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NUMERICAL SOLUTIONS OF PARABOLIC PROBLEMS ON UNBOUNDED 3-D SPATIAL DOMAIN *1)

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Abstract

In this paper, the numerical solutions of heat equation on 3-D unbounded spatial domain are considered. An artificial boundary Γ is introduced to finite the computational domain. On the artificial boundary Γ, the exact boundary condition and a series of approximating boundary conditions are derived, which are called artificial boundary conditions. By the exact or approximating boundary condition on the artificial boundary, the original problem is reduced to an initial-boundary value problem on the bounded computational domain, which is equivalent or approximating to the original problem. The finite difference method and finite element method are used to solve the reduced problems on the finite computational domain. The numerical results demonstrate that the method given in this paper is effective and feasible.

Mathematics subject classification: 35K05, 65M06, 65M60.
Key words: Heat equation, Artificial boundary, Exact boundary conditions, Finite element method.

1. Introduction

Numerical solutions of heat equation on unbounded 3-D spatial domains are considered. This kind of problems originate from the heat transfer, fluid dynamics, astrophysics, finance or other areas of applied mathematics. Because of the unboundedness of the physical domains, how to numerically solve these problems efficiently is real a challenge.

Strain [14] developed a method to solve the parabolic equations on unbounded domains, which combines the fast Gauss transform with an adaptive refinement scheme. This method can solve heat equation with large timesteps, especially for highly nonuniform or discontinuous initial data.

Artificial boundary method [3, 4, 10, 11] is a powerful tool of the numerical solution for the boundary-valued problems on unbounded domains. By introducing an artificial boundary, the domain is divided into two parts, a finite computational domain and an infinite domain. A suitable boundary condition is imposed on the artificial boundary, such that the solution of the problem with the suitable boundary condition on the artificial boundary on the finite computational domain is a good approximation of the original problem.

For the elliptic problems on unbounded domains, there are many approaches to construct artificial boundary condition to solve them [5, 10, 11, 12], but for the parabolic problems on unbounded domains there are only a few results related to the artificial boundary conditions. L. Halpern and J. Rauch[7] proposed a family of artificial boundary conditions for parabolic equations on unbounded domains, which are local in time, and there are many auxiliary functions involved in the artificial boundary conditions. C. J. Zhu and Q. K. Du [15] studied the

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parabolic problem on an unbounded domain by a semi-discrete approach in time. On each time step, they used the nature boundary element method to solve an elliptic problem on unbounded domain. Recently, H. Han and Z. Huang [8, 9] gave the exact boundary conditions for the heat problems on unbounded domains in one dimension and in two dimensions. Furthermore, a series of artificial boundary conditions are given. Han and Zheng [13] derived the nonreflecting boundary conditions for acoustic problems in three dimensions.

In this paper, the exact boundary condition is derived on the given artificial boundary Γ for the parabolic problem on unbounded three dimensional spatial domain, that is, the relationship between $\frac{\partial u}{\partial n}\Big|_\Gamma$ and $\frac{\partial u}{\partial t}\Big|_\Gamma$ is given. Moreover, a series of artificial boundary conditions with high accuracy are obtained. By the artificial boundary conditions, a family of approximate problems of the original problem on the bounded computational domain are constructed. The stability of the approximate problem is proved. Finally, numerical examples manifest the feasibility and effectiveness of the given method.

2. The Artificial Boundary Condition

Let $D \subset \mathbb{R}^3$ denote a bounded domain, namely $D \subset B(0,a) = \{x \in \mathbb{R}^3 \mid ||x|| \le a\}$ with $a > 0$. Suppose

$$D^c = \mathbb{R}^3 \backslash \overline{D}, \quad \Omega_c^T = D^c \times (0,T], \quad \Gamma_0 = \partial D \times (0,T].$$

Consider the following initial-boundary value problem:

$$\frac{\partial u}{\partial t} - \triangle u = f(x,t), \qquad (x,t) \in \Omega_c^T \tag{2.1}$$

$$u\Big|_{\Gamma_0} = g(x,t), \qquad (x,t) \in \Gamma_0, \tag{2.2}$$

$$u\Big|_{t=0} = u_0(x), \qquad x \in D^c, \tag{2.3}$$

$$u \to 0, \qquad \text{when } ||x|| \to +\infty, \tag{2.4}$$

where $f(x,t), g(x,t)$ and $u_0(x)$ are given smooth functions and $f(x,t)$, $u_0(x)$ vanish outside the ball $B(0,a)$, namely

$$f(x,t) = 0, \quad u_0(x) = 0, \text{ if } ||x|| \ge a.$$

We introduce an artificial boundary $\Gamma = \{(x,t) \mid ||x|| = b, 0 < t \le T\}$ with $b > a$ to divide domain Ω_c^T into two parts,

$$\begin{aligned} \Omega_b^T &= \{(x,t) \mid x \in D^c \text{ and } ||x|| < b, 0 < t < T\}, \\ \Omega_e^T &= \{(x,t) \mid ||x|| \ge b, 0 < t \le T\}. \end{aligned}$$

If we can seek a suitable boundary condition on Γ, problem (2.1)-(2.4) can be reduced to a problem on the bounded computational domain Ω_i^T. In the sphere coordinate, the restriction of the solution $u(r,\theta,\phi,t)$ of problem (2.1)-(2.4) on the unbounded domain Ω_e^T satisfies

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial r^2} + \frac{2}{r}\frac{\partial u}{\partial r} + \frac{1}{r^2}\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial u}{\partial\theta}) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 u}{\partial\phi^2}, \quad (r,\theta,\phi,t) \in \Omega_e^T, \tag{2.5}$$

$$u|_{r=b} = u(b,\theta,\phi,t), \tag{2.6}$$

$$u|_{t=0} = 0, \tag{2.7}$$

$$u \to 0, \quad \text{when } \; r \to +\infty, \tag{2.8}$$

where $\Omega_e^T = \{r > b, \theta \in [0,\pi], \phi \in [0,2\pi], t \in [0,T]\}$.

Since $u(b,\theta,\phi,t)$ is unknown, problem (2.5)-(2.8) is an uncompleted posed problem; it can't be solved independently. If $u(b,\theta,\phi,t)$ is given, problem (2.5)-(2.8) is well posed, so the solution $u(r,\theta,\phi,t)$ of (2.5)-(2.8) can be given by $u(b,\theta,\phi,t)$.

