\tilde{t})(u^n,\mu^n)\right. \\ &\left. +(-1)^j I_1[\beta_j(1-z)]\mathcal{F}(\tilde{t})(u^{n+1}_{[m]},\mu^{n+1}_{[m]})\right\} \end{aligned}\right. \tag{59}$$

for $m \in \mathbb{Z}_+$.

We next analyse the convergence of the algorithm (58–59).

Theorem 7 *Let f satisfy Assumptions 1 and 2. Subject to the conditions*

$$\Delta t^2 L(R,\rho(A)) \leq 1 \qquad \textit{and} \qquad \Delta t(1+\Delta t)\sum_{j=0}^{r}\sum_{\tilde{t}\in \mathrm{SENT}^f_{j+2}} \alpha(\tilde{t}) < 1,$$

the iterative procedure (58–59) is convergent.

Proof Subject to Assumptions 2 and (59), it is true that

$$\begin{aligned}&\|u^{n+1}_{[m+1]} - u^{n+1}_{[m]}\|\\ &\leq \Delta t^2 \sum_{j=0}^{r}\sum_{\tilde{t}\in \mathrm{SENT}^f_{j+2}} \alpha(\tilde{t})\Delta t^j L(R,\rho(A)^{\lfloor \frac{j}{2}\rfloor})\Big(\|u^{n+1}_{[m]} - u^{n+1}_{[m-1]}\| + \|\mu^{n+1}_{[m]} - \mu^{n+1}_{[m-1]}\|\Big),\\ &\|\mu^{n+1}_{[m+1]} - \mu^{n+1}_{[m]}\|\\ &\leq \Delta t \sum_{j=0}^{r}\sum_{\tilde{t}\in \mathrm{SENT}^f_{j+2}} \alpha(\tilde{t})\Delta t^j L(R,\rho(A)^{\lfloor \frac{j}{2}\rfloor})\Big(\|u^{n+1}_{[m]} - u^{n+1}_{[m-1]}\| + \|\mu^{n+1}_{[m]} - \mu^{n+1}_{[m-1]}\|\Big).\end{aligned}$$

Summing up the above expression and noting that $\Delta t^2 L(R,\rho(A)) \leq 1$ results in

$$\begin{aligned}&\|u^{n+1}_{[m+1]} - u^{n+1}_{[m]}\| + \|\mu^{n+1}_{[m+1]} - \mu^{n+1}_{[m]}\|\\ &\leq \Delta t(1+\Delta t)\sum_{j=0}^{r}\sum_{\tilde{t}\in \mathrm{SENT}^f_{j+2}} \alpha(\tilde{t})\Big(\|u^{n+1}_{[m]} - u^{n+1}_{[m-1]}\| + \|\mu^{n+1}_{[m]} - \mu^{n+1}_{[m-1]}\|\Big).\end{aligned}$$

An inductive argument yields

$$\begin{aligned}&\|u^{n+1}_{[m+1]} - u^{n+1}_{[m]}\| + \|\mu^{n+1}_{[m+1]} - \mu^{n+1}_{[m]}\|\\ &\leq \left[\Delta t(1+\Delta t)\sum_{j=0}^{r}\sum_{\tilde{t}\in \mathrm{SENT}^f_{j+2}} \alpha(\tilde{t})\right]^m \Big(\|u^{n+1}_{[1]} - u^{n+1}_{[0]}\| + \|\mu^{n+1}_{[1]} - \mu^{n+1}_{[0]}\|\Big).\end{aligned}$$

The condition $\Delta t(1+\Delta t)\sum_{j=0}^{r}\sum_{\tilde{t}\in \mathrm{SENT}^f_{j+2}} \alpha(\tilde{t}) < 1$ leads to

$$\lim_{m\to+\infty}\big(\|u^{n+1}_{[m+1]} - u^{n+1}_{[m]}\| + \|\mu^{n+1}_{[m+1]} - \mu^{n+1}_{[m]}\|\big) = 0. \tag{60}$$

and the iterative procedure (58–59) is convergent. □

8 Numerical experiments

In this section, we derive two practical time integration formulæ and use them to illustrate the solution of two nonlinear wave equations.

As the first example of a symmetric time-stepping integrator for (1–2), we take $r = 1$ in (12–13), and this results in

$$\beta_0(z) = (1-z)^2(1+2z), \quad \beta_1(z) = z(1-z)^2 \tag{61}$$

–the corresponding time integration formula is determined by (61) and (16–19) and denoted by Brik1.

