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Multi-domain boundary knot method for ultra-thin coating problems

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Abstract: This paper develops a multi-domain boundary knot method (BKM) formulation to solve the heat conduction problems of ultra-thin coatings. This approach overcomes the troublesome singular integration difficulty in the boundary element method in the simulation of such ultra-thin coating problems. Our numerical results show that the present BKM is very promising with sufficient accuracy in predicting the temperature distributions and the other physical quantities in thin coated layers even when the thickness ranges from 10^{-1}m to 10^{-9}m. The present method can also easily be extended to the three-dimensional problems.

Keywords: Boundary knot method; multidomain; ultra-thin coating; singularity; heat conduction

1 Introduction

Thin coatings often outperform their substrate counterparts in terms of the heat and wear-resistance properties. As the coating deposition techniques and advanced coating materials have greatly been improved in recent decades, an increasing number of thin-coating films has been designed and employed to improve the machining performances in industrial applications (Bhushan, B. Chemical, 1999; Rhodes J, Walker AC, 1987; Hollaway LC, Zhang L, Photiou NK, Teng J et al, 2006). Consequently, there is a high demand in the accurate numerical simulation of heat conduction in ultra-thin coatings. For instance, it is known that the cutting temperature field plays a key role in the tool performance indicators such as the accuracy of the equipment surface, tool wear and lifespan, chip formation, surface quality,

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and cutting forces (Zhang Yaoming, Gu Yan, Jeng-Tzong Chen, 2010; Du F, Lovell MR, Wu TW, 2001).

The standard numerical methods such as the finite element and the finite difference methods have been applied to the simulation of heat transfer in thin coatings. However, their computational costs grow exponentially with the increasing aspect ratio of thin structures. As an alternative approach, the boundary element method (BEM) (Zhang Yaoming, Gu Yan, Jeng-Tzong Chen ,2010 ; Stephenson DA, Jen TC, Lavine AS ,1994 ; Stephenson DA, Jen TC, Lavine AS ,1997; Du F, Lovell MR, Wu TW, 2001) has long been considered to avoid such drawbacks. However, the standard BEM involves singular and nearly singular integrals, which need very carefully to be performed in the analysis of thin body or ultra-thin coating problems. Moreover, surface meshing of three-dimensional (3D) thin body domains remains a nontrivial task.

In order to alleviate the mesh generation, recent decades have witnessed a fast development of meshless techniques which require neither domain nor boundary meshing. Generally, the meshless methods can be divided into the domain-type or boundary-type techniques, depending on whether their basis functions satisfy the governing equations of interest. As an alternative boundary-type meshless method competing with the BEM, the method of fundamental solutions (MFS) has in recent decades attracted increasing attentions, since the method avoids the challenging singular integration in the BEM and is mathematical simple, easy-to-implement, accurate, integration-free, and spectral convergent (Golberg MA, Chen CS, 1998; Li Ming, Chen CS, Hon YC, 2011). However, the artificial boundary outside the physical domain required in the MFS is largely placed by trial and error approach and can cause numerical instability, especially for domains with a complex boundary (Kitagawa T., 1991; Balakrishnan K, Ramachandran PA. 2001).

The boundary knot method (BKM) (Chen W, Wang FZ., 2010; Chen W, Fu ZJ, Wei X., 2009) is a recently developed method to circumvent this major drawback of the MFS while keeping all its merits being mathematically simple, easy-to-program, truly meshless, and integration-free. This method employs the non-singular general solutions instead of the singular fundamental solutions to avoid the singularity and the artificial boundary.

In this study, we make the first attempt to extend the BKM to the heat conduction analysis of ultra-thin coatings. Considering different mechanical properties of each layer material, a multi-domain BKM formulation is developed to handle a wide range of coating thickness. Our numerical experiments show that the BKM solution outperforms the BEM (Zhang Yaoming, Gu Yan, Jeng-Tzong Chen, 2010) in terms of the accuracy and efficiency. We find that the BKM keeps a high accuracy even when the coatings are very thin at micro- or nano-scales

A brief outline of the rest of this paper is as follows. In Section 2, we briefly present the basic formulation of the BKM method. And then Section 3 proposes a multi-domain BKM formulation to analyze the ultra-thin layer problems, followed by Section 4, where the accuracy and stability of the proposed method are tested by two benchmark problems. Section 5 concludes this paper with some remarks.