Let

$$u(b,\theta,\phi,t) = \frac{a_{00}(t)}{2} + \sum_{n=1}^{\infty}\left\{\frac{a_{n0}(t)}{2}P_n^0(\cos\theta) + \sum_{m=1}^{n} P_n^m(\cos\theta)\Big(a_{nm}(t)\cos m\phi + b_{nm}(t)\sin m\phi\Big)\right\}, \tag{2.9}$$

where $P_n^m(\cos\theta)$, $(n=1,2,\cdots,m=1,2,\cdots,n)$ are the Associate *Legendre* functions[1] and

$$a_{nm}(t) = \frac{(2n+1)(n-m)!}{2\pi(n+m)!}\int_0^{2\pi}\int_0^{\pi} u(b,\xi,\psi,t)P_n^m(\cos\xi)\cos m\psi\sin\xi d\xi d\psi, \tag{2.10}$$

$$b_{nm}(t) = \frac{(2n+1)(n-m)!}{2\pi(n+m)!}\int_0^{2\pi}\int_0^{\pi} u(b,\xi,\psi,t)P_n^m(\cos\xi)\sin m\psi\sin\xi d\xi d\psi. \tag{2.11}$$

Let the solution of problem (2.5)–(2.8), $u(r,\theta,\phi,t)$, be

$$u(r,\theta,\phi,t) = \frac{u_{00}(r,t)}{2} + \sum_{n=1}^{\infty}\left\{\frac{u_{n0}(r,t)}{2}P_n^0(\cos\theta) + \sum_{m=1}^{n} P_n^m(\cos\theta)\Big(u_{nm}(r,t)\cos m\phi + v_{nm}(r,t)\sin m\phi\Big)\right\}. \tag{2.12}$$

Substituting (2.12) into (2.5), we obtain:
(i) $u_{00}(r,t)$ satisfies the following initial-boundary value problem:

$$\frac{\partial u_{00}}{\partial t} = \frac{\partial^2 u_{00}}{\partial r^2} + \frac{2}{r}\frac{\partial u_{00}}{\partial r}, \quad r>b, 0<t\le T, \tag{2.13}$$

$$u_{00}|_{r=b} = a_{00}(t), \tag{2.14}$$

$$u_{00}|_{t=0} = 0, \tag{2.15}$$

$$u_{00}\to 0, \quad \text{when} \;\; r\to+\infty. \tag{2.16}$$

(ii) $u_{nm}(r,t)$ (or $v_{nm}(r,t)$) satisfies the following initial-boundary value problem:

$$\frac{\partial G}{\partial t} = \frac{\partial^2 G}{\partial r^2} + \frac{2}{r}\frac{\partial G}{\partial r} - \frac{n(n+1)}{r^2}G, \quad r>b, 0<t\le T, \tag{2.17}$$

$$G|_{r=b} = a_{nm}(t)(\text{or } b_{nm}(t)), \tag{2.18}$$

$$G|_{t=0} = 0, \tag{2.19}$$

$$G\to 0, \quad \text{when} \;\; r\to+\infty. \tag{2.20}$$

In [2], we have the solution $u_{00}(r,t)$ of problem (2.13)–(2.16), which is given by:

$$u_{00}(r,t) = \frac{2b}{r\sqrt{\pi}}\int_{\frac{r-b}{2\sqrt{t}}}^{\infty} a_{00}\big(t-\frac{(r-b)^2}{4\mu^2}\big)e^{-\mu^2}d\mu, \tag{2.21}$$

and

$$\frac{\partial u_{00}}{\partial r}(b,t) = -\frac{1}{b}u_{00}|_{r=b} - \frac{1}{\sqrt{\pi}}\int_0^t \frac{\partial a_{00}(\lambda)}{\partial\lambda}\frac{1}{\sqrt{t-\lambda}}d\lambda. \tag{2.22}$$

We now consider the initial-boundary value problem (2.17)–(2.20). First consider the following simplified problem:

$$\frac{\partial G_n}{\partial t} = \frac{\partial^2 G_n}{\partial r^2} + \frac{2}{r}\frac{\partial G_n}{\partial r} - \frac{n(n+1)}{r^2}G_n, \quad r>b, 0<t\le T, \tag{2.23}$$

$$G_n|_{r=b} = 1, \tag{2.24}$$

$$G_n|_{t=0} = 0, \tag{2.25}$$

$$G_n\to 0, \quad \text{when} \;\; r\to+\infty. \tag{2.26}$$

Let

$$G_n(r,t) = e^{-\mu^2 t} w(r). \tag{2.27}$$

Substituting (2.27) into (2.23), we have

$$\frac{\partial^2 w}{\partial r^2} + \frac{2}{r}\frac{\partial w}{\partial r} + (\mu^2 - \frac{n(n+1)}{r^2})w = 0. \tag{2.28}$$

Equation (2.28) has two independent solutions:

$$\left.\begin{aligned} w_1(\mu r) &= \sqrt{\tfrac{\pi}{2\mu r}} J_{n+1/2}(\mu r), \\ w_2(\mu r) &= \sqrt{\tfrac{\pi}{2\mu r}} Y_{n+1/2}(\mu r). \end{aligned}\right\} \tag{2.29}$$

Let

$$G_*(r,t) = \frac{2}{\pi}\int_0^\infty e^{-\mu^2 t}\frac{w_1(\mu r)w_2(\mu b) - w_1(\mu b)w_2(\mu r)}{w_1^2(\mu b) + w_2^2(\mu b)}\frac{d\mu}{\mu}. \tag{2.30}$$

It is straight to check that $G_*(r,t)$ satisfies equation (2.23) and

$$\begin{aligned} G_*(r,t)|_{r=b} &= 0, \\ G_*(r,t)|_{t=0} &= \lim_{t\to+0} G_*(r,t) \\ &= \frac{2}{\pi}\int_0^\infty \frac{w_1(\mu r)w_2(\mu b) - w_1(\mu b)w_2(\mu r)}{w_1^2(\mu b) + w_2^2(\mu b)}\frac{d\mu}{\mu} \\ &= \frac{2}{\pi}\left(\frac{b}{r}\right)^{1/2}\int_0^\infty \frac{J_{n+1/2}(\mu r)Y_{n+1/2}(\mu b) - Y_{n+1/2}(\mu r)J_{n+1/2}(\mu b)}{J^2_{n+1/2}(\mu b) + Y^2_{n+1/2}(\mu b)}\frac{d\mu}{\mu} \\ &= -\left(\frac{b}{r}\right)^{n+1}, \quad r > b. \end{aligned}$$

