

# **A general algorithm for the numerical evaluation of domain integrals in 3D boundary element method for transient heat conduction**

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## **Abstract**

In this paper, a general algorithm is proposed for evaluating domain integrals in 3D boundary element method. These integrals are involved in the solution of transient heat conduction problems when using a time-dependent boundary integral equation method named as pseudo-initial condition method. Accurate evaluation of domain integrals is of great importance to the successful implementation of this method. However, as the time-dependent kernel in the domain integral is close to singular when small time step is used, a straightforward application of Gaussian quadrature may produce large errors, and thus lead to instability of the analysis. To overcome this drawback, a coordinate transformation coupled with an element subdivision technique is presented. The coordinate transformation makes the integrand of domain integral more smooth; meanwhile, the element subdivision technique considers the relations between the size of the element and the time step. With the proposed method, more Gaussian points are shifted towards the source point, thus more accurate results can be obtained. Numerical examples demonstrate that the calculation accuracy of domain

integrals and the stability of analysis for transient heat conduction problems are improved by the proposed algorithm when small time step is used.

**Keywords:** domain integrals; stability analysis; transient heat conduction; boundary element method; element subdivision technique

## 1. Introduction

The transient heat conduction analysis is widely applied to the practical engineering problem. The main numerical methods for the transient heat conduction problem are the finite difference method (FDM), the finite element method (FEM) and the boundary element method (BEM). Compared to FDM and FEM, the BEM [1-10] is a more attractive method to analyze this problem. The BEM using a time-dependent fundamental solution for transient heat conduction problem can be classified into two schemes. One is the time convolution method and the other is the pseudo-initial condition method. Compared to the time convolution method, the pseudo-initial condition method is more efficient because no time convolution is required. When using the pseudo-initial condition method, the temperature computed in the previous step is considered as the initial condition in current step. Thus, the domain integral of this pseudo-initial condition is required in this method.

Although the domain integrals in the pseudo-initial condition method are actually regular in nature, they can't be evaluated accurately and efficiently by the standard Gaussian quadrature when small time step is used. This is because as the time step decreased progressively, the integrand in the domain integral (the time-dependent fundamental solution) varies dramatically near the source point. When the time step approaches zero, the time-dependent kernel is close to singular. We may call these integrals as pseudo-singular integrals. The difficulty of numerically integrating a function with such behavior can introduce numerical unstable problems into the solution, as reported in [11-14]. Thus accurate calculation of the domain integrals is important to the successful implementation of the pseudo-initial condition method.

However, much literature focus on the nearly singular integrals [15-20] and singular integrals [21-27], and little literature refer to these pseudo-singular domain integrals. Gao [28-29] proposed a radial integration method which converted the domain

integrals into equivalent boundary integrals. This method is not so efficient to solve large scale problems. Wrobel *et al* [30] introduced a semi-analytical integration scheme using polar coordinates. Their method is applicable primarily to the two-dimensional problems and a linear variation of the potential must be assumed in each cell.

In our method, firstly a coordinate transformation denoted as  $(\alpha, \beta, \gamma)$  transformation is introduced. It is an extension of Zhang's [31]  $(\alpha, \beta)$  transformation. With the coordinate transformation, the integrand in the domain integrals are smoothed out, which is advantageous for the numerical calculation of the pseudo-singular domain integrals. Furthermore, an element subdivision technique is proposed considering the position of the source point, the shape of the element, the property of the time-dependent fundamental solution and the relations between the size of the element and the time step. With the element subdivision technique, integration elements are divided into several pyramidal and hexahedral patches. The domain integrals on the pyramidal patches have a large impact on the whole integrals, and thus we focus on these integrals on pyramidal patches. In our numerical implementation, the  $(\alpha, \beta, \gamma)$  transformation is applied on pyramidal patches. Using the coordinate transformation, the integrands of domain integrals which vary drastically can be accurately calculated by our method even if the time step is very small. And for hexahedral patches, the standard Gaussian quadrature is employed. Numerical examples are presented to verify our method. Results demonstrate the accuracy and efficiency of our method.

