Accurate numerical evaluation of domain integrals in 3D boundary element method for transient heat conduction problem

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Abstract

This paper presents an improved approach for the numerical evaluation of domain integrals that appear in the solution of transient heat conduction problems when using a time-dependent boundary integral equation method. An implementation of this method requires the accurate evaluation of the domain integrals. As the time step value is very small, the integrand in the domain integral is close to singular, thus rendering accurate evaluation of the integral difficult. First a closest point is introduced when the source point is close to, but not on the cell in the present method. Then a coordinate transformation coupled with a cell subdivision technique is proposed considering the position of the source point or the closest point and the relations between the size of the cell and the time step value. With the new method, accurate evaluation of domain integrals can be obtained. Numerical examples have demonstrated the accuracy and efficiency of the proposed method.

Keywords: domain integrals; cell subdivision; transient heat conduction; boundary element method.

1. Introduction

The boundary element method (BEM) [1-13] is an efficient tool for the analysis of the transient heat conduction problem. The pseudo-initial condition method is a boundary integral equation formulation based on the time-dependent fundamental solution. When using this method for the transient heat conduction problem, the temperature computed in the previous step is considered as the initial condition in current step. Therefore, the domain integrals of this pseudo-initial condition are required in the pseudo-initial condition method. The integrand in the domain integral is a regular function, but as the time step approaches to zero, it is close to singular [1]. When small time step is used, a straightforward computation using Gaussian quadrature can produce large errors, and thus lead to instability of the analysis as reported in [14-17]. Thus, accurate numerical evaluation of the domain integral is of crucial importance for the successful implementation of the pseudo-initial condition method.

Various methods have been proposed to cope with these integrals. Gao [18-20] presented a radial integration method which converted the domain integrals into equivalent boundary integrals. Wrobel *et al* [21] proposed a semi-analytical integration method based on polar coordinates. But this method is mainly applied to the two-dimensional problems. Recently, the present authors [22] developed a method for three-dimensional problems. But the case that the source point locates outside the cell is not considered in this method.

Though the source point is not on the cell, the domain integrals can't be evaluated accurately and efficiently by standard Gaussian quadrature when the time step value is small. In present paper, firstly a closest point is introduced when the source point is close to the cell. It is very convenient to implement the coordinate transformation and the cell subdivision technique by using the closest point instead of source point when the source point locates outside the cell. Then, a coordinate transformation denoted as (α,β,γ) transformation is proposed. The transformation is an extension of Zhang's [23] (α,β) transformation. With the transformation, the integrand in the domain integral becomes smoother. Thus, the computational accuracy can be improved. Finally, we presented the cell subdivision technique. The integrand in the domain

integral varies dramatically around the source point or closest point when the time step is small. We subdivided the volume cell into the pyramidal and hexahedral patches considering the position of the source point or the closest point and the relations between the size of the cell and the time step value. With the subdivision technique, more integration points are shifted towards the source point or the closest point, and thus more accurate results can be obtained. Through introducing a closest point, we can evaluate the domain integrals in a uniform method no matter whether the source point locates on the cell or not. Numerical results demonstrate the accuracy and efficiency of our method.

The outline of the rest of this paper is as follows. Section 2 introduces the boundary integral equation and the domain integral. And then the concept of closest point, (α,β,γ) transformation and the cell subdivision technique are presented in Section 3. After that, several numerical examples are given in Section 4. Finally, the conclusion is provided in Section 5.

2. General description

2.1 The boundary integral equation

In this section, we discuss BEM solutions for the three-dimensional diffusion equation

$$\nabla^2 u(\mathbf{x},t)-\frac{1}{k}\frac{\partial u(\mathbf{x},t)}{\partial t}=0 \tag{1}$$