The last equality is from [[6], formula 6.542]. Let

$$G_n(r,t) = \left(\frac{b}{r}\right)^{n+1} + G_*(r,t), \tag{2.31}$$

then $G_n(r,t)$ is the solution of problem (2.23)–(2.26). By Duhamel's theorem we obtain the solution $u_{nm}(r,t)$ (or $v_{nm}(r,t)$) of problem (2.17)–(2.20)

$$\begin{aligned} u_{nm}(r,t) &= \int_0^t a_{nm}(\lambda)\frac{\partial}{\partial t}G_n(r,t-\lambda)d\lambda \\ &= -\int_0^t a_{nm}(\lambda)\frac{\partial}{\partial \lambda}G_n(r,t-\lambda)d\lambda \\ &= -a_{nm}(\lambda)G_n(r,t-\lambda)\Big|_{\lambda=0}^{\lambda=t} + \int_0^t \frac{da_{nm}(d\lambda)}{\lambda}G_n(r,t-\lambda)d\lambda \\ &= \int_0^t \frac{da_{nm}(\lambda)}{d\lambda}G_n(r,t-\lambda)d\lambda. \end{aligned} \tag{2.32}$$

Similarly we have

$$v_{nm}(r,t) = \int_0^t \frac{db_{nm}(\lambda)}{d\lambda}G_n(r,t-\lambda)d\lambda. \tag{2.33}$$

Furthermore we get

$$\frac{\partial u_{nm}}{\partial r}\Big|_{r=b} = \int_0^t \frac{da_{nm}(\lambda)}{d\lambda}\frac{\partial G_n(r,t-\lambda)}{\partial r}d\lambda\Big|_{r=b} \tag{2.34}$$

$$= -\frac{n+1}{b}a_{nm}(t) - \frac{4}{\pi^2 b}\int_0^t \frac{da_{nm}(\lambda)}{d\lambda}\left[\int_0^\infty \frac{e^{-\mu^2(t-\lambda)}\,d\mu}{\mu[J^2_{n+1/2}(\mu b) + Y^2_{n+1/2}(\mu b)]}\right]d\lambda \tag{2.35}$$

On the other hand,

$$\begin{aligned}\frac{4\sqrt{t}}{\pi^2 b}\int_0^\infty \frac{e^{-\mu^2 t}}{\mu[J^2_{n+1/2}(\mu b)+Y^2_{n+1/2}(\mu b)]}d\mu &= \frac{4}{\pi^2}\frac{\sqrt{t}}{b}\int_0^\infty \frac{e^{-\xi^2 t/b^2}}{J^2_{n+1/2}(\xi)+Y^2_{n+1/2}(\xi)}\frac{d\xi}{\xi}\\ &\equiv H_{n+1/2}(t/b^2). \end{aligned}\tag{2.36}$$

Combining (2.35) and (2.36), we have

$$\frac{\partial u_{nm}}{\partial r}\Big|_{r=b} = -\frac{n+1}{b}a_{nm}(t) - \int_0^t \frac{\partial a_{nm}(\lambda)}{\partial \lambda}\frac{H_{n+1/2}(\frac{t-\lambda}{b^2})}{\sqrt{t-\lambda}}d\lambda. \tag{2.37}$$

Similarly we obtain

$$\frac{\partial v_{nm}}{\partial r}\Big|_{r=b} = -\frac{n+1}{b}b_{nm}(t) - \int_0^t \frac{\partial b_{nm}(\lambda)}{\partial \lambda}\frac{H_{n+1/2}(\frac{t-\lambda}{b^2})}{\sqrt{t-\lambda}}d\lambda. \tag{2.38}$$

From (2.12), we have the exact boundary condition on Γ_b:

$$\begin{aligned}\frac{\partial u}{\partial r}\Big|_{r=b} &= \frac{1}{2}\frac{\partial u_{00}}{\partial r}\Big|_{r=b}\\ &\quad+\sum_{n=1}^{\infty}\left[\frac{1}{2}\frac{\partial u_{n0}}{\partial r}P_n^0(\cos\theta)+\sum_{m=1}^{n}P_n^m(\cos\theta)\left(\frac{\partial u_{nm}}{\partial r}\cos m\phi+\frac{\partial v_{nm}}{\partial r}\sin m\phi\right)\right]_{r=b}\\ &= -\frac{1}{2b}a_{00}(t)-\frac{1}{2\sqrt{\pi}}\int_0^t\frac{\partial a_{00}(\lambda)}{\partial\lambda}\frac{1}{\sqrt{t-\lambda}}d\lambda\\ &\quad+\sum_{n=1}^{\infty}\left\{\frac{1}{2}\left[-\frac{n+1}{b}a_{n0}(t)-\int_0^t\frac{da_{n0}(\lambda)}{d\lambda}\frac{H_{n+1/2}(\frac{t-\lambda}{b^2})}{\sqrt{t-\lambda}}d\lambda\right]P_n^0(\cos\theta)\right.\\ &\quad+\sum_{m=1}^{n}\left[-\frac{n+1}{b}\Big(a_{nm}(t)\cos m\phi+b_{nm}(t)\sin m\phi\Big)\right.\\ &\quad\left.\left.-\int_0^t\left(\frac{da_{nm}(\lambda)}{d\lambda}\cos m\phi+\frac{db_{nm}(\lambda)}{d\lambda}\sin m\phi\right)\frac{H_{n+1/2}(\frac{t-\lambda}{b^2})}{\sqrt{t-\lambda}}d\lambda\right]P_n^m(\cos\theta)\right\}\\ &\equiv \Phi_\infty\left(u\big|_\Gamma,\frac{\partial u}{\partial t}\big|_\Gamma\right).\end{aligned}\tag{2.39}$$

where $\Gamma=\{(x,t)\mid ||x||=b, 0<t\le T\}$. By the addition theorem of *Legendre* functions [6]:

$$P_n(\cos\gamma)=P_n^0(\cos\xi)P_n^0(\cos\theta)+2\sum_{m=1}^{n}\frac{(n-m)!}{(n+m)!}P_n^m(\cos\xi)P_n^m(\cos\theta)\cos m(\psi-\phi),$$

where

$$\cos\gamma=\cos\xi\cos\theta+\sin\xi\sin\theta\cos(\psi-\phi),$$

we can simplify the formula in (2.39) into:

$$\begin{aligned}\frac{\partial u}{\partial r}\Big|_{r=b} &= -\frac{1}{4\pi b}\int_S u(b,\xi,\psi,t)dS_{\xi,\psi}-\frac{1}{4\pi^{3/2}}\int_0^t\int_S\frac{\partial u(b,\xi,\psi,\lambda)}{\partial\lambda}dS_{\xi,\psi}\frac{1}{\sqrt{t-\lambda}}d\lambda\\ &\quad-\sum_{n=1}^{\infty}\left\{\frac{(n+1)(2n+1)}{4\pi b}\int_S u(b,\xi,\psi,t)P_n(\cos\gamma)dS_{\xi,\psi}\right.\\ &\quad\left.+\frac{2n+1}{4\pi}\int_0^t\int_S\frac{\partial u(b,\xi,\psi,\lambda)}{\partial\lambda}P_n(\cos\gamma)dS_{\xi,\psi}\frac{H_{n+1/2}(\frac{t-\lambda}{b^2})}{\sqrt{t-\lambda}}d\lambda\right\}\\ &\equiv \Phi_\infty\left(u\big|_\Gamma,\frac{\partial u}{\partial t}\big|_\Gamma\right).\end{aligned}\tag{2.40}$$