This paper is organized as follows. In section 2, the boundary integral equation and the domain integral are described. Section 3 introduces the  $(\alpha, \beta, \gamma)$  transformation and the element subdivision technique. Numerical examples are given in Section 4. The paper ends with conclusions 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

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

The boundary integral equation for transient heat conduction in an isotropic, homogeneous medium  $\Omega$  bounded by  $\Gamma$  is as follows:

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

where  $\mathbf{y}$  and  $\mathbf{x}$  are the source and the field points, respectively.  $c(\mathbf{y})$  is a function of the solid angle of the boundary at point  $\mathbf{y}$ .  $k$  denotes the diffusion coefficient,  $t_0$  stands for the initial time and  $u_0(\mathbf{x}, t_0)$  is the initial condition.

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

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

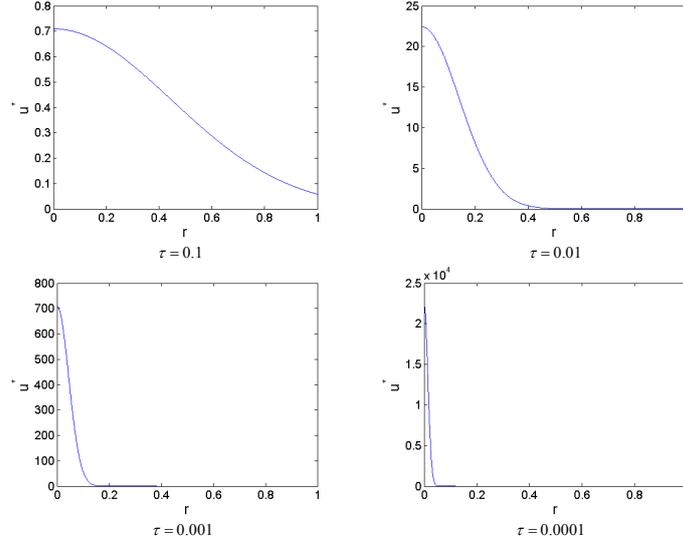
where  $\tau = t_F - t$  and  $r$  represents the Euclidean distance between the source and the field points.

## 2.2 The domain integral

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

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

The initial condition  $u_0(\mathbf{x}, t_0)$  is a well-behaved function. As the time step approaches zero, the integrand in the domain integral (the time-dependent fundamental solution  $u^*$ ) is close to singular, its limit being a Dirac delta function [1] as shown in Fig. 1. It can be seen that the function  $u^*$  becomes less smooth with the time step decreasing. A very large yet finite value occurs at the source point as the time step is small. Thus these pseudo-singular domain integrals can not be accurately calculated by the standard Gaussian quadrature when small time step is used.



**Fig. 1.** Variation of  $u^*$  with  $r$  for several values of time steps.

### 3. New method for evaluating the domain integrals

#### 3.1 The $(\alpha, \beta, \gamma)$ transformation

In this section, we first introduce the  $(\alpha, \beta, \gamma)$  transformation. The transformation is used in the following sub-pyramids, which is a method for solving the singular integrals. To construct the  $(\alpha, \beta, \gamma)$  coordinate system as shown in Fig. 2, the following mapping is used:

$$\begin{cases} x_\gamma = x_1 + (x_2 - x_1)\alpha + (x_4 - x_1)\beta \\ y_\gamma = y_1 + (y_2 - y_1)\alpha + (y_4 - y_1)\beta \\ z_\gamma = z_1 + (z_2 - z_1)\alpha + (z_4 - z_1)\beta \end{cases} \quad \alpha, \beta \in [0, 1] \quad (5a)$$

$$\begin{cases} x = x_0 + (x_\gamma - x_0)\gamma \\ y = y_0 + (y_\gamma - y_0)\gamma \\ z = z_0 + (z_\gamma - z_0)\gamma \end{cases} \quad \gamma \in [0, 1] \quad (5b)$$

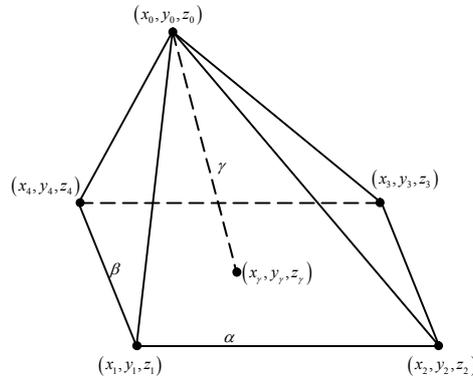
Combining Eqs.(5a)-(5b), the expression for obtaining coordinates  $(x, y, z)$  can be written as:

$$\begin{cases} x = x_0 + [(x_1 - x_0) + (x_2 - x_1)\alpha + (x_4 - x_1)\beta]\gamma \\ y = y_0 + [(y_1 - y_0) + (y_2 - y_1)\alpha + (y_4 - y_1)\beta]\gamma \\ z = z_0 + [(z_1 - z_0) + (z_2 - z_1)\alpha + (z_4 - z_1)\beta]\gamma \end{cases} \quad (6)$$

