Journal of Computational Mathematics, Vol.25, No.6, 2007, 730–745.

# APPROXIMATION, STABILITY AND FAST EVALUATION OF EXACT ARTIFICIAL BOUNDARY CONDITION FOR THE ONE-DIMENSIONAL HEAT EQUATION*

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**Abstract**

In this paper we consider the numerical solution of the one-dimensional heat equation on unbounded domains. First an exact semi-discrete artificial boundary condition is derived by discretizing the time variable with the Crank-Nicolson method. The semi-discretized heat equation equipped with this boundary condition is then proved to be unconditionally stable, and its solution is shown to have second-order accuracy. In order to reduce the computational cost, we develop a new fast evaluation method for the convolution operation involved in the exact semi-discrete artificial boundary condition. A great advantage of this method is that the unconditional stability held by the semi-discretized heat equation is preserved. An error estimate is also given to show the dependence of numerical errors on the time step and the approximation accuracy of the convolution kernel. Finally, a simple numerical example is presented to validate the theoretical results.

*Mathematics subject classification:* 65N12, 65M12, 26A33.
*Key words:* Heat equation, Artificial boundary conditions, Fast evaluation, Unbounded domains.

## 1. Introduction

There are a large number of problems modeled by partial differential equations defined on unbounded domains. When numerically solving this kind of problems, a common practice is to limit the computation to a finite domain by introducing artificial boundaries. To make complete the "truncated" problem on the finite domain, artificial boundary conditions (ABCs) should be designed and applied. They are called exact if the solution of the truncated problem is exactly the same as that of the original problem on the unbounded domain. ABCs were first derived by Engquist and Majda [8] for hyperbolic systems. Since then, their idea has been extended and refined for numerous applications. Givoli [10] and Tsynkov [20] made thorough reviews on this topic.

This paper is concerned with the numerical issues related to the heat equation on one-dimensional unbounded domains. Much attention has been paid on the numerical solution to the Schrödinger equation, both linear [1, 2, 4, 6, 13, 15, 21] and nonlinear [3, 23]. Comparatively, the attention paid on the heat equation is much less [12, 14, 19, 22]. Actually, these two equations share many similarities. One lies in the fact that for one-dimensional problems on unbounded domains, both their exact ABCs (in a form of Dirichlet-to-Neumann mapping) involve the nonlocal half-order derivative operator. To well understand these two equations with exact ABCs, a key point is to explore the properties of this operator. Correspondingly, to

* Received July 24, 2006; final revised May 9, 2007; accepted May 15, 2007.

well resolve their solutions numerically, a key point is to approximate the half-order derivative operator by an efficient and stable method.

So far, there are two different numerical methods for evaluating this half-order derivative operator. The first one was proposed by Baskakov and Popov [6]. They approximated the integrands with piecewise linear interpolating functions at the discrete time points. This idea presents a 1.5th-order approximation to the half-order derivative operator, but its generalization has to be very careful. Mayfield [18] showed that even cooperated with the classical unconditionally stable Crank-Nicolson scheme for the interior discretization of the Schrödinger equation, this idea adapted for the exact ABCs in the Neumann-to-Dirichlet form can only guarantee the stability on some disjoined intervals of $\Delta t/\Delta x^2$ ($\Delta t$ is the time step, and $\Delta x$ the spatial step). Comparatively, when cooperated with a delicately designed finite difference scheme for the heat equation, Wu and Sun [22] proved the unconditional stability. Another idea to approximate the half-order derivative operator was proposed by Yevick et. al [21], Antoine and Besse [2]. The starting point is the semi-discretization of time variable with the Crank-Nicolson method for the Schrödinger equation on the whole space. By using the $\mathcal{Z}$-transform, an exact semi-discrete ABC is then derived. There are two highlights about this method. First, it presents an approximation of second-order accuracy for the half-order derivative operator, which is more accurate than the direct integration method. Second, the reduced problem with this semi-discrete ABC is unconditionally stable. Moreover, if a conforming Galerkin method is employed for the spatial discretization, this stability is automatically maintained.

No matter which method is employed, the approximate discrete half-order derivative operator involves convolution operations. If the number of time steps is large, these operations become very costly, which justifies the use of fast evaluation methods. Two candidates have been appeared in the literature. The first one was proposed by Jiang and Greengard [15]. They divided the convolution into a local part and a history part. The local part is approximated with the Baskakov-Popov method, while the history part is approximated by a sum of convolutions with decaying exponential kernels, thus fast evaluation is straightforward. The second method was given by Arnold et. al [5]. Based on their discrete transparent boundary conditions, they approximated convolution coefficients with a sum of exponentials directly. These exponentials were determined by equating a number of elements with their corresponding convolution coefficients. Both of these two methods work well for some problems, as their numerical tests demonstrated, but up to now, neither of them can ensure stability in a rigorous mathematical way.

In this paper, following the idea of [2, 21], we will derive the exact semi-discrete ABC for the one-dimensional heat equation. Stability of the reduced problem will be proved, and we will show that this semi-discrete approximation is of second-order accuracy, which is superior to the scheme proposed by Wu and Sun [22]. A new fast evaluation method will be proposed for the half-order derivative operator. We will rigorously prove its stability and present an error estimate which shows the dependence of numerical error on the time step and the approximating accuracy of the convolution kernel.

## 2. Preliminary

The $\mathcal{Z}$-transform of a complex sequence $\mathbf{f} = \{f_0, f_1, \cdots\}$ is defined as the power series

$$\mathcal{Z}\{\mathbf{f}\}(z) = \sum_{n=0}^{+\infty} f_n z^{-n}. \tag{2.1}$$

Its radius of convergence is denoted by $R(\mathcal{Z}\{\mathbf{f}\})$. We will use the following Plancherel theorem for the $\mathcal{Z}$-transform.

**Lemma 2.1.** *Let* $\mathbf{f} = \{f_0, f_1, \cdots\}$ *and* $\mathbf{g} = \{g_0, g_1, \cdots\}$ *be two complex sequences. If* $R(\mathcal{Z}\{\mathbf{f}\}) < 1$ *and* $R(\mathcal{Z}\{\mathbf{g}\}) < 1$*, then*

$$\sum_{n=0}^{+\infty} f_n \bar{g}_n = \frac{1}{2\pi}\int_0^{2\pi} \mathcal{Z}\{\mathbf{f}\}(e^{i\varphi})\overline{\mathcal{Z}\{\mathbf{g}\}(e^{i\varphi})}d\varphi. \tag{2.2}$$

*Moreover, if* $R(\mathcal{Z}\{\mathbf{f}\}) < 1$ *and* $R(\mathcal{Z}\{\mathbf{g}\}) = 1$*, then for any* $\rho$ *satisfying* $R(\mathcal{Z}\{\mathbf{f}\}) < \rho < 1$ *we have*

$$\sum_{n=0}^{+\infty} f_n \bar{g}_n = \frac{1}{2\pi}\int_0^{2\pi} \mathcal{Z}\{\mathbf{f}\}(\rho e^{i\varphi})\overline{\mathcal{Z}\{\mathbf{g}\}(\rho^{-1}e^{i\varphi})}d\varphi. \tag{2.3}$$

The following embedding result is standard.

