

A DISCREPANCY PRINCIPLE FOR THE SOURCE POINTS LOCATION IN USING THE MFS FOR SOLVING THE BHCP

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Based on the discrepancy principle, we develop in this paper a new method of choosing the location of source points to solve the backward heat conduction problem (BHCP) by using the method of fundamental solutions (MFS). The standard Tikhonov regularization technique with the L curve method for an optimal regularized parameter is adopted for solving the resultant highly ill-conditioned system of linear equations. Numerical verifications of the proposed computational method are presented for both the one-dimensional and the two-dimensional BHCP.

Keywords: Method of fundamental solutions; backward heat conduction problem.

1. Introduction

The method of fundamental solutions (MFS) was introduced by Kupradze and Aleksidze [1964]. In the last decade, it has been successfully used in multivariate interpolation and in solution of partial differential equations (PDEs) [Golberg and Chen (1999)], e.g. the solutions to potential problems by Mathon and Johnston [1977], the exterior Dirichlet problem for acoustic equations by Kress and Mohsen [1986], the general second order linear elliptic PDEs by Clements [1998] and the homogeneous diffusion problems by Young et al. [2004]. Recently, Hon and Wei applied the MFS to solve the Cauchy problem of heat equations in the one-dimensional Hon and Wei (2004) and multidimensional cases [Hon and Wei (2005)]. The recent development of the MFS and related methods can be found in the paper of Fairweather and Karageorghis [1998]. The conditions for the uniqueness of the backward heat conduction problem (BHCP) had been investigated by Miranker [1961].

It is known that the location of source points in the MFS plays a very important role in the accuracy of the method. Until recently the placement of the source points fell mainly into two categories: on a circle containing the solution domain

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[Kress and Mohsen (1986)] and a line below the initial time for parabolic equations [Hon and Wei (2004, 2005); Mera (2005)]. Most researchers choose the radius of the circle based on trial and error. In this paper, we try to develop a new method for choosing the radius of the circle based on the discrepancy principle. For numerical illustration, we apply the method to solve the BHCP, which is also called the final boundary value problem.

The solution of the BHCP does not continuously depend on the final temperature data see Payne (1975), which means that any small change in the given final temperature data may induce enormous change in the solution (see for instance Miranker [1961]). In other words, the BHCP is a typical ill-posed problem. Stable approximation by using regularization techniques was provided by Cannon [1964] and Han et al. [1995]. A method based on perturbation of the original parabolic heat equation was proposed by Lattes and Lions [1969] and Lesnic et al. [1998]. Some iterative solution methods were also developed for solving the BHCP. Recently, Mera [2005] applied the MFS to solve the BHCP. In his paper, he placed the source points on a line below the initial time. In this paper, we offer a new method of choosing the location of source points which is different from the method proposed by Mera [2005]. Numerical verification of our proposed method indicates that this scheme improves the accuracy of the computation. To solve the highly ill-conditioned resultant system of linear equations in our computation, we adapt the use of the standard Tikhonov regularization technique with the L curve method | Hansen and O'Leary (1993); Hansen (1992a, 1992b); Hansen (2000)] for an optimal regularization parameter.

2. Formulation of the Problem

In the real life physical heat conduction problem, we have to determine the temperature distribution from collected temperature data at a particular time T and certain fixed boundary conditions. Assume that the function u(x,t) satisfies the heat conduction equation

$$\frac{\partial}{\partial t}u(x,t) = \nabla^2 u(x,t), \quad (x,t) \in \Omega \times (0,T), \tag{2.1}$$

with the final condition

$$u(x,T) = f(x), \quad x \in \Omega, \tag{2.2}$$

and the measured Dirichlet boundary condition

$$u(x,t) = g(x,t), \quad x \in \Gamma, 0 < t < T, \tag{2.3}$$

where f(x), g(x,t) are known functions, the domain $\Omega \in \Re^d$, d=1,2, and $\Gamma=\partial\Omega$ is the boundary of the domain.