The Jacobian of the transformation from the  $(x, y, z)$  system to the  $(\alpha, \beta, \gamma)$  system is

$$Jb = \gamma^2 \begin{vmatrix} x_2 - x_1 & y_2 - y_1 & z_2 - z_1 \\ x_3 - x_1 & y_3 - y_1 & z_3 - z_1 \\ x_1 - x_0 & y_1 - y_0 & z_1 - z_0 \end{vmatrix} \quad (7)$$

With the  $(\alpha, \beta, \gamma)$  transformation, the rapid variations of the integrand are smoothed out in some degree. Thus, the computational accuracy of the domain integrals can be improved.



**Fig. 2.** The  $(\alpha, \beta, \gamma)$  coordinate transformation.

### 3.2 Element subdivision

To further improve the computational accuracy of the domain integrals, an element subdivision technique is proposed in this part. As shown in Fig.1, a large spike occurs in the integrand near the source point as the time step value is small. Thus the steep slopes produced by the integrand require that integration points be shifted towards the source point in order to calculate more accurately the integral under consideration. The detailed analysis is as follows.

Firstly we study the probability density function of normal distribution

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{x^2}{2\sigma^2}\right) \quad (8)$$

$$\int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{x^2}{2\sigma^2}\right) dx = 1 \quad (9)$$

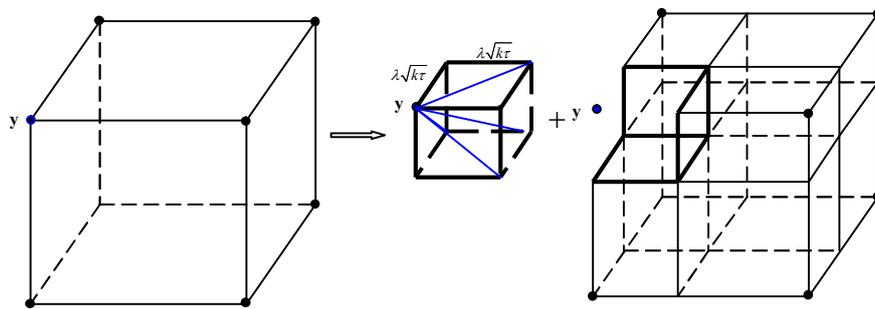
From Eq. (8), it can be noted that the form of the probability density function is

almost like that of the time-dependent fundamental solution  $u^*$ . As all we know, the integral value of Eq. (9) 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  $\sigma$  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 the above analysis, the following element subdivision technique is introduced as shown in Fig. 3:

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

The advantage of the proposed element subdivision technique is that more integration points are shifted towards the source point. Using the element subdivision technique coupled with the  $(\alpha, \beta, \gamma)$  transformation, the domain integrals can be accurately calculated.



**Fig. 3.** The subdivision of hexahedron element (the source point is on the vertex of the element).

#### 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:

$$I = \int_{\Omega} \frac{1}{(4\pi k\tau)^{1.5}} \exp\left(-\frac{r^2}{4k\tau}\right) d\Omega \quad (10)$$

The coefficient  $k$  in Eq. (10) is assumed to be 1 and the dimensionless parameter  $\lambda$  is 8. The  $(\alpha, \beta, \gamma)$  transformation with  $15 \times 15 \times 15$  Gaussian points is used on the sub-pyramids and  $5 \times 5 \times 5$  point Gaussian quadrature is used on the sub-hexahedrons.