**Lemma 2.2.** $H^1[x_L, x_R]$ *is continuously embedded into* $C[x_L, x_R]$*, i.e., there exists a constant* $C_1$ *dependent only on the length of interval* $[x_L, x_R]$*, such that*

$$||f||_{\infty,[x_L,x_R]} \leq C_1 ||f||_{1,[x_L,x_R]}, \ \forall f \in H^1[x_L, x_R]. \tag{2.4}$$

To prove the stability property, we will use the discrete Gronwall inequality [16].

**Lemma 2.3.** *If* $x_j, j = 0, \cdots, N$ *is a sequence of real numbers with*

$$|x_j| \leq \delta + M\sum_{j=0}^{i-1} |x_j|, \ i = 1, \cdots, N, \tag{2.5}$$

*where* $M$ *and* $\delta$ *are two positive real numbers, then*

$$|x_i| \leq (M|x_0| + \delta)\exp[iM], \ i = 1, \cdots, N. \tag{2.6}$$

## 3. Approximation and Stability of an Exact ABC

We consider the heat equation of the form

$$\partial_t u = \partial_{xx} u + f(x,t), \ x \in \mathbf{R}, \ 0 < t \leq T_f, \tag{3.1}$$

$$\lim_{x\to\infty} u(x,t) = 0, \ 0 < t \leq T_f, \tag{3.2}$$

$$u(x,0) = u_0(x), \ x \in \mathbf{R}. \tag{3.3}$$

Here, $T_f$ denotes the ending time point. We assume that both the source function $f$ and the initial function $u_0$ are compactly supported in an interval $[x_L, x_R]$, with $x_L < x_R$. It is known that with this assumption, an exact boundary condition can be built at the artificial boundary $\{x_L, x_R\} \times (0, T_f]$, which is introduced for limiting the computational domain. Applying this boundary condition leads to a reduced problem, of which the solution is the same as that of the original one (3.1)-(3.3) being restricted to $[x_L, x_R] \times (0, T_f]$:

$$\partial_t u = \partial_{xx} u + f(x,t), \ x \in [x_L, x_R], \ 0 < t \leq T_f, \tag{3.4}$$

$$\partial_\nu u + \partial_t^{\frac{1}{2}} u = 0, \ x \in \{x_L, x_R\}, \ 0 < t \leq T_f, \tag{3.5}$$

$$u(x,0) = u_0(x), \ x \in [x_L, x_R]. \tag{3.6}$$

Here, $\partial_\nu = -\partial_x$ if $x = x_L$, and $\partial_\nu = \partial_x$ if $x = x_R$. $\partial_t^{\frac{1}{2}}$ denotes the half-order derivative operator defined as

$$\partial_t^{1/2} v = \frac{1}{\sqrt{\pi}} \partial_t \int_0^t \frac{v(s)}{\sqrt{t-s}} ds. \tag{3.7}$$

The readers are referred to [11] for detail.

Now we turn to the numerical solution of the problem (3.4)-(3.6). For brevity and simplicity, we only consider the time discretization. All the results can be modified correspondingly without difficulty if a conforming Galerkin method is employed for the spatial discretization. Generally speaking, to obtain the approximate solution of the problem (3.4)-(3.6), there are two questions which must be answered. The first one is how to discretize the governing heat equation (3.4). As to this point, a common approach is to use the Crank-Nicolson scheme, which is also the choice used in this paper. The second question is how to approximate the half-order derivative operator $\partial_t^{\frac{1}{2}}$ involved in the artificial boundary condition (3.5). So far, there are two different methods. Baskakov and Popov [6] used the piecewise linear interpolation to approximate the integrating function in the definition of half-order derivative operator (3.7), thus derived a discretization with 1.5th-order accuracy. Based on the Crank-Nicolson discretization in time for the Schrödinger equation on the whole space, Yevick, Friese and Schmidt [21], Antoine and Besse [2] derived an approximation of $\partial_t^{\frac{1}{2}}$ with second-order accuracy. Following their idea, we will design an exact semi-discrete ABC for the heat equation in the following.

Let $\Delta t$ be the time step, and let $N = [T_f/\Delta t]$ be the total number of time steps. Besides, we let $G_n(\cdot) \sim g(\cdot, t_n)$, with $t_n = n\Delta t$ for any given function $g(\cdot, t)$. The Crank-Nicolson scheme reads for the whole-space problem (3.1)-(3.3) as

$$\frac{U_n - U_{n-1}}{\Delta t} = \frac{\partial_{xx} U_n + \partial_{xx} U_{n-1}}{2} + \frac{F_n + F_{n-1}}{2}, \ x \in \mathbf{R}, \ 1 \le n \le N, \tag{3.8}$$

$$\lim_{x\to\infty} U_n(x) = 0, \ 1 \le n \le N, \tag{3.9}$$

$$U_0(x) = u_0(x), \ x \in \mathbf{R}. \tag{3.10}$$

Due to our assumption on the source function $f$ and the initial function $u_0$, on the spatial domain $(-\infty, x_L] \cup [x_R, +\infty)$, the above problem is simplified as

$$\frac{U_n - U_{n-1}}{\Delta t} = \frac{\partial_{xx} U_n + \partial_{xx} U_{n-1}}{2}, \ x \in (-\infty, x_L] \cup [x_R, \infty), \ 1 \le n \le N, \tag{3.11}$$

$$\lim_{x\to\infty} U_n(x) = 0, \ 1 \le n \le N, \tag{3.12}$$

$$U_0(x) = 0, \ x \in (-\infty, x_L] \cup [x_R, \infty). \tag{3.13}$$

Performing the $\mathcal{Z}$-transform on both sides of equation (3.11) and using (3.13), we get

$$\partial_{xx} \mathcal{Z}\{\mathbf{U}\} = \frac{2}{\Delta t} \frac{1 - z^{-1}}{1 + z^{-1}} \mathcal{Z}\{\mathbf{U}\},$$

where $\mathbf{U} = \{U_0, U_1, \cdots\}$. This equation has two general solutions. Subject to the infinity condition (3.12), the solution must behave like

$$\mathcal{Z}\{\mathbf{U}\} \sim \exp\left(-x \sqrt[+]{\frac{2}{\Delta t} \frac{1 - z^{-1}}{1 + z^{-1}}}\right), \quad x \in [x_R, +\infty),$$

and

$$\mathcal{Z}\{\mathbf{U}\} \sim \exp\left(x \sqrt[+]{\frac{2}{\Delta t} \frac{1 - z^{-1}}{1 + z^{-1}}}\right), \quad x \in [-\infty, x_L].$$

Thus an exact relation can be set up as

$$\partial_\nu \mathcal{Z}\{\mathbf{U}\} + \sqrt[+]{\frac{2}{\Delta t}\frac{1-z^{-1}}{1+z^{-1}}}\,\mathcal{Z}\{\mathbf{U}\} = 0,\ x \in \{x_L, x_R\}.$$

By the inverse $\mathcal{Z}$-transform we arrive at

$$\partial_\nu U_n + D_t^{\frac{1}{2}} U_n = 0,\ x \in \{x_L, x_R\}, \tag{3.14}$$

where $D_t^{\frac{1}{2}}$ is defined as

$$D_t^{\frac{1}{2}} v_n = \sqrt{\frac{2}{\Delta t}} \sum_{m=0}^{n} \alpha_m v_{n-m},$$

with $\{v_0, v_1, \cdots\}$ being any given sequence, and

$$\alpha_m = \begin{cases} \beta_k = \dfrac{(2k)!}{2^{2k}(k!)^2}, & m = 2k, \\ -\beta_k, & m = 2k+1. \end{cases} \tag{3.15}$$

Here, the sequence $\{\alpha_0, \alpha_1, \cdots\}$ is just the inverse $\mathcal{Z}$-transform of $\sqrt[+]{\frac{1-z^{-1}}{1+z^{-1}}}$, see [2]. Eq. (3.14) forms an exact ABC for the semi-discrete problem (3.8)-(3.10). Since (3.8) is an approximation of the continuous equation (3.1), $D_t^{\frac{1}{2}}$ must be some approximation of $\partial_t^{\frac{1}{2}}$. This is indeed true. The following lemma can be found in Lubich [17].