In practical application, the Dirichlet boundary condition (2.3) and the final condition (2.2) are given only at some scattered data points. Assume that these data are collected at the discrete points $(x_i, t_i), i = 1, ..., m$, on $\Omega \times T$ satisfying

the final condition (2.2) and (x_i, t_i) , $i = m+1, \ldots, m+n$ on $\Gamma \times [0, T]$ satisfying the boundary condition (2.3). We also call these discrete points (x_i, t_i) , $i = 1, \ldots, m+n$, the collocation points.

3. Method of Fundamental Solutions

Here, we choose N source points $\{(\eta_j, \tau_j)\}_{j=1}^N$, which are uniformly located on $\partial \Upsilon \times [-\delta t, T]$, where Υ is an extended domain containing the domain Ω , which satisfies $\partial \Upsilon \cap \partial \Omega = \emptyset$. See Fig. 1 for the one-dimensional case.

The fundamental solution to the problem (2.1) is given as follows:

$$K(x,t) = \frac{H(t)}{(4\pi t)^{\frac{d}{2}}} e^{\frac{\|x\|}{4t}},$$
(3.1)

where H(t) is the Heaviside function and d = 1, 2 is the dimension of the space. The basis functions are given as follows:

$$\phi_j(x,t) = K(x - \eta_j, t - \tau_j) \ j = 1, \dots, N,$$
 (3.2)

which satisfies the PDE (2.1). The above choice of source points ensures that the basis function ϕ does not have a singularity in the domain Ω .

Based on the idea of the method of fundamental solutions given by Hon and Wei [2004, 2005] and Mera [2005], the solution to the BHCP is sought in the following

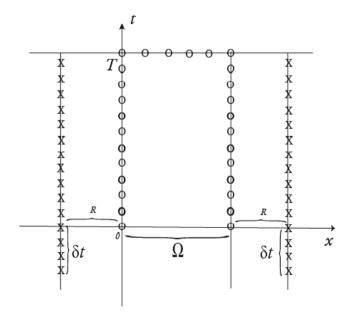


Fig. 1. \times represents source points (η_j, τ_j) , and \circ collocation points.

form:

$$u(x,t) \approx \tilde{u}(x,t) = \sum_{j=1}^{N} \lambda_j \phi_j(x,t), \tag{3.3}$$

where λ_i are unknown coefficients to be determined. For this choice of basis functions the approximated solution \tilde{u} already satisfies the heat equation (2.1) and the coefficients $\lambda_j, j = 1, ..., N$, are determined such that \tilde{u} satisfies the boundary condition (2.3) and the final condition (2.2). We obtain the following system of linear algebraic equations for the unknown λ_j :

$$\tilde{u}(x_i, t_i) = \sum_{j=1}^{N} \lambda_j \phi_j(x_i, t_i) = \begin{cases} f(x_i) & i = 1, 2, \dots, m, \\ g(x_i, t_i) & i = m + 1, m + 2, \dots, m + n. \end{cases}$$
(3.4)

In matrix form, the values of the unknown coefficients λ_j can be obtained from solving the matrix equation

$$A\lambda = b, (3.5)$$

where A is an $(n+m) \times N$ square matrix,

$$A_{ij} = \phi_i(x_i, t_i),$$

and b is an n+m vector,

$$b = \begin{pmatrix} f(x_i) \\ g(x_i, t_i) \end{pmatrix}.$$

Since the original problem (2.1)–(2.2) is highly ill-posed, the ill-conditioning of the matrix A in Eq. (3.5) persists. In other words, most standard numerical methods cannot achieve good accuracy in solving the matrix equation (3.5) due to the bad conditioning of A. In fact, the condition number of A increases dramatically with respect to the total number of collocation points. Several regularization methods have been developed for solving these kinds of ill-conditioning problems [Hansen and O'Leary (1993); Hansen (1992a, 1992b, 2000)]. In our computation we adapt the standard Tikhonov regularization Tikhonov and Arsenin (1977) to solve the matrix equation (3.5). The Tikhonov-regularized solution λ_{α} for Eq. (3.5) is defined as the solution to the following least squares problem:

$$\min_{\lambda} \{ \|A\lambda - b\|^2 + \alpha^2 \|\lambda\|^2 \}, \tag{3.6}$$

where $\| \bullet \|$ denotes the usual Euclidean norm and α is called the regularization parameter.