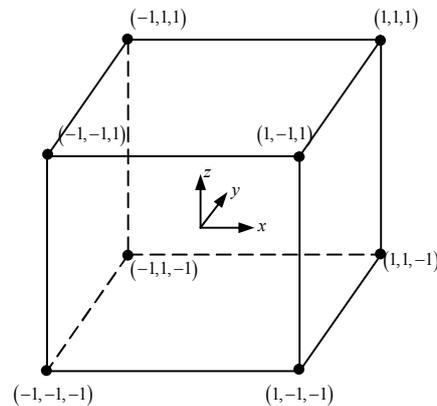
The numerical values obtained by our method will be compared to ‘exact’ values in terms of the relative error defined by

$$\text{Relative Error} = \left| \frac{I_{\text{numerical}} - I_{\text{exact}}}{I_{\text{exact}}} \right| \quad (11)$$

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

#### 4.1 Example 1

In this example, the domain integral of Eq. (10) is evaluated over a hexahedron element 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.4. The coordinate of the source point is set at  $(1, 1, 1)$ . The relative errors of various methods with different time steps are compared in Table 1.  $\tau$  represents the time step value.  $5 \times 5 \times 5$  means straightforward Gaussian quadrature with  $5 \times 5 \times 5$  Gaussian points. The  $(\alpha, \beta, \gamma)$  transformation combined with the element subdivision technique is denoted as  $(\alpha, \beta, \gamma)$ .



**Fig. 4.** The node coordinates of hexahedron element.

A number of interesting points can be drawn from Table 1:

- As the time step is large, accurate numerical results can be obtained by applying Gaussian quadrature straightforward, and better accuracy can be obtained with more Gaussian points.
- The standard Gaussian quadrature becomes inefficient and inaccurate to evaluate the domain integral when the time step is smaller than 0.001.
- Using the proposed method, the domain integral can be accurately and efficiently calculated within a wide range of the time step  $\tau$ .

As illustrated in this example, when the time step is very small, the domain integrals can not be accurately calculated by the standard Gaussian quadrature. However, with our method, high computational accuracy can be obtained within a wide range of the time step  $\tau$ .

**Table 1**

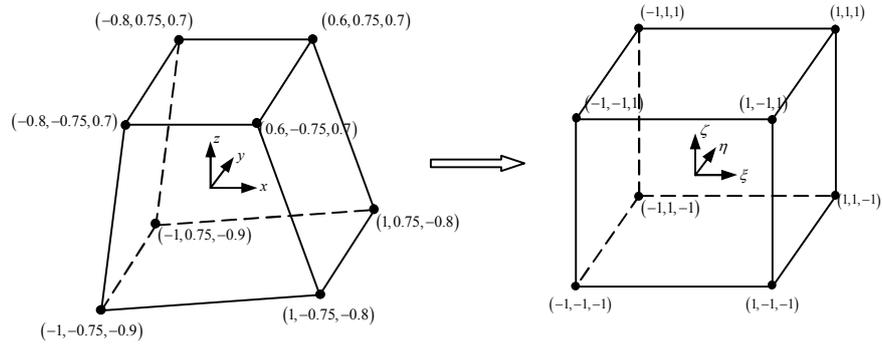
Relative errors for integral  $I$  on hexahedron element with the node coordinates of  $(-1, -1, -1), (1, -1, -1), (1, 1, -1), (-1, 1, -1), (-1, -1, 1), (1, -1, 1), (1, 1, 1), (-1, 1, 1)$ . Errors less than  $1 \times 10^{-12}$  are indicated with a '-'.

$\tau$	0.1	0.01	0.001	0.0001	0.00001
Exact	0.1249970959413	0.125	0.125	0.125	0.125
5×5×5	1.61E-03	2.80E-01	8.97E-01	1.00E+00	1.00E+00
10×10×10	4.31E-09	5.73E-04	9.73E-02	6.78E-01	1.00E+00
15×15×15	-	4.16E-06	1.42E-02	7.72E-01	9.97E-01
20×20×20	-	4.44E-09	1.48E-03	8.06E-02	1.01E-01
30×30×30	-	-	1.26E-06	1.07E-02	4.09E-01
$(\alpha, \beta, \gamma)$	1.76E-11	1.82E-08	4.45E-08	4.45E-08	4.45E-08

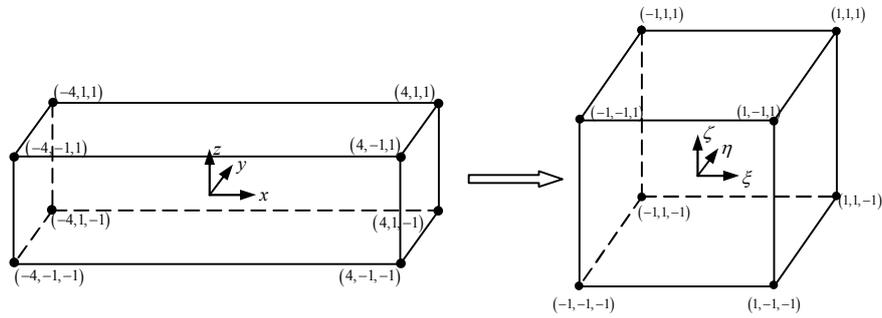
#### 4.2 Example 2

For a more general example, different locations of the source points on the hexahedron elements with different shape are considered as shown in Fig.5 and Fig.6. The relative errors with different time steps are compared in Table 2 and Table 3. The

coordinate in the tables is the local coordinate of the source point.