**Lemma 3.1.** *If $v \in C^2[0, T_f]$ with $v(0) = v'(0) = 0$, then for any $n \geq 0$ with $n\Delta t \leq T_f$, it holds*

$$|\partial_t^{\frac{1}{2}} v(t_n) - D_t^{\frac{1}{2}} v_n| \leq C_2 \max_{t \in [0, T_f]} |v''(t)| \Delta t^2.$$

*Here, $v_n = v(t_n)$, and $C_2$ is a constant independent of any parameter.*

Now applying the semi-discrete ABC (3.14), we derive a semi-discrete problem defined only on the finite interval $[x_L, x_R]$,

$$\frac{U_n - U_{n-1}}{\Delta t} = \frac{\partial_{xx} U_n + \partial_{xx} U_{n-1}}{2} + \frac{F_n + F_{n-1}}{2},\ x \in [x_L, x_R],\ 1 \leq n \leq N, \tag{3.16}$$

$$\partial_\nu U_n + D_t^{\frac{1}{2}} U_n = 0,\ x \in \{x_L, x_R\},\ 0 \leq n \leq N, \tag{3.17}$$

$$U_0(x) = u_0(x),\ x \in [x_L, x_R]. \tag{3.18}$$

**Lemma 3.2.** *Let $\mathbf{v} = \{v_0, v_1 \cdots\}$ be a real sequence. For any nonnegative integer $n$, we have*

$$\sum_{m=0}^{n} v_m D_t^{1/2} v_m \geq 0.$$

*Proof.* For any fixed $n$, we define the sequence $\mathbf{V} = \{V_0, V_1, \cdots\}$ as

$$V_m = \begin{cases} v_m, & m \leq n, \\ 0, & m > n. \end{cases}$$

Since

$$\sum_{m=0}^{n} v_m D_t^{1/2} v_m = \sum_{m=0}^{+\infty} V_m D_t^{1/2} V_m,$$

if we can show the right hand side is not less than zero, this lemma is then proved.

It is obvious that $R(\mathcal{Z}\{\mathbf{V}\})$ equals zero since $\mathbf{V}$ has at most finite nonzero elements. Let $\alpha = \{\alpha_0, \alpha_1, \cdots\}$. It is straightforward to verify that $R(\mathcal{Z}\{\alpha\}) = 1$. Thus then, if denoting

$$\mathbf{W} = \{D_t^{\frac{1}{2}} V_0, D_t^{\frac{1}{2}} V_1, \cdots\},$$

we have $R(\mathcal{Z}\{\mathbf{W}\}) = 1$, since

$$D_t^{\frac{1}{2}} V_m = \frac{2}{\sqrt{2\Delta t}} \alpha_m * V_m,$$

with $*$ denoting the convolution operation. For any $\rho \in [\frac{1}{2}, 1)$, by the Plancherel theorem (see Lemma 2.1) for the $\mathcal{Z}$-transform, we have

$$\sum_{m=0}^{+\infty} V^m D_t^{1/2} V^m = \frac{1}{2\pi} \Re \int_0^{2\pi} \overline{\mathcal{Z}\{\mathbf{V}\}(\rho e^{i\varphi})} \mathcal{Z}\{\mathbf{W}\}(\rho^{-1} e^{i\varphi}) d\varphi$$
$$= \frac{1}{2\pi} \Re \int_0^{2\pi} \overline{\mathcal{Z}\{\mathbf{V}\}(\rho e^{i\varphi})} \mathcal{Z}\{\mathbf{V}\}(\rho^{-1} e^{i\varphi}) \sqrt[+]{\frac{2}{\Delta t} \frac{1 - \rho e^{-i\varphi}}{1 + \rho e^{-i\varphi}}} d\varphi. \tag{3.19}$$

When $\rho \to 1$, then function $\sqrt[+]{\frac{2}{\Delta t} \frac{1 - \rho e^{-i\varphi}}{1 + \rho e^{-i\varphi}}}$ is singular at $\varphi = \pi$. But fortunately, this singularity is weak. Thus for any $\epsilon > 0$, there exists a constant $\delta > 0$, such that for any $\rho \in [\frac{1}{2}, 1]$, it holds that

$$\int_{\pi-\delta}^{\pi+\delta} \sqrt[+]{\frac{2}{\Delta t} \frac{1 - \rho e^{-i\varphi}}{1 + \rho e^{-i\varphi}}} d\varphi < \epsilon.$$

Since $R(\mathcal{Z}\{\mathbf{V}\}) = 0$, the function $\overline{\mathcal{Z}\{\mathbf{V}\}(\rho e^{i\varphi})} \mathcal{Z}\{\mathbf{V}\}(\rho^{-1} e^{i\varphi})$ is bounded by some constant $M > 0$, and uniformly continuous in the annular domain $\left\{z : \frac{1}{2} \le |z| \le 2\right\}$. Consequently,

$$\sum_{m=0}^{+\infty} V^m D_t^{1/2} V^m$$
$$= \frac{1}{2\pi} \Re \lim_{\rho \to 1^-} \left( \int_0^{\pi-\delta} + \int_{\pi-\delta}^{\pi+\delta} + \int_{\pi+\delta}^{2\pi} \right) \overline{\mathcal{Z}\{\mathbf{V}\}(\rho e^{i\varphi})} \mathcal{Z}\{\mathbf{V}\}(\rho^{-1} e^{i\varphi}) \sqrt[+]{\frac{2}{\Delta t} \frac{1 - \rho e^{-i\varphi}}{1 + \rho e^{-i\varphi}}} d\varphi$$
$$\ge \frac{1}{2\pi} \Re \left( \int_0^{\pi-\delta} + \int_{\pi+\delta}^{2\pi} \right) |\mathcal{Z}\{\mathbf{V}\}(e^{i\varphi})|^2 \sqrt[+]{\frac{2}{\Delta t} \frac{1 - e^{-i\varphi}}{1 + e^{-i\varphi}}} d\varphi - \frac{M\epsilon}{2\pi}$$
$$\ge \frac{1}{2\pi} \Re \int_0^{2\pi} |\mathcal{Z}\{\mathbf{V}\}(e^{i\varphi})|^2 \sqrt[+]{\frac{2}{\Delta t} \frac{1 - e^{-i\varphi}}{1 + e^{-i\varphi}}} d\varphi - \frac{2M\epsilon}{2\pi} \ge -\frac{2M\epsilon}{2\pi}.$$