2 BKM formulation

This section will give a brief introduction to the BKM formulation through an illustrative case:

$$L\{u_h(x)\} = 0, x \in \Omega \tag{1}$$

$$u_h(x) = G(x), x = B_f \tag{2a}$$

$$\frac{\partial u_h(x)}{\partial n} = F(x), x = B_q \tag{2b}$$

where $L\{\}$ represents a linear differential operator, u_h denotes the homogeneous solution, $x \in R^d$, d=2, 3, Ω means the entire domain, $B = B_q + B_f$ is the boundary of the domain Ω, and $G(x)$and $F(x)$are Dirichlet and Neumann boundary conditions along the boundaries B_f and B_q, respectively.

Unlike the DR-BEM (Chen W, Tanaka M. A ,2002; Wang Fuzhang, Chen Wen and Jiang Xirong, 2009; Nardini D, Brebbia, CA, 1983) and the MFS where the singular fundamental solution is employed to represent the homogeneous solution, the BKM approximates the homogeneous solution by using the nonsingular general solution μ as the basis function as shown in the following formula

$$u_h(x) = \sum_{k=1}^{M} \alpha_k \mu(r_k) \tag{3}$$

where the subscript k is the index of the source points on the boundary, M is the number of knots on the boundary, α_k denotes the desired coefficients, μ is the nonsingular general solution, and $r_k = \|x - x_k\|$ is the Euclidean distance norm.

3 BKM for coating problems

In this section, the multi-domain BKM is presented for the steady-state heat conduction in a two-layer coating. And then we discuss the efficiency and validity of the present scheme in details.

3.1 Mutlidomain BKM formulation

Consider the steady-state heat conduction in a layered system with an ultra-thin coating as shown in Figure 1. Here, $\Omega = \Omega_1 \cup \Omega_2$, where Ω_1 and Ω_2 are the homogenous and isotropic subdomains, respectively. The boundary of the subdomain Ω_1 is denoted by B_1, while the boundary of the subdomain Ω_2 is represented by B_2. The contact interface of the two subdomains is B_I. The temperature field in the thin coating structure is governed by the Laplace equation

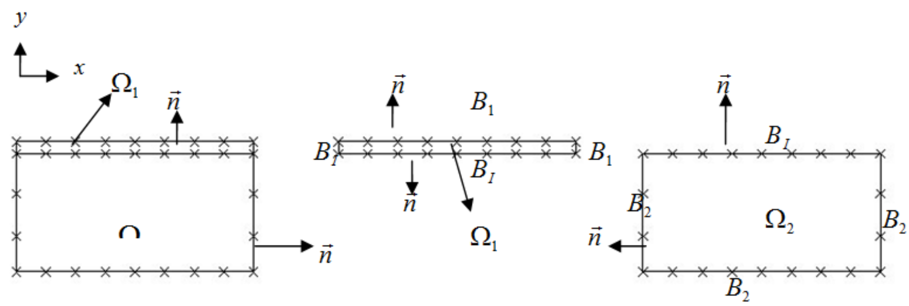

Figure 1: Boundary discretization of two subdomains

$$\Delta T_h(x) = 0, \; x \in \Omega \tag{4}$$

where Δ represents the Laplace operator and T_h denotes temperature variable. The boundary conditions are given by

$$T_h(x) = G(x), x \in B_q \tag{5}$$

$$\frac{\partial T_h(x)}{\partial n} = F(x), x \in B_f \tag{6}$$

where $G(x)$ and $F(x)$ are Dirichlet and Neumann boundary conditions, respectively. B is the boundary of the domain, B_I the interface of the domain, i.e., $B = B_2 \cup B_1 \cup B_I$.

On B_1 and B_1 of Ω_1 as shown in Fig. 1, the following discretized equations of the

BKM can be obtained via the BKM formula (3):

$$[G^1]\begin{pmatrix}\{\alpha^1\}\\ \{\alpha_I^1\}\end{pmatrix}=\{T^1\} \tag{7a}$$

$$[G_I^1]\begin{pmatrix}\{\alpha^1\}\\ \{\alpha_I^1\}\end{pmatrix}=\{T_I^1\} \tag{7b}$$

$$[F^1]\begin{pmatrix}\{\alpha^1\}\\ \{\alpha_I^1\}\end{pmatrix}=\{Q^1\} \tag{7c}$$

$$[F_I^1]\begin{pmatrix}\{\alpha^1\}\\ \{\alpha_I^1\}\end{pmatrix}=\{Q_I^1\} \tag{7d}$$

where G_I^1 and F_I^1 are the boundary conditions formed by Eq. (2) on B_1, G^1 and F^1 are the boundary conditions formed by Eq. (2) on B_I, T_I^1 and B_1 are the interface temperature and the normal derivative (flux) of the temperature on B_1, B_2 and B_2 are the unknown coefficients on B_2 and B_1, respectively, and T^1 and Q^1 denote the temperature and the normal derivative of the temperature on B_1.