The boundary integral equation for transient heat conduction in an isotropic, homogeneous medium Ω bounded by Γ is as follows:

$$\begin{aligned} &c(\mathbf{y})u(\mathbf{y},t_F)+k\int_{t_0}^{t_F}\int_{\Gamma}u(\mathbf{x},t)q^*(\mathbf{y},\mathbf{x},t_F,t)d\Gamma(\mathbf{x})dt \\ &=k\int_{t_0}^{t_F}\int_{\Gamma}q(\mathbf{x},t)u^*(\mathbf{y},\mathbf{x},t_F,t)d\Gamma(\mathbf{x})dt+\int_{\Omega}u_0(\mathbf{x},t_0)u^*(\mathbf{y},\mathbf{x},t_F,t_0)d\Omega(\mathbf{x}) \end{aligned} \tag{2}$$

where $\mathbf{y}$ and $\mathbf{x}$ are the source point and the field point, respectively. $c(\mathbf{y})$ is a function of the solid angle of the boundary at point $\mathbf{y}$. k denotes the diffusion coefficient. t_0 and t_F stand for the initial time and the end time of one step, respectively. t represents the time between t_0 and t_F. u^* and q^* are the time-dependent fundamental solution and its derivative with respect to the unit

outward normal at the boundary. u_0 is the initial temperature.

The time-dependent fundamental solution u^* is given by:

$$u^* = \frac{1}{(4\pi k\tau)^{1.5}} \exp\left(-\frac{r^2}{4k\tau}\right) \tag{3}$$

where r represents the distance between the source point and the field point. τ is the time step, as follows:

$$\tau = t_F - t_0 \tag{4}$$

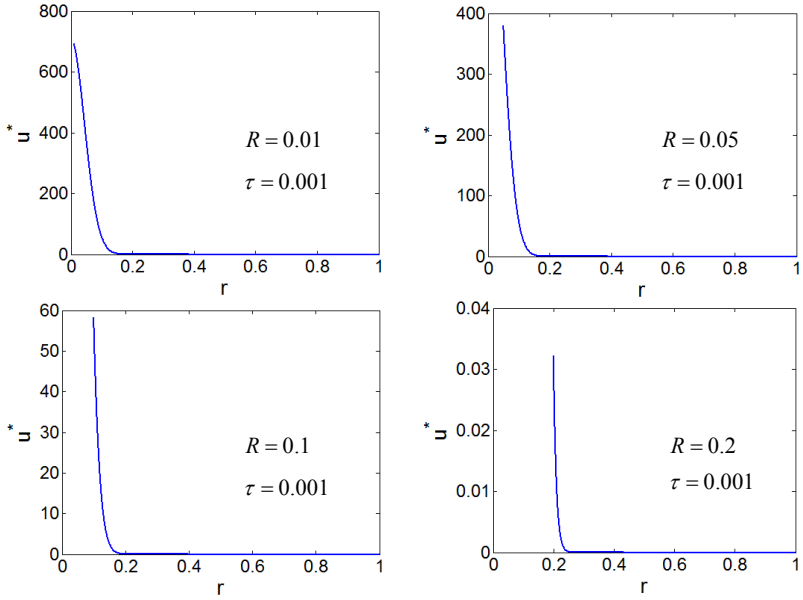

Fig. 1. Variation of the function u^* with r for $\tau = 0.001$.

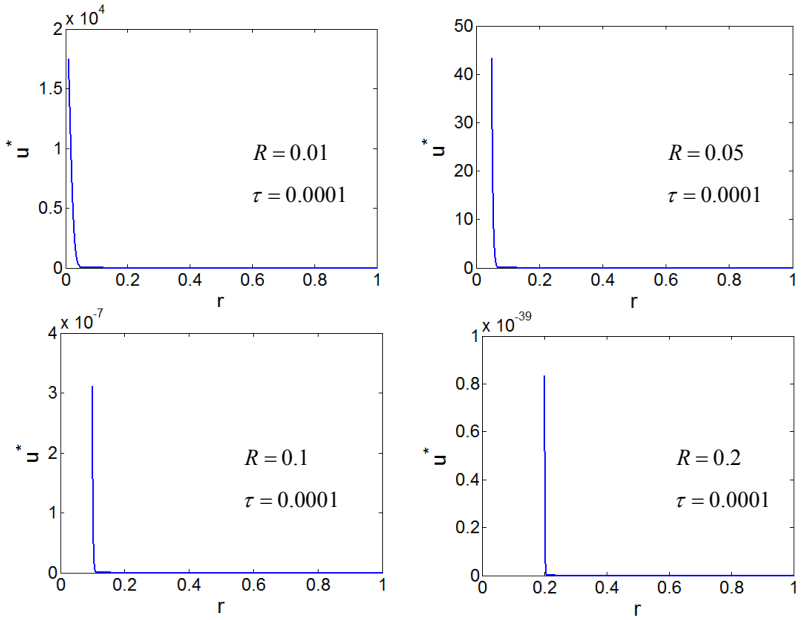

Fig. 2. Variation of function u^* with r for $\tau = 0.0001$.