The proof is complete taking $\epsilon \to 0$. $\square$

**Theorem 3.1.** *Let $U_n$ be the solution of the following problem:*

$$\frac{U_n - U_{n-1}}{\Delta t} = \frac{\partial_{xx} U_n + \partial_{xx} U_{n-1}}{2} + A_{n-\frac{1}{2}}, \quad x \in [x_L, x_R], \quad 1 \le n \le N, \tag{3.20}$$
$$\partial_\nu U_n + \mathcal{M} U_n = B_n, \ x \in \{x_L, x_R\}, \ 0 \le n \le N, \tag{3.21}$$
$$U_0(x) = u_0(x), \ x \in [x_L, x_R], \tag{3.22}$$

*where $\mathcal{M}$ is a linear operator from the sequence space to itself and satisfies*

$$\sum_{m=0}^{n} f_m \mathcal{M} f_m \ge 0$$

*for any real sequence $\{f_0, f_1, \cdots\}$. If $\Delta t \le \frac{1}{4}$, then we have the estimate*

$$||U_n||_0^2 \le C_3 \left( ||u_0||_0^2 + \Delta t \sum_{x\in\{x_L,x_R\}} \sum_{m=0}^{n} |B_m|^2 + \Delta t \sum_{m=1}^{n} ||A_{m-\frac{1}{2}}||_0^2 \right), \tag{3.23}$$

*where $C_3$ depends only on the length of interval $[x_L, x_R]$ and the ending time point $T_f$.*

*Proof.* Multiplying both sides of equation (3.20) with $U_{n-\frac{1}{2}} = (U_n + U_{n-1})/2$, and integrating with respect to $x$ on $[x_L, x_R]$, we have

$$\begin{aligned}
&\frac{||U_n||_0^2 - ||U_{n-1}||_0^2}{2\Delta t} \\
=\ & (\partial_{xx} U_{n-\frac{1}{2}}, U_{n-\frac{1}{2}}) + (A_{n-\frac{1}{2}}, U_{n-\frac{1}{2}}) \\
=\ & -||\partial_x U_{n-\frac{1}{2}}||_0^2 + \sum_{x\in\{x_L,x_R\}} (B_{n-\frac{1}{2}} - \mathcal{M} U_{n-\frac{1}{2}}, U_{n-\frac{1}{2}}) + (A_{n-\frac{1}{2}}, U_{n-\frac{1}{2}}) \\
\le\ & -||\partial_x U_{n-\frac{1}{2}}||_0^2 + \sum_{x\in\{x_L,x_R\}} \left( \frac{1}{4C_1^2} |U_{n-\frac{1}{2}}|^2 + C_1^2 |B_{n-\frac{1}{2}}|^2 \right) \\
& - \sum_{x\in\{x_L,x_R\}} U_{n-\frac{1}{2}} \mathcal{M} U_{n-\frac{1}{2}} + \frac{1}{2} ||U_{n-\frac{1}{2}}||_0^2 + \frac{1}{2} ||A_{n-\frac{1}{2}}||_0^2 \\
\le\ & ||U_{n-\frac{1}{2}}||_0^2 + C_1^2 \sum_{x\in\{x_L,x_R\}} |B_{n-\frac{1}{2}}|^2 - \sum_{x\in\{x_L,x_R\}} U_{n-\frac{1}{2}} \mathcal{M} U_{n-\frac{1}{2}} + \frac{1}{2} ||A_{n-\frac{1}{2}}||_0^2.
\end{aligned}$$

Summing up with $n$ and using the assumption on $\mathcal{M}$ gives

$$\begin{aligned}
&\frac{||U_n||_0^2 - ||u_0||_0^2}{2\Delta t} \\
\le\ & \sum_{m=1}^{n} ||U_{m-\frac{1}{2}}||_0^2 + C_1^2 \sum_{x\in\{x_L,x_R\}} \sum_{m=1}^{n} |B_{m-\frac{1}{2}}|^2 + \frac{1}{2} \sum_{m=1}^{n} ||A_{m-\frac{1}{2}}||_0^2 \\
\le\ & \sum_{m=0}^{n} ||U_m||_0^2 + C_1^2 \sum_{x\in\{x_L,x_R\}} \sum_{m=0}^{n} |B_m|^2 + \frac{1}{2} \sum_{m=1}^{n} ||A_{m-\frac{1}{2}}||_0^2.
\end{aligned}$$

Consequently,

$$\begin{aligned}
(1 - 2\Delta t)||U_n||_0^2 \le\ & ||u_0||_0^2 + 2\Delta t \sum_{m=0}^{n-1} ||U_m||_0^2 \\
& + 2\Delta t C_1^2 \sum_{x\in\{x_L,x_R\}} \sum_{m=0}^{n} |B_m|^2 + \Delta t \sum_{m=1}^{n} ||A_{m-\frac{1}{2}}||_0^2.
\end{aligned}$$

Since $\Delta t \le \frac{1}{4}$, we have

$$||U_n||_0^2 \le 2||u_0||_0^2 + \sum_{m=0}^{n-1} ||U_m||_0^2 + C_1^2 \sum_{x\in\{x_L,x_R\}} \sum_{m=0}^{n} |B_m|^2 + \frac{1}{2} \sum_{m=1}^{n} ||A_{m-\frac{1}{2}}||_0^2.$$

Using the discrete Gronwall's inequality Lemma 2.3, the desired inequality (3.23) is obtained with $C_3 = \max(2, C_1^2) \exp(T_f)$. Here we use the fact that $N\Delta t \le T_f$. $\square$

Thanks to Lemma 3.2 and Theorem 3.1, we have

**Theorem 3.2.** *The semi-discrete problem* (3.16)-(3.18) *is stable in the* $L^2$ *sense. Thus it admits at most one solution.*

**Theorem 3.3.** *Let* $u$ *be the solution of the continuous problem* (3.1)-(3.3)*, and assume that* $u$ *is sufficiently smooth. If* $U_n$ *is the solution of the semi-discrete problem* (3.16)-(3.18) *and* $\Delta t \le \frac{1}{4}$*, we have*

$$||e_n||_0 \le C_4 \Delta t^2, \tag{3.24}$$

*where* $e_n = u_n - U_n$*,* $C_4$ *is a constant independent of* $\Delta t$*, but dependent on* $T_f$*, the length of interval* $[x_L, x_R]$ *and the solution* $u$*.*