As the second example, letting $r = 2$ in (12–13), we have

$$\beta_0(z) = (1-z)^3(1+3z+6z^2), \quad \beta_1(z) = z(1-z)^3(1+3z), \quad \beta_2(z) = \frac{1}{2}z^2(1-z)^3, \tag{62}$$

and denote the corresponding time integration formula determined by (62) and (16–19) by Brik2.

For comparison we briefly describe a number of standard finite difference schemes and the method-of-lines schemes for the nonlinear Klein–Gordon equation (see, e.g. [4,16,42]), which we use with very small steps as our reference solution.

1. Standard finite difference schemes

Let u_j^n be the approximation of $u(x_j, t_n)$, $j = 0, 1, \dots, M, n = 0, 1, \dots, N$, and introduce standard central difference operators

$$\delta_t^2 u_j^n = \frac{u_j^{n+1} - 2u_j^n + u_j^{n-1}}{\Delta t^2} \qquad \text{and} \qquad \delta_x^2 u_j^n = \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta x^2}.$$

We consider three frequently used *finite difference schemes* to discretise (1–2):

- A explicit finite difference scheme Expt-FD
$$\delta_t^2 u_j^n - a^2 \delta_x^2 u_j^n = f(u_j^n);$$
- Semi-implicit finite difference scheme Simpt-FD
$$\delta_t^2 u_j^n - \frac{a^2}{2}\big(\delta_x^2 u_j^{n+1} + \delta_x^2 u_j^{n-1}\big) = f(u_j^n);$$
- Compact finite difference scheme Compt-FD
$$\Big(I + \frac{\Delta x^2}{12}\delta_x^2\Big)\delta_t^2 u_j^n - \frac{a^2}{2}\big(\delta_x^2 u_j^{n+1} + \delta_x^2 u_j^{n-1}\big) = \Big(I + \frac{\Delta x^2}{12}\delta_x^2\Big) f(u_j^n).$$

2. Method-of-lines schemes

Method-of-lines approximations for (1–2) separate between two stages, first space and then time discretisation. We approximate the spatial differential operator $\mathcal{A}$ to obtain a semi-discrete scheme of the form $u''(t) + Au(t) = f\big(u(t)\big)$, where A is a symmetric and positive semi-definite matrix. Subsequently, we use an ODE solver to deal with the semi-discrete scheme. The time integrators we select for comparison are

- Gauss2s4: the two-stage Gauss method of order four from [21];
- RKN3s4: the three-stage Runge–Kutta–Nyström method of order four from [21];
- IRKN2s4: the two-stage implicit symplectic Runge–Kutta–Nyström method of order four derived in [43];
- ERKN3s4: the three-stage extended Runge–Kutta–Nyström method of order four presented in [47];
- SV: classical Strömer–Verlet formula [21];
- ISV: improved Strömer–Verlet formula given in [48].

For the time integrators Brik1 and Brik2 derived in this paper we use the tolerance 10^{-15} and choose $m = 2$ in the waveform relaxation algorithm (58–59), which means just one iteration at each step. Therefore, these two methods can be implemented at lower cost. It should be noted that when the error of a method under consideration is very large for some Δt, we do not plot the corresponding points in efficiency curves.

Problem 1 We consider the nonlinear Klein–Gordon equation

$$\frac{\partial^2 u(x,t)}{\partial t^2} - a^2 \frac{\partial^2 u(x,t)}{\partial x^2} + au(x,t) - bu^3(x,t) = 0,$$

in the region $(x,t) \in [-10,10] \times [0,T]$ with the initial conditions

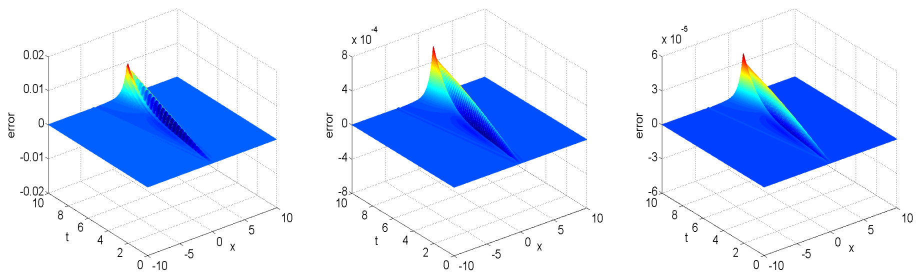
$$u(x,0) = \sqrt{\frac{2a}{b}}\operatorname{sech}(\lambda x), \qquad u_t(x,0) = c\lambda\sqrt{\frac{2a}{b}}\operatorname{sech}(\lambda x)\tanh(\lambda x),$$