The determination of a suitable value of the regularization parameter α is crucial and is still under intensive research [Tikhonov and Arsenin (1977); Tautenhahn and Hämarik (1999)]. In our computation we use the L curve method, which is a kind of noise-free rules, to determine a suitable value of α . The L curve method was first developed by Lawson and Hanson [1974] and also applied by Chen *et al.* [1995] for solving the deconvolution problem. Hansen and O'Leary [1993] investigated the

properties of regularized systems under different values of α . The L curve method is sketched in the following:

Define a curve

$$L = \{ (\log(\|\lambda_{\alpha}\|^{2}), \log(\|A\lambda_{\alpha} - b\|^{2})), \alpha > 0 \}.$$
(3.7)

This curve is known as the L curve and a suitable regularization parameter α is the one that corresponds to a regularized solution near the "corner" of the L curve [Hansen (1992a, 1992b, 2000)].

In our computation, we used the Matlab code developed by Hansen [1994] for solving the discrete ill-conditioned system (3.5). Denote the regularized solution of (3.5) by λ^{α^*} . The approximated solution \tilde{u}_{α}^* for the BHCP problem (2.1)–(2.2) is then given as

$$\tilde{u}_{\alpha^*}(x,t) = \sum_{j=1}^{N} \lambda_j^* \phi_j(x,t).$$
 (3.8)

Bakushinskii [1985] proved that the convergence of x^{δ}_{α} cannot be guaranteed in using the free-noise rule. To the knowledge of the authors, there is still no convergence proof available in using other methods to determine the regularization parameter, such as Morozov's discrepancy principle and the monotone error rule Tautenhahn and Hämarik (1999). Nevertheless, these methods perform well in practice (see for instances Hanke and Hansen [1993] and Gellrich and Hofmann [1993]). The numerical results given in the following section indicate that the proposed scheme is feasible and efficient.

4. The Location and the Number of Source Points

For simplicity, the analysis of the choice of parameters is investigated only in the one-dimensional situation. Without loss of generality we assume that the spatial domain Ω is the interval [0,1] and we fix m=20 and n=40 in the following computation for the one-dimensional case.

An optimal placement of the location of source points is still an open problem for the MFS. Golberg and Chen [1997] suggested that the source points are chosen to be equally distributed around a circle of radius R, which is not suitable for problems with a nonsmooth domain. Mera [2005] chose the source points on a line below the initial time in solving the BHCP, which is similar to the method presented by Hon and Wei [2004]. More details can be found in the recent works Alves and Antunes (2005, 2008); Chen, Lee, Yu and Shieh (2008).

The discrepancy principle, which is a posteriori choice of the regularization parameter, was introduced by Morozov in 1966. It has been proven that the principle is suitable both for numerical computations and for convergence theories.

In this paper, we choose the location of source points on a position which has the same distance, R, away from the boundary of the domain. In other words, we

choose the source points located on $\partial \Upsilon \times [-\delta t, T]$, where $\partial \Upsilon$ is the boundary of interval [-R, 1+R] in the one-dimensional case. Based on the idea of the discrepancy principle, we fix the radius R of the source points through

$$\parallel A * \lambda_{R^*,\delta}^{\alpha^*} - \tilde{b} \parallel = \delta, \tag{4.1}$$

where $\lambda_{R^*,\delta}^{\alpha^*}$ is the regularized solution to (3.5) for $R=R^*$ in the MFS and δ is the noisy level. Hence, the location of source points depends in the parameters δt and R. The following investigation shows that the accuracy of the method increases with respect to an increase in the value of δt and R^* in the MFS.