*Proof.* By the Taylor expansion and Lemma 3.1, we have

$$\begin{aligned}&\frac{u_n - u_{n-1}}{\Delta t} = \frac{\partial_{xx}u_n + \partial_{xx}u_{n-1}}{2} + \frac{F_n + F_{n-1}}{2} + A_{n-\frac{1}{2}},\ x \in [x_L, x_R],\ 1 \le n \le N,\\ &\partial_\nu u_n + D_t^{\frac{1}{2}} u_n = B_n,\ x \in \{x_L, x_R\},\ 0 \le n \le N,\end{aligned}$$

with

$$||A_{n-\frac{1}{2}}||_0 \le C\Delta t^2, \quad |B_n| \le C\Delta t^2.$$

Here, the constant $C$ is independent of $\Delta t$. The error function $e_n$ satisfies

$$\frac{e_n - e_{n-1}}{\Delta t} = \frac{\partial_{xx}e_n + \partial_{xx}e_{n-1}}{2} + A_{n-\frac{1}{2}},\ x \in [x_L, x_R],\ 1 \le n \le N, \tag{3.25}$$

$$\partial_\nu e_n + D_t^{\frac{1}{2}} e_n = B_n,\ x \in \{x_L, x_R\},\ 0 \le n \le N, \tag{3.26}$$

$$e_0(x) = 0. \tag{3.27}$$

The desired result (3.24) can be obtained by applying Lemma 3.2 and Theorem 3.1. □

## 4. Fast Evaluation

At the $n$-th time step, solving the semi-discrete problem (3.16)-(3.18) necessitates evaluating the convolution involved in $D_t^{\frac{1}{2}} U_n$, which requires $\mathcal{O}(n)$ operations. If a direct solver with $\mathcal{O}(M)$ operations is adopted, the total computational cost will be $\mathcal{O}(N^2 + NM)$. When $N$ becomes large, this cost becomes very expensive. In this case, a fast evaluation method is indispensable.

The spirit of fast evaluation of the half-order derivative, both continuous and discretized, lies in approximating the kernel function or the kernel sequence with a sum of exponentials. Based on the integral equality

$$\frac{1}{\sqrt{t}} = \frac{2}{\sqrt{\pi}} \int_0^\infty e^{-s^2 t} ds,$$

Jiang and Greengard [15] derived a sum of exponentials to approximate the kernel function $1/\sqrt{t}$ by using the piecewise Gauss-Legendre quadrature. Arnold et. al [5] proposed another method which uses a sum of exponentials to directly approximate the discrete convolution coefficients involved in the discrete transparent boundary condition. These exponentials are determined by equating a first number of elements with their corresponding convolution coefficients. In this work, we propose a new method. Given a small error tolerance $\epsilon$, if we design an approximation for the sequence of convolution coefficients $\{\beta_0, \beta_1, \cdots\}$ such that

$$\tilde{\beta}_k = \sum_{j=1}^{L} w_j e^{-s_j k}, \quad s_j > 0, \quad |\beta_k - \tilde{\beta}_k| \le \epsilon, \quad k = 0, 1, \cdots, [N/2], \tag{4.1}$$

we can approximate the half-order derivative by

$$\tilde{D}_t^{\frac{1}{2}} v_n = \frac{2}{\sqrt{2\Delta t}} \sum_{m=0}^{n} \tilde{\alpha}_m v_{n-m}, \tag{4.2}$$

with $\mathbf{v} = \{v_0, v_1, \cdots\}$ being a sequence and

$$\tilde{\alpha}_m = \begin{cases} \tilde{\beta}_k, & m = 2k, \\ -\tilde{\beta}_k, & m = 2k+1. \end{cases} \tag{4.3}$$

Consequently, we derive another approximate semi-discrete problem by replacing $D_t^{\frac{1}{2}}$ in (3.16)-(3.18) with $\tilde{D}_t^{\frac{1}{2}}$

$$\frac{\tilde{U}_n - \tilde{U}_{n-1}}{\Delta t} = \frac{\partial_{xx}\tilde{U}_n + \partial_{xx}\tilde{U}_{n-1}}{2} + \frac{F_n + F_{n-1}}{2}, \; x \in [x_L, x_R], \; 1 \le n \le N, \tag{4.4}$$

$$\partial_\nu \tilde{U}_n + \tilde{D}_t^{\frac{1}{2}} \tilde{U}_n = 0, \; x \in \{x_L, x_R\}, \; 0 \le n \le N, \tag{4.5}$$

$$\tilde{U}_0(x) = u_0(x), \; x \in [x_L, x_R]. \tag{4.6}$$

Define

$$\mathcal{F}_{odd}(w, s; \mathbf{v}, k) = \sum_{m=1}^{k} w e^{-sm} v_{2k+1-2m}, \qquad \mathcal{F}_{even}(w, s; \mathbf{v}, k) = \sum_{m=1}^{k} w e^{-sm} v_{2k-2m}.$$

Obviously $\mathcal{F}_{odd}(w, s; \mathbf{v}, 0) = \mathcal{F}_{even}(w, s; \mathbf{v}, 0) = 0$. In addition, we have the recursion relations

$$\mathcal{F}_{odd}(w, s; \mathbf{v}, k) = e^{-s}\left[w v_{2k-1} + \mathcal{F}_{odd}(w, s; \mathbf{v}, k-1)\right],$$
$$\mathcal{F}_{even}(w, s; \mathbf{v}, k) = e^{-s}\left[w v_{2k-2} + \mathcal{F}_{even}(w, s; \mathbf{v}, k-1)\right].$$

The summation term in (4.2) is then computed within $\mathcal{O}(L)$ operations with

$$\sum_{m=2}^{n} \tilde{\alpha}_m v_{n-m} = \begin{cases} \sum_{j=1}^{L} \mathcal{F}_{even}(w_j, s_j; \mathbf{v}, k) - \sum_{j=1}^{L} \mathcal{F}_{odd}(w_j, s_j; \mathbf{v}, k-1), & n = 2k, \\ \sum_{j=1}^{L} \mathcal{F}_{odd}(w_j, s_j; \mathbf{v}, k) - \sum_{j=1}^{L} \mathcal{F}_{even}(w_j, s_j; \mathbf{v}, k), & n = 2k+1, \end{cases}$$

which leads to a final scheme with $\mathcal{O}(N(L+M))$ operations. This is a remarkable saving of computational cost compared with the direct evaluation when $N$ is large.

**Lemma 4.1.** *For any real sequence $\mathbf{v} = \{v_0, v_1, \cdots\}$, and any nonnegative integer $n$, we have*

$$\sum_{m=0}^{n} v^m \tilde{D}_t^{1/2} v^m \ge 0,$$

*if both $w_j$ and $s_j$ in formula* (4.1) *are positive.*

*Proof.* The $\mathcal{Z}$-transform of sequence $\tilde{\alpha} = \{\tilde{\alpha}_0, \tilde{\alpha}_1, \cdots\}$ is

$$\begin{aligned} \sum_{m=0}^{\infty} \tilde{\alpha}_m z^{-m} &= \sum_{m=0}^{\infty} \tilde{\beta}_m z^{-2m} - \sum_{m=0}^{\infty} \tilde{\beta}_m z^{-2m-1} \\ &= \sum_{j=1}^{L} w_j \left( \sum_{m=0}^{\infty} e^{-s_j m} z^{-2m} - \sum_{m=0}^{\infty} e^{-s_j m} z^{-2m-1} \right) \\ &= \sum_{j=1}^{L} w_j \frac{1 - z^{-1}}{1 - e^{-s_j} z^{-2}}, \end{aligned}$$

and its radius of convergence is

$$R(\mathcal{Z}\{\tilde{\alpha}\}) = \max(e^{-s_0}, e^{-s_1}, \cdots, e^{-s_L}) < 1.$$

