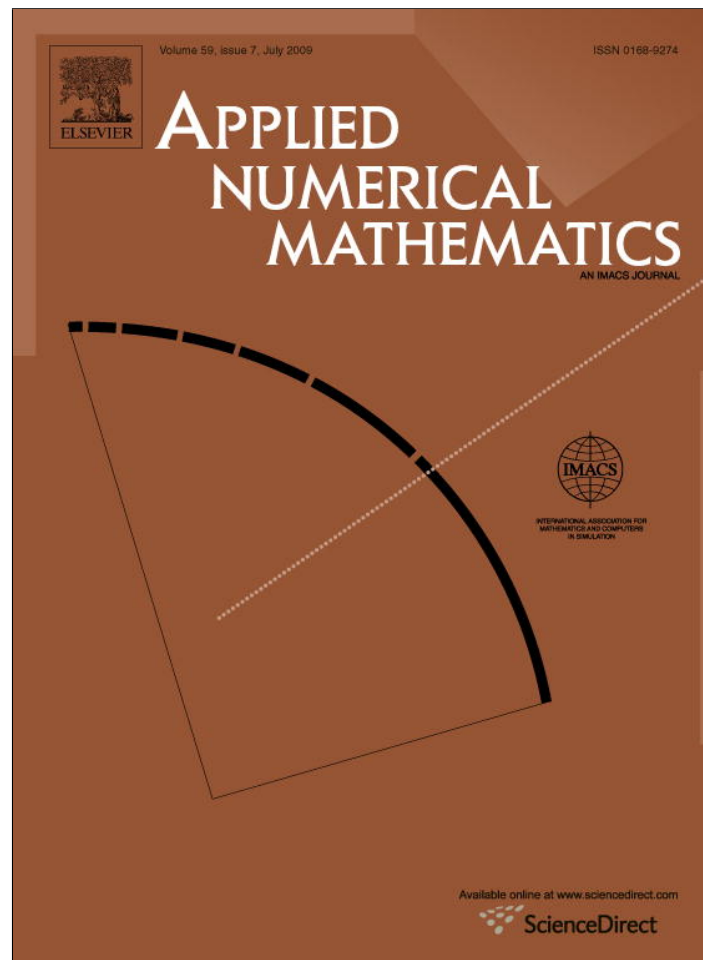


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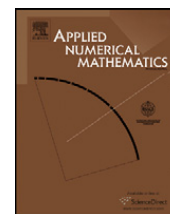
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An analysis of the finite-difference method for one-dimensional Klein–Gordon equation on unbounded domain [☆]

Houde Han ^{*}, Zhiwen Zhang

Department of Mathematical Sciences, Tsinghua University, Beijing 100084, PR China

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ABSTRACT

The numerical solution of the one-dimensional Klein–Gordon equation on an unbounded domain is analyzed in this paper. Two artificial boundary conditions are obtained to reduce the original problem to an initial boundary value problem on a bounded computational domain, which is discretized by an explicit difference scheme. The stability and convergence of the scheme are analyzed by the energy method. A fast algorithm is obtained to reduce the computational cost and a discrete artificial boundary condition (DABC) is derived by the Z -transform approach. Finally, we illustrate the efficiency of the proposed method by several numerical examples.

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1. Introduction

The Klein–Gordon equation arises in relativistic quantum mechanics and field theory, which is of great importance for the high energy physicists [15], and is used to model many different phenomena, including the propagation of dislocations in crystals and the behavior of elementary particles. The one-dimensional Klein–Gordon equation is given by the following partial differential equation:

$$\hbar^2 \frac{\partial^2 u}{\partial t^2} - \hbar^2 c^2 \frac{\partial^2 u}{\partial x^2} + m^2 c^4 u = f(x, t), \quad \forall x \in \mathbb{R}^1, t > 0, \quad (1.1)$$

where $u = u(x, t)$ represents the wave density at position x and time t , \hbar is the Planck constant, c and m are particle velocity and particle mass, respectively.

There are a lot of studies on the numerical solution of initial and initial-boundary problems of the linear or nonlinear Klein–Gordon equation. For example, Khalifa and Elgamel [22] developed a numerical scheme based on a finite element method for the nonlinear Klein–Gordon equation with Dirichlet boundary condition on a bounded domain, which shows the overflow solution as expected. Duncan [6] analyzed three finite difference approximations of the initial nonlinear Klein–Gordon equation, showed they are directly related to symplectic mappings and tested the schemes on the traveling wave and periodic breather problems over long time intervals. However, when we wish to solve the Klein–Gordon numerically on an unbounded domain, these methods will face essential difficulties. Since the unboundedness of the physical domain in our problem, the standard finite element method or finite difference method can't be used directly.

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^{*} Corresponding author.

E-mail addresses: hhan@math.tsinghua.edu.cn (H. Han), zhangzhiwen02@mails.tsinghua.edu.cn (Z. Zhang).

The artificial boundary condition (ABC) method is a powerful approach to reduce the problems on the unbounded domain to a bounded computational domain. In the well-known paper of Engquist and Majda [12], absorbing boundary conditions using Padé approximation of a pseudo-differential operator on a line-type boundary for the wave equation are derived. Higdon [20,21] developed radiation boundary conditions for the numerical modeling of dispersive waves. By specifying the wavenumber and frequency parameters, the boundary conditions based on compositions of simple first-order differential operators was got. His formulas can be applied without modification to higher-dimensional problem. Low-order local ABCs may have low accuracy, whereas high-order local ABCs are usually hard to implement because they typically involve high-order derivatives [13]. The local ABCs may generate some nonphysical reflection at the artificial boundary and the well-posedness of the resulting truncated initial-boundary problem is still open in general. Nonlocal artificial boundary conditions have the potential of being more accurate than the local ones. Han and Zheng [19] obtained three kinds of exact nonreflecting boundary conditions for exterior problems of wave equations in two and three-dimensional space by an approach based on Duhamel's principle. X. Antoine and C. Besse [2] obtained a nonreflecting boundary conditions for the one-dimensional Schrödinger equation. X. Antoine, C. Besse and V. Mouysset [3] also generalized their approach to simulate the two-dimensional Schrödinger equation using nonreflecting boundary conditions. Han and Huang [16], Han, Yin and Huang [18] derived the exact nonreflecting boundary conditions for two- and three-dimensional Schrödinger equations. Han and Yin [17] also derived the exact nonreflecting boundary conditions for two- and three-dimensional Klein–Gordon equations. Generally speaking, the exact boundary conditions require more computational cost. In order to overcome this disadvantage, a fast algorithm is given in our paper.

The organization of this article is the following: In Section 2 we introduce two artificial boundaries and find the artificial boundary conditions, then reduce the original problem to an equivalent problem on the bounded computational domain. In Section 3, a finite-difference scheme for the reduced problem is given and its stability and convergence are analyzed. A fast algorithm is obtained in Section 4 to reduce the computational cost. In Section 5, a discrete artificial boundary condition (DABC) is derived by the Z-transform approach. Some numerical results will be given in Section 6 to demonstrate the accuracy and efficiency of the proposed methods.

2. The artificial boundary condition

In this section, we study the numerical approximation of a dispersive wave solution $u(x, t)$, to the equation with a source term on an unbounded domain. More precisely, we consider the following linear Klein–Gordon equation on $\mathbb{R}^1 \times [0, T]$:

$$\frac{\partial^2 u}{\partial t^2} - a^2 \frac{\partial^2 u}{\partial x^2} + b^2 u = f(x, t), \quad \forall x \in \mathbb{R}^1, \quad t \in [0, T], \tag{2.1}$$

$$u|_{t=0} = \varphi_0(x), \quad \forall x \in \mathbb{R}^1, \tag{2.2}$$

$$u_t|_{t=0} = \varphi_1(x), \quad \forall x \in \mathbb{R}^1. \tag{2.3}$$

Here a, b are two real constants. Assume $\varphi_0(x), \varphi_1(x)$ and $f(x, t)$ satisfying: $\text{Supp}\{\varphi_0(x)\} \subset [x_l, x_r]$, $\text{Supp}\{\varphi_1(x)\} \subset [x_l, x_r]$ and $\text{Supp}\{f(x, t)\} \subset [x_l, x_r] \times [0, T]$. For simplicity of the deduction, we take $x_l = -1$ and $x_r = 1$.