where $\lambda = \sqrt{a/(a^2-c^2)}$ and $a, b, a^2 - c^2 > 0$. The exact solution of Problem 1 is given by

$$u(x,t) = \sqrt{\frac{2a}{b}}\operatorname{sech}(\lambda(x-ct)).$$

The real parameter $\sqrt{2a/b}$ represents the amplitude of a soliton which travels with velocity c. The potential function is $V(u) = au^2/2 - bu^4/4$ [34]. We use the parameters $a = 0.3$, $b = 1$ and $c = 0.25$ which are similar to those in [34].

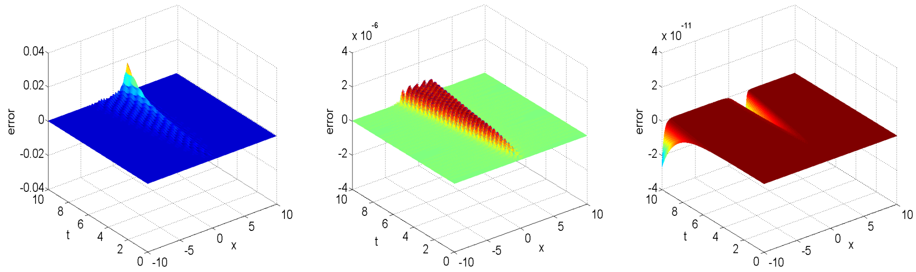
In Figs 2 and 3, we integrate the Problem 1 on the region $(x,t) \in [-10,10] \times [0,10]$ using the time integrator BRIK2, coupled with the fourth-order symmetric finite difference (SFD) and Fourier spectral collocation (FSC). The error graphs are shown there with the stepsize $\Delta t = 0.01$ and several values of M. Numerical results demonstrate that the accuracy of the spatial discretisation is consistent with our theory. It is evident that Fourier spectral collocation method is superior..



(a) M=200 (b) M=400 (c) M=800

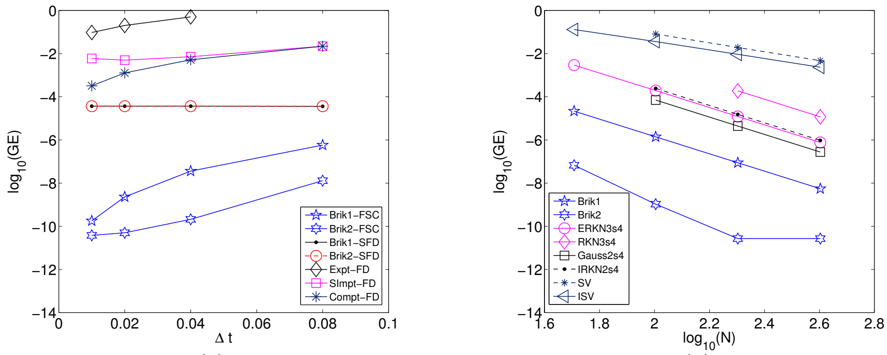
Fig. 2 The errors for Problem 1 obtained by combining the time integrator Brik2 with the fourth-order finite difference spatial discretisation for $\Delta t = 0.01$ with $M = 200, 400$ and 800.

To compare our methods with classical finite difference and method-of-lines schemes, we integrate the problem in the region $(x,t) \in [-10,10] \times [0,10]$ with different time stepsizes Δt and the numbers of the spatial nodal values M. The



(a) M=100 (b) M=200 (c) M=400

Fig. 3 The errors for Problem 1 obtained by combining the time integrator Brik2 with Fourier spectral collocation method for $\varDelta t = 0.01$ with $M = 200, 400$ and 800.