Defining the sequence $\mathbf{V} = \{V_0, V_1, \cdots\}$ by

$$V_m = \begin{cases} v_m, & m \le n, \\ 0, & m > n, \end{cases}$$

and using the Plancherel theorem for the $\mathcal{Z}$ transform (see Lemma 2.1), we have

$$\begin{aligned}
&\sum_{m=0}^{n} v_m \tilde{D}_t^{1/2} v_m = \sum_{m=0}^{+\infty} V_m \tilde{D}_t^{1/2} V_m \\
&= \frac{1}{2\pi} \sum_{j=1}^{L} w_j \Re \int_0^{2\pi} |\mathcal{Z}\{\mathbf{V}\}(e^{i\varphi})|^2 \frac{2}{\sqrt{2\Delta t}} \frac{1-e^{-i\varphi}}{1-e^{-s_j}e^{-2i\varphi}} d\varphi \\
&= \frac{1}{2\pi} \sum_{j=1}^{L} w_j \int_0^{2\pi} |\mathcal{Z}\{\mathbf{V}\}(e^{i\varphi})|^2 \frac{2}{\sqrt{2\Delta t}} \frac{1-\cos\varphi + e^{-s_j}(\cos\varphi - \cos 2\varphi)}{|1-e^{-s_j}e^{-2i\varphi}|^2} d\varphi.
\end{aligned}$$

If $\cos\varphi \ge \cos 2\varphi$, then

$$1-\cos\varphi + e^{-s_j}(\cos\varphi - \cos 2\varphi) \ge 0.$$

Otherwise, owing to our assumption on $s_j$ we have

$$1-\cos\varphi + e^{-s_j}(\cos\varphi - \cos 2\varphi) \ge 1-\cos\varphi + e^{-0}(\cos\varphi - \cos 2\varphi) \ge 0.$$

The proof ends since $w_j > 0$. $\square$

Using Lemma 4.1 and Theorem 3.1, we get

**Theorem 4.1.** *The approximate semi-discrete problem* (4.4)-(4.6) *is stable in the $L^2$ sense, and it admits at most one solution.*

**Theorem 4.2.** *Let $u$ be the solution of the continuous problem* (3.1)-(3.3), *and assume $u$ is smooth enough. If $\tilde{U}^n$ is the solution of the approximate semi-discrete problem* (4.4)-(4.6), *we have*

$$||\,\tilde{e}^n||_0 \le C_5(\Delta t^2 + \epsilon/\Delta t^{1.5}),$$

*where $\tilde{e}_n = u_n - \tilde{U}_n$, $C_5$ is a constant independent of $\Delta t$ and $\epsilon$.*

*Proof.* By the Taylor expansion and Lemma 3.1, we have

$$\begin{aligned}
&\frac{u_n - u_{n-1}}{\Delta t} = \frac{\partial_{xx}u_n + \partial_{xx}u_{n-1}}{2} + \frac{F_n + F_{n-1}}{2} + A_{n-\frac{1}{2}},\ x \in (x_L, x_R),\ 1 \le n \le N, \\
&\partial_\nu u_n + \tilde{D}_t^{\frac{1}{2}} u_n = \tilde{B}_n,\ x \in \{x_L, x_R\},\ 0 \le n \le N,
\end{aligned}$$

with $||A_{n-\frac{1}{2}}||_0 = \mathcal{O}(\Delta t^2)$. Since

$$\begin{aligned}
\tilde{B}_n &= \tilde{D}_t^{\frac{1}{2}} u(x,t_n) - \partial_t^{\frac{1}{2}} u(x,t_n) \\
&= \tilde{D}_t^{\frac{1}{2}} u(x,t_n) - D_t^{\frac{1}{2}} u(x,t_n) + D_t^{\frac{1}{2}} u(x,t_n) - \partial_t^{\frac{1}{2}} u(x,t_n) \\
&= \frac{2}{\sqrt{2\Delta t}} \sum_{m=0}^{n} (\tilde{\alpha}_m - \alpha_m) u(x,t_{n-m}) + D_t^{\frac{1}{2}} u(x,t_n) - \partial_t^{\frac{1}{2}} u(x,t_n),
\end{aligned}$$

and $n \le N \le T_f/\Delta t$, by Lemma 3.1 and (4.1), we have

$$|\tilde{B}_n| \le C\left(\epsilon/\Delta t^{1.5} + \Delta t^2\right),$$

where $C$ is a constant independent of $\epsilon$ and $\Delta t$. The proof ends by using Lemma 4.1 and Theorem 3.1. $\square$

**Remark 4.1.** When $\epsilon = \mathcal{O}(\Delta t^{3.5})$, the error decays at the same rate with respect to $\Delta t$ as that for direct evaluation of convolution.

Now we explain our idea to derive a sum of decaying exponentials satisfying (4.1). Since

$$\beta_k = \frac{\Gamma(2k+1)}{2^{2k}\Gamma(k+1)^2},$$

using the Legendre duplication formula (see p. 29 and p. 41 in [7]) yields

$$\beta_k = \frac{1}{\sqrt{\pi}}\frac{\Gamma(k+\frac{1}{2})}{\Gamma(k+1)} = \frac{2}{\pi}\int_0^{\pi/2} \sin^{2k}\theta d\theta. \tag{4.7}$$

The approximation relation (4.1) is easy to build, since one can approximate the integral in Eq. (4.7) by a numerical quadrature scheme. For example, provided $\{w_j^*, s_j^*\}_{j=1}^L$ are the points and weights of an $L$-point numerical quadrature scheme on $[0, \pi/2]$, we then have

$$\tilde{\beta}_k = \frac{2}{\pi}\sum_{j=1}^{L} w_j^* \sin^{2k} s_j^*,$$

which is indeed a sum of decaying exponentials with

$$w_j = \frac{2}{\pi}w_j^*, \quad s_j = -2\ln\sin s_j^*.$$

Notice that these $w_j$ and $s_j$ are positive, which fulfills the requirement of Lemma 4.1. Fig. 4.1 shows the errors if $L$-point Gauss-Legendre quadrature rule is employed on the integration interval $[0, \pi/2]$. When $L = 100$, the error is always less than $3.6 \times 10^{-6}$ even if $N_f$ is as large as $10^6$. It can be further reduced to $1.1 \times 10^{-10}$ if $L$ is set to be 200.

Given the number of time steps $N$ and an error tolerance $\epsilon$, how to determine the optimal number of decaying exponentials surely has its theoretical importance. We do not intend to study this problem in this paper. Alternatively, we present here an applicable idea to make the sum of decaying exponentials as small as possible.

Since the error increases with the number of time steps, see Fig. 4.1, and the integration function $\sin^{2k}\theta$ becomes nearly singular at point $\theta = \pi/2$. We may place more points near $\theta = \pi/2$. Our idea is as follows. First, we express the integrating interval $[0, \pi/2]$ as the union of $M$ dyadic intervals and one residual interval containing the nearly singular point $\theta = \pi/2$, i.e.,

$$[0, \pi/2] = \bigcup_{j=1}^{M}\left[(1-2^{j-1})\times\frac{\pi}{2}, (1-2^j)\times\frac{\pi}{2}\right]\bigcup\left[(1-2^M)\times\frac{\pi}{2}, \frac{\pi}{2}\right].$$

On each of the dyadic intervals, we use $L_1$-point Gauss-Legendre quadrature rule, and on the residual interval, we use the same rule but different number of integrating points, say $L_2$, which is usually larger than $L_1$. Thus the total number of integrating points is $L = M \times L_1 + L_2$.