This is the exact boundary condition satisfied by the solution of problem (2.1)-(2.4). Therefore, problem (2.1)-(2.4) is equivalent to the following initial-boundary value problem on the bounded domain $\Omega_i^T = \{(r,\theta,\phi,t) \in \Omega_i^T \mid r < b\}$ with $\Omega_i = \{(r,\theta,\phi) \in D^c, r < b\}$.

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial r^2} + \frac{1}{r}\frac{\partial u}{\partial r} + \frac{1}{r^2}\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial u}{\partial\theta}) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 u}{\partial\phi^2}, \quad (r,\theta,\phi,t) \in \Omega_i^T \tag{2.41}$$

$$u|_{\Gamma_0} = g(\theta,\phi,t), \tag{2.42}$$

$$\frac{\partial u}{\partial r}\Big|_{r=b} = \Phi_\infty\left(u\big|_\Gamma, \frac{\partial u}{\partial t}\big|_\Gamma\right), \tag{2.43}$$

$$u|_{t=0} = 0. \tag{2.44}$$

If we take the first few terms of the above summation, namely for $N = 0, 1, 2, \cdots$

$$\begin{aligned}\frac{\partial u}{\partial r}\Big|_{r=b} &= -\frac{1}{4\pi b}\int_S u(b,\xi,\psi,t)dS_{\xi,\psi} - \frac{1}{4\pi^{3/2}}\int_0^t\int_S \frac{\partial u(b,\xi,\psi,\lambda)}{\partial\lambda}dS_{\xi,\psi}\frac{1}{\sqrt{t-\lambda}}d\lambda \\ &\quad -\sum_{n=1}^N\Bigg\{\frac{(n+1)(2n+1)}{4\pi b}\int_S u(b,\xi,\psi,t)P_n(\cos r)dS_{\xi,\psi} \\ &\quad +\frac{2n+1}{4\pi}\int_0^t\int_S\frac{\partial u(b,\xi,\psi,\lambda)}{\partial\lambda}P_n(\cos r)dS_{\xi,\psi}\frac{H_{n+1/2}(\frac{t-\lambda}{b^2})}{\sqrt{t-\lambda}}d\lambda\Bigg\} \\ &\equiv \Phi_N\left(u\big|_\Gamma, \frac{\partial u}{\partial t}\big|_\Gamma\right).\end{aligned} \tag{2.45}$$

Using boundary condition (2.45) instead of (2.43), we obtain a series of approximate problems.

3. Stability Analysis of the Reduced Problems on the Bounded Computational Domain

We firstly concentrate on the approximate problem for $N = 0, 1, 2, \cdots$,

$$\frac{\partial u}{\partial t} = \triangle u, \quad (x,t) \in \Omega_b^T, \tag{3.1}$$

$$u|_{\Gamma_0} = g(\theta,\phi,t), \tag{3.2}$$

$$\frac{\partial u}{\partial r}\Big|_{r=b} = \Phi_N\left(u\big|_\Gamma, \frac{\partial u}{\partial t}\big|_\Gamma\right), \tag{3.3}$$

$$u|_{t=0} = u_0(x). \tag{3.4}$$

Suppose that $u(r,\theta,\phi,t)$ is a solution of problem (3.1)-(3.4), then

Lemma 3.1. *The following inequality holds:*

$$\int_0^t\int_0^{2\pi}\int_0^\pi \Phi_N\left(u\big|_\Gamma, \frac{\partial u}{\partial t}\big|_\Gamma\right)u\big|_\Gamma b^2\sin\theta d\theta d\phi d\tau \le 0. \tag{3.5}$$

Proof. Recall that

$$\begin{aligned}u(b,\theta,\phi,t) &= \frac{a_{00}(t)}{2} + \sum_{n=1}^\infty\Bigg\{\frac{a_{n0}(t)}{2}P_n^0(\cos\theta) \\ &\quad + \sum_{m=1}^n P_n^m(\cos\theta)\Big(a_{nm}(t)\cos m\phi + b_{nm}(t)\sin m\phi\Big)\Bigg\}.\end{aligned} \tag{3.6}$$

Substituting (3.6) into (2.45), we can get

$$\begin{aligned}\Phi_N(u\big|_\Gamma, \frac{\partial u}{\partial t}\big|_\Gamma) \quad &\equiv \quad -\frac{1}{2b}a_{00}(t) - \frac{1}{2\sqrt{\pi}}\int_0^t \frac{\partial a_{00}(\lambda)}{\partial \lambda}\frac{1}{\sqrt{t-\lambda}}d\lambda \\ &+\sum_{n=1}^{N}\Bigg\{\frac{1}{2}\left[-\frac{n+1}{b}a_{n0}(t) - \int_0^t \frac{da_{n0}(\lambda)}{d\lambda}\frac{H_{n+1/2}(\frac{t-\lambda}{b^2})}{\sqrt{t-\lambda}}d\lambda\right]P_n^0(\cos\theta) \\ &+\sum_{m=1}^{n}\Bigg[-\frac{n+1}{b}\Big(a_{nm}(t)\cos m\phi + b_{nm}(t)\sin m\phi\Big) \\ &-\int_0^t \left(\frac{da_{nm}(\lambda)}{d\lambda}\cos m\phi + \frac{db_{nm}(\lambda)}{d\lambda}\sin m\phi\right)\frac{H_{n+1/2}(\frac{t-\lambda}{b^2})}{\sqrt{t-\lambda}}d\lambda\Bigg]P_n^m(\cos\theta)\Bigg\} \\ &\equiv \quad W_0(a_{00}) + \sum_{n=1}^{N}\frac{W_n(a_{n0}(t))}{2}P_n^0(\cos\theta) + \\ &\sum_{n=1}^{N}\sum_{m=1}^{n}\Big\{W_n(a_{nm}(t))\cos m\phi + W_n(b_{nm}(t))\sin m\phi\Big\}P_n^m(\cos\theta), \qquad (3.7)\end{aligned}$$

with

$$\begin{aligned}W_0(f(t)) &= -\frac{1}{2b}f(t) - \frac{1}{2\sqrt{\pi}}\int_0^t \frac{\partial f(\lambda)}{\partial\lambda}\frac{1}{\sqrt{t-\lambda}}d\lambda, \\ W_n(f(t)) &= -\frac{n+1}{b}f(t) - \int_0^t \frac{df(\lambda)}{d\lambda}\frac{H_{n+1/2}(\frac{t-\lambda}{b^2})}{\sqrt{t-\lambda}}d\lambda.\end{aligned}$$