(a) (b)

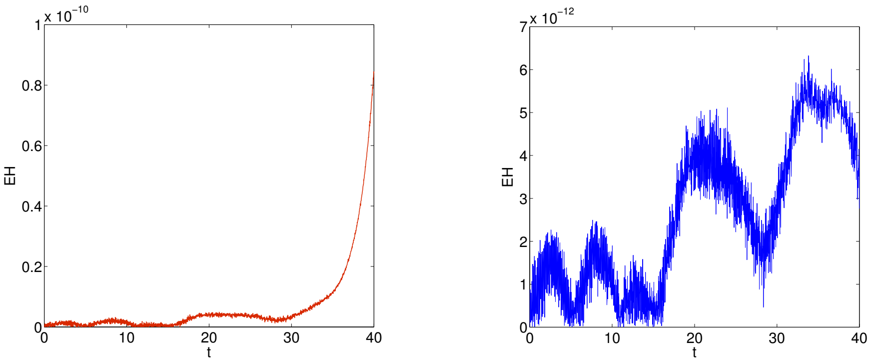
Fig. 4 The efficiency curves for Problem 1: (a) comparison with standard finite difference schemes, (b) comparison with method-of-lines schemes.

numerical results are shown in Fig. 4. We compare our methods with the standard finite difference schemes with stepsizes $\varDelta t = 0.01 \times 2^{3-j}$ for $j = 0, 1, 2, 3$ and $M = 1000$ for the finite difference schemes Expt-FD, SImpt-FD and Compt-FD, $M = 800$ for Brik1-SFD and Brik2-SFD and $M = 400$ for Brik1-FSC and Brik2-FSC. Global error $\mathrm{GE} = \|u(t_n) - u^n\|_\infty$ are plotted to logarithmic scale in Fig. 4(a).

In comparison with the method-of-lines schemes, we discretise the spatial derivative by Fourier spectral collocation method with fixed $M = 400$ and integrate the Klein–Gordon equation with $\varDelta t = 0.2/2^j$ for $j = 0, 1, 2, 3$. The efficiency curves (accuracy versus the computational cost measured by the number of function evaluations required by each method) are shown in Fig. 4(b).

In conclusion, Fig. 4 demonstrates that Brik1 and Brik2, combined with Fourier spectral collocation, enjoy much better accuracy and are more practical than main methods in the literature.

Fig. 5 displays the error in the semi-discrete energy conservation law, $\mathrm{EH} = |\tilde{E}(t) - \tilde{E}(t_0)|$, as a function of the time-step. It can be observed there that the error of Brik1 is $\approx 10^{-10}$, while that of Brik2 is $\approx 10^{-12}$.



(a) Brik1 (b) Brik2

Fig. 5 Discrete energy conservation by Brik1 and Brik2 with the spatial discretisation by Fourier spectral collocation with $M = 800$ up to $T = 40$, using $\varDelta t = 0.02$.

Problem 2 We consider the sine-Gordon equation

$$\frac{\partial^2 u}{\partial t^2}(x,t) - \frac{\partial^2 u}{\partial x^2}(x,t) + \sin(u(x,t)) = 0$$

in the region $-20 \leq x \leq 20$, $0 \leq t \leq T$, subject to the initial conditions

$$u(x,0) = 0, \qquad u_t(x,0) = 4\text{sech}(x/\sqrt{1+c^2})/\sqrt{1+c^2},$$

where $\kappa = 1/\sqrt{1+c^2}$. The exact solution is

$$u(x,t) = 4\arctan\left(c^{-1}\sin(ct/\sqrt{1+c^2})\text{sech}(x/\sqrt{1+c^2})\right).$$

This is the well-known *breather solution* of the sine-Gordon equation and represents a pulse-type structure of a soliton. The parameter c is the velocity and we choose $c = 0.5$. The potential function is $V(u) = 1 - \cos(u)$. Problem 2 is integrated by Brik2, coupled either with the fourth-order symmetric finite difference SFD or Fourier spectral collocation FSC. The error graphs are shown in Figs 6 and 7 with $\varDelta t = 0.01$ and several values of M. They demonstrate how the accuracy of the spatial discretisation varies with M, and also indicate that FSC is decisively superior to SFD.

Efficiency curves are displayed in Fig. 8. To compare our methods with a standard finite difference scheme, in Fig. 8 (a) we integrate the problem $\varDelta t = 0.04, 0.03, 0.02, 0.01$. We use $M = 1000$ for the finite difference scheme Expt-FD, SImpt-FD and Compt-FD, $M = 400$ for the Brik1-SFD and Brik2-SFD and $M = 200$ for the Brik1-FSC and Brik2-FSC.