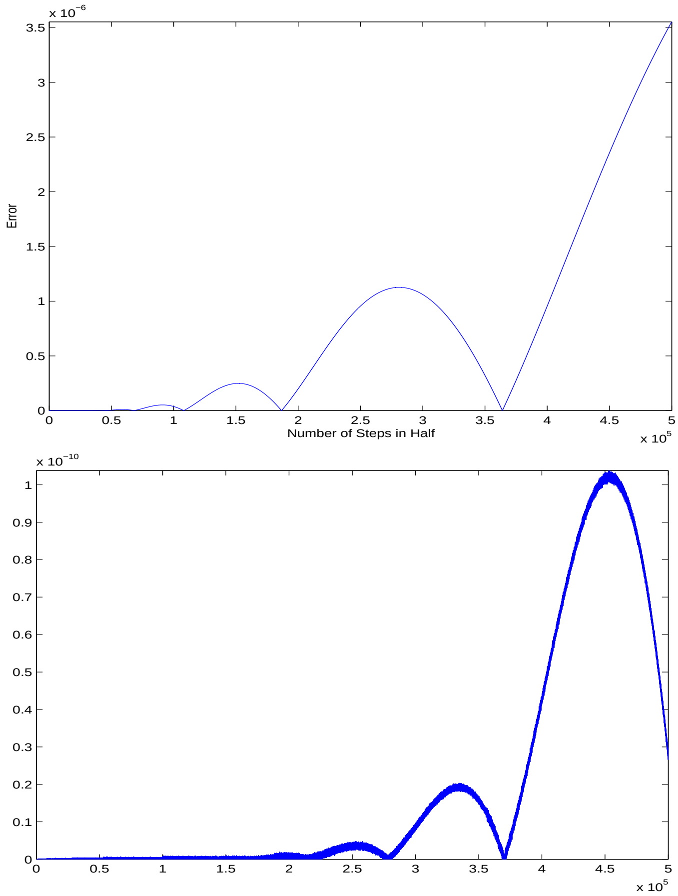


Fig. 4.1. Error between the exact convolution coefficient $\beta_k$ and its approximation $\tilde{\beta}_k$, which is derived by the direct $L$-point Gauss-Legendre quadrature scheme on $[0, \pi/2]$. Top: $L = 100$. Bottom: $L = 200$

Fig. 4.2 shows the relative error with $M = 5$, $L_1 = 9$, $L_2 = 36$, which gives a total number of $L = 81$. The maximal error is less than $5.0 \times 10^{-11}$, which is a significant improvement compared with the direct Gauss-Legendre quadrature method. We point out that this set of parameters $M$, $L_1$ and $L_2$ is only determined by our numerical tests. They are not supposed to be the optimal choice, even for this specific method.

We close this section by making a comparison between the proposed fast evaluation method and those already existing in the literature. We will refer to the method of Jiang and Greengard [15] as Jiang-Greengard, the method of Arnold, Ehrhardt and Sofronov [5] as Arnold-Ehrhardt-Sofronov, and the present one as Zheng in the following.

1. Stability: Zheng is the only one given a rigorous proof for the unconditional stability. For the other two methods, this issue is still open to the author's knowledge.
2. Number of exponentials: Given an accuracy $\epsilon$, to determine the number of exponentials for approximating the kernel is of course an important issue. Jiang-Greengard is the only one gives a theoretical analysis on this issue. As to Arnold-Ehrhardt-Sofronov and Zheng, this number has to be determined by trial and error up to this time.
3. Complexity of implementation: All three methods need only to compute the exponentials once. Comparatively, Arnold-Ehrhardt-Sofronov is the most difficult one to implement.

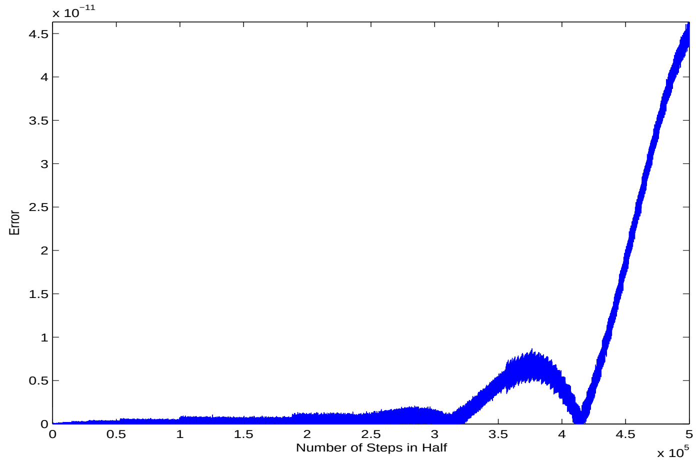


Fig. 4.2. Error between the exact convolution coefficient $\beta_k$ and its approximation $\tilde{\beta}_k$, which is a sum of decaying exponentials. The decaying exponentials are derived by the piecewise Gauss-Legendre quadrature rule. The total number is $L = 81$.

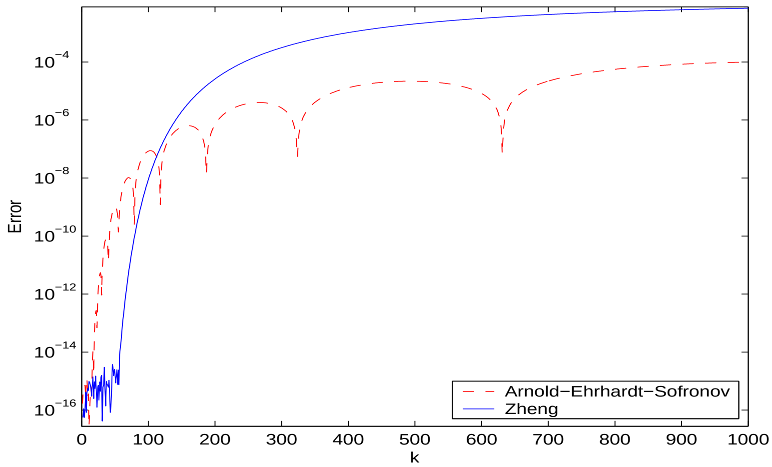


Fig. 4.3. Error of approximate convolution coefficients. $L = 20$. Zheng's exponentials are obtained by using the 20-point Gauss-Legendre quadrature rule on $[0, \frac{\pi}{2}]$. Error $= |\tilde{\beta}_k - \beta_k|$.

Table 4.1: Condition number of the Padé approximation for $g(x) = \sum_{k=0}^{\infty} \beta_k x^k$.

| $L$ | 4 | 6 | 8 | 10 | 12 |
|---|---|---|---|---|---|
| Condition Number | $2.0 \times 10^4$ | $2.2 \times 10^7$ | $2.5 \times 10^{10}$ | $2.8 \times 10^{13}$ | $1.1 \times 10^{15}$ |

This is because a Padé approximation should be performed in Arnold-Ehrhardt-Sofronov, and this treatment becomes much ill-conditioned as the number of exponentials increases. Table 4.1 lists the condition number of the coefficient matrix used to determine the Padé rational function. See [9] for the algorithm description. This disadvantage prohibits large values of $L$.