Similarly, for B_2 and B_I on Ω_2, we also have

$$[G^2]\begin{pmatrix}\{\alpha^2\}\\ \{\alpha_I^2\}\end{pmatrix}=\{T^2\} \tag{8a}$$

$$[G_I^2]\begin{pmatrix}\{\alpha^2\}\\ \{\alpha_I^2\}\end{pmatrix}=\{T_I^2\} \tag{8b}$$

$$[F^2]\begin{pmatrix}\{\alpha^2\}\\ \{\alpha_I^2\}\end{pmatrix}=\{Q^2\} \tag{8c}$$

$$[F_I^2]\begin{pmatrix}\{\alpha^2\}\\ \{\alpha_I^2\}\end{pmatrix}=\{Q_I^2\} \tag{8d}$$

where G_I^2 and F_I^2 are the boundary conditions formed by Eq. (2) on B_I, G^2 and F^2 are the boundary conditions formed by Eq. (2) on B_2, T_I^2 and Q_I^2 represent the interface temperature and the normal derivative of the temperature on B_I, receptively, T^2 and Q^2 are the temperature and the normal derivative of the temperature on the subdomain Ω_2, and α^2 and α_I^1 are the unknown coefficients for B_2 and B_I.

For a well-posed boundary value problem, there is only one unknown, either T or Q, at each nodal point on the boundaries. However, along the interface B_I, both T and Q are unknowns. In order to solve the problem, the following continuity conditions at the interface must be satisfied.

(a) Continuity of temperature

$$T_1^2 = T_1^2 \tag{9}$$

(b) Continuity of normal flux

$$k_1 Q_1^1 = -k_1 Q_1^2 \tag{10}$$

Where k_1 and k_2 denote the coefficients of the heat conductivity of the two subdomains, respectively. According to the continuity conditions (9) and (10) at the interface, equations (5) and (6) can be discretized by

$$\begin{bmatrix} [G^1] & [0] \\ [G_I^1] & [0] \\ [F_I^1] & \frac{k_2}{k_1}[F_I^2] \\ [0] & G^2 \end{bmatrix} \begin{pmatrix} \varphi^1 \\ \varphi_I^1 \\ \varphi^2 \\ \varphi_I^2 \end{pmatrix} = \begin{bmatrix} [T^1] \\ [0] \\ [0] \\ [T^2] \end{bmatrix} \tag{11}$$

The above formulation can easily be extended to the multilayer problems. The boundary and interface unknowns can simultaneously be solved by equations (11). Once the boundary unknowns are evaluated, the temperature distributions at any internal point can be calculated via equation (3).

3.2 Implementation procedure

The BKM has a clear distinction from the BEM for ultra-thin coating problems in that the former employs the nonsingular general solution, whose expression for steady-state heat conduction equation is given by

$$u_h = e^{-c(x^2-y^2)}\cos(2cxy) \tag{12}$$

where c is a problem-dependent shape parameter. Some schemes are developed to determine the appropriate shape parameter, such as the golden section search algorithm (Kontoni DPN, Partridge PW, Brebbia CA, 1991; Chen, JT, Wong FC, 1998) . In this study, we will use the direct search method (Kontoni DPN, Partridge PW, Brebbia CA, 1991).to obtain the optimal shape parameter c. Below we give the key steps in the BKM solution of the heat conduction problem in the multi-layer thin coating problems.

Step 1. For n_b collocation boundary points $\{x\}_{i=1}^{n_b}$ in B_q, we set a step size ζ and an ending point m.

Step 2. For $w = 1$ to m/ζ:

(1) Solve equations (7) and (8) by using the BKM with $c = w\zeta$.

(2) Evaluate the BKM numerical solution $\tilde{u}$ with test points n_t on the boundary B_q and then calculate the relative error of μ. Since the analytical solution is usually not available in practice, this study uses the residual error of the governing equation and Dirichlet boundary condition for the error in μ. More details can be found in Kontoni DPN, Partridge PW, Brebbia CA(1991).