In Fig. 8(b) we compare our methods with method-of-lines schemes The problem is integrated over the time interval $[0, 40]$ with fixed $M = 200$ and time stepsizes $\varDelta t = 0.4/2^j$ for $j = 0, 1, 2, 3$. It can be observed that the time integrators Brik1 and Brik2, coupled with the Fourier spectral collocation, are again superior.

Numerical results in Fig. 9 represent the error of the semi-discrete energy conservation law. It can be seen that the error is bounded. The errors obtained by Brik1 and Brik2 reach the magnitudes of 10^{-7} and $\approx 10^{-10}$ respectively.

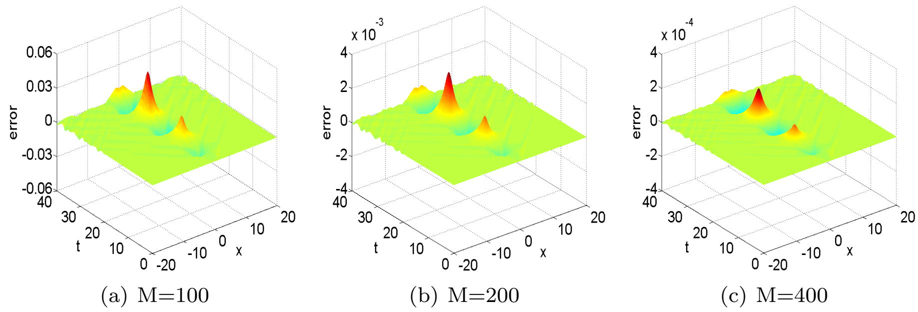


Fig. 6 The error for the sine-Gorden equation, blending the time integrator Brik2 with fourth-order finite difference spatial discretisation for $\Delta t = 0.01$ and $M = 100, 200, 400$.

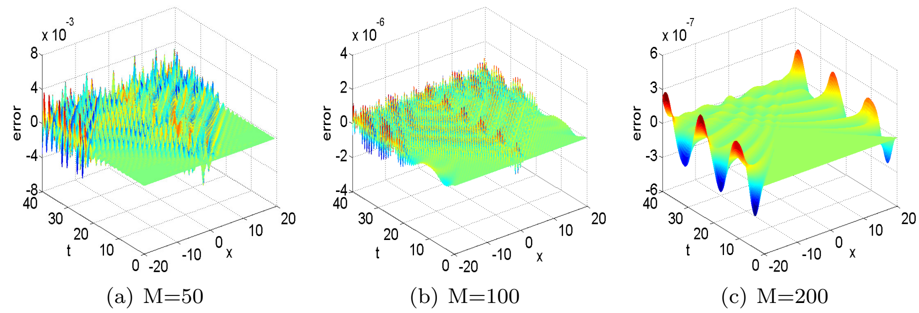
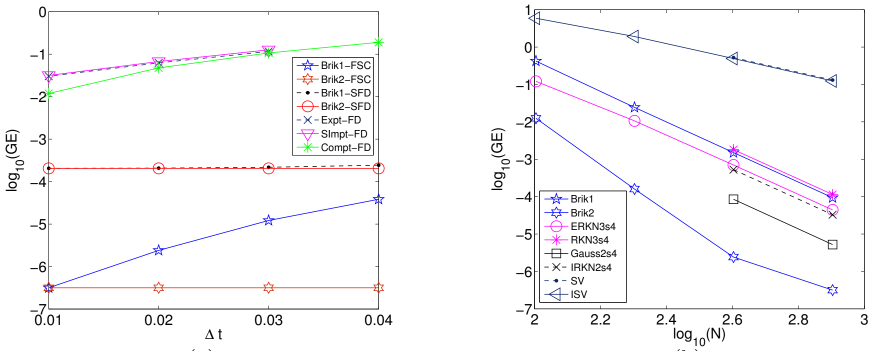


Fig. 7 The errors blending the time integrator Brik2 with Fourier spectral method for $\Delta t = 0.01$ and $M = 50, 100, 200$.