4. Accuracy: Compared with Arnold-Ehrhardt-Sofronov, Zheng generally provides more accurate numerical approximations. Figs. 4.3 and 4.4 show the errors of approximate con-

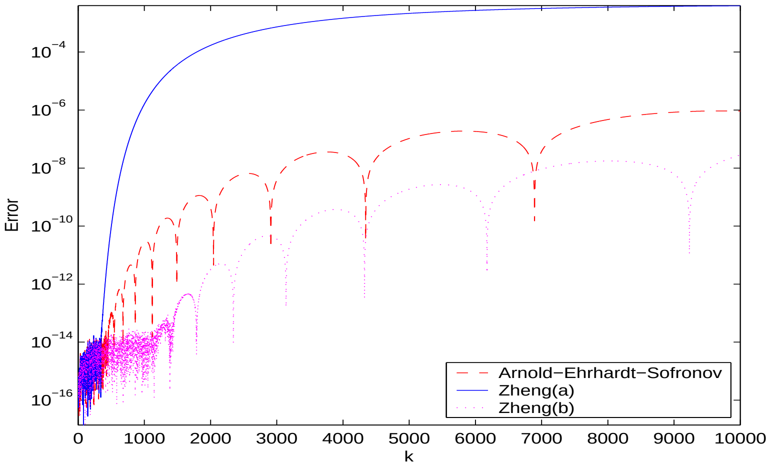


Fig. 4.4. Error of approximate convolution coefficients. $L = 50$. Zheng(a) uses the 50-point Gauss-Legendre quadrature rule on $[0, \frac{\pi}{2}]$, and Zheng(b) uses the 20-point Gauss-Legendre quadrature rule on $[0, \frac{\pi}{4}]$ and 30-point on $[\frac{\pi}{4}, \frac{\pi}{2}]$. Error $= |\tilde{\beta}_k - \beta_k|$.

volution coefficients when $L = 20$ and $L = 50$. The exponentials for Arnold-Ehrhardt-Sofronov are determined with the arbitrary precision algorithm of Maple. The advantage of Zheng over Arnold-Ehrhardt-Sofronov is clearly demonstrated. We remark that if $k \le L$, the coefficients $\tilde{\beta}_k$ obtained by Arnold-Ehrhardt-Sofronov are theoretically exact. This explains why the results of Arnold-Ehrhardt-Sofronov are better at the initial stage. Also notice that when this event happens, the absolute error is very small.

5. Universality: Arnold-Ehrhardt-Sofronov presents a general idea for fast evaluating the discrete convolution. Jiang-Greengard and Zheng are specially designed for the half-order derivative operator.

## 5. Numerical Example

We consider the one-dimensional heat equation

$$\partial_t u = \partial_{xx} u, \ x \in \mathbf{R}, \ 0 < t \le T_f, \tag{5.1}$$

$$u(x,0) = \frac{1}{\sqrt{4t_0}} \exp\left(-\frac{x^2}{4t_0}\right), \tag{5.2}$$

where $t_0$ is a positive constant. It can be verified that the exact solution of this problem is

$$u(x,t) = \frac{1}{\sqrt{4(t+t_0)}} \exp\left(-\frac{x^2}{4(t+t_0)}\right).$$

We set $t_0 = 0.25$ and $T_f = 10$, and take the computational domain as $[-5, 5]$. The error is defined as

$$\mathrm{Err} = \frac{||u(\cdot, T_f) - U_N(\cdot)||_0}{||u(\cdot, T_f)||_0}.$$

For the spatial discretization, we use the $p$-version finite element method. For the problem with analytical solutions, this method usually presents numerical solutions with exponentially

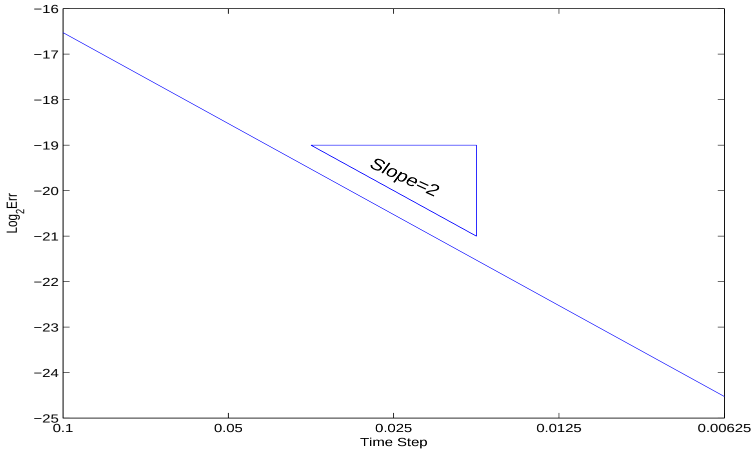


Fig. 5.1. Error in time.

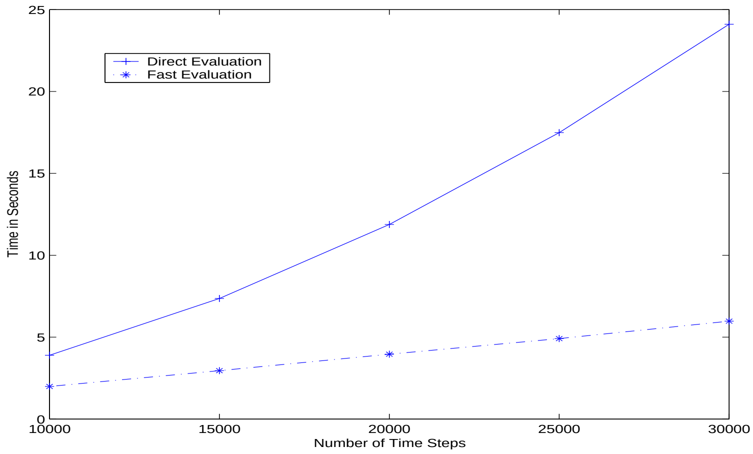


Fig. 5.2. Comparison of computational cost.

decaying accuracy. The computational domain is divided into four elements with same size. The finite element subspace is set to be continuous piecewise polynomial space with degree of 8. For the linear system, we use the direct solver based on the LU-decomposition. All the computation is performed on a notebook PC with a 1.7GHz CPU and a 768M memory.

We plot the error in Fig. 5.1 with different time steps. A second-order degeneracy of error can be clearly observed. We remark that the error from the finite element discretization is neglectable, since a further-refined mesh presents almost the same numerical solutions. To demonstrate the superiority of the fast evaluation method, we plot in Fig. 5.2 the computation time in seconds. One can see that the computation cost increases linearly with the number of time steps when the fast evaluation is used for the convolution involved in the artificial boundary condition. It is also observed that the computational time increases much faster when the direct evaluation is employed.

**Acknowledgments.** This work is supported partially by the National Natural Science Foundation of China under Grant No. 10401020, the Alexander von Humboldt Foundation, and the Key Project of China *High Performance Scientific Computation Research 2005CB321701.*

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