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The method of fundamental solutions and condition number analysis for inverse problems of Laplace equation

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Abstract

This paper investigates the applications of the method of fundamental solutions together with the conditional number analysis to solve various inverse 2D Laplace problems involving under-specified and/or over-specified boundary conditions. Through the method of fundamental solutions and the condition number analysis, it is numerically found that solutions of inverse Laplace problems can be obtained without iteration or regularization for small noise levels, since the method of fundamental solutions is a boundary-type meshless numerical method that can automatically satisfy the governing equation. However for larger values of noise levels regularization is still necessary to obtain promising result. The present paper mainly focuses on the two types of numerical predictions of inverse 2D Laplace problems: (1) Cauchy problem, and (2) shape identification problem. Good quantitative agreement with the analytical solutions and other numerical methods for small perturbed boundary data is observed by using present meshless numerical scheme.

Keywords: Inverse problems; Cauchy problems; Ill-posed problems; Laplace equation; Method of fundamental solutions; Condition number analysis; Perturbed boundary data

1. Introduction

Mathematical solutions of boundary value problems (BVPs) usually consider well-posed problems, which are defined by the uniqueness and existence of the solution, and continuous dependence on the input data [1]. It is not always possible in many engineering or science fields to set up well-posed problems. For example, in groundwater flows, boundary conditions specified along geological features may not form a closed boundary. However, distributed monitoring wells often exist to provide observations of the piezometric heads in the interested domain. These kinds of problems are often considered to be ill-posed BVPs.

Inverse problems are ubiquitously found in many fields, such as heat conduction analysis [2,3], Cauchy problems [4–7], crack and defect detections [8] and medical applications, etc. These ill-posed problems traditionally must be treated using viable methods such as regularization techniques, objective functionals and experimental

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procedures [2–8]. Mera et al. [5] have given a detail study on various regularization methods used to solve the Cauchy problems.

The method of fundamental solutions (MFS) first proposed by Kupradze and Aleksidze in 1964 [9], has become a versatile boundary-type meshless numerical scheme to solve well-posed problems. This method is free from the treatments of singularities, meshes, and numerical integrations [10–12]. The concept of the MFS is to decompose the solutions of the partial differential equations by the superposition of their fundamental solutions with proper source intensities. The intensities are thus the unknown parameters to be determined by the method of collocation through known augmented data on the boundary or even in the domain.

Meshless numerical methods have also been applied to study inverse problems. Cheng and Cabral [13] applied domain-type meshless scheme of the radial basis function collocation method (RBFCM) to solve general ill-posed boundary value problems of Laplace equation without regularizations or iterations for small noisy boundary data. Marin and Lesnic [14] also applied the MFS to obtain the solution of a Cauchy problem associated with the 2D linear elasticity. Marin [15] further extended the scheme to solve a Cauchy problem involving 3D Helmholtz equations. However in all the above-mentioned last two works, the Tikhonov regularization technique had been adopted to solve the resulted equation system. Ramachandran [16] on the other hand used the singular value decomposition (SVD) technique to solve the linear equations. In the present study we will apply the MFS together with the condition number analysis to solve several ill-posed BVPs including the Cauchy problem. Furthermore it is numerically found that no regularizations or iterations are necessary for all kinds of inverse problems by implementing the condition number analysis if noise level is kept small.

Inverse problems, especially Cauchy problems, are very difficult to solve both numerically and analytically since their solutions do not depend continuously on the prescribed boundary conditions [17]. The system of linear algebraic equations obtained by discretizing the inverse problem is usually ill-conditioned [4,5]. The capability of equation solver has been significantly improved in recent years. We found that high accuracy is achieved in our numerical experiments by the applications of the MFS for inverse problems when the condition number of the resultant linear equations system approaches the limit of the equation solver. The condition number is dependent on the solution scheme and numerical precision. When the MFS together with the analysis of condition number is applied to solve inverse problems with small noise range, no iteration or regularization procedures are needed. However regularization is still necessary in general for larger values of noise levels such as 1% perturbation.