Combining (3.6) and (3.7), we obtain

$$\begin{aligned}&\int_0^t\int_0^{2\pi}\int_0^{\pi}\Phi_N\left(u\big|_\Gamma, \frac{\partial u}{\partial t}\big|_\Gamma\right)u\big|_\Gamma b^2\sin\theta d\theta d\phi d\tau = \\ &2\pi b^2\int_0^t\Bigg\{\frac{W_0(a_{00}(\tau))}{2}a_{00}(\tau) + \sum_{n=1}^{N}\frac{1}{2n+1}N_n(a_{n0}(\tau))a_{n0}(\tau) + \\ &\sum_{n=1}^{N}\sum_{m=1}^{n}\frac{(n+m)!}{(2n+1)(n-m)!}\Big\{W_n(a_{nm}(\tau))a_{nm}(\tau) + W_n(b_{nm}(\tau))b_{nm}(\tau)\Big\}\Bigg\}d\tau \qquad (3.8)\end{aligned}$$

On the other hand, we consider the following auxiliary problem on the domain $\{(r,t) \mid b \le r < +\infty, 0 \le t \le T\}$ for $n = 0, 1, 2, \cdots, N$:

$$\begin{aligned}\frac{\partial G_n}{\partial t} &= \frac{\partial^2 G_n}{\partial r^2} + \frac{2}{r}\frac{\partial G_n}{\partial r} - \frac{n(n+1)}{r^2}G_n, \quad r > b, 0 < t \le T, &(3.9)\\ G_n|_{r=b} &= a_{nm}(t), &(3.10)\\ G_n|_{t=0} &= 0, &(3.11)\\ G_n \to 0, &\quad \text{when} \quad r \to +\infty. &(3.12)\end{aligned}$$

From (2.37) we have

$$\frac{\partial G_n}{\partial r}|_{r=b} = W_n(a_{nm}(t)). \qquad (3.13)$$

Multiplying $r^2G_n(r,t)$ on equation (3.8), integrating by parts on $[b,+\infty) \times [0,t]$ and using (3.11)-(3.12), we have

$$\begin{aligned}\int_b^\infty \frac{|G_n(r,t)|^2}{2}r^2dr \quad &= \quad -\int_0^t b^2\frac{\partial G_n(b,\tau)}{\partial r}G_n(b,\tau)d\tau. \\ &-\int_0^t\int_b^\infty\left[(r\frac{\partial G_n(r,\tau)}{\partial r})^2 + (n^2+n)G_n^2(r,\tau)\right]drd\tau. \qquad (3.14)\end{aligned}$$

Namely

$$\int_b^\infty \frac{|G_n|^2}{2} r^2 dr + \int_0^t \int_b^\infty \left[r^2 (\frac{\partial G_n(r,\tau)}{\partial r})^2 + n(n+1) G_n^2(r,\tau) \right] dr d\tau$$

$$= \quad - \int_0^t b^2 \frac{\partial G_n(b,\tau)}{\partial r} G_n(b,\tau) d\tau. \tag{3.15}$$

This means

$$\int_0^t \frac{\partial G_n(b,\tau)}{\partial r} G_n(b,\tau) d\tau = \int_0^t W_n(a_{nm}(\tau)) a_{nm}(\tau) d\tau \leq 0. \tag{3.16}$$

Similarly we have

$$\int_0^t W_n(b_{nm(\tau)}) b_{nm}(\tau) d\tau \leq 0. \tag{3.17}$$

Combining (3.8), (3.16) and (3.17), we complete the proof of the lemma.

For the approximate problem (3.1)-(3.4), we have the following stability estimate:

Theorem 3.1. *Suppose that u is a solution of problem (3.1)-(3.4), then the following stability holds:*

$$\int_{\Omega_b} |u(x,t)|^2 dx \leq \int_{\Omega_b} |u_0(x)|^2 dx, \quad 0 \leq t \leq T. \tag{3.18}$$

Proof. For simpleness, only consider the case $g = 0$. Multiplying u on the equation (3.1) and integrating by parts on Ω_b^T, we obtain:

$$\frac{1}{2} \int_{\Omega_b} |u(x,t)|^2 dx dt = \frac{1}{2} \int_{\Omega_b} |u_0(x)|^2 dx + \int_0^t \int_\Gamma \frac{\partial u(r,t)}{\partial r}\big|_\Gamma u(r,t)\big|_\Gamma dS dt - \int_0^t \int_{\Omega_b} \frac{\partial u}{\partial r} \frac{\partial u}{\partial r} dx dt \tag{3.19}$$

From the lemma, we know that

$$\int_0^t \int_\Gamma \frac{\partial u(r,t)}{\partial r}\big|_\Gamma u(r,t)\big|_\Gamma dS dt \leq 0.$$

This means

$$\int_{\Omega_b} |u(x,t)|^2 dx \leq \int_{\Omega_b} |u_0(x)|^2 dx, \quad 0 \leq t \leq T.$$

From estimate (3.18), we have:

Theorem 3.2. *The approximate problem (3.1)-(3.4) at most has one solution.*

Let $N \to \infty$ in (3.3), one gets

Corollary 3.1. *The reduced problem (2.41)-(2.44) at most has one solution.*

4. Numerical Examples

In order to demonstrate the effectiveness of the artificial boundary conditions given in this paper, three numerical examples are discussed. Two kinds of numerical methods, finite element method(FEM) and finite difference method(FDM), are used to solve these examples.