In order to reduce the problem (2.1)–(2.3) to a bounded computational domain, we introduce two artificial boundaries,

$$\Sigma_r = \{(x, t) \mid x = 1, \quad 0 \leq t \leq T\},$$

$$\Sigma_l = \{(x, t) \mid x = -1, \quad 0 \leq t \leq T\},$$

which divide $\mathbb{R}^1 \times [0, T]$ into three parts,

$$D_l = \{(x, t) \mid -\infty \leq x \leq -1, \quad 0 \leq t \leq T\},$$

$$D_i = \{(x, t) \mid -1 \leq x \leq 1, \quad 0 \leq t \leq T\},$$

$$D_r = \{(x, t) \mid 1 \leq x \leq +\infty, \quad 0 \leq t \leq T\}.$$

The bounded domain D_i is our computational domain. Consider the restriction of $u(x, t)$ on the unbounded domain D_r . $u(x, t)$ satisfies,

$$\frac{\partial^2 u}{\partial t^2} - a^2 \frac{\partial^2 u}{\partial x^2} + b^2 u = 0, \quad \forall (x, t) \in D_r, \tag{2.4}$$

$$u|_{\Sigma_r} = u(1, t) \equiv g_1(t), \tag{2.5}$$

$$u|_{t=0} = 0, \quad x \geq 1, \tag{2.6}$$

$$u_t|_{t=0} = 0, \quad x \geq 1. \tag{2.7}$$

Since $u(1, t)$ is unknown, the problem (2.4)–(2.7) is incomplete, which cannot be solved independently. If $u|_{\Sigma_r} = u(1, t) \equiv g_1(t)$ is given, the problem above has a unique solution. Let

$$U(x, s) = \mathcal{L}(u(x, t)) = \int_0^{+\infty} e^{-st} u(x, t) dt, \quad \text{Re } s > 0,$$

denotes the Laplace transform of the unknown solution $u(x, t)$. By (2.4)–(2.7) it satisfies,

$$s^2 U(x, s) - a^2 U_{xx}(x, s) + b^2 U(x, s) = 0, \quad 1 < x < +\infty, \tag{2.8}$$

$$U(1, s) = G(s) \equiv \mathcal{L}(g_1(t)) = \int_0^{+\infty} e^{-st} g_1(t) dt, \tag{2.9}$$

$$|U(x, s)| < +\infty, \quad x \rightarrow +\infty. \tag{2.10}$$

Eq. (2.8) is a second-order linear ODE with constant coefficient, its general solution is given by

$$U(x, s) = c_1(s) \exp\left(-\frac{\sqrt{s^2 + b^2}}{a}(x - 1)\right) + c_2(s) \exp\left(\frac{\sqrt{s^2 + b^2}}{a}(x - 1)\right).$$

The condition (2.10) implies $c_2(s) \equiv 0$, and we obtain

$$U(x, s) = c_1(s) \exp\left(-\frac{\sqrt{s^2 + b^2}}{a}(x - 1)\right), \tag{2.11}$$

here the roots with positive real parts are taken. The partial derivative with respect to x yields,

$$\frac{\partial U(x, s)}{\partial x} = -\frac{\sqrt{s^2 + b^2}}{a} c_1(s) \exp\left(-\frac{\sqrt{s^2 + b^2}}{a}(x - 1)\right). \tag{2.12}$$

Combining (2.11) and (2.12) on the artificial boundary Σ_r , we arrive at

$$\frac{\partial U(1, s)}{\partial x} = -\frac{\sqrt{s^2 + b^2}}{a} U(1, s) = -\frac{1}{a\sqrt{s^2 + b^2}} (s^2 U(1, s) + b^2 U(1, s)). \tag{2.13}$$

By the table of Laplace transform (see page 1108 of [14]), we obtain

$$\mathcal{L}^{-1}\left(\frac{1}{\sqrt{s^2 + b^2}}\right) = J_0(bt),$$

$$\mathcal{L}^{-1}(s^2 U(1, s) + b^2 U(1, s)) = \frac{\partial^2 u(1, t)}{\partial t^2} + b^2 u(1, t).$$

Then, by the convolution theorem of Laplace transforms, from (2.13) we obtain:

$$\begin{aligned} \frac{\partial u(1, t)}{\partial x} &= -\frac{1}{a} \int_0^t J_0(bt - b\tau) \left[\frac{\partial^2 u(1, \tau)}{\partial \tau^2} + b^2 u(1, \tau) \right] d\tau \\ &= -\frac{1}{a} \frac{\partial u(1, t)}{\partial t} - \frac{b}{a} \int_0^t J_0'(bt - b\tau) \frac{\partial u(1, \tau)}{\partial \tau} d\tau - \frac{b^2}{a} \int_0^t J_0(bt - b\tau) u(1, \tau) d\tau \\ &= -\frac{1}{a} \frac{\partial u(1, t)}{\partial t} - \frac{b^2}{a} \int_0^t [J_0''(bt - b\tau) + J_0(bt - b\tau)] u(1, \tau) d\tau. \end{aligned}$$

We get the artificial boundary condition of the problem (2.1)–(2.3) on Σ_r . Similarly we can get the artificial boundary condition on Σ_l , with $t \in [0, T]$. Hence, we can reduce the initial boundary value problem on the computational domain D_i .

$$\frac{\partial^2 u}{\partial t^2} - a^2 \frac{\partial^2 u}{\partial x^2} + b^2 u = f(x, t), \quad \forall (x, t) \in [-1, 1] \times [0, T], \tag{2.14}$$

$$u|_{t=0} = \varphi_0(x), \quad u_t|_{t=0} = \varphi_1(x), \quad \forall x \in [-1, 1], \tag{2.15}$$

$$\frac{\partial u(1, t)}{\partial t} + a \frac{\partial u(1, t)}{\partial x} = -b^2 \int_0^t [J_0''(bt - b\tau) + J_0(bt - b\tau)] u(1, \tau) d\tau, \tag{2.16}$$

$$\frac{\partial u(-1, t)}{\partial t} - a \frac{\partial u(-1, t)}{\partial x} = -b^2 \int_0^t [J_0''(bt - b\tau) + J_0(bt - b\tau)] u(-1, \tau) d\tau. \tag{2.17}$$

Let $\mathbf{J}(x) = \mathbf{J}_0(x) + \mathbf{J}_0''(x)$, where $\mathbf{J}(x)$ is a special function. By some basic recursion formulas of Bessel functions (see page 242 of [1]), we have

$$\mathbf{J}(x) := \mathbf{J}_0(x) + \mathbf{J}_0''(x) = \mathbf{J}_0(x) - (\mathbf{J}_1'(x))' = \frac{1}{2}(\mathbf{J}_0(x) + \mathbf{J}_2(x)).$$

The artificial boundary conditions (2.16), (2.17) will have two simple forms:

$$\frac{\partial u(1, t)}{\partial t} + a \frac{\partial u(1, t)}{\partial x} = -b^2 \int_0^t \mathbf{J}(bt - b\tau) u(1, \tau) d\tau, \tag{2.18}$$

$$\frac{\partial u(-1, t)}{\partial t} - a \frac{\partial u(-1, t)}{\partial x} = -b^2 \int_0^t \mathbf{J}(bt - b\tau) u(-1, \tau) d\tau. \tag{2.19}$$

Moreover, let $\mathbf{F}(x)$ denotes the primitive of $\mathbf{J}(x)$:

$$\mathbf{F}(x) = \int_0^x \mathbf{J}(s) ds = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!k!(2k+2)} \left(\frac{x}{2}\right)^{2k+1} + \sum_{k=0}^{\infty} \frac{(-1)^k x}{k!(k+2)!(2k+3)} \left(\frac{x}{2}\right)^{2k+3}.$$

Integrating by parts in Eqs. (2.18) and (2.19), we obtain another two equivalent forms of boundary conditions. The new forms will bring some convenience for the proof of stability and convergence.

$$\frac{\partial u(1, t)}{\partial t} + a \frac{\partial u(1, t)}{\partial x} = -b \int_0^t \mathbf{F}(bt - b\tau) \frac{\partial u(1, \tau)}{\partial \tau} d\tau. \tag{2.20}$$

$$\frac{\partial u(-1, t)}{\partial t} - a \frac{\partial u(-1, t)}{\partial x} = -b \int_0^t \mathbf{F}(bt - b\tau) \frac{\partial u(-1, \tau)}{\partial \tau} d\tau. \tag{2.21}$$

Next, we discuss the uniqueness and stability estimate of the reduced problem (2.14)–(2.17). Multiply Eq. (2.1) by $\frac{\partial u}{\partial t}$ and integrate with respect to $x \in [-1, 1]$ for fixed $t \in (0, T]$, using the boundary condition (2.16), (2.17), we get

$$\begin{aligned} & \frac{d}{dt} \left\{ \frac{1}{2} \int_{-1}^1 \left[\left(\frac{\partial u(x, t)}{\partial t} \right)^2 + a^2 \left(\frac{\partial u(x, t)}{\partial x} \right)^2 + b^2 u^2(x, t) \right] dx \right\} + a^2 \frac{\partial u(1, t)}{\partial t} \mathbf{B}(u(1, t)) + a^2 \frac{\partial u(-1, t)}{\partial t} \mathbf{B}(u(-1, t)) \\ & = \int_{-1}^1 f(x, t) \frac{\partial u(x, t)}{\partial t} dx. \end{aligned} \tag{2.22}$$

Here

$$\mathbf{B}(v(t)) = \frac{1}{a} \frac{dv(t)}{dt} + \frac{b^2}{a} \int_0^t [J_0''(bt - b\tau) + J_0(bt - b\tau)] v(\tau) d\tau.$$