9 Conclusions and a discussion

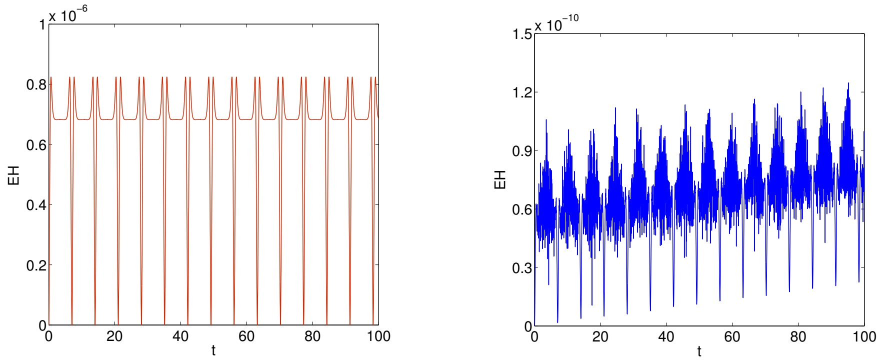
In this paper we have derived and analysed a novel class of time-stepping methods for the nonlinear Klein–Gordon equation (1–2). These new methods are based on the operator-variation-of-constants formula (8), introduced on the Hilbert space $L^2(\mathbf{\Omega})$. It is an implicit method. A class of time integration formulæ (20) has been designed by applying a two-point Hermite interpolation to nonlinear integrals that feature in the operator-variation-of-constants formula. It has been shown that such formulæ can have arbitrarily high order and be symmetric. We have also discussed the choice of the positive semi-definite differential matrix to approximate the spatial differential operator. Sstability and convergence for the fully discrete scheme have been proved in both linear and nonlinear settings. The fully discrete scheme is implicit and and we have solved it with the waveform relaxation algorithm (58–59) and analysed its convergence. Numerical experiments carried out in this paper clearly demonstrate that the new methods are decisively superior to both standard finite difference and method-of-lines schemes.

The methodology presented in this paper can be extended to a range of other nonlinear wave equations. Some of the more immediate possibilities of extensions of our work are



(a) (b)

Fig. 8 Efficiency curves for Problem 2: (a) comparison with standard finite difference schemes, (b) comparison with method-of-lines schemes.



(a) Brik1 (b) Brik2

Fig. 9 Energy conservation by Brik1 and Brik2, both blended with FSC, using $M = 200$, $\Delta t = 0.02$ and $T = 100$.

1. *High dimensional problems.* Although the equation (1) is univariate, our method can be extended to Klein–Gordon equations in a moderate number d of space dimensions,

$$u_{tt} - a^2 \Delta u = f(u), \qquad t_0 \le t \le T, \quad \mathbf{x} \in [-\pi, \pi]^d, \tag{63}$$

where $u = u(\mathbf{x}, t)$ and $\Delta = \sum_{i=1}^{d} \frac{\partial^2}{\partial x_i^2}$, with periodic boundary conditions. A large dimension d requires combining our time integration formula (20) with other spatial approximate techniques, such as *sparse grids* [10] or *discrete FFT* [8,9].

2. *Neumann and Dirichlet boundary problems.* In this paper we only consider the problems (1) equipped with periodic boundary conditions (2). Our approach can be extended to problems with Neumann and Dirichlet boundary conditions in the domain $\mathbf{\Omega} = [0, \pi]^d$. To this end we might discretise space with *discrete Fast Sine Transformation* for Dirichlet boundary conditions and *discrete Fast Cosine Transformation* for the Neumann boundary case. Such transforms have been

heavily studied in this context [36]. We expect to report related new work in the near future.

3. Our approach also can be directly applied to the computation of the *the damped nonlinear Klein–Gordon equation*

$$\begin{cases} u_{tt} + \alpha(x)u_t - \beta\Delta u + u + f'(u) = 0, & (x,t) \in \mathbf{\Omega} \times [t_0, +\infty), \\ u(x,t_0) = \varphi_1(x),\ u_t(x,t_0) = \varphi_2(x), & x \in \bar{\mathbf{\Omega}}, \end{cases} \tag{64}$$

where $\mathbf{\Omega}$ is a C^1 domain in $\mathbb{R}^d$, β represents the amplitude of the diffusion and the damper $\alpha : \mathbf{\Omega} \to [0,\infty)$ is effective uniformly about the spatial infinity,

$$\alpha(x) \geq 0, \qquad \alpha \in L^\infty(\mathbf{\Omega}), \qquad \liminf_{|x|\to\infty} \alpha(x) > 0.$$

The damper $\alpha(x)$ need satisfy appropriate conditions which guarantee that the total energy defined by

$$E(t) = \int_{\mathbf{\Omega}} \Big[|u_t|^2 + |\nabla u|^2 + |u|^2 + 2f(u)\Big]\mathrm{d}x$$

decays uniformly.