In real data measurement, we can collect only the perturbed data (Gaussian-distributed random vector) $\tilde{f}(x_i)$, i = 1, ..., m, and $\tilde{g}(x_i, t_i)$, i = m + 1, ..., m + n, which satisfy

$$\sqrt{\frac{1}{m} \left(\sum_{i=1}^{m} (f(x_i) - \tilde{f}(x_i))^2 \right)} \le \delta \cdot \max|f|, \tag{4.2}$$

and

$$\sqrt{\frac{1}{n} \left(\sum_{i=1}^{n} (g(x_{i+m}, t_{i+m}) - \tilde{g}(x_{i+m}, t_{i+m}))^2 \right)} \le \delta \cdot \max|g|, \tag{4.3}$$

where δ is the tolerated noise level.

In order to estimate the computational error of the numerical approximation, we choose some extra test points to compute the root mean square error (RMSE):

RMSE =
$$\sqrt{\frac{1}{M} \sum_{i=1}^{M} (\tilde{u}(\bar{x}_i, 0) - u(\bar{x}_i, 0))^2},$$
 (4.4)

where M is the total number of test points on the domain Ω , and $\{\bar{x}_i\}_{i=1}^M$ is a set of test points which are uniformly distributed in Ω . In our computations, we take M=40 in the one-dimensional case.

For simplicity, the m+n collocation points are uniformly distributed on the boundary $\partial\Omega\times[0,T]$ and $\Omega\times\{T\}$. The N source points are taken to be uniformly distributed on the source points location $\partial\Upsilon\times[-\delta t,T]$. We denote h as the distance between two source points.

To analyze the choice of parameters and verify the effect of the proposed algorithm, we choose the following benchmark function used in the papers of Lattes [1969], Lesnic [1998] and Mera [2005]:

$$u(x,t) = e^{-\pi^2 t} \sin(\pi x),$$
 (4.5)

which has a severe behavior since u(x,t) decays to zero rapidly as t increases.

Firstly, we investigate the convergence of our proposed numerical algorithm with respect to the value of δt . In our computations, we fix T=0.5, h=0.5, R=2.5 and $\delta=0.03$. Figure 2 shows that the RMSE of the numerical solution decreases

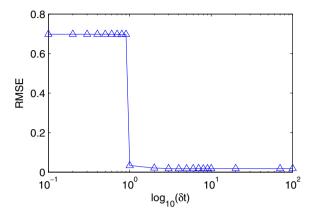


Fig. 2. The RMSE with respect to parameter $\log_{10}(\delta t)$ for T=0.5, h=0.5, R=2 and $\delta=0.03$.

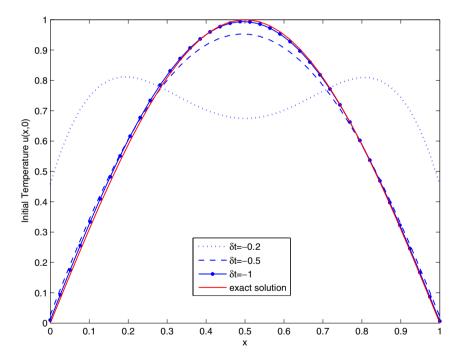


Fig. 3. The numerical solution for the initial temperature obtained with T=0.5, N=40, $R=2, \delta=0.03$ and various $\delta t.$

dramatically with respect to the increase in the value of δt until the value of δt reaches 1. Figure 3 presents numerical solutions for the initial temperature obtained in the MFS with various δt . It can be seen that the numerical solution already approaches the exact solution excellently when $\delta t = 1$. For this reason, we always

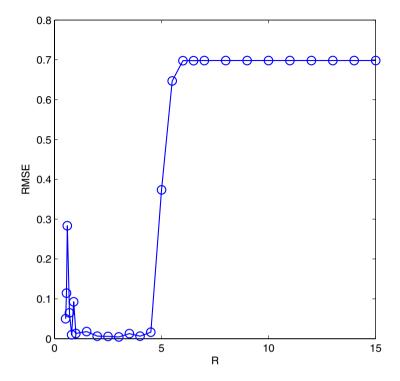


Fig. 4. The RMSE with respect to parameter R for $T = 0.5, \delta t = 1, N = 40$ and $\delta = 0.03$.

choose $\delta t = 1$ in the one-dimensional case. It was found that in general the MFS produces accurate numerical solutions for other test cases even when δt is large.