2.2 The domain integral

The domain integral involved in Eq. (2) can be written as:

$$I = \int_{\Omega} u_0(\mathbf{x},t_0)u^*(\mathbf{y},\mathbf{x},t_F,t_0)d\Omega(\mathbf{x}) = \int_{\Omega} u_0(\mathbf{x},t_0)\frac{1}{(4\pi k\tau)^{1.5}}\exp\left(-\frac{r^2}{4k\tau}\right)d\Omega(\mathbf{x}) \qquad (5)$$

The initial temperature $u_0(\mathbf{x},t_0)$ is a regular function. As the time step approaches zero, the time-dependent fundamental solution u^* becomes less and less smooth, its limit being a Dirac delta function [1]. When the source point locates outside the cell, domain integrals can also not be calculated accurately by the standard Gaussian quadrature using small time step. *k* denotes the diffusion coefficient and is assumed to be 1 in Fig. 1 and Fig. 2. *R* represents the minimum distance from the source point to the cell. And *r* represents the distance between the source point and the field point. It can be seen that steep slopes produced by the function u^* require more Gauss points to evaluate more accurately the integral under consideration.

3. New method for evaluating the domain integrals

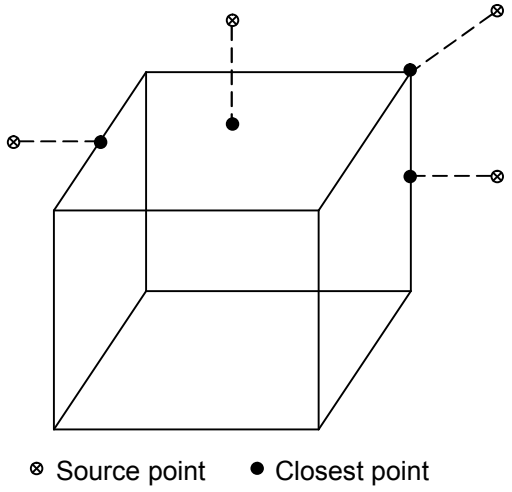

Fig. 3. Several typical position of the closest point

3.1 The closest point

In this section, we first introduce the concept of the closest point. From previous analysis, it can be obtained that when the time step value is small, a straightforward application of Gaussian quadrature can produce large errors even the source point is not on the cell. The method proposed in the paper [22] is efficient for evaluating the

domain integrals, but it doesn't consider the source point locating outside the cell. It is very inconvenient to implement the coordinate transformation and the cell subdivision technique when the source point is not on the cell. Therefore, a closest point is introduced. For the sake of simplicity, the closest point is obtained according to the minimum distance in the local coordinate system. Fig. 3 shows several typical position of the closest point.

3.2 The (α,β,γ) transformation

The (α,β,γ) transformation is used in the pyramidal patch as shown in Fig. 4. (x_0,y_0,z_0) is the source point or the closest point. (x_1,y_1,z_1), (x_2,y_2,z_2), (x_3,y_3,z_3) and (x_4,y_4,z_4) are the node coordinates of the cell.

To construct the (α,β,γ) coordinate system, the following mapping is used:

$$\begin{cases} x_\gamma = x_1 + (x_2 - x_1)\alpha + (x_4 - x_1)\beta \\ y_\gamma = y_1 + (y_2 - y_1)\alpha + (y_4 - y_1)\beta \\ z_\gamma = z_1 + (z_2 - z_1)\alpha + (z_4 - z_1)\beta \end{cases} \quad \alpha,\beta \in [0,1] \tag{6a}$$

$$\begin{cases} x = x_0 + (x_\gamma - x_0)\gamma \\ y = y_0 + (y_\gamma - y_0)\gamma \\ z = z_0 + (z_\gamma - z_0)\gamma \end{cases} \quad \gamma \in [0,1] \tag{6b}$$