Acknowledgements The first author Changying Liu is sincerely thankful to Numerical Analysis Group in University of Cambridge since the work was partly done when he was studying at this group as a visiting Ph.D. student in 2015.

References

1. Ablowitz, M.J., Kruskal, M.D., Ladik, J.F.: Solitary wave collisions. *SIAM J. Appl. Math.* **36**, 428–437 (1979).
2. Abramowitz, M., Stegun, I.: *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*. Dover publications (1964).
3. Bader, P., Iserles, A., Kropielnicka, K., Singh, P.: Effective approximation for the semiclassical Schrödinger equation, *Found. Comput. Math.* **14**, 689–720 (2014).
4. Bao, W.Z., Dong, X.C.: Analysis and comparison of numerical methods for the Klein–Gordon equation in the nonrelativistic limit regime. *Numer. Math.* **120**, 189–229 (2012).
5. Bank, R., Graham, R.L., Stoer, J., Varga, R., Yserentant, H.: *High Order Difference Methods for Time Dependent PDEs,* Springer-Verlag, Berlin Heidelberg (2008).
6. Bátkai, A., Farkas, B., Csomós, P., Ostermann, A.: Operator semigroups for numerical analysis, 15th Internet Seminar. (2011).
7. Brenner, P., van Wahl, W.: Global classical solutions of nonlinear wave equations. *Math. Z.* **176**, 87–121 (1981).
8. Briggs, W.L., Henson, V.E.: *The DFT: An Owner's Manual for the Discrete Fourier Transform.* SIAM, Philadelphia (2000).
9. Bueno-Orovio, A., Pérez-García, V.M., Fenton, F.H.: Spectral methods for partial differential equations in irregular domains: the spectral smoothed boundary method. *SIAM J. Sci. Comput.* **28**, 886–900 (2006).
10. Bungartz, H.-J., Griebel, M.: Sparse grids, *Acta Numerica* **13**, 147–269 (2004).
11. Cao, W., Guo, B.: Fourier collocation method for solving nonlinear Klein–Gordon equation. *J. Comput. Phys.* **108**, 296–305 (1993).
12. Cohen, D., Hairer, E., Lubich, C.: Conservation of energy, momentum and actions in numerical discretizations of non-linear wave equations. *Numer. Math.* **110**, 113–143 (2008).
13. Cox, S., Matthews, P.: Exponential time differencing for stiff systems, *J. Comput. Phys.* **176**, 430–455 (2002).