To investigate the effect of the choice of R in our computations, we fix $\delta t=1$, N=20 and $\delta=0.03$. Figure 4 displays the RMSE as a function of the parameter R. It can be observed from the figure that the RMSE does not decrease with respect to an increase or decrease in the value of R as other parameters. In this case the R^* computed by our method is 1.96, which is located within the range for optimal convergence.

The following numerical results indicate that this choice of the location of source points performs well in all of the following examples and better than the method given in the paper of Mera [2005].

Lastly, we investigate the convergence of the numerical solution with respect to the total number (N) of source points. Here, we fix T=0.5, $\Upsilon=[-2,3]$, $\delta t=1$ and $\delta=0.03$. The source points are chosen to be uniformly distributed on the location $\partial \Upsilon \times [-\delta t, T]$. Figure 5 displays the RMSE as a function of the parameter N. It can be seen that the RMSE of the numerical solution decreases dramatically with respect to an increase in the value of N until the value of N reaches 20. Figure 6 shows that for N=20 the numerical solution already approximates the exact solution very well.

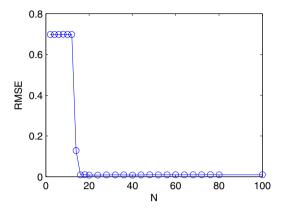


Fig. 5. The RMSE with respect to parameter N for $T=0.5, \delta t=1, R=2$ and $\delta=0.03$.

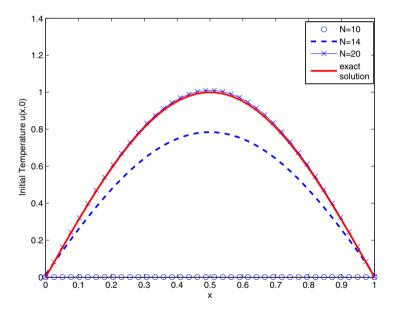


Fig. 6. The numerical solution for the initial temperature obtained with the final time T=0.5, $\delta t=1, R=2, \delta=0.03$ and various N.

5. Numerical Solutions for the BHCP

In this section, both the one-dimensional and the two-dimensional BHCP will be considered, in Secs. 5.1 and 5.2, respectively.

5.1. Numerical example for the one-dimensional BHCP

For numerical verification, we use in this section the proposed method to solve the BHCP in both the one-dimensional and the two-dimensional case. In the computation, a different noise level δ will be used. We always choose $\delta t = 1, N = 20$ and $R = R^*$, which is chosen by using the proposed discrepancy principle given in the last section. The numerical approximation to the solution u(x,0) with a different noise level δ is displayed in Fig. 7. It can be seen that even for large $\delta = 0.1$ our proposed method produces an accurate numerical solution. Figures 8–10 display the approximation to u(x,t) and its error in the domain Ω with noise level $\delta = 0.03$ and T=1. Again, it can be seen that our method performs well in this example.

Next, we investigate the performance of our method in comparison with the result given in the paper of Mera [2005], in which he compares his method with other numerical methods, such as the boundary element method (BEM) and the finite difference method (FDM).

Figure 11 displays the numerical solutions obtained by using our proposed method with $\delta t = 1$ and $R = R^*$ and Mera's method in comparison with the exact solution. Both numerical results are obtained for the finite time T=1, the noise level $\delta = 0.03$, the number of collocation points m = 20, n = 40, and the number of source points N=40. It can be seen that our method outperforms Mera's method under the same parameter setting and requires a similar computational cost. The comparison has been made by using various other numerical examples, and similar results have been obtained.