Combining Eqs. (6a)-(6b), the expression for obtaining coordinates (x,y,z) can be written as:

$$\begin{cases} x = x_0 + \left[(x_1 - x_0) + (x_2 - x_1)\alpha + (x_4 - x_1)\beta\right]\gamma \\ y = y_0 + \left[(y_1 - y_0) + (y_2 - y_1)\alpha + (y_4 - y_1)\beta\right]\gamma \\ z = z_0 + \left[(z_1 - z_0) + (z_2 - z_1)\alpha + (z_4 - z_1)\beta\right]\gamma \end{cases} \quad \alpha,\beta,\gamma \in [0,1] \tag{7}$$

The Jacobian of the transformation from the (x,y,z) system to the (α,β,γ) system is

$$Jb = \gamma^2 \begin{vmatrix} x_2 - x_1 & y_2 - y_1 & z_2 - z_1 \\ x_3 - x_1 & y_3 - y_1 & z_3 - z_1 \\ x_1 - x_0 & y_1 - y_0 & z_1 - z_0 \end{vmatrix} \tag{8}$$

With the (α, β, γ) transformation, the variations of the integrand become smoother. Thus, the computational accuracy of the domain integrals can be improved.

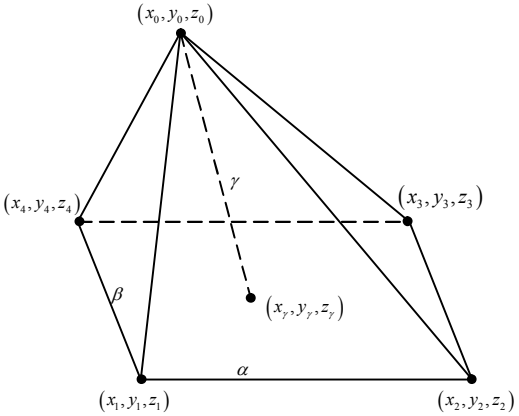

Fig. 4. The (α, β, γ) coordinate transformation.

3.3 The cell subdivision technique

To further improve the computational accuracy of the domain integrals, a cell subdivision technique is proposed in this part. As shown in Fig. 1 and Fig. 2, a steep slope occurs in the integrand near the closest point as the time step value is small. Thus, more integration points should be shifted towards the closest point in order to calculate more accurately the integral under consideration. The detailed analysis is as follows.

Firstly we see the following probability density function of normal distribution.

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{x^2}{2\sigma^2} \right) \tag{9}$$

$$\int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{x^2}{2\sigma^2} \right) dx = 1 \tag{10}$$

From Eq. (9), it can be noted that the form of the probability density function is almost like that of the time-dependent fundamental solution u^*. As all we know, the integral value of Eq. (10) mainly concentrates in the interval $[-3\sigma, 3\sigma]$. This also applies similarly to the evaluation of the domain integral for the time-dependent

fundamental solution. Then a length parameter $\lambda\sqrt{k\tau}$ is introduced, and $\sqrt{k\tau}$ is similar to σ in the probability density function. The length parameter $\lambda\sqrt{k\tau}$ is the real distance in the global coordinate system, not in the local coordinate system.

Through introducing the closest point, the domain integrals can be evaluated in a uniform method no matter whether the source point is on the cell or not. The cell subdivision technique is presented as follows:

- Firstly, a cube region with the length of $2\lambda\sqrt{k\tau}$ is constructed to well cover the source point or the closest point on the integration cell. If the cube region beyond the boundary of the cell, taking that as the boundary of the cube region.
- Secondly, sub-pyramids are created in cube region considering the position of the source point or the closest point and sub-hexahedrons are constructed in the remaining regions of the cell.

Fig.5 shows the subdivision of hexahedron cell when the source point or the closest point is on the vertex of the cell. The advantage of the proposed cell subdivision technique is that more integration points are shifted towards the source point or the closest point. With the cell subdivision technique coupled with the (α,β,γ) transformation, the domain integrals can be accurately calculated.