(3) Calculate the error of μ at the test points at the iteration w.

Step 3. Find w in Step 2 and the minimum error of μ at the w-th iteration, then the optimal shape parameter will be $c = w\zeta$.

4 Numerical results and discussions

4.1 4.1 A thin coating on a shaft

As depicted in Fig. 2, a circular shaft with a thin coating is considered. The heat conductivities of the subdomains Ω_1 and Ω_2 are supposed to be the same. $r_1 = 2$ and $r_2 = 6$ are the inner and outer radii of the subdomain Ω_2. The subdomain Ω_1 is considered to be the coating with an outer radius $r_3 = 7$. The boundaries of both domains are supposed to satisfy the Dirichlet boundary condition. The analytical solution is $T = x^2 - y^2 + 6$. We uniformly distribute 8 test knots along the boundary of $r_4 = 3.5$ and $r_5 = 6.5$.

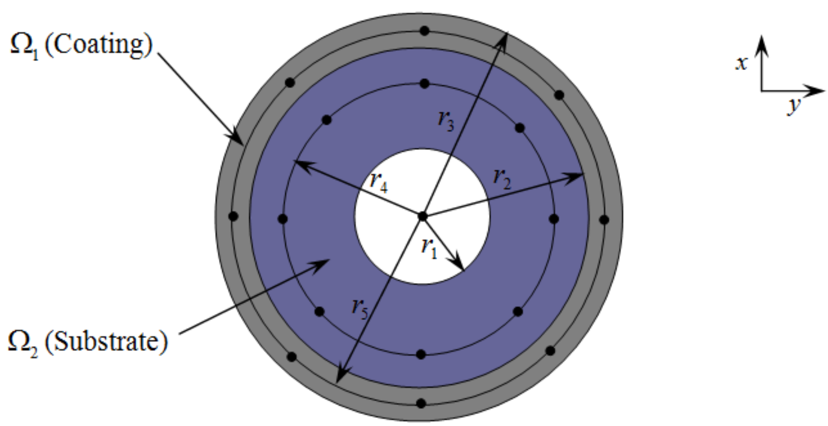

Figure 2: Cross section of a shaft with a thin coating

To simplify the problem, we assume that the two subdomains have the same material constants and heat conductivities. In the practice, however, the situations are more complicated. This case is considered only to verify the validity of the BKM with an available analytical solution.

5 to 100 uniform knots are applied along each boundary of the two domains, which means that the total number of the knots ranges from 15 to 300. The following

averaged relative error is used in this study

$$\varepsilon = \frac{1}{N}\sqrt{\sum_{k=1}^{N}(\frac{T-\bar{T}}{T})} \tag{13}$$

The temperatures and the heat fluxes at points situated on $r_4 = 3.5$ and $r_5 = 6.5$ (see Fig. 2) are displayed in Figs. 3 and 4. The shape parameter is c=0.01 in this case. The results demonstrate that the calculated temperature and heat flux are reliable. The solution accuracy is improved as the number of the knots increases.

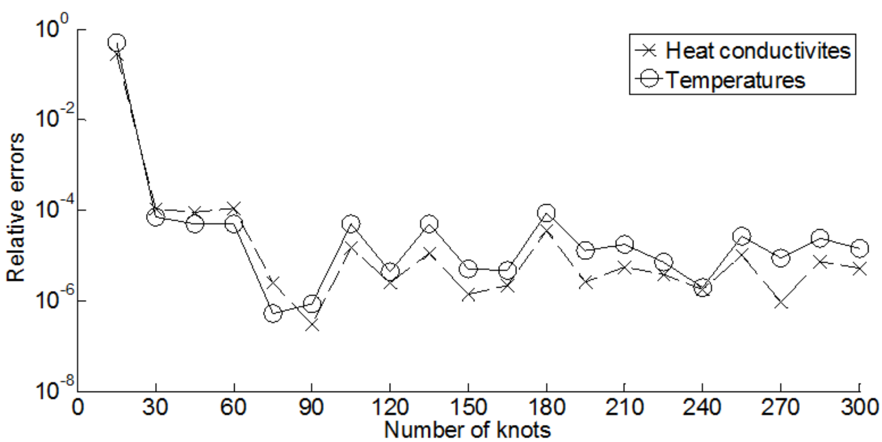

Figure 3: Relative errors of the computed temperatures and heat fluxes on $r_4 = 3.5$ as shown in Fig. 2