**Fig. 5.** The node coordinates of hexahedron element.



**Fig. 6.** The node coordinates of hexahedron element.

Table 2 show that good results can be obtained by the method based on  $(\alpha, \beta, \gamma)$  transformation considering the different positions of the source points. And the proposed method is not sensitive to the position of the source point. From Table 3, it can be seen that even the integration element with poor shape can be accurately calculated.

**Table 2**

Relative errors for integral  $I$  with different position of the source points on hexahedron element with the node coordinates of  $(-1, -0.75, -0.9)$ ,  $(1, -0.75, -0.8)$ ,  $(1, 0.75, -0.8)$ ,  $(-1, 0.75, -0.9)$ ,  $(-0.8, -0.75, 0.7)$ ,  $(0.6, -0.75, 0.7)$ ,  $(0.6, 0.75, 0.7)$ ,  $(-0.8, 0.75, 0.7)$ . Errors less than  $1 \times 10^{-12}$  are indicated with a '-'.

$\tau$	0.1	0.01	0.001	0.0001	0.00001
(1.0, 0.0, 0.0)	-	6.97E-09	2.48E-08	3.83E-08	3.91E-08
(0.9, 0.9, 0.9)	-	2.36E-09	2.92E-08	2.89E-08	4.14E-08
(0.2, 0.4, 0.8)	-	2.80E-08	2.01E-08	3.74E-08	4.34E-08
(0.0, 0.0, 0.0)	-	1.48E-09	1.68E-08	3.69E-08	3.69E-08

**Table 3**

Relative errors for integral  $I$  with different position of the source points on hexahedron element with the node coordinates of  $(-4, -1, -1), (4, -1, -1), (4, 1, -1), (-4, 1, -1), (-4, -1, 1), (4, -1, 1), (4, 1, 1), (-4, 1, 1)$ .

$\tau$	0.1	0.01	0.001	0.0001	0.00001
(1.0, 0.0, 0.0)	5.73E-08	9.02E-09	4.25E-08	4.76E-08	4.45E-08
(0.9, 0.9, 0.9)	6.34E-09	1.53E-08	3.29E-08	2.10E-08	4.19E-08
(0.2, 0.4, 0.8)	4.81E-09	6.10E-10	2.83E-08	4.75E-08	4.45E-08
(0.0, 0.0, 0.0)	1.13E-07	8.55E-09	3.92E-08	4.75E-08	4.45E-08

#### 4.3 Example 3

In this case, the initial condition  $u_0(\mathbf{x}, t_0)$  is no longer assumed to be 1 and it is always expressed as interpolation of the shape function. So the following integrals are considered.

$$I_1 = \int_{\Omega} N \frac{1}{(4\pi k\tau)^{1.5}} \exp\left(-\frac{r^2}{4k\tau}\right) d\Omega \quad (12)$$

where  $N$  is the shape function of the hexahedron element.

The integration element with the node coordinates is shown in Fig.5 and the source point is set at  $(0.9, 0.9, 0.9)$ . The relative errors with different time steps are compared in Table 4.

It can be seen from Table 4 that adding the shape function to the integrand of domain integrals almost has no influence on the calculation accuracy. This indicates the  $(\alpha, \beta, \gamma)$  transformation is effective and it doesn't make the well behaved function for instance the shape function worse. Compared with the method of calculating the integrals directly with  $20 \times 20 \times 20$  Gaussian points, more accurate results can be obtained with the proposed algorithm, and it can keep high accuracy even for very small time step.