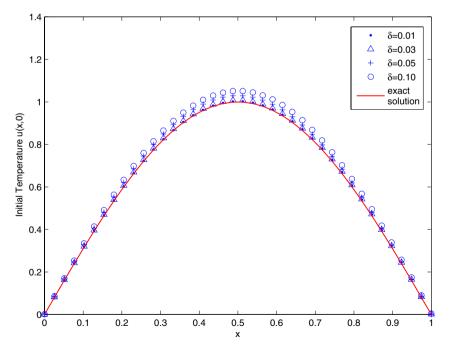


Fig. 7. The numerical solution $\tilde{u}(x,0)$ for $T=0.5, \delta t=1, N=20, R=1.96$ and noise levels $\delta = 0.01(\bullet), \ \delta = 0.03(\triangle), \ \delta = 0.05(+), \ \delta = 0.1(\circ).$

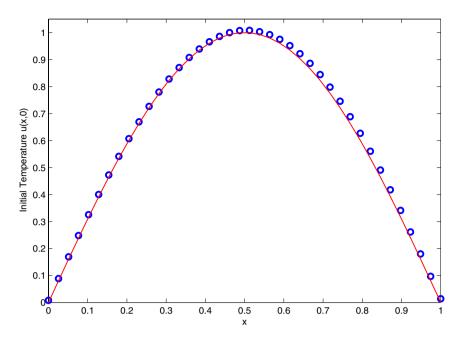


Fig. 8. The exact solution (-) and the numerical solution (o) for the initial temperature obtained with $T=1, \delta t=1, N=40, R=R^*=5.3$ and $\delta=0.03$.

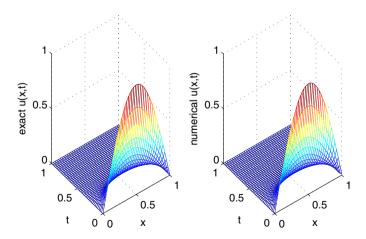


Fig. 9. The exact solution u(x,t) (left) and the approximate $\tilde{u}(x,t)$ (right) obtained with $T=1, \delta t=1, N=40, R=R^*=5.3$ and $\delta=0.03$.

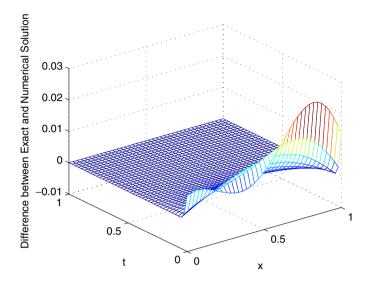


Fig. 10. The difference between the exact and the numerical solution to u(x,t) for T=1, $\delta t=1,$ N=40, $R=R^*=5.3$ and $\delta=0.03$.

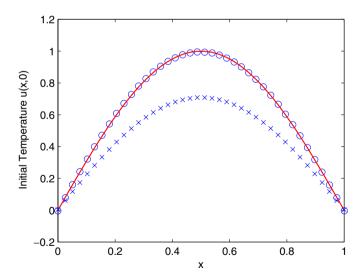


Fig. 11. The numerical solution u(x,0) obtained by our method (o) and the method in the paper of Mera [2005] (×), and the exact solution (-) for final time T=0.7 and noise level $\delta=0.05$.

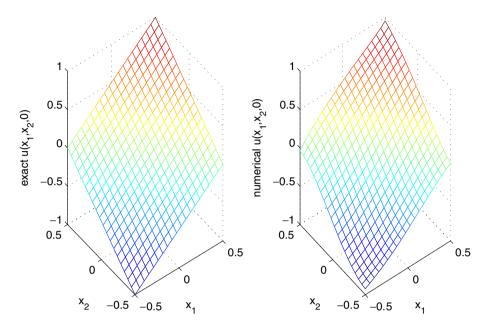


Fig. 12. The exact solution $u(x_1, x_2, 0) = x_1 + x_2$ (left) and its approximation $\tilde{u}(x_1, x_2, 0)$ (right) with $T = 1, \delta t = 1, N = 400, R = 0.11$ and $\delta = 0.05$.

Numerical results in the last subsection also indicate that the proposed method performs very well even for the large final time T=1, which is larger than the maximum T=0.7 used in the paper of Mera [2005].