4.2 A rectangular plate of a 2D solid with a thin coating

This case is a simplified engineering problem and has been investigated by the BEM (Zhang Yaoming, Gu Yan, Jeng-Tzong Chen, 2010). We make a direct comparison between the present BKM and the BEM for this case. As shown in Fig. 5, a $2\times 1m^2$ rectangular region of a 2D solid with a thin coating is considered. The thickness of the thin coating is defined as h, and the structure is the approximate representation of a real machining process. In2001, Du F, Lovell MR, Wu TW (2001) considered a similar coating test case, in which the exact solution is $T = x_2/(1+h)$. By contrast, the test case presented in this paper is more general, and thus the numerical results are expected to be more accurate if the example in (Du F, Lovell MR, Wu TW 2007) is revisited.

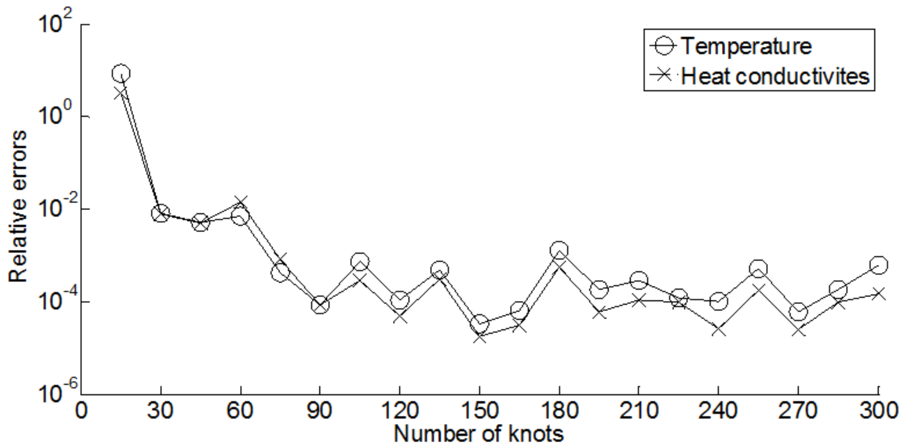

Figure 4: Relative errors of the computed temperatures and heat fluxes on $r_5 = 6.5$ as shown in Fig. 2

In this case, the subdomain Ω_1 is considered to be the coating layer while Ω_2 is the substrate. Heat conductivities of the subdomains Ω_1 and Ω_2 are respectively r_3r_1 and r_2. For the subdomain r_4, 10 uniform knots are applied on each horizontal side, and 1 knot is used on each vertical side. For the subdomain r_5, 10 knots are applied on each horizontal side in conjunction with 8 on the vertical side. In total, the number of knots is 48. We obtain the optimal shape parameter c via the direct search method as described above in Section 3.2. When the coating thickness Ω_2 ranges from 10^{-1}m to 10^{-9}m, the optimal fluxes $\partial T/\partial n$ at point D(1.5,1) of the interface of both subdomain Ω_1 and Ω_2 are listed in Table 1.

The temperatures and the heat fluxes $\partial T/\partial n$ at point E (0.5,1+h/2) as shown in Fig. 5 are respectively displayed in Fig. 6 and Table 2. It can be observed that the BKM shows a higher accuracy than the BEM when the coating thickness h ranges from 10^{-1}m to 10^{-9}m.

In this example, we find that the value of the shape parameter should be larger than 0.7 when h=10^{-9}m. Otherwise, the results will generally tend worse as the shape parameter increases. To gain some helpful insight into the choice of the shape parameter, 10 uniform knots along the line y=1+h/2 as shown in Fig. 5 are distributed to analyze the influence of the shape parameter on the solution accuracy and stability. Figs. 7 and 8 show the temperatures and the heat fluxes on the line y=1+h/2 with the shape parameters c= 0.2, 0.6, 1 and 1.4 for different coating thicknesses h. Figs. 9 and 10 illustrate the temperatures and the heat fluxes with