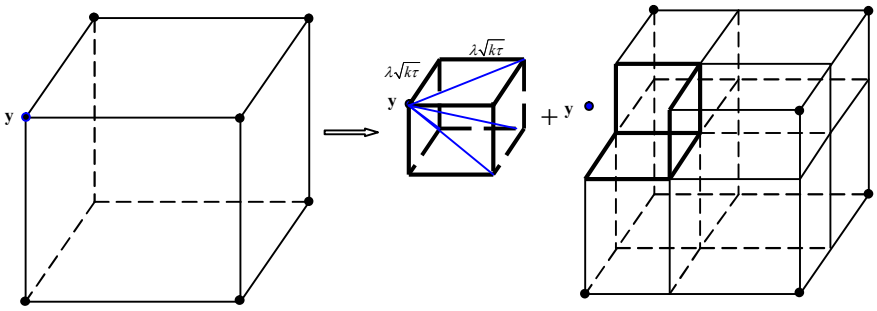

Fig. 5. The subdivision of hexahedron cell.

4. Numerical examples

To verify the accuracy and efficiency of our method, several examples are presented in this section. The domain integrals of the following form are considered:

$$I=\int_{\Omega}\frac{1}{(4\pi k\tau)^{1.5}}\exp\left(-\frac{r^2}{4k\tau}\right)d\Omega \tag{11}$$

The coefficient k in Eq. (11) is assumed to be 1 and the dimensionless parameter λ is 8. The (α,β,γ) transformation with 15×15×15 Gaussian points is used on the sub-pyramids and 5×5×5 point Gaussian quadrature is used on the sub-hexahedrons. The numerical values obtained by our method will be compared to 'exact' values in terms of the relative error defined by

$$\text{Relative Error} = \left| \frac{I_{\text{numerical}} - I_{\text{exact}}}{I_{\text{exact}}} \right| \tag{12}$$

where $I_{\text{numerical}}$ and I_{exact} are the numerical and 'exact' values of the integral under consideration, respectively. The accuracy of I_{exact} is to 10^{-12}.

4.1 Example 1

In the first example, the domain integral of Eq. (11) is evaluated over a hexahedron cell with the node coordinates of (-1, -1, -1), (1, -1, -1), (1, 1, -1), (-1, 1, -1), (-1, -1, 1), (1, -1, 1), (1, 1, 1), (-1, 1, 1) as shown in Fig.6. The coordinate of the source point is set at (1.01, 0, 0). The relative errors of various methods with different time steps are compared in Table 1. τ represents the time step value. 5×5×5 means straightforward Gaussian quadrature with 5×5×5 Gauss points. The (α,β,γ) transformation combined with the cell subdivision technique is denoted as (α,β,γ).

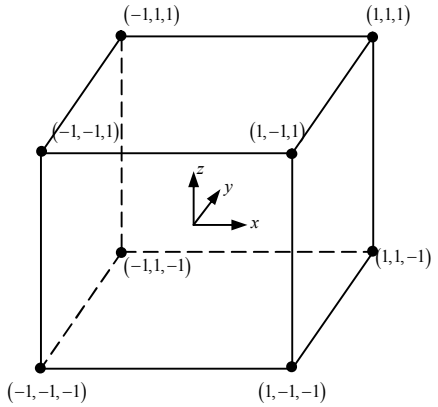

Fig. 6. The node coordinates of hexahedron cell.

Table 1

Relative errors for integral *I* on hexahedron cell with the node coordinates of (-1, -1, -1), (1, -1, -1), (1, 1, -1), (-1, 1, -1), (-1, -1, 1), (1, -1, 1), (1, 1, 1), (-1, 1, 1). Errors less

than 10^{-12} are indicated with a '-'.

τ	0.1	0.01	0.001	0.0001	0.00001
5×5×5	2.02E-03	1.82E+00	7.94E+00	1.00E+00	1.00E+00
10×10×10	3.01E-09	5.54E-02	1.00E+00	1.00E+00	1.00E+00
15×15×15	-	5.77E-04	2.27E+00	3.42E+01	6.10E-01
30×30×30	-	-	9.54E-02	1.00E+00	1.00E+00
(α,β,γ)	-	1.09E-08	2.95E-08	3.01E-08	3.15E-08

It can be seen from Table 1 that when the time step value is small, a straightforward computation using Gaussian quadrature can produce large errors even with 30×30×30 Gauss points, while accurate and stable results can be obtained by our method. As illustrated in this example, it is necessary to consider the problem that the source point locates outside the cell when small time step is used. And the proposed method is efficient for solving this problem by introducing a closest point.