The present work contributes to the applications of the MFS and condition number analysis to solve 2D inverse Laplace problems of the following two types of problems: (1) Cauchy problem, and (2) shape identification problem. The following sections will discuss the details about the governing equations, numerical procedures, the results and discussions and concluding remarks.

2. Governing equations

For Cauchy problems, we discuss the steady-state heat conduction in an isotropic homogeneous media. We consider an isotropic medium in an open bounded domain $\Omega \subset \mathbb{R}^2$, and assume that Ω is bounded by a surface Γ. In the absence of heat generation and other modes of heat transfer, the governing equation for steady-state heat conduction or a field potential in the domain is given by the following Laplace equation [4]:

$$\nabla^2 T(\mathbf{x}) = 0, \quad \mathbf{x} \in \Omega \tag{1}$$

where T is the temperature or a field potential to be solved and $\mathbf{x}$ is the spatial coordinates of the problem. For the Cauchy problem, Eq. (1) has to be solved subjected to the following boundary conditions:

$$\begin{aligned} T|_{\Gamma_1} &= f_1 \\ T|_{\Gamma_2} &= f_2 \\ \partial_n T|_{\Gamma_2} &= q_2 \\ \partial_n \Gamma|_{\Gamma_3} &= q_3 \end{aligned} \tag{2}$$

where f_1 & f_2 are the prescribed boundary temperatures on Γ_1 & Γ_2, and q_2 & q_3 are prescribed heat fluxes on Γ_2 & Γ_3. No boundary conditions are specified on Γ_0. Moreover, $\Gamma = \Gamma_0 + \Gamma_1 + \Gamma_2 + \Gamma_3$, with Γ_i disjoint from each

other, and Γ_0 & Γ_2 are nonempty sets. It can be found from Eq. (2) that the boundary Γ_2 is over-specified, while Γ_0 is under-specified.

A necessary condition for the inverse Cauchy problem given by Eqs. (1) and (2) to be identifiable is that measure $(\Gamma_2) > $ measure (Γ_0). Although the problem has a unique solution, it is well-known that the solution is unstable with respect to a small perturbation on the over-specified boundary Γ_2 [16]. Therefore, Cauchy problems are ill-posed inverse problems.

In this study the Laplace equation (1) is also adopted to other types of inverse problems: for example such as shape identification problem. The accuracy and stability of the scheme will be examined later, since these problems often occur in practical engineering or medical applications.

3. The method of fundamental solutions (MFS)

The main advantages of the MFS widely used in recent years to solve BVPs are it does not require a discretized computational domain, and it offers numerical solution without dealing with singularities and numerical integrations. To obtain the required coefficients for interpolating the field variables at the interior part of the computational domain, the MFS only needs the boundary values of the field variables at certain nodes on the boundary.

By the principle of the MFS, the numerical solution for the field variable such as temperature is given by a general formulation expressed by

$$T(\mathbf{x}) = \sum_{i=1}^{N} \alpha_i G(\mathbf{x}, \mathbf{s}_i) \tag{3}$$

where α_i represents the intensities of sources that are used to determine the interior values of the field variable. $G(\mathbf{x}, \mathbf{s}_i)$ is the fundamental solution or the free space Green's function of the Laplacian operator. These coefficients are determined by the method of collocation using the known boundary values for the well-posed BVPs and also the internal data for the ill-posed inverse problems. To avoid the singularity of the fundamental solution G, the N prescribed source points $\mathbf{s}_i$ are located outside the computational domain. This paper will further address details to determine the positions of N source points through the condition number analysis.

For the 2D Laplace equation, the expression for $G(\mathbf{x}, \mathbf{s}_i)$ in Eq. (3) is given by

$$G(\mathbf{x}, \mathbf{s}_i) = \frac{-1}{2\pi} \ln(|\mathbf{x} - \mathbf{s}_i|). \tag{4}$$

In Eq. (3), we are able to obtain a system of linear algebraic equations if we can properly collocate the equation by the prescribed boundary data of Eq. (2) or even the given internal data for some inverse problems. The final expression for the determination of the coefficients α