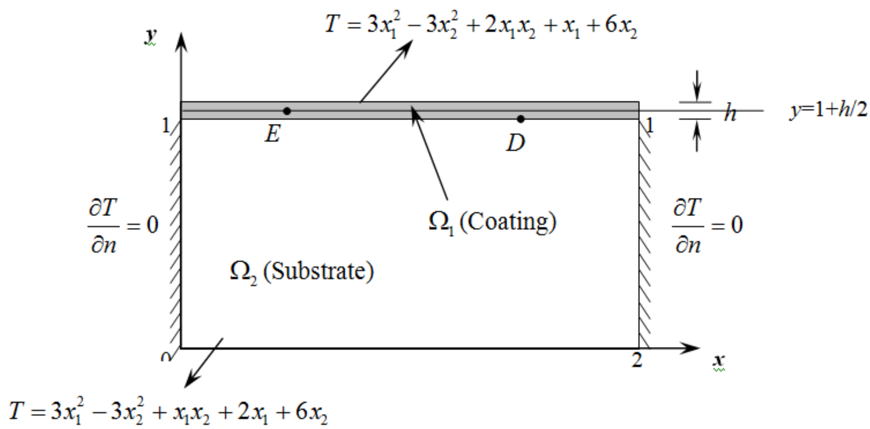

Figure 5

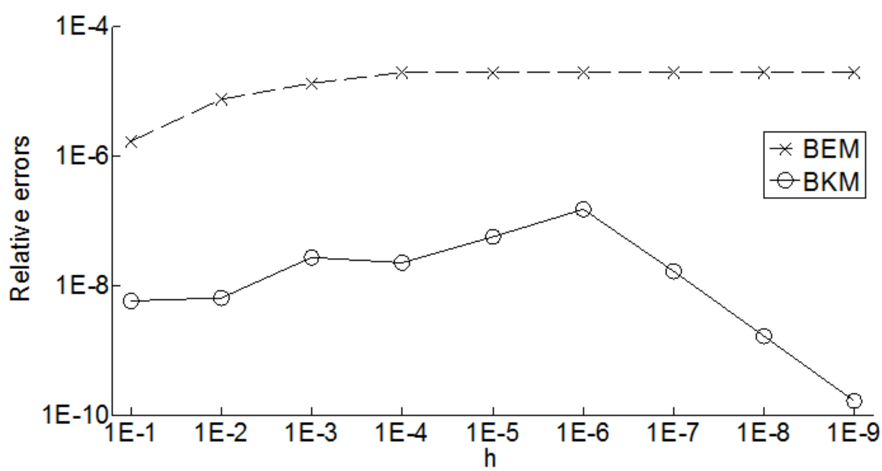

Figure 6: Relative errors of the calculated temperatures at point E as shown in Fig. 5

Table 1: Results of normal fluxes $\partial T/\partial n$ at point D on the interface of the subdomains Ω_1 and Ω_2 as shown in Fig. 5

Thickness (m)	Exact	BEM	Relative error	BKM	Optimal c	Relative error
1.0E-1	3.00	2.999972	9.28E-6	3.000000059	0.283	1.98E-8
1.0E-2	3.00	2.999787	7.08E-5	2.999999988	0.386	3.72E-9
1.0E-3	3.00	3.000048	1.62E-5	2.999999966	0.408	1.10E-8
1.0E-4	3.00	3.000024	8.15E-6	2.999999965	0.621	1.17E-8
1.0E-5	3.00	2.998634	4.55E-5	2.999999990	0.506	3.32E-9
1.0E-6	3.00	2.998325	5.58E-4	2.999999969	0.657	1.03E-8
1.0E-7	3.00	2.999276	2.41E-4	3.000000055	0.563	1.83E-8
1.0E-8	3.00	2.998910	3.63E-4	3.000000477	0.884	1.59E-7
1.0E-9	3.00	3.001953	6.51E-4	2.999999832	0.754	5.61E-8

Table 2: Results of heat fluxes $\partial T/\partial n$ at point E in the subdomain Ω_1 as shown in Fig. 5

h [m]	Exact	BEM	Relative error	BKM	Optimal c	Relative error
1.0E-1	6.100000	6.099934	1.08E-5	6.100000	0.252	1.56E-8
1.0E-2	6.010000	6.007734	3.77E-4	6.009996	0.389	1.82E-8
1.0E-3	6.001000	5.997616	5.64E-4	6.001047	0.484	2.77E-8
1.0E-4	6.000100	5.996694	5.68E-4	6.000642	0.331	2.26E-8
1.0E-5	6.000010	5.996604	5.68E-4	6.000009	0.451	5.73E-8
1.0E-6	6.000001	5.996595	5.68E-4	6.000002	0.541	1.51E-7
1.0E-7	6.000000	5.996595	5.68E-4	6.000002	0.384	3.01E-7
1.0E-8	6.000000	5.996594	5.68E-4	6.000006	0.521	9.52E-7
1.0E-9	6.000000	5.996594	5.68E-4	6.000122	0.905	2.03E-5

h=10^{-2}m, 10^{-4}m, 10^{-6}m and 10^{-8}m for a variable shape parameter c.