**Table 4**

Relative errors for integral  $I_1$  on hexahedron element with the node coordinates of

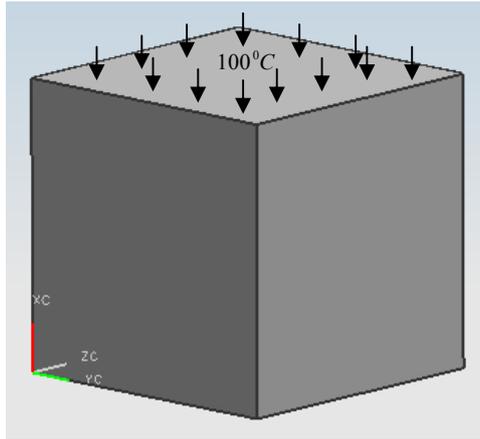
(-1, -0.75, -0.9), (1, -0.75, -0.8), (1, 0.75, -0.8), (-1, 0.75, -0.9), (-0.8, -0.75, 0.7), (0.6, -0.75, 0.7), (0.6, 0.75, 0.7), (-0.8, 0.75, 0.7). Errors less than  $1 \times 10^{-12}$  are indicated with a '-'.

$\tau$	0.1	0.01	0.001	0.0001	0.00001
Exact	0.0102024503	0.0031484778	0.0023039226	0.0023738299	0.0023748831
20×20×20	-	1.20E-10	2.71E-03	6.00E-02	7.22E-01
30×30×30	-	-	1.33E-06	4.97E-02	9.99E-01
$(\alpha, \beta, \gamma)$	-	1.13E-08	9.01E-08	5.06E-08	4.50E-08

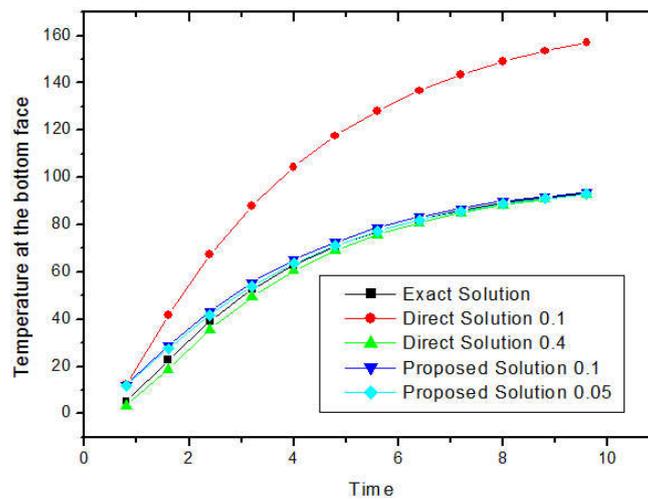
#### 4.4 Example 4

To further demonstrate the effectiveness of the proposed method, the following example is presented. A 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  $20 \text{ kg/m}^3$ ,  $2 \text{ kJ/(m} \cdot \text{ }^\circ\text{C)}$  and  $0.8 \text{ kJ/(kg} \cdot \text{ }^\circ\text{C)}$ , respectively. The length of the cube is 1m. A uniform temperature  $100^\circ\text{C}$  is imposed suddenly on the top face of the cube. The initial temperature of the cube is  $0^\circ\text{C}$ . In this application, the variation history of the temperature from 0h to 9.6h at the bottom face is concerned. To illustrate the accuracy of the method, numerical results are compared with the existing analytical solution to the considered problem as shown in Fig.8. 'Direct Solution 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  $(\alpha, \beta, \gamma)$  transformation combined with the element subdivision technique are used for calculating the integrals and the time step is also 0.1h.

In Fig.8, it can be noted that the direct solutions start to become unstable when the time step is less than 0.1h. This illustrates the calculation accuracy of domain integrals influence on stability of pseudo-initial condition method. With our method, the pseudo-singular domain integrals can be evaluated accurately and thus good results are obtained.



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



**Fig. 8.** The temperature at the bottom face.

## 5. Conclusion

A general algorithm for the evaluation of the domain integrals which arise in 3D boundary element method for transient heat conduction problems was proposed in this paper. Employing the proposed method, the domain integrals can be effectively and accurately calculated. Furthermore, an element subdivision technique takes into account the position of the source point, the shape of the integration element and the relations between the size of element and the time step. Thus even the time step is very small, accurate results can still be obtained by our method. Accurate calculation of these integrals is of great importance to the successful implementation of the pseudo-initial condition method. Thus the stability of the analysis can be improved with the proposed algorithm when small time step is used. Numerical examples were presented and results demonstrated the accuracy and efficiency of our method.

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