4.2 Example 2

In this example, the integration cell is the same as described in example 1. The source point moves close to the cell. The coordinates in Table 2 and Table 3 are the position of the source point. The relative errors in Table 2 and Table 3 are obtained by the proposed method and a straightforward Gaussian quadrature with 20×20×20 Gauss points, respectively.

Table 2

Relative errors for integral *I* by the proposed method on hexahedron cell with the node coordinates of (-1, -1, -1), (1, -1, -1), (1, 1, -1), (-1, 1, -1), (-1, -1, 1), (1, -1, 1), (1, 1, 1), (-1, 1, 1).

τ	0.1	0.01	0.001	0.0001
(1.1, 0, 0)	-	1.03E-08	2.65E-08	1.31E-08
(1.05, 0, 0)	-	1.13E-08	2.77E-08	3.13E-08
(1.01, 0, 0)	-	1.09E-08	2.95E-08	3.01E-08
(1.005, 0, 0)	-	1.08E-08	3.35E-08	3.12E-08
(1.001, 0, 0)	-	1.07E-08	3.87E-08	3.97E-08

Table 3

Relative errors for integral I by a straightforward Gaussian quadrature with 20×20×20 Gauss points on hexahedron cell with the node coordinates of (-1, -1, -1), (1, -1, -1), (1, 1, -1), (-1, 1, -1), (-1, -1, 1), (1, -1, 1), (1, 1, 1), (-1, 1, 1).

τ	0.1	0.01	0.001	0.0001
(1.1, 0, 0)	-	1.70E-06	6.03E-01	1.00E+00
(1.05, 0, 0)	-	1.70E-06	6.03E-01	1.00E+00
(1.01, 0, 0)	-	1.70E-06	6.03E-01	1.00E+00
(1.005, 0, 0)	-	1.70E-06	6.03E-01	1.00E+00
(1.001, 0, 0)	-	1.70E-06	6.03E-01	1.00E+00

Table 2 and Table 3 show that the relative errors don't change for a certain time step value when the source point moves close to the cell in the two methods. As the time step decrease, a straightforward application of Gaussian quadrature would produce large errors no matter whether the source point locates close to the cell or not. But with our proposed method, good results can be obtained with a wide range of time steps.

4.3 Example 3

A more general example is presented in this part. The domain integrals of the following form are considered:

$$I_1 = \int_{\Omega} N \frac{1}{\left(4\pi k\tau\right)^{1.5}} \exp\left(-\frac{r^2}{4k\tau}\right) d\Omega \tag{13}$$

where N is the shape function of the hexahedron cell.

Different locations of the source points are considered. The integration cell is shown in Fig. 6. The relative errors for different locations of the source points and time steps are compared in Table 4.

Table 4

Relative errors for integral I_1 by the proposed method on hexahedron cell with the node coordinates of (-1, -1, -1), (1, -1, -1), (1, 1, -1), (-1, 1, -1), (-1, -1, 1), (1, -1, 1), (1, 1, 1), (-1, 1, 1). Errors less than 10^{-12} are indicated with a '-'.

τ	0.1	0.01	0.001	0.0001
(1.01, 1.02, 1.03)	1.27E-11	5.15E-09	7.90E-09	3.16E-09
(1.01, 0.0, 1.03)	2.02E-12	7.80E-10	1.86E-08	1.41E-08
(1.01, 0.1, 0.2)	-	5.26E-09	2.67E-08	3.02E-08
(0.0, -1.04, -1.05)	7.22E-12	1.58E-08	1.41E-08	7.78E-08
(0.0, 0.0, -1.05)	-	1.19E-08	2.03E-08	1.95E-08

From Table 4 it can be seen that the relative errors almost don't change with position of the source point when adding the shape function into the domain integral. These illustrate the proposed method is a robust algorithm for evaluating the domain integrals.