From Figs.7 and 8 one can find that the accuracy of the BKM solution drops as$c$decreases for h=10^{-1}m. This indicates that better BKM solution for h=10^{-1}m, which is thicker than others, will be obtained as the shape parameter$c$ decreases. With the shape parameter c=0.2 and c=0.6, we can not get the correct BKM solution for h=10^{-9}m. This indicates that the shape parameter should be larger for very thin coating problems.

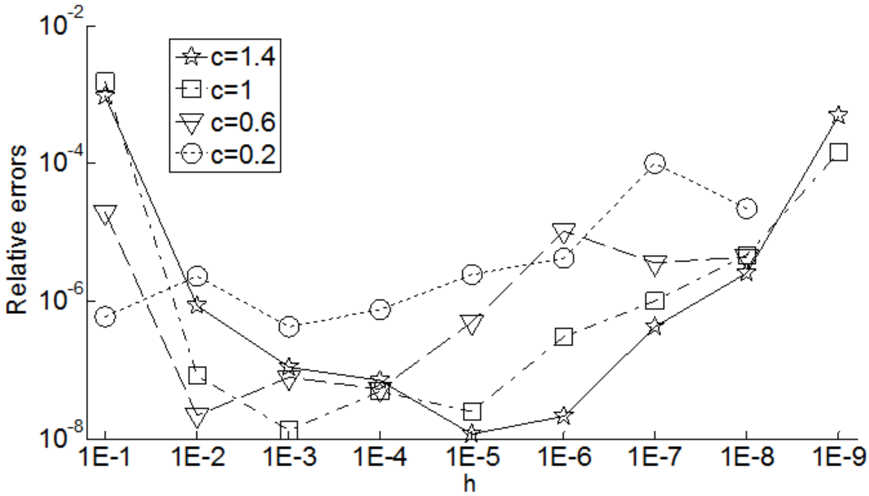

Figure 7: The temperature along the line $y = 1 + h/2$ as shown in Fig. 5

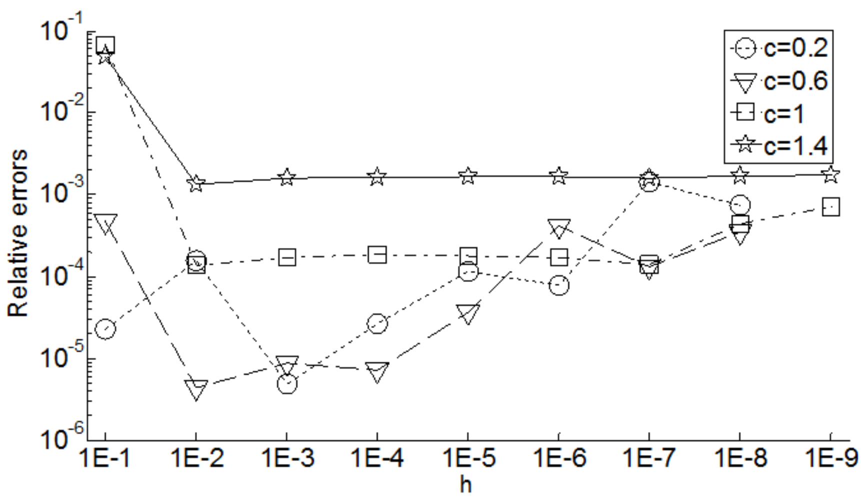

Figure 8: The heat fluxes along the line y=1+h/2 as shown in Fig. 5

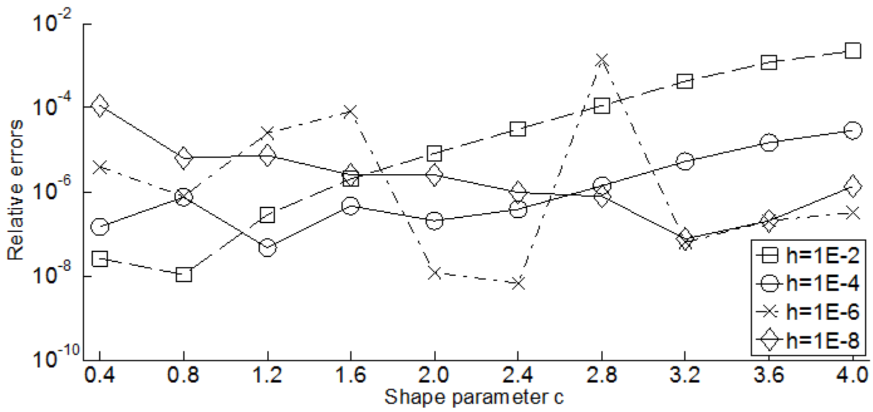

Figure 9: The temperature along the line$y = 1 + h/2$ as shown Fig. 5

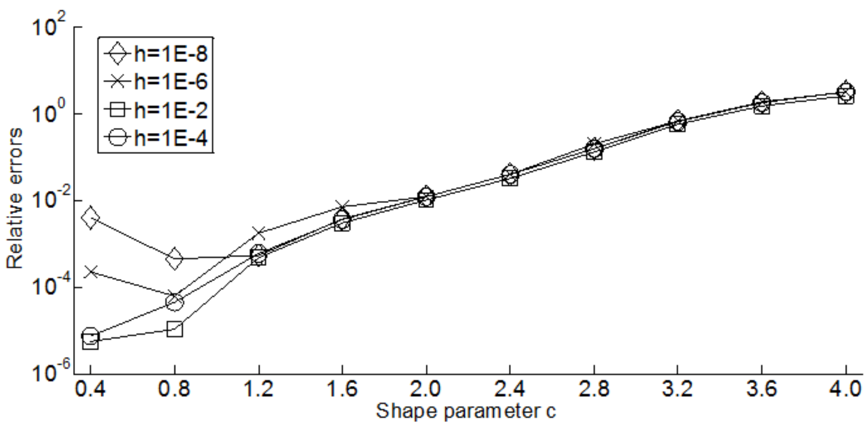

Figure 10: The heat fluxes along the line$y = 1 + h/2$ as shown in Fig. 5

From Figs.9 and 10, we can find that the BKM solution gets worse as the h drops for c=0.4. This indicates that small value of c leads a better BKM solution in a thicker thickness.From Figs.9 and 10, we can also find that the BKM solution are getting worse when the shape parameter c increases with a fixed thickness h. From all numerical experiments reported above, we observe that the shaper parameter $c$should increase as h decreases, however, $c<0.6$ always leads to good results except when the thickness is $h=10^{-9}$. For the coating thickness $h=10^{-9}$the shape parameter should be selected around c=1.

1. Conclusions