Example 1. Let's consider an initial-boundary value problem on the domain out of a sphere:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial r^2} + \frac{2}{r}\frac{\partial u}{\partial r} + \frac{1}{r^2}\frac{1}{\sin\theta}\frac{\partial}{\partial \theta}(\sin\theta \frac{\partial u}{\partial \theta}) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2 u}{\partial \phi^2}, \quad (r,\theta,\phi,t) \in \Omega_c^T, \tag{4.1}$$

$$u|_{r=a} = g(\theta,\phi,t), \tag{4.2}$$

$$u|_{t=0} = 0, \tag{4.3}$$

$$u \to 0, \quad \text{when} \quad r \to +\infty. \tag{4.4}$$

where $a = 1$, $T = 1$, $g(\theta, \phi, t) = \frac{1}{8(\pi t)^{\frac{3}{2}}} e^{-a^2/4t}$. The exact solution of problem (4.1)–(4.4) is

$$u(r, \theta, \phi, t) = \frac{1}{8(\pi t)^{\frac{3}{2}}} e^{-r^2/4t}. \tag{4.5}$$

First, Crank-Nicholson difference scheme is used to solve problem (4.1)–(4.4). The interval $[0, T]$ is divided into L equal parts:

$$0 = t_0 < t_1 < \cdots < t_L = T. \tag{4.6}$$

An artificial boundary $\Gamma_b = \{(r, \theta, \phi, t) \mid r = b, 0 < t \leq T\}$ with $b = 2$ is introduced to finite Ω_c^T and a bounded computational domain $\Omega_0^T = \{(r, \theta, \phi, t) \,|\, a < r < b, 0 < t < T\}$ is obtained. Then we divide the interval $[a, b]$ of r-axis into M equal parts, the interval $[0, \pi]$ into J equal parts and the interval $[0, 2\pi]$ into K equal parts:

$$a = r_0 < \cdots < r_M = b, \quad 0 = \theta_0 < \cdots < \theta_J = \pi. \quad 0 = \phi_0 < \cdots < \phi_K = 2\pi \tag{4.7}$$

Let $\tau = T/L$, $h = (b-a)/M$,$\delta = \pi/J$ and $\epsilon = 2\pi/K$. In this example we choose $N = 0$. Now we have the following formula by Crank-Nicholson scheme:

$$\frac{u_{i+1,j,k}^{n+1} - 2u_{i,j,k}^{n+1} + u_{i-1,j,k}^{n+1} + u_{i+1,j,k}^{n} - 2u_{i,j,k}^{n} + u_{i-1,j,k}^{n}}{2h^2} + \frac{u_{i+1,j,k}^{n+1} - u_{i-1,j,k}^{n+1} + u_{i+1,j,k}^{n} - u_{i-1,j,k}^{n}}{hr_i} +$$

$$\frac{u_{i,j+1,k}^{n+1} - 2u_{i,j,k}^{n+1} + u_{i,j-1,k}^{n+1} + u_{i,j+1,k}^{n} - 2u_{i,j,k}^{n} + u_{i,j-1,k}^{n}}{2r_i^2\delta^2} + \frac{u_{i,j+1,k}^{n+1} - u_{i,j-1,k}^{n+1} + u_{i,j+1,k}^{n} - u_{i,j-1,k}^{n}}{2r_i^2\delta \tan\theta_j}$$

$$+ \frac{1}{\sin^2\phi_k} \frac{u_{i,j,k+1}^{n+1} - 2u_{i,j,k}^{n+1} + u_{i,j,k-1}^{n+1} + u_{i,j,k+1}^{n} - 2u_{i,j,k}^{n} + u_{i,j,k-1}^{n}}{2r_i^2\epsilon^2} - \frac{u_{i,j,k}^{n+1} - u_{i,j,k}^{n}}{\tau} = 0,$$

$$1 \leq i \leq M,\ 1 \leq j \leq J,\ 0 \leq n \leq L-1,\ 1 \leq k \leq K;$$

$$u_{i,j,k}^{0} = 0, \qquad 0 \leq i \leq M,\ 1 \leq j \leq J,\ 1 \leq k \leq K;$$

$$u_{0,j,k}^{n} = g(\theta_j, \epsilon_k, t_n), \qquad 1 \leq n \leq L,\ 1 \leq j \leq J,\ 1 \leq k \leq K;$$

where $t_n = n\tau, r_i = ih, \theta_j = j\delta, \phi_k = k\epsilon$ and the artificial boundary conditions on Γ_b are given by numerical integrals of $\Phi_0(u|_{\Gamma_b}, \frac{\partial u}{\partial t}|_{\Gamma_b})$. For different M, J ,L and K, we have the results in the first column of Table. 1. In Fig.1, we give the error function $|u(b, \theta, \phi, t) - u_h(b, \theta, \phi, t)|$ for $t \in [0, T]$ with $\theta = \pi/3, \phi = \pi/3$.

Table 1: The results of Example 1.

	FDM	FEM
M	$\lVert u - u_h\rVert_{1,\Omega}/\lVert u\rVert_{1,\Omega}$	$\lVert u - u_h\rVert_{1,\Omega}/\lVert u\rVert_{1,\Omega}$
8	2.6674e-1	2.4610e-1
16	1.3412e-1	1.2624e-1
32	6.6020e-2	6.3601e-2
64	3.4168e-2	3.2338e-2

Furthermore, we use finite element method to solve problem (4.1)–(4.4). To do so, we should give the variational form of problem (4.1)–(4.4):

$$\left.\begin{array}{l} \text{Find } u \in U, \text{ such that} \\ \dfrac{d}{dt}(u, v)_{\Omega_0} + a(u, v) = 0, \forall v \in V, \end{array}\right\} \tag{4.8}$$