4.4 Example 4

A real transient heat conduction problem is considered in this example. The cube is heated on the top face and other faces are insulated as shown in Fig.7. The density, heat conductivity and heat capacity are $20kg/m^3$, $2kJ/(m.h^0C)$ and $0.8kJ/(kg.^0C)$, respectively. The length of the cube is 1m. A uniform temperature 100^0C is imposed suddenly on the top face of the cube. The initial temperature of the cube is 0^0C. In this application, the variation history of the temperature from 0h to 9.6h at the bottom face is concerned. 96 boundary linear quadrilateral elements with 150 nodes and 64 volume linear hexahedral cells with 125 nodes are used. To illustrate the accuracy of the proposed method, numerical results are compared with the existing analytical solution to the considered problem as shown in Fig. 8. 'Regular Gaussian 0.1' means that the domain integrals are evaluated using the Gaussian quadrature directly and the time step is 0.1h. 'Proposed Solution 0.1' represents that (α,β,γ) transformation combined with the cell subdivision technique is used for calculating the integrals and the time step is 0.1h.

Fig. 8 shows that the 'Regular Gaussian' solutions start to become unstable when the time step is less than 0.1h. With our method, the domain integrals can be evaluated accurately and thus good results are obtained for a wide range of time steps.

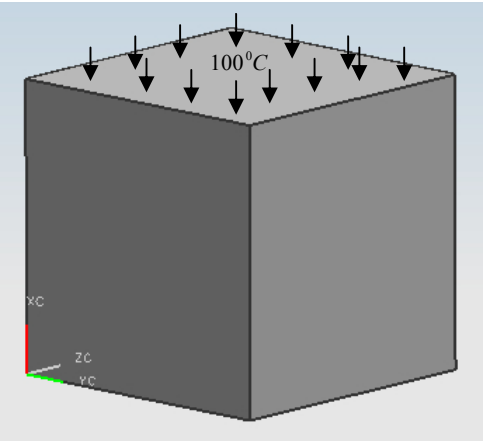

Fig. 7. The cube is heated on the top face.

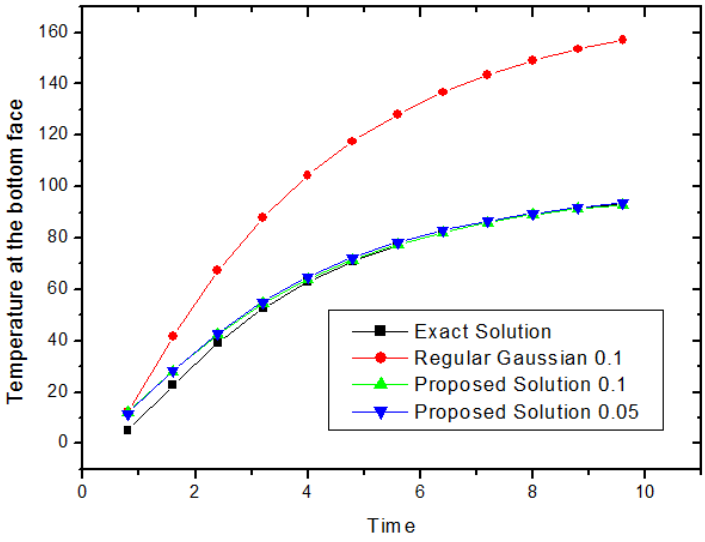

Fig. 8. The temperature at the bottom face.

5. Conclusion

An improved approach for the numerical evaluation of domain integrals that appear in the BEM solution for transient heat conduction problems is presented in this paper. With the proposed method, the domain integrals can be evaluated accurately and efficiently no matter whether the source point locates on the integration cell or not. Firstly through introducing a closest point, the numerical evaluation of the domain integrals can be implemented by a uniform method. Then using the (α,β,γ) transformation and the cell subdivision technique, more Gauss points are shifted towards the source point or the closest point, and thus more accurate results are obtained. The accurate numerical evaluation of the domain integrals can improve the stability of the pseudo-initial condition method for the transient heat conduction when

small time step is used. Numerical examples are presented and results demonstrate the accuracy and efficiency of our method.

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