This study makes the first attempt to apply the BKM for the heat conduction analysis in thin coating problems, and a multi-domain BKM scheme is also developed for this simulation. In literature, the BEM is reported to be a convenient method to simulate this kind of ultra-thin coating problems (Zhang Yaoming, Gu Yan, Jeng-Tzong Chen, 2010). This study shows the numerical comparisons between the BKM and the BEM. We find that the BKM has the following advantages in the solution of steady-state heat conduction problems in ultra-thin coating systems.

- Since the BKM based method employs the nonsingular general solution rather than the singular fundamental solution, the temperatures and other physical quantities could be accurately evaluated even when the thickness to length ratio of the coated film is as small as the order of 10^{-9}m. This is more than sufficient for modeling most thin coatings at the micro- or nano-scales.

- This study investigates both the temperature and its gradients through numerical examples, which indicate that the BKM has some advantages compared to the BEM in terms of the accuracy and efficiency for the heat conduction analysis in ultra-thin coating systems. It is worth noting that the BKM is much easier to program than the BEM.

- We made a detailed study on the efficiency of the BKM through the shape parameter c in terms of the thickness of coating. Our empirical finding is that the shape parameter c increases as the thickness of the coating decrease, and the BKM solution gets better. We observed that the shape parameter c from 0 to 0.6 always leads to accurate BKM results except for the case of the coating thickness $h=10^{-9}$m. For $h=10^{-9}$m the shape parameter usually should be around c=1.

Our further work along this line is to apply the BKM to more cases to investigate its applicability and efficiency. In particular, we will apply the BKM to more challenging multi-layered coating systems and thermal effects.

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