14. Dodd, R.K., Eilbeck, I.C., Gibbon, J.D., Morris, H.C.: *Solitons and Nonlinear Wave Equations.* Academic London (1982).
15. Drazin, P.J., Johnson, R.S.: *Solitons: An Introduction.* Cambridge University Press, Cambridge UK (1989).
16. Duncan, D.B.: Symplectic finite difference approximations of the nonlinear Klein–Gordon equation, *SIAM J. Numer. Anal.* **34**, 1742–1760 (1997).
17. Dyn, N.: On the existence of Hermite–Birkhoff quadrature formulas of Gaussian type, *J. Approx. Theory.* **31**, 22–32 (1981).
18. Ginibre, J., Velo, G.: The global Cauchy problem for the nonlinear Klein–Gordon equation. *Math. Z.* **189**, 487–505 (1985).
19. Grundy, R.E.: Hermite interpolation visits ordinary two-point boundary value problems, *ANZIAM J.* **48**, 533–552 (2007).
20. Guo, B.-Y., Li, X., Vázquez, L.: A Legendre spectral method for solving the nonlinear Klein–Gordon equation, *Comp. Appl. Math.* **15**, 19–36 (1996).
21. Hairer, E., Lubich, C., Wanner, G.: *Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations* (2nd edn). Springer, Berlin, Heidelberg (2006).
22. Hesthaven, J.S., Gottlieb, S., Gottlieb, D.: *Spectral Methods for Time-Dependent Problems.* Cambridge Monographs on Applied and Computational Mathematics, Cambridge University Press (2007).
23. Hochbruck, M., Ostermann, A.: Explicit exponential Runge–Kutta methods for semilinear parabolic problems, *SIAM J. Numer. Anal.* **43**, 1069–1090 (2005).
24. Hochbruck, M., Ostermann, A.: Exponential Runge–Kutta methods for parabolic problems, *Appl. Numer. Math.* **53**, 323–339 (2005).
25. Hochbruck, M., Ostermann, A.: Exponential integrators, *Acta Numerica* **19**, 209–286 (2010).
26. Ibrahim, S., Majdoub, M., Masmoudi, N.: Global solutions for a semilinear, two-dimensional Klein–Gordon equation with exponential-type nonlinearity, *Commun. Pure Appl. Math.* **59**, 1639–1658 (2006).
27. Iserles, A.: *A First Course in the Numerical Analysis of Differential Equations* (2nd edn), Cambridge University Press, Cambridge (2008).
28. Janssen, J., Vandewalle, S.: On SOR waveform relaxation methods, *SIAM J. Numer. Anal.* **34**, 2456–2481 (1997).
29. Jetter, K.: Uniqueness of Gauss–Birkhoff quadrature formulas, *SIAM J. Numer. Anal.* **24**, 147–154 (1987).
30. Kassam, A.-K., Trefethen, L.N.: Fourth-order time stepping for stiff PDEs, *SIAM J. Sci. Comput.* **26**, 1214–1233 (2005).
31. Khanamiryan, M.: Quadrature methods for highly oscillatory linear and nonlinear systems of ordinary differential equations, Part I, *BIT* Numer. Math. **48**, 743–762 (2008).
32. Kosecki, R.: The unit condition and global existence for a class of nonlinear Klein–Gordon equations. *J. Differ. Eqns* **100**, 257–268 (1992).
33. Li, S., Vu-Quoc, L.: Finite difference calculus invariant structure of a class of algorithms for the nonlinear Klein–Gordon equation, *SIAM J. Numer. Anal.* **32**, 1839–1875 (1995).
34. Liu, C., Shi, W., Wu, X.: An efficient high-order explicit scheme for solving Hamiltonian nonlinear wave equations, *Appl. Math. Comput.* **246**, 696–710 (2014).
35. Lubich, C., Ostermann, A.: Multigrid dynamic iteration for parabolic equations, *BIT* **27**, 216–234 (1987).
36. Mulholland, L.S., Huang, W. Z., Sloan, D. M.: Pseudospectral solution of near-singular problems using numerical coordinate transformations based on adaptivity. *SIAM J. Sci. Comput.* **19**, 1261–1289 (1998).
37. Nikolov, G.: Existence and uniqueness of Hermite–Birkhoff Gaussian quadrature formulas, *Calcolo* **26**, 41–59 (1989).
38. Pascual, P.J., Jiménez, S., Vázquez, L.: *Numerical Simulations of a Nonlinear Klein–Gordon Model. Applications. Computational Physics (Granada, 1994).* Lecture Notes in Physics, vol. **448**. pp. 211–270. Springer, Berlin (1995).
39. Phillips, G. M.: Explicit forms for certain Hermite approximations,*BIT* **13**, 177–180 (1973).
40. Shen, J., Tang, T., Wang, L.L.: *Spectral Methods: Algorithms, Analysis, Applications*. Springer, Berlin (2011).
41. Strauss, W.A.: *Nonlinear Wave Equations*. Regional Conference Series in Mathematics, Vol. **73**, AMS, Providence, RI, (1989).

42. Sun, Z. Z.: *Numerical Methods of Partial Differential Equations* (2nd edn, in Chinese), Science Press, Beijing (2012).
43. Tang, W.S., Ya, Y.J., Zhang, J.J.: High order symplectic integrators based on continuous-stage Runge-Kutta Nyström methods, `arXiv:`1510.04395.
44. Tourigny, Y.: Product approximation for nonlinear Klein–Gordon equations. *IMA J. Numer. Anal.* **9**, 449–462 (1990).
45. Vandewalle, S.: *Parallel Multigrid Waveform Relaxation for Parabolic Problems.* Teubner Scripts on Numerical Mathematics, B. G. Teubner, Stuttgart, (1993).
46. Wang, B., Liu, K., Wu, X.: A Filon-type asymptotic approach to solving highly oscillatory second–order initial value problems, *J. Comput. Phys.* **243**, 210–223 (2013).
47. Wu, X., You, X., Wang, B.: *Structure-Preserving Algorithms for Oscillatory Differential Equations.* Springer-Verlag, Berlin Heidelberg (2013).
48. Wu, X., Liu, K., Shi, W.: *Structure-Preserving Algorithms for Oscillatory Differential Equations II.* Springer-Verlag, Heidelberg (2015).