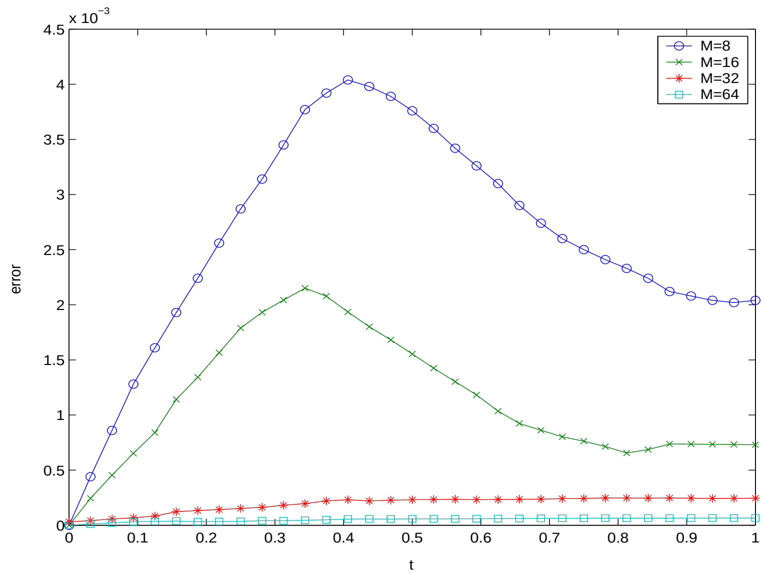

Fig. 1: The numerical result of example 1

where

$$\Omega_0 = \{(r,\theta,\phi) \mid a<r<b,\ 0\le\theta\le\pi,\ 0\le\phi\le 2\pi\}, \tag{4.9}$$

$$\begin{aligned}
(u,v)_{\Omega_0} &= \int_{\Omega_0} uvr^2\sin\theta\ drd\theta d\phi, && (4.10)\\
a(u,v) &= \int_{\Omega_0}\{\frac{\partial u}{\partial r}\frac{\partial v}{\partial r} - \frac{1}{r}\frac{\partial u}{\partial r}v + \frac{1}{r^2}\frac{\partial u}{\partial \theta}\frac{\partial v}{\partial \theta} - \frac{\cos\theta}{r^2\sin\theta}\frac{\partial u}{\partial \theta}v\\
&+ \frac{1}{r^2\sin^2\theta}\frac{\partial u}{\partial \phi}\frac{\partial v}{\partial \phi}\}r^2\sin\theta drd\theta d\phi - \int_0^{2\pi}\int_0^{\pi}(\frac{\partial u}{\partial r}v)|_{r=b}b^2\sin\theta d\theta d\phi, && (4.11)\\
U &= \Big\{w(r,\theta,\phi,t)\Big| t\in[0,T], w(\cdot,\cdot,\cdot,t), \frac{\partial w}{\partial t}(\cdot,\cdot,\cdot,t)\in H^1(\Omega_0), \text{and}\\
& w(r,\theta,\phi,0)=0, w\big|_{r=a} = g(\theta,\phi,t), w(r,\theta,0,t) = w(r,\theta,2\pi,t)\Big\}, && (4.12)\\
V &= \Big\{v(r,\theta,\phi)\in H^1(\Omega_0)\ \Big|\ v(a,\theta,\phi)=0, v(r,\theta,0)=v(r,\theta,2\pi)\Big\}. && (4.13)
\end{aligned}$$

If we give a partition of Ω_0 such as (4.7), we can construct the finite dimension subspace V_h of V by using piecewise trilinear functions:

$$V_h = \Big\{p_h(r,\theta,\phi)\in C^0(\Omega_0)\ \Big|\ p_h|_{[r_{i-1},r_i]\times[\theta_{j-1},\theta_j]\times[\phi_{k-1},\phi_k]} \in P_{111}(r,\theta,\phi)\Big\},$$

where $P_{111}(r,\theta,\phi)$ is the space of trilinear functions with $p_h(r,\theta,0)=p_h(r,\theta,2\pi)$ and $1\le i\le M,\ 1\le j\le J, 1\le k\le K$. Let $\{N_1(r,\theta,\phi), N_1(r,\theta,\phi),\cdots,N_M(r,\theta,\phi)\}$ is a basis of space V_h with $M=\dim V_h$, and

$$\begin{aligned}
U_h &= \Big\{w_h(r,\theta,\phi,t)\Big|\ w_h(r,\theta,\phi,t) = \sum_{i=1}^{M}\alpha_i(t)N_i(r,\theta,\phi)\\
&\quad \text{and}\ \ w_h(a,\theta_j,\phi_k,t) = g(\theta_j,\phi_k,t), \alpha_i\in H^1([0,T]), \alpha_i(0)=0\Big\},\\
V_h^0 &= \{v_h(r,\theta,\phi)\in V_h \mid v_h(a,\theta,\phi)=0, v_h(r,\theta,0)=v_h(r,\theta,2\pi)\}.
\end{aligned}$$

Then we will solve the following approximation problem of (4.8):

$$\left.\begin{array}{l}\text{Find } u_h \in U_h, \text{ such that}\\ \dfrac{d}{dt}(u_h, v_h)_{\Omega_0} + a(u_h, v_h) = 0, \forall v_h \in V_h^0,\end{array}\right\} \tag{4.14}$$

From variational problem (4.14), we obtain an initial value problem of ordinary differential equations containing functions $\alpha_1(t), \cdots, \alpha_M(t)$. Then we can obtain $\alpha_1(t), \cdots, \alpha_M(t)$ from the initial value problem (4.14) by numerical method. The numerical results are shown in the second column of Table.1.

Example 2. Consider the same problem in Example 1 with another boundary condition

$$g(\theta, \phi, t) = \frac{1}{8(\pi t)^{\frac{3}{2}}} e^{-\frac{(r\sin\theta\cos\phi - x_0)^2 + (r\sin\theta\cos\phi - y_0)^2 + (r\cos\theta - z_0)^2}{4t}}$$

where $(x_0, y_0, z_0) = (0.5, 0.5, 0.5)$. We introduce an artificial boundary Γ_b with $b = 2$ to bounded the domain Ω_c^T Finite element method similar to that in Example 1 is used to solve this example. For different choices of N, the order of the artificial boundary condition in (2.45), errors $\|u - u_h\|_{1,\Omega}/\|u\|_{1,\Omega}$ are shown in Table 2.

Table 2: The results of Example 2

	$N=0$		$N=2$		$N=4$	
M	FDM	FEM	FDM	FEM	FDM	FEM
8	3.1130e-1	2.9592e-1	1.9184e-1	1.8592e-1	1.4401e-1	1.3592e-1
16	2.5075e-1	2.4119e-1	9.7369e-2	9.4319e-2	7.4747e-2	6.8319e-2
32	1.8521e-1	1.7143e-1	4.9782e-2	4.7765e-2	3.8673e-2	3.5461e-2
64	1.7438e-1	1.6732e-1	2.5241e-2	2.3321e-2	1.9162e-2	1.7435e-2

	$N=7$		$N=12$	
M	FDM	FEM	FDM	FEM
8	1.3531e-1	1.3032e-1	1.3078e-1	1.2473e-1
16	6.8863e-2	6.4568e-2	6.4484e-2	6.0259e-2
32	3.4883e-2	3.2182e-2	3.1486e-2	3.0093e-2
64	1.6853e-2	1.5346e-2	1.5185e-2	1.4528e-2

In Fig. 2, the error function $|u(b, \theta, \phi, t) - u_h(b, \theta, \phi, t)|$ for $t \in [0, T]$ with $\theta = \pi/3, \phi = \pi/3$ are demonstrated.

Example 3. Consider the following problem:

$$\frac{\partial u}{\partial t} - \triangle u = 0, \qquad (x, t) \in \Omega_c^T \tag{4.15}$$

$$u\Big|_{\Gamma_0} = g(x, t), \qquad (x, t) \in \Gamma_0, \tag{4.16}$$

$$u\Big|_{t=0} = 0, \tag{4.17}$$

$$u \to 0 \qquad \text{when } ||x|| \to +\infty, \tag{4.18}$$

where Γ_0 is the boundary of $\Omega = \{(x_1, x_2, x_3) \in \mathbb{R}^3, |x_i| \le 1, i = 1, 2, 3\} \times [0, T]$ and $\Omega_c^T = \mathbb{R}^3 \times [0, T] \backslash \Omega$

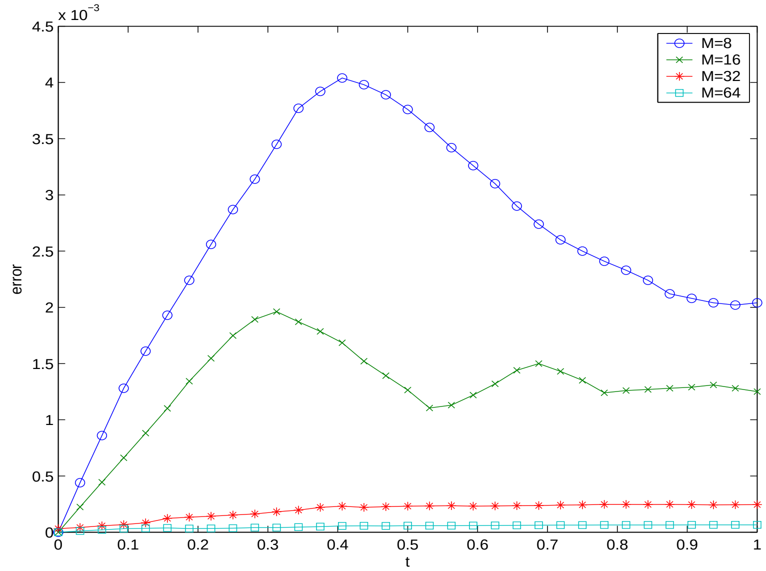

Fig. 2: The numerical result of example 2

The exact solution is

$$u(x_1,x_2,x_3,t)=\frac{1}{8(\pi t)^{\frac{3}{2}}}e^{-\frac{(x_1-x_1^0)^2+(x_2-x_2^0)^2+(x_3-x_3^0)^2}{4t}}$$

with $(x_1^0,x_2^0,x_3^0)=(0.5,0.5,0.5)$. The boundary condition is given by the exact solution. The standard finite element method is used to solve this problem. For different choices of N and $b=3$, the results of $\|u-u_h\|_{1,\Omega}/\|u\|_{1,\Omega}$ at $(x,y,z)=(1.5,1.5,1.5)$ are shown in Table 3.

Table 3: The errors for artificial boundaries with different accuracy

M	$N=0$	$N=1$	$N=3$	$N=6$	$N=9$
8	2.8628e-1	2.1532e-1	1.9653e-1	1.7891e-1	1.6962e-1
16	2.2846e-1	1.2457e-1	1.1462e-1	1.0641e-1	9.8843e-2
32	1.6862e-1	6.4392e-2	5.6673e-2	5.0843e-2	4.9273e-2
64	1.2463e-1	3.3648e-2	2.7356e-2	2.5143e-2	2.4762e-2

Table 4: The result for different artificial boundaries

Mesh size	b=2	b=3	b=4	b=5
1/4	2.3364e-1	1.9884e-1	1.8634e-1	1.8023e-1
1/8	1.4973e-1	1.2859e-2	1.2256e-1	1.18262-1
1/16	7.6462e-2	6.4328e-2	6.1638e-2	5.9634e-2
1/32	3.8288e-2	3.2232e-2	3.0934e-2	2.9783e-2

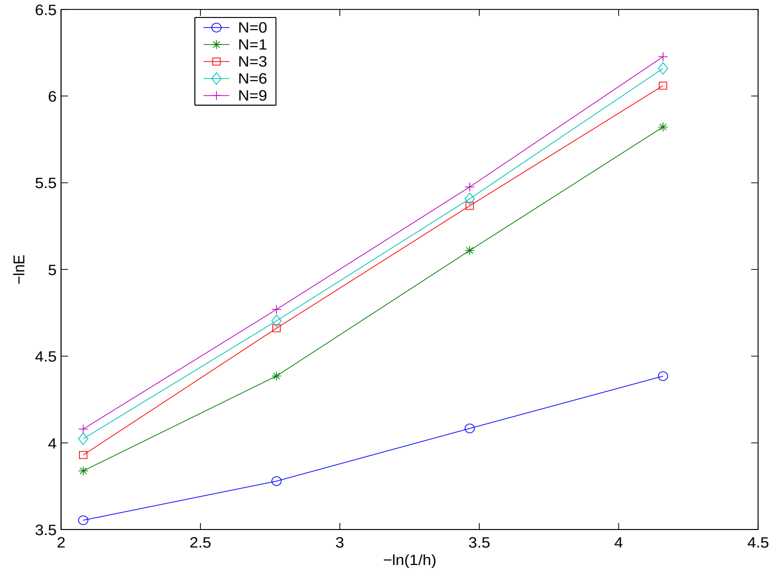

Fig. 3: The convergent rate of the artificial boundary conditions with different accuracy

To know the relation between the errors and the location of artificial boundary condition, we select different artificial boundaries, namely b=2, 3, 4, 5. The error function $\|u-u_h\|_{1,\Omega}/\|u\|_{1,\Omega}$ at $(x_1, x_2, x_3) = (1.5, 1.5, 1.5)$ are shown in Table.4. In this example, N is chosen to be 4.

Fig.3 demonstrates the convergent rates of the artificial boundary conditions with different accuracy.

5. Conclusion

The exact boundary condition and a family of artificial boundary conditions of heat equation on unbounded domains in 3-D spatial space are provided. By them the reduced problems on bounded computational domain are obtained, which is equivalent or approximate to the original problem. Furthermore the stability analysis of the reduced problems is given. The good performance of the numerical examples shows that the given method is feasible and effective.

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