5.2. Numerical example for the two-dimensional BHCP

In this subsection, it will be seen that our proposed method also performs well in solving the two-dimensional BHCP. The total number of source points is chosen to be N=400 in this computation.

In order to verify the effectiveness of our method, we consider the exact solution given by $u(x_1, x_2, t) = x_1 + x_2$. In the computation, we choose m = 64 and n = 196 collocation points which are uniformly distributed on the boundary of the solution domain $\Omega \times [\delta t, T]$, where $\Omega = [-0.5, 0.5] \times [-0.5, 0.5]$, and N = 400 source points which are uniformly distributed in $\partial \Upsilon \times [0, T]$, where $\Upsilon = [-R - 0.5, R + 0.5] \times [-R - 0.5, R + 0.5]$ and $\delta t = 1$. We also fix the final time T = 1. The boundary data are perturbed with noise level $\delta = 0.05$.

Figure 12 presents the comparison between the exact solution $u(x_1, x_2, 0)$ and the numerical solution obtained by our method. The error function between the exact solution and the numerical solution is displayed in Fig. 13. It can be seen that the numerical solution obtained by our method has a good approximation to the exact solution even for the two-dimensional BHCP and the large finite time T=1.

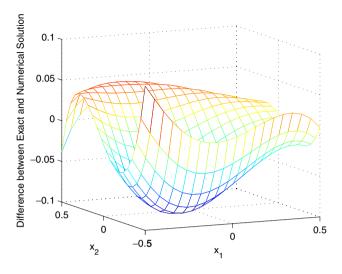


Fig. 13. The difference between the exact and the numerical solution to $u(x_1, x_2, 0)$ for $\delta t = 1, N = 400, R = 0.11, \delta = 0.05$.

To further explore the application of the proposed method for solving the twodimensional BHCP, we consider the example

$$u(x_1, x_2, t) = \sin\left(\frac{1}{\sqrt{2}}\pi(x_1 + x_2)\right)e^{-\pi^2 t},\tag{5.1}$$

which is a typical example for testing the efficiency of solving the two-dimensional BHCP. Here, we choose the same parameters used in the last example. The exact solution $u(x_1, x_2, 0)$ and the numerical solution obtained by using our method are displayed in Fig. 14. The error between the exact solution and the numerical solution

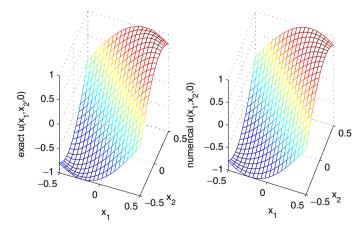


Fig. 14. The exact solution $u(x_1, x_2, 0) = \sin(\frac{1}{\sqrt{2}}\pi(x_1 + x_2))$ (left) and its approximation $\tilde{u}(x_1, x_2, 0)$ (right) with $T = 1, \delta t = 1, N = 400, R = 0.11$ and $\delta = 0.05$.

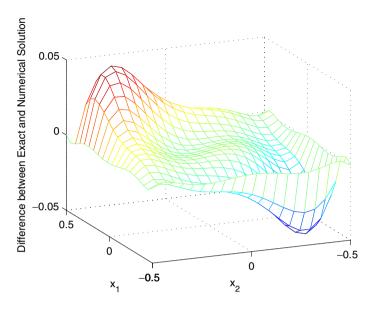


Fig. 15. The difference between the exact and the numerical solution to $u(x_1, x_2, 0)$ for $\delta t = 1$, $N = 400, R = 0.11, \delta = 0.05$.

is shown in Fig. 15. It can be found that our method also produces an accurate solution in this severe example.

6. Conclusion

Based on the idea of the discrepancy principle, we develop in this paper a new computational method for choosing the location of source points to solve the backward heat conduction problem by using the method of fundamental solutions. Numerical results indicate that the proposed method gives an accurate and reliable scheme and performs better than other existing methods. Finally, the method can be readily extended to solve problems in complex and irregular domains.

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