We introduce two auxiliary functions $W^{(1)}(x, t)$ and $W^{(2)}(x, t)$, which satisfy the following problems, respectively:

$$W_{tt}^{(1)} - a^2 W_{xx}^{(1)} + b^2 W^{(1)} = 0, \quad \forall (x, t) \in D_r,$$

$$W^{(1)}|_{\Sigma_r} = u(1, t), \quad 0 \leq t \leq T,$$

$$W^{(1)}|_{t=0} = 0, \quad 1 < x < +\infty,$$

$$W_t^{(1)}|_{t=0} = 0, \quad 1 < x < +\infty$$

and

$$W_{tt}^{(2)} - a^2 W_{xx}^{(2)} + b^2 W^{(2)} = 0, \quad \forall (x, t) \in D_l,$$

$$W^{(2)}|_{\Sigma_l} = u(-1, t), \quad 0 \leq t \leq T,$$

$$W^{(2)}|_{t=0} = 0, \quad -\infty < x < -1,$$

$$W_t^{(2)}|_{t=0} = 0, \quad -\infty < x < -1.$$

Through a similar analysis, we obtain,

$$a^2 \frac{\partial u(1, t)}{\partial t} \mathbf{B}(u(1, t)) = \frac{d}{dt} \left\{ \frac{1}{2} \int_1^{+\infty} \left[\left(\frac{\partial W^{(1)}(x, t)}{\partial t} \right)^2 + a^2 \left(\frac{\partial W^{(1)}(x, t)}{\partial x} \right)^2 + b^2 (W^{(1)}(x, t))^2 \right] dx \right\}, \quad (2.23)$$

and

$$a^2 \frac{\partial u(-1, t)}{\partial t} \mathbf{B}(u(-1, t)) = \frac{d}{dt} \left\{ \frac{1}{2} \int_{-\infty}^{-1} \left[\left(\frac{\partial W^{(2)}(x, t)}{\partial t} \right)^2 + a^2 \left(\frac{\partial W^{(2)}(x, t)}{\partial x} \right)^2 + b^2 (W^{(2)}(x, t))^2 \right] dx \right\}. \quad (2.24)$$

We introduce $\mathbb{E}(t)$ and $\mathbb{F}(t)$ as following,

$$\begin{aligned} \mathbb{E}(t) &= \frac{1}{2} \int_{-1}^1 \left[\left(\frac{\partial u(x, t)}{\partial t} \right)^2 + a^2 \left(\frac{\partial u(x, t)}{\partial x} \right)^2 + b^2 u^2(x, t) \right] dx \\ &\quad + \frac{1}{2} \int_1^{+\infty} \left[\left(\frac{\partial W^{(1)}(x, t)}{\partial t} \right)^2 + a^2 \left(\frac{\partial W^{(1)}(x, t)}{\partial x} \right)^2 + b^2 (W^{(1)}(x, t))^2 \right] dx \\ &\quad + \frac{1}{2} \int_{-\infty}^{-1} \left[\left(\frac{\partial W^{(2)}(x, t)}{\partial t} \right)^2 + a^2 \left(\frac{\partial W^{(2)}(x, t)}{\partial x} \right)^2 + b^2 (W^{(2)}(x, t))^2 \right] dx, \end{aligned} \quad (2.25)$$

$$\mathbb{F}(t) = \frac{1}{2} \int_{-1}^1 (f(x, t))^2 dx. \quad (2.26)$$

Combining (2.22)–(2.26) and using Cauchy–Schwarz inequality, we obtain,

$$\frac{d}{dt} \mathbb{E}(t) \leq \mathbb{E}(t) + \mathbb{F}(t), \quad 0 \leq t \leq T. \quad (2.27)$$

Using the Gronwall inequality from inequality (2.27) and noticing that,

$$\mathbb{E}(0) = \frac{1}{2} \int_{-1}^1 [(\varphi_1(x))^2 + a^2 (\varphi_1'(x))^2 + b^2 (\varphi_0(x))^2] dx.$$

we get the stability estimate for the solution of the reduced problem (2.14)–(2.17):

$$\begin{aligned} &\int_{-1}^1 \left[\left(\frac{\partial u(x, t)}{\partial t} \right)^2 + a^2 \left(\frac{\partial u(x, t)}{\partial x} \right)^2 + b^2 u^2(x, t) \right] dx \\ &\leq \int_{-1}^1 [(\varphi_1(x))^2 + a^2 (\varphi_1'(x))^2 + b^2 (\varphi_0(x))^2] dx + \int_0^t \int_{-1}^1 e^{t-\tau} (f(x, \tau))^2 dx d\tau. \end{aligned} \quad (2.28)$$

Then, we obtain the following stability estimate of the reduced problem (2.14)–(2.17).

Theorem 2.1. *The reduced problem (2.14)–(2.17) has at most one solution $u(x, t)$ on the bounded computational domain D_i , and $u(x, t)$ continuously depends on the initial value $\{\varphi_0(x), \varphi_1(x)\}$, and $f(x, t)$.*

From Theorem 2.1, we know that the reduced problem (2.14)–(2.17) is equivalent to the original problem (2.1)–(2.3). Namely, the solution of the reduced problem (2.14)–(2.17) is the restriction of the solution of original problem (2.1)–(2.3) on the bounded domain D_i , vice versa.

3. Analysis of the difference scheme

In this section, we consider the finite difference approximation of the reduced problem (2.14)–(2.17) on the bounded domain D_i . We divide the domain D_i by a set of lines parallel to the x - and t -axes to form a grid. We write $h = 1/I$ and $\tau = T/N$ for the line spacings, where I and N are two positive integers. The crossing points Ω_h^τ are called the grid points,

$$\Omega_h^\tau = \{(x_i, t_n) \mid x_i = -1 + ih, \quad i = 0, 1, \dots, 2I; \quad t_n = n\tau, \quad n = 0, 1, \dots, T/\tau\}.$$

Suppose $\mathbf{U} = \{u_i^n \mid 0 \leq i \leq 2I, n \geq 0\}$ is a grid function on Ω_h^τ . For the simplicity, assume the constants $a = b = 1$. Introduce the following notations [24]:

$$\begin{aligned} u_{i-1/2}^n &= \frac{1}{2}(u_{i-1}^n + u_i^n), & u_i^{n-1/2} &= \frac{1}{2}(u_i^n + u_i^{n-1}), \\ \delta_x u_{i-1/2}^n &= \frac{1}{h}(u_i^n - u_{i-1}^n), & \delta_t u_i^{n-1/2} &= \frac{1}{\tau}(u_i^n - u_i^{n-1}), \\ \delta_x^0 u_i^n &= \frac{1}{2h}(u_{i+1}^n - u_{i-1}^n), & \delta_t^0 u_i^n &= \frac{1}{2\tau}(u_i^{n+1} - u_i^{n-1}), \\ \delta_x^2 u_i^n &= \frac{1}{h^2}(u_{i+1}^n - 2u_i^n + u_{i-1}^n), & \delta_t^2 u_i^n &= \frac{1}{\tau^2}(u_i^{n+1} - 2u_i^n + u_i^{n-1}). \end{aligned}$$

We denote the value of the solution $u(x, t)$ at the grid point (x_i, t_n) by U_i^n and $f_i^n = f(x_i, t_n)$. Using the Taylor expansion, it follows from (2.14), (2.15), (2.21), (2.20) that:

$$\delta_t^2 U_i^n - \delta_x^2 U_i^n + U_i^n = f_i^n + R_i^n, \quad 1 \leq i \leq 2I - 1, \quad n \geq 1, \tag{3.1}$$

$$U_i^0 = \phi_0(ih), \quad 0 \leq i \leq 2I, \tag{3.2}$$

$$U_i^1 = U_i^0 + \tau \phi_1(ih) + S_i^1, \quad 0 \leq i \leq 2I, \tag{3.3}$$

$$\delta_t U_{2l}^{n+1/2} + \delta_x U_{2l-1/2}^n = - \sum_{m=1}^n \delta_t^0 U_{2l}^m \int_{(m-1)\tau}^{m\tau} \mathbf{F}(n\tau - s) ds + P_{2l}^n, \quad n \geq 2, \tag{3.4}$$

$$\delta_t U_0^{n+1/2} - \delta_x U_{1/2}^n = - \sum_{m=1}^n \delta_t^0 U_0^m \int_{(m-1)\tau}^{m\tau} \mathbf{F}(n\tau - s) ds + Q_0^n, \quad n \geq 2. \tag{3.5}$$

If the solution $u(x, t)$ is smooth enough, there exists a constant C , such that

$$|R_i^n| \leq C(h^2 + \tau^2), \quad |S_i^1| \leq C\tau^2, \quad |P_{2l}^n| \leq C(h + \tau), \quad |Q_0^n| \leq C(h + \tau).$$

Omitting the truncation errors in (3.1)–(3.5), we construct a finite difference scheme of the reduced problem (2.14)–(2.17):

$$\delta_t^2 u_i^n - \delta_x^2 u_i^n + u_i^n = f_i^n, \quad 1 \leq i \leq 2I - 1, \quad n \geq 1, \tag{3.6}$$

$$u_i^0 = \phi_0(ih), \quad 0 \leq i \leq 2I, \tag{3.7}$$

$$u_i^1 = u_i^0 + \tau \phi_1(ih), \quad 0 \leq i \leq 2I, \tag{3.8}$$

$$\delta_t u_{2l}^{n+1/2} + \delta_x u_{2l-1/2}^n = - \sum_{m=1}^n \delta_t^0 u_{2l}^m \int_{(m-1)\tau}^{m\tau} \mathbf{F}(n\tau - s) ds, \quad n \geq 2, \tag{3.9}$$

$$\delta_t u_0^{n+1/2} - \delta_x u_{1/2}^n = - \sum_{m=1}^n \delta_t^0 u_0^m \int_{(m-1)\tau}^{m\tau} \mathbf{F}(n\tau - s) ds, \quad n \geq 2. \tag{3.10}$$

This is an explicit scheme with global boundary conditions. In the following, we consider the stability and convergence of the scheme. Multiplying (3.6) by $2h\delta_t^0 u_i^n$ and summing up for i from 1 to $2I - 1$, we obtain

$$\sum_{i=1}^{2I-1} 2h\delta_t^0 u_i^n (\delta_t^2 u_i^n - \delta_x^2 u_i^n + u_i^n) = \sum_{i=1}^{2I-1} 2h\delta_t^0 u_i^n f_i^n. \tag{3.11}$$

After some calculation, we get

$$\sum_{i=1}^{2I-1} 2h\delta_t^0 u_i^n \delta_t^2 u_i^n = \frac{h}{\tau} \sum_{i=1}^{2I-1} \{(\delta_t u_i^{n+1/2})^2 - (\delta_t u_i^{n-1/2})^2\}. \tag{3.12}$$

Using the summation by parts formula and the boundary condition (3.9)–(3.10), we have

$$\begin{aligned} - \sum_{i=1}^{2I-1} 2h\delta_t^0 u_i^n \delta_x^2 u_i^n &= \frac{h}{\tau} \sum_{i=0}^{2I-1} \delta_x u_{i+1/2}^{n+1} \delta_x u_{i+1/2}^n - \frac{h}{\tau} \sum_{i=0}^{2I-1} \delta_x u_{i+1/2}^n \delta_x u_{i+1/2}^{n-1} + 2\delta_x u_{1/2}^n \delta_t^0 u_0^n - 2\delta_x u_{2I-1/2}^n \delta_t^0 u_{2I}^n \\ &= \frac{h}{\tau} \sum_{i=0}^{2I-1} \delta_x u_{i+1/2}^{n+1} \delta_x u_{i+1/2}^n - \frac{h}{\tau} \sum_{i=0}^{2I-1} \delta_x u_{i+1/2}^n \delta_x u_{i+1/2}^{n-1} \end{aligned}$$

$$\begin{aligned}
 & + 2\delta_t^0 u_0^n \left\{ \delta_t u_0^{n+1/2} + \sum_{m=1}^n \delta_t^0 u_0^m \int_{(m-1)\tau}^{m\tau} \mathbf{F}(n\tau - s) ds \right\} \\
 & + 2\delta_t^0 u_{2l}^n \left\{ \delta_t u_{2l}^{n+1/2} + \sum_{m=1}^n \delta_t^0 u_{2l}^m \int_{(m-1)\tau}^{m\tau} \mathbf{F}(n\tau - s) ds \right\} \\
 \equiv & \mathbf{I}_1 + \mathbf{I}_2 + \mathbf{I}_3.
 \end{aligned} \tag{3.13}$$

Notice that,

$$\begin{aligned}
 \mathbf{I}_2 & = 2\delta_t^0 u_0^n \left\{ \delta_t u_0^{n+1/2} + \sum_{m=1}^n \delta_t^0 u_0^m \int_{(m-1)\tau}^{m\tau} \mathbf{F}(n\tau - s) ds \right\} \\
 & = 2\delta_t^0 u_0^n \left\{ \delta_t^0 u_0^n + \sum_{m=1}^n \delta_t^0 u_0^m \int_{(m-1)\tau}^{m\tau} \mathbf{F}(n\tau - s) ds \right\} + 2\delta_t^0 u_0^n \{ \delta_t u_0^{n+1/2} - \delta_t^0 u_0^n \} \\
 & \equiv \mathbf{I}_2^A + \mathbf{I}_2^B.
 \end{aligned}$$

Similarly,

$$\mathbf{I}_3 \equiv \mathbf{I}_3^A + \mathbf{I}_3^B.$$

Using the linear interpolation to construct a continuous function $\tilde{u}(1, t)$, which satisfies $\tilde{u}_t(1, t) = \delta_t^0 u_0^m$, $t \in [m\tau - \tau, m\tau)$. According to the stability estimate of the continuous case in Section 2, we obtain

$$\mathbf{I}_2^A = 2\delta_t^0 u_0^n \left\{ \delta_t^0 u_0^n + \sum_{m=1}^n \delta_t^0 u_0^m \int_{(m-1)\tau}^{m\tau} \mathbf{F}(n\tau - s) ds \right\} \geq 0. \tag{3.14}$$

It is easy to check,

$$\mathbf{I}_2^B = 2\delta_t^0 u_0^n \{ \delta_t u_0^{n+1/2} - \delta_t^0 u_0^n \} = \frac{1}{2} \{ (\delta_t u_0^{n+1/2})^2 - (\delta_t u_0^{n-1/2})^2 \}.$$

By the same technique, we obtain that \mathbf{I}_3^A is also nonnegative, and

$$\mathbf{I}_3^B = 2\delta_t^0 u_{2l}^n \{ \delta_t u_{2l}^{n+1/2} - \delta_t^0 u_{2l}^n \} = \frac{1}{2} \{ (\delta_t u_{2l}^{n+1/2})^2 - (\delta_t u_{2l}^{n-1/2})^2 \}.$$

The third term in the left of Eq. (3.11) is easy,

$$\sum_{i=1}^{2l-1} 2h\delta_t^0 u_i^n u_i^n = \frac{h}{\tau} \sum_{i=1}^{2l-1} u_i^n u_i^{n+1} - \frac{h}{\tau} \sum_{i=1}^{2l-1} u_i^{n-1} u_i^n. \tag{3.15}$$

We introduce an auxiliary quantity \tilde{E} ,

$$\begin{aligned}
 \tilde{E} & \equiv \frac{s}{2} h (\delta_t u_0^{n+1/2})^2 + h \sum_{i=1}^{2l-1} (\delta_t u_i^{n+1/2})^2 + \frac{s}{2} h (\delta_t u_{2l}^{n+1/2})^2 + h \sum_{i=0}^{2l-1} \delta_x u_{i+1/2}^{n+1} \delta_x u_{i+1/2}^n + h \sum_{i=1}^{2l-1} u_i^n u_i^{n+1} \\
 & = \frac{s}{2} h (\delta_t u_0^{n+1/2})^2 + h \sum_{i=1}^{2l-1} (\delta_t u_i^{n+1/2})^2 + \frac{s}{2} h (\delta_t u_{2l}^{n+1/2})^2 + h \sum_{i=0}^{2l-1} (\delta_x u_{i+1/2}^{n+1/2})^2 - \frac{h}{4} \sum_{i=0}^{2l-1} (\delta_x u_{i+1/2}^{n+1} - \delta_x u_{i+1/2}^n)^2 \\
 & \quad + h \sum_{i=1}^{2l-1} (u_i^{n+1/2})^2 - \frac{h\tau^2}{4} \sum_{i=1}^{2l-1} (\delta_t u_i^{n+1/2})^2 \\
 & = \frac{s}{2} h (\delta_t u_0^{n+1/2})^2 + \left(1 - s^2 - \frac{\tau^2}{4} \right) h \sum_{i=1}^{2l-1} (\delta_t u_i^{n+1/2})^2 + \frac{s}{2} h (\delta_t u_{2l}^{n+1/2})^2 + s^2 h \sum_{i=1}^{2l-1} (\delta_t u_i^{n+1/2})^2 \\
 & \quad - \frac{hs^2}{4} \sum_{i=0}^{2l-1} (\delta_t u_{i+1/2}^{n+1} - \delta_t u_{i+1/2}^n)^2 + h \sum_{i=0}^{2l-1} (\delta_x u_{i+1/2}^{n+1/2})^2 + h \sum_{i=1}^{2l-1} (u_i^{n+1/2})^2 \\
 & \geq \alpha h \sum_{i=0}^{2l} (\delta_t u_i^{n+1/2})^2 + h \sum_{i=0}^{2l-1} (\delta_x u_{i+1/2}^{n+1/2})^2 + h \sum_{i=1}^{2l-1} (u_i^{n+1/2})^2 > 0,
 \end{aligned} \tag{3.16}$$

where

$$s = \frac{\tau}{h \in (0, 1)}, \quad \alpha = \min\left(\frac{s}{2}, 1 - s^2 - \frac{\tau^2}{4}\right) > 0.$$

The right hand of Eq. (3.11) is bounded by:

$$\begin{aligned} \sum_{i=1}^{2l-1} 2h\delta_t^0 u_i^n f_i^n &= h \sum_{i=1}^{2l-1} f_i^n (\delta_t u_i^{n+1/2} + \delta_t u_i^{n-1/2}) \\ &\leq \left(\frac{1}{2} - \frac{s^2}{2} - \frac{\tau^2}{8}\right) h \sum_{i=1}^{2l-1} \{(\delta_t u_i^{n-1/2})^2 + (\delta_t u_i^{n+1/2})^2\} + \frac{h}{1 - s^2 - \tau^2/4} \sum_{i=1}^{2l-1} (f_i^n)^2. \end{aligned} \tag{3.17}$$

Assume $s^2 + \frac{\tau^2}{4} < 1$, according to the definition of \tilde{E}_n , we obtain the inequality

$$\tilde{E}_n \geq \left(1 - s^2 - \frac{\tau^2}{4}\right) h \sum_{i=1}^{2l-1} (\delta_t u_i^{n-1/2})^2. \tag{3.18}$$

Combining the expressions (3.12)–(3.18), we get

$$\begin{aligned} \tilde{E}_n &\leq \tilde{E}_{n-1} + \frac{\tau}{2}(\tilde{E}_n + \tilde{E}_{n-1}) + \frac{\tau}{1 - s^2 - \tau^2/4} \|f^n\|^2, \\ \tilde{E}_n &\leq \frac{1 + \tau/2}{1 - \tau/2} \tilde{E}_{n-1} + \frac{\tau}{(1 - \tau/2)(1 - s^2 - \tau^2/4)} \|f^n\|^2. \end{aligned}$$

When $\tau \leq \frac{2}{3}$, we have

$$\tilde{E}_n \leq \left(1 + \frac{3\tau}{2}\right) \tilde{E}_{n-1} + \frac{\tau}{2(1 - \tau/2)(1 - s^2 - \tau^2/4)} \|f^n\|^2.$$

By discrete Gronwall inequality (see page 11 of [23]), we arrive at

$$\begin{aligned} \tilde{E}_n &\leq \tilde{E}_0 \prod_{k=0}^{n-1} \left(1 + \frac{3\tau}{2}\right) + \sum_{k=1}^n \frac{\tau}{2(1 - \tau/2)(1 - s^2 - \tau^2/4)} \|f^{k+1}\|^2 \left(1 + \frac{3\tau}{2}\right)^{n-1-k} \\ &\leq e^{\frac{3}{2}n\tau} \left\{ \tilde{E}_0 + \frac{\tau}{2(1 - \tau/2)(1 - s^2 - \tau^2/4)} \sum_{k=1}^n \|f^k\|^2 \right\}. \end{aligned} \tag{3.19}$$

From (3.16) and (3.19), we obtain the stability theory of the scheme (3.6)–(3.10).

Theorem 3.1 (stability of the scheme). Suppose $\{u_i^n\}$ is the solution of difference scheme (3.6)–(3.10), $s = \tau/h \in (0, 1)$ and $\alpha = \min(\frac{s}{2}, 1 - s^2 - \frac{\tau^2}{4}) > 0$. Let

$$E_n = \alpha h \sum_{i=0}^{2l} (\delta_t u_i^{n+1/2})^2 + h \sum_{i=0}^{2l-1} (\delta_x u_{i+1/2}^{n+1/2})^2 + h \sum_{i=1}^{2l-1} (u_i^{n+1/2})^2$$

denotes the energy norm at n th time. We have the following estimate,

$$E_n \leq \tilde{E}_n \leq e^{\frac{3}{2}n\tau} \left\{ \tilde{E}_0 + \frac{\tau}{2(1 - \tau/2)(1 - s^2 - \tau^2/4)} \sum_{k=1}^n \|f^k\|^2 \right\}.$$

Where, $\|f^k\|^2 = \sum_{i=1}^{2l-1} h(f_i^k)^2$.

Since the difference scheme (3.6)–(3.10) is a system of linear algebraic equation at each time level, it is easy to obtain,

Lemma 3.1. The difference scheme (3.6)–(3.10) has a unique solution.

Next, we turn to analyze the convergence of the difference scheme. Let $e_i^n = U_i^n - u_i^n$ denotes the error on the grid point (x_i, t_n) . Subtracting (3.1)–(3.5) from (3.6)–(3.10), we can obtain the error equation:

$$\delta_t^2 e_i^n - \delta_x^2 e_i^n + e_i^n = r_i^n, \quad 1 \leq i \leq 2l - 1, \quad n \geq 1, \tag{3.20}$$

$$e_i^0 = 0, \quad 0 \leq i \leq 2l, \tag{3.21}$$

$$e_i^1 = s_i^1, \quad 0 \leq i \leq 2l, \tag{3.22}$$

$$\delta_t e_{2l}^{n+1/2} + \delta_x e_{2l-1/2}^n = - \sum_{m=1}^n \delta_t^0 e_{2l}^m \int_{(m-1)\tau}^{m\tau} \mathbf{F}(n\tau - s) ds + p_{2l}^n, \quad n \geq 2, \tag{3.23}$$

$$\delta_t e_0^{n+1/2} - \delta_x e_{1/2}^n = - \sum_{m=1}^n \delta_t^0 e_0^m \int_{(m-1)\tau}^{m\tau} \mathbf{F}(n\tau - s) ds + q_0^n, \quad n \geq 2. \tag{3.24}$$

Where there exists a constant c , such that

$$|r_i^n| \leq c(h^2 + \tau^2), \quad |s_i^1| \leq c\tau^2, \quad |p_{2l}^n| \leq c(h + \tau), \quad |q_0^n| \leq c(h + \tau). \tag{3.25}$$

Using the same technique in the proof of Theorem 3.1, we can obtain the following convergence theory.

Theorem 3.2 (convergence of the scheme). Let \mathcal{E}_n denotes the energy norm of the error at n th time level, $s = \tau/h \in (0, 1)$, and $\alpha = s/2$.

$$\mathcal{E}_n = \alpha h \sum_{i=0}^{2l} (\delta_t u_i^{n+1/2})^2 + h \sum_{i=0}^{2l-1} (\delta_x u_{i+1/2}^{n+1/2})^2 + h \sum_{i=1}^{2l-1} (u_i^{n+1/2})^2$$

we have the estimate,

$$\mathcal{E}_n \leq e^{\frac{3}{2}n\tau} \left\{ \tilde{\mathcal{E}}_0 + \frac{\tau}{1 - \tau/2} \sum_{k=1}^{k=n} \left\{ \frac{(q_0^n)^2}{\alpha h} + \frac{(p_{2l}^n)^2}{\alpha h} + \sum_{i=1}^{2l-1} \frac{h(r_i^n)^2}{\alpha} \right\} \right\}.$$

It follows from (3.21), (3.22) and (3.25) that,

$$\begin{aligned} \tilde{\mathcal{E}}_0 &= \frac{s}{2} h (\delta_t e_0^{1/2})^2 + h \sum_{i=1}^{2l-1} (\delta_t e_i^{1/2})^2 + \frac{s}{2} h (\delta_t e_{2l}^{1/2})^2 + h \sum_{i=0}^{2l-1} \delta_x e_{i+1/2}^1 \delta_x e_{i+1/2}^0 + h \sum_{i=1}^{2l-1} e_i^1 e_i^0 \\ &= O(2lh\tau^2) = O(\tau^2), \end{aligned}$$

and

$$\sum_{k=1}^{k=n} \left\{ \frac{(q_0^n)^2}{\alpha h} + \frac{(p_{2l}^n)^2}{\alpha h} + \sum_{i=1}^{2l-1} \frac{h(r_i^n)^2}{\alpha} \right\} \sim O(1).$$

Hence, the energy norm of the absolute error \mathcal{E}_n have one order convergence.

4. The fast algorithm

The artificial boundary conditions need to compute the convolution terms, which are very expensive for numerical computation. We recall the boundary condition (2.18) and take $a = b = 1$,

$$\frac{\partial u(1, t)}{\partial x} + \frac{\partial u(1, t)}{\partial t} = - \int_0^t \mathbf{J}(t - \tau) u(1, \tau) d\tau.$$

Where the special function $\mathbf{J}(t - \tau)$ can be defined by the series:

$$\begin{aligned} \mathbf{J}(t - \tau) &= \frac{1}{2} \{ \mathbf{J}_0(t - \tau) + \mathbf{J}_2(t - \tau) \} = \frac{1}{2} + \sum_{l=0}^{+\infty} \frac{(-1)^{l+1}}{(l+1)!(l+2)!2^{2l+3}} (t - \tau)^{2+2l} \\ &\equiv \frac{1}{2} + \sum_{l=0}^{+\infty} \alpha_l (t - \tau)^{2+2l}. \end{aligned} \tag{4.1}$$

The coefficients $\{\alpha_l\}$ decay in a rate of $O((l!)^{-2})$, so we just choose the first $\frac{K}{2} - 1$ (K is a positive even number) terms in (4.1) to approximate the special function $\mathbf{J}(t - \tau)$. Then we obtain a approximate boundary condition of the original boundary condition (2.18):

$$\begin{aligned} \frac{\partial u(1, t)}{\partial x} + \frac{\partial u(1, t)}{\partial t} &= - \int_0^t \left\{ \sum_{l=0}^{K/2-1} \alpha_l (t - \tau)^{2+2l} \right\} u(1, \tau) d\tau - \frac{1}{2} \int_0^t u(1, \tau) d\tau \\ &= - \sum_{l=0}^{K/2-1} \int_0^t \left\{ \alpha_l \sum_{j=0}^{2(l+1)} C_{2(l+1)}^j (-1)^j t^j \tau^{2(l+1)-j} \right\} u(1, \tau) d\tau - \frac{1}{2} \int_0^t u(1, \tau) d\tau \\ &\equiv \sum_{l=0}^K P_l(t) \int_0^t \tau^l u(1, \tau) d\tau, \end{aligned} \tag{4.2}$$

here $\{P_l(t), l = 0, 1, 2, \dots, K\}$ are given polynomials of time t . The advantage of this algorithm is that we just need to deal with a series of integrations $\{\int_0^t \tau^l u(1, \tau) d\tau, l = 0, 1, 2, \dots, K\}$, instead of the convolution term. Since

$$\int_0^{t_n} \tau^l u(1, \tau) d\tau = \int_0^{t_{n-1}} \tau^l u(1, \tau) d\tau + \int_{t_{n-1}}^{t_n} \tau^l u(1, \tau) d\tau, \quad l = 0, 1, 2, \dots, K.$$

In practical computation, at the n th time level we just need to save the previous integration value, and do one step integral calculus. Our numerical example shows that this algorithm is very efficiency.

5. Discrete artificial boundary conditions

In this section we discuss how to get the discrete artificial BCs (DABC) for the Klein–Gordon equation. This approach was introduced by A. Arnold in [4] for Schrödinger equation, and M. Ehrhardt in [8] for parabolic equation. After that Arnold and Ehrhardt used this approach to find the discrete artificial BCs for other equations in [5,11,25]. [5] deals with a generalized Schrödinger equation appearing in acoustics. [25] deals with a parabolic equation. [11] deals with a Schrödinger–Poisson system. A Princeton group also adapted this approach to systems of wave equations for materials with cracks [7].

Instead of discretizing the analytic ABC like (3.9) and (3.10), we construct DABCs of the fully discretized whole-space problem. Reconsider the original initial value problem (2.1), (2.2), for simplicity assuming $a = b = 1$ again. We mimic the derivation of the analytic ABC in Section 2 on a discrete level. First choose two integers I and N , and choose T as a fixed computational time. Let h denotes spatial mesh, τ denotes time mesh, respectively.

$$h = 1/I, \quad \tau = T/N.$$

With the uniform grid points $\{(x_i, t_n) \mid x_i = -1 + ih, i \in \mathbf{Z}, t_n = n\tau, n \in \mathbf{N}\}$ and the approximations $u_i^n \sim u(x_i, t_n)$ and $f_i^n \sim f(x_i, t_n)$, the discretized Klein–Gordon equation on the unbounded domain $(-\infty, +\infty) \times [0, T]$ reads:

$$(u_i^{n+1} - 2u_i^n + u_i^{n-1}) - \alpha(u_{i+1}^n - 2u_i^n + u_{i-1}^n) + \tau^2 u_i^n = \tau^2 f_i^n, \quad i = 0, \pm 1, \pm 2, \dots, n = 1, 2, \dots, \tag{5.1}$$

$$u_i^0 = \phi_0(x_i), \quad u_i^1 = u_i^0 + \tau \phi_1(x_i), \quad i = 0, \pm 1, \pm 2, \dots, \tag{5.2}$$

with

$$\alpha = \left(\frac{\tau}{h}\right)^2.$$

Assume $\phi_0(x)$, $\phi_1(x)$, and $f(x, t)$ have the same compact support as in Section 2, we get

$$\begin{aligned} u_i^0 &= 0, \quad u_i^1 = 0, \quad i = 2I, 2I + 1, 2I + 2, \dots, \quad i = 0, -1, -2, \dots, \\ f_i^n &= 0, \quad i = 2I, 2I + 1, 2I + 2, \dots, \quad i = 0, -1, -2, \dots, \quad n = 0, 1, \dots \end{aligned}$$

We try to find the boundary condition on Σ_{2I+1}^h and Σ_{-1}^h ,

$$\begin{aligned} \Sigma_{2I+1}^h &= \{(x_{2I+1}, t_n) \mid n = 0, 1, \dots\}, \\ \Sigma_{-1}^h &= \{(x_{-1}, t_n) \mid n = 0, 1, \dots\}. \end{aligned}$$

First consider the restriction of the problem (5.1), (5.2) for $i \geq 2I$, which satisfies the following difference equation.

$$(u_i^{n+1} - 2u_i^n + u_i^{n-1}) - \alpha(u_{i+1}^n - 2u_i^n + u_{i-1}^n) + \tau^2 u_i^n = 0, \quad i = 2I + 1, 2I + 2, \dots, n = 1, 2, \dots, \tag{5.3}$$

$$u_i^0 = \phi_0(x_i), \quad u_i^1 = u_i^0 + \tau \phi_1(x_i), \quad i = 2I + 1, 2I + 2, \dots \tag{5.4}$$

Since $\{u_{2I}^n \mid n = 2, 3, \dots\}$ are unknown on the boundary Γ_{2I+1}^h , the problem (5.3), (5.4) is incomplete, which cannot be solved independently. Assume $\{u_{2I}^n \mid n = 2, 3, \dots\}$ are given, then the difference equation above has a unique solution. This problem is defined on the half-infinite domain. To solve it, we use the Z-transform method (see page 1127 of [14]):

Let

$$\mathbf{Z}\{u_i^n\} = U_i(z) := \sum_{n=0}^{\infty} u_i^n z^{-n}, \quad z \in \mathbb{C}, |z| > R_u,$$

where R_u denotes the convergence radius of this Laurent series. $\mathbf{Z}\{u_i^n\}$ is called the Z-transform of the sequence $\{u_i^n\}$ for each fixed index i . According to the initial condition and default $u_i^{-1} = 0$, we have

$$\mathbf{Z}\{u_i^{n+1}\} = zU_i(z), \quad \mathbf{Z}\{u_i^{n-1}\} = \frac{1}{z}U_i(z).$$

The difference equation (5.3) becomes

$$zU_i(z) - 2U_i(z) + \frac{1}{z}U_i(z) - \alpha(U_{i+1}(z) - 2U_i(z) + U_{i-1}(z)) + \tau^2 U_i(z) = 0, \quad i = 2I + 1, 2I + 2, \dots$$

Then $\{U_i^n \mid i = 2I, 2I + 1, 2I + 2, \dots\}$ satisfy the following problem

$$-\alpha U_{i+1} + \beta(z)U_i(z) - \alpha U_{i-1} = 0, \quad i = 2I + 1, 2I + 2, \dots, \tag{5.5}$$

$$U_i(z) \rightarrow 0, \quad i \rightarrow +\infty, \tag{5.6}$$

where $\beta(z) = z + \frac{1}{z} + c$, $c = \tau^2 + 2(\frac{\tau}{h})^2 - 2$. Eq. (5.5) is a homogeneous 2nd order difference equation with constant coefficients, of which the solution has the form:

$$U_i(z) = (\lambda(z))^{i-1} U_{2I}(z), \quad i = 2I, 2I + 1, 2I + 2, \dots \tag{5.7}$$

Then $\lambda(z)$ satisfies

$$\alpha \lambda^2(z) - \beta(z)\lambda(z) + \alpha = 0. \tag{5.8}$$

By Eq. (5.8) and the assumptions (5.6), (5.7), we get:

$$\begin{aligned} \lambda(z) &= \frac{\beta(z) - \sqrt{\beta^2(z) - 4\alpha^2}}{2\alpha} = \frac{z + 1/z + c - \sqrt{z^2 + r_1 z + r_2 + r_3/z + 1/z^2}}{2\alpha} \\ &= \frac{z + 1/z + c - z\sqrt{1 + r_1/z + r_2/z^2 + r_3/z^3 + 1/z^4}}{2\alpha} \\ &\equiv \frac{z + 1/z + c - zS(z)}{2\alpha}, \end{aligned} \tag{5.9}$$

where $r_1 = r_3 = 2c$, $r_2 = 2 + c^2 - 4\alpha^2$ are three constants. First, we try to find the Laurent expansion of $S(z)$. Observe that $S'(z)$ satisfies,

$$S'(z) = \frac{-r_1/z^2 - 2r_2/z^3 - 3r_3/z^4 - 4/z^5}{2S(z)},$$

hence

$$2S'(z) \left(1 + \frac{r_1}{z} + \frac{r_2}{z^2} + \frac{r_3}{z^3} + \frac{1}{z^4}\right) = \left(-\frac{r_1}{z^2} - \frac{2r_2}{z^3} - \frac{3r_3}{z^4} - \frac{4}{z^5}\right) S(z). \tag{5.10}$$

Next, we assume that $S(z) = 1 + \sum_{n \geq 1} a_n z^{-n}$ and $S'(z) = -\sum_{n \geq 1} n a_n z^{-n-1}$, using the formula (5.10) we can obtain a recursion relation of a_n for $n \geq 5$,

$$a_n = \frac{1}{2n} \{ (3 - 2n)r_1 a_{n-1} + (6 - 2n)r_2 a_{n-2} + (9 - 2n)r_3 a_{n-3} + (12 - 2n)a_{n-4} \},$$

with

$$a_1 = \frac{r_1}{2}, \quad a_2 = \frac{r_2}{2} - \frac{a_1 r_1}{4}, \quad a_3 = \frac{r_3}{2} - \frac{a_2 r_1}{2}, \quad a_4 = \frac{1}{2} + \frac{a_1 r_3}{8} - \frac{a_2 r_2}{4} - \frac{5a_3 r_1}{8}.$$

According to (5.9), we obtain the Laurent series of $\lambda(z) = \sum_{n=0}^{+\infty} \lambda_n z^{-n}$:

$$\lambda_0 = \frac{c - a_1}{2\alpha}, \quad \lambda_1 = \frac{1 - a_2}{2\alpha}, \quad \lambda_n = -\frac{a_{n+1}}{2\alpha}, \quad n \geq 2.$$

From Fig. 1 we can see that the absolute value of λ_n decline very quickly. The method of computing the Laurent coefficients through an ODE was first given in Section 2 of Chapter 1 in [10]. Now, we get the inverse transform of $\lambda(z)$

$$\mathbf{Z}^{-1}\{\lambda(z)\} = \{\lambda_n\}.$$

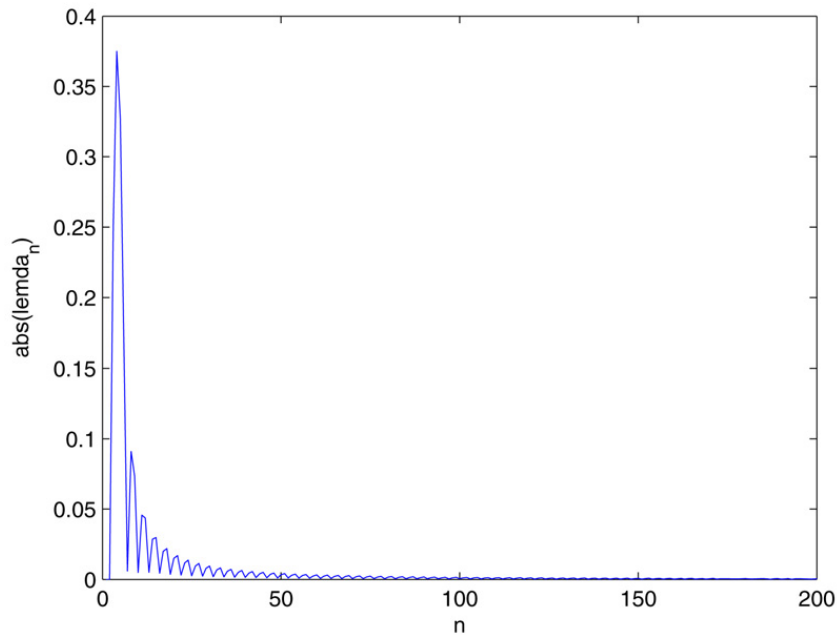


Fig. 1. The decay tendency of the coefficient $\{\lambda_n\}$, here $h = 0.01$, $\tau = 0.005$.

According to the formula (5.7) and the convolution theorem for Z-transforms, we get

$$u_{2l+1}^n = \sum_{k=0}^n \lambda_{n-k} u_{2l}^k, \quad n = 2, 3, \dots$$

This is the DABC on the boundary Σ_{2l+1}^h , we are trying to find. Similarly, we can get the DABC on the boundary Σ_{-1}^h as following

$$u_{-1}^n = \sum_{k=0}^n \lambda_{n-k} u_0^k, \quad n = 2, 3, \dots$$

In practical, we can make some tables for the coefficients $\{\lambda_n | n \geq 0\}$ before starting the numerical computations.

Using our DABCs, the numerical solution on the computational domain D_i exactly equals the restriction of the discrete whole-space solution on the computational domain. Therefore, this scheme prevents any numerical reflections at the boundary.

Remark 5.1. According to our calculation, these coefficients $\{\lambda_n\}$ are exact, the numerical error of the DABC method is just equal to the discretization error of (5.1), (5.2) on the unbounded domain $\mathbf{R}^1 \times [0, T]$. Hence the DABC method has the second order convergence.

Remark 5.2. One can also compute explicit solution to inhomogeneous 2nd order difference equation with constant coefficients, see [9]. So with only very minor changes, we can also deal with the Klein–Gordon equation with initial data that is not supported within the computational domain.

6. Numerical tests

To show the effectiveness of different boundary conditions, ABC, DABC and the fast algorithm (FAST) are given in this paper. We present some numerical examples in this section. In Example 1, we consider the Klein–Gordon equation without source term, the exact solution is given, and the numerical solutions are compared with the exact solution. The second example is the Klein–Gordon equation with source term, simultaneously we compare the computational time of the different schemes for Example 2. We also test the relation between the numerical accuracy of the fast algorithm and the optimal strategy of choosing K , especially, we test the long time performance of the fast algorithm (FAST).

Example 1. We consider the Klein–Gordon equation without source term:

$$\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} + u = 0, \quad \forall x \in \mathbf{R}^1, t \geq 0,$$

Table 1

Computational errors and convergence rate of the difference schemes for Example 1 ($t = 0.5$ s).

Mesh size	ABC	FAST	DABC
1/20	1.8342E-1 ...	1.8389E-1 ...	2.4531E-1 ...
1/40	4.8302E-2 1.8986	4.8426E-2 1.8987	6.6407E-2 1.8470
1/80	1.3002E-2 1.8573	1.3035E-2 1.8574	1.8219E-2 1.8224
1/160	2.9430E-3 2.2090	2.9505E-3 2.2091	4.3234E-3 2.1069

Table 2

Computational errors and convergence rate of the difference schemes for Example 1 ($t = 1.0$ s).

Mesh size	ABC	FAST	DABC
1/20	8.8304E-2 ...	8.8387E-2 ...	6.8669E-2 ...
1/40	2.1502E-2 2.0533	2.1550E-2 2.0506	1.4306E-2 2.3999
1/80	5.4552E-3 1.9707	5.4717E-3 1.9692	3.9813E-3 1.7966
1/160	1.3212E-3 2.0644	1.3257E-3 2.0635	1.3178E-3 1.5104

Table 3

Computational errors and convergence rate of the difference schemes for Example 2 ($t = 1.0$ s).

Mesh size	ABC	FAST	DABC
1/20	8.2727E-2 ...	8.3344E-2 ...	6.9831E-2 ...
1/40	2.0447E-2 2.0229	2.0659E-2 2.0171	1.5699E-2 2.2240
1/80	5.2655E-3 1.9516	5.3282E-3 1.9386	4.4639E-3 1.7584
1/160	1.2735E-3 2.0672	1.2890E-3 2.0667	1.3693E-3 1.6975

$$u|_{t=0} = \begin{cases} \sin(5\pi x), & |x| \leq 1, \\ 0, & |x| > 1, \end{cases}$$

$$u_t|_{t=0} = 0, \quad \forall x \in \mathbb{R}^1$$

which has the exact solution:

$$u(x, t) = \frac{1}{2} \{ \phi_0(x+t) + \phi_0(x-t) \} - \frac{t}{2} \int_{x-t}^{x+t} \phi_0(\xi) \frac{J_1(\sqrt{t^2 - (x-\xi)^2})}{\sqrt{t^2 - (x-\xi)^2}} d\xi,$$

where $\phi_0(x) = u|_{t=0}$. The solution represents two waves propagating to the left and right respectively with amplitudes gradually decreasing. To evaluate the quality of numerical solution, we define an error function as

$$E(t) = \frac{\|u_{\text{num}}(\cdot, t) - u_{\text{exa}}(\cdot, t)\|_{L^2}}{\|u_{\text{exa}}(\cdot, t)\|_{L^2}}.$$

The relative error and convergence rates of Example 1 are shown in Table 1 ($t = 0.5$ s) and Table 2 ($t = 1.0$ s). It can be observed that the errors decay with a nearly-optimal convergence rate of 4 when the mesh is refined by a factor 2. When the computation time $t = 2$, all the original wave will propagate out the computational domain.

Example 2. Secondly, we consider the same Klein–Gordon equation with source term, which will physically effect the wave propagations.

$$\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} + u = 10 \cos(5t) \sin(3\pi x), \quad \forall x \in \mathbb{R}^1, t \geq 0,$$

$$u|_{t=0} = \begin{cases} \sin(5\pi x), & |x| \leq 1, \\ 0, & |x| > 1, \end{cases}$$

$$u_t|_{t=0} = 0, \quad \forall x \in \mathbb{R}^1.$$

In this example, the “exact solution” is given on a very fine mesh ($h = \frac{1}{640}$, $\tau = \frac{h}{2}$). The relative error and convergence rates of Example 2 are shown in Table 3 ($t = 1.0$ s) and Table 4 ($t = 1.5$ s). It can be observed that the errors decay with a nearly-optimal convergence rate of 4 when the mesh is refined by a factor 2.

Fig. 2 shows the wave amplitudes of difference schemes at fixed times, left one is for Example 1 ($t = 1.0$ s) and right one is for Example 2 ($t = 1.5$ s). Compared with the left one, we can find that the external force can generate new wave, when the original wave propagate out the computational domain.

Table 4

Computational errors and convergence rate of the difference schemes for Example 2 ($t = 1.5$ s).

Mesh size	ABC	FAST	DABC
1/20	1.4313E-1 ...	1.4944E-1 ...	2.2887E-1 ...
1/40	3.5462E-2 2.0181	3.7102E-2 2.0140	6.2109E-2 1.8425
1/80	9.2490E-3 1.9170	9.6787E-3 1.9166	1.6798E-2 1.8486
1/160	2.1870E-3 2.1145	2.2838E-3 2.1189	4.1326E-3 2.0323

Table 5

Computational time of different scheme for Example 2 ($t = 1.0$ s).

h (mesh size)	ABC	DABC	FAST
1/10	0.18536	0.00055	0.00357
1/20	0.81051	0.00099	0.00420
1/40	3.34773	0.00311	0.00533
1/80	13.6388	0.00638	0.00853
1/160	55.5626	0.02028	0.01427
1/320	229.469	0.07662	0.03335

Table 6

The relation between computational accuracy and K , for fixed mesh size $h = 1/320$.

Terminal time	K	Time cost (seconds)	Error
$T = 1$	$K = 2$	0.109000	4.26576e-009
$T = 2$	$K = 4$	0.297000	1.15538e-009
$T = 3$	$K = 6$	0.453000	2.036991e-010
$T = 4$	$K = 8$	0.610000	2.384202e-011
$T = 5$	$K = 8$	0.766000	1.027745e-009
$T = 6$	$K = 10$	0.953000	1.200938e-010
$T = 7$	$K = 10$	1.125000	3.230213e-009
$T = 8$	$K = 12$	1.328000	4.558574e-010
$T = 9$	$K = 12$	1.469000	8.079006e-009
$T = 10$	$K = 14$	1.688000	1.235935e-009
$T = 12$	$K = 16$	2.328000	2.918184e-009
$T = 16$	$K = 20$	2.687000	1.304432e-009
$T = 20$	$K = 26$	3.796000	2.365757e-009

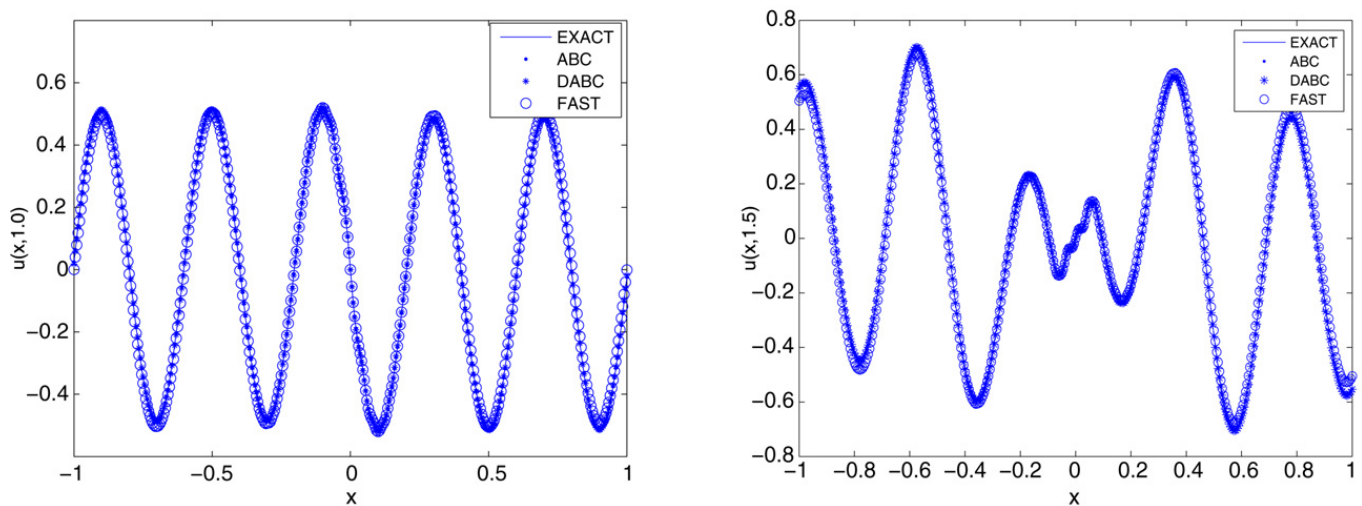


Fig. 2. Wave amplitudes of different schemes at fixed times, left is for Example 1 ($t = 1.0$ s), right is for Example 2 ($t = 1.5$ s).

Table 5 shows computational time of difference scheme for Example 2 ($t = 1.0$ s). The ABC method is very expensive for numerical computation, when the mesh is very fine. The FAST algorithm improves the efficiency dramatically, and the DABC method is very fast too.

Table 6 shows the relation between computational accuracy of the fast algorithm and the optimal strategy of choosing K , here the Error function is defined by

$$Error(T) = \|u_{num}(\cdot, T) - u_{exa}(\cdot, T)\|_{L^2}.$$

In Eq. (4.2) of Section 4, we truncate the power series expansion of the special function $\mathbf{J}(t - \tau)$ to obtain a fast algorithm.

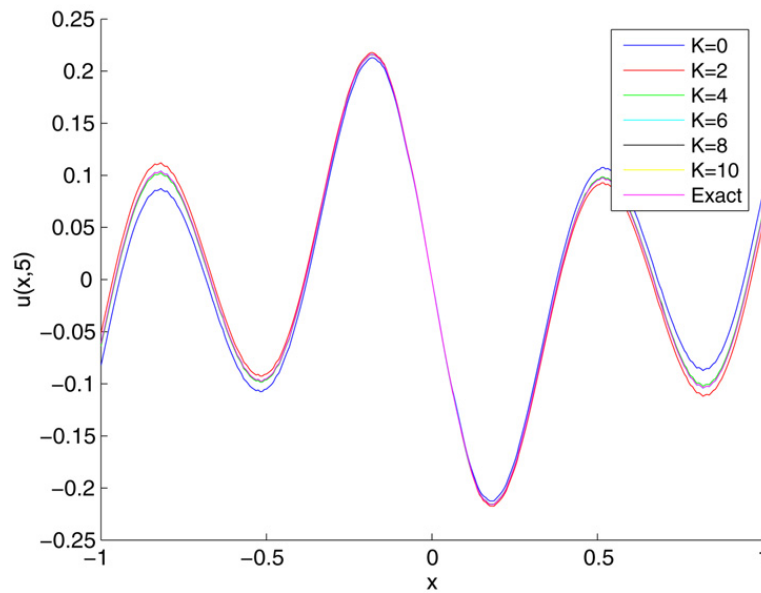


Fig. 3. The relationship between the choosing of K and the accuracy of the result for Example 2 with the fixed time $t = 5$, $h = 1/160$.

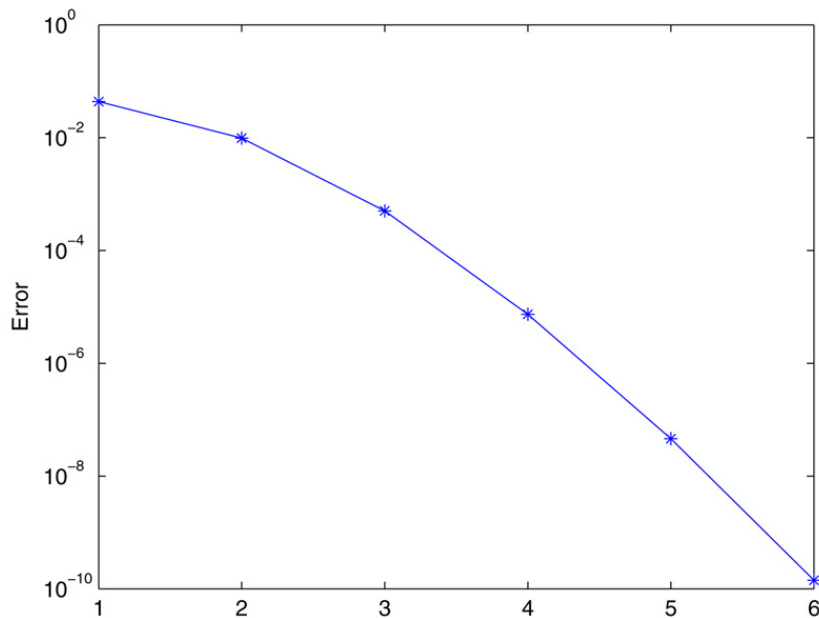


Fig. 4. The decay rate of the error in L_2 norm in choosing different K for Example 2 with the fixed time $t = 5$. From left to right, $K = 0, 2, 4, 6, 8, 10$, $h = 1/160$.

Numerical tests indicate that the numerical accuracy of the fast algorithm highly depends on the computational time t and the choosing of truncation term number K . When the computational time is not very long compared with the spatial domain $[-1, 1]$, only using few terms (with K small) can get a very high accuracy. For long time computation, in order to get the same accuracy, we must increase the term number K accordingly.

Fig. 3 shows the relation between computational accuracy and the different number K . For the fixed time $t = 5$, we can see that when $K \geq 4$, the numerical solution is almost the same with the exact solution. Fig. 4 shows the convergence rate between the numerical solution and the exact solution for different K . Fig. 5 shows the long time propagation of the Klein–Gordon equation.

7. Conclusion

In this paper, we analyze the finite difference method for the one-dimensional Klein–Gordon equation on the unbounded domain. Two artificial boundary conditions are obtained to reduce the original problem to an initial boundary value problem on a bounded computational domain, which is discretized by an explicit difference scheme. The stability and convergence of the scheme are analyzed by the energy method. A fast algorithm is obtained to reduce the computational cost and a

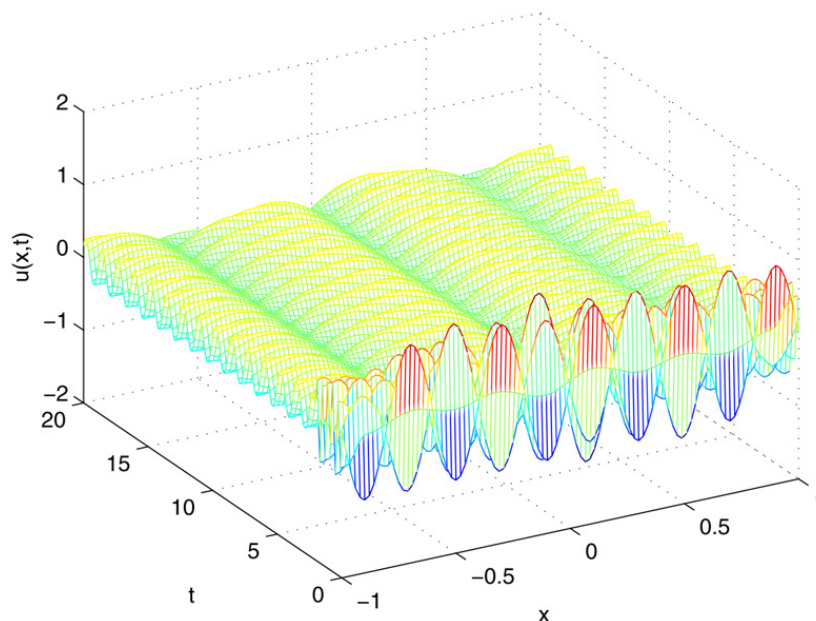


Fig. 5. Long time ($t = 20$ s) computation of Example 2.

discrete artificial boundary condition (DABC) is derived by the Z-transform approach. Finally, we illustrate the efficiency of the proposed method by several numerical examples. The artificial boundary condition for the multi-dimensional and nonlinear Klein–Gordon equation will be considered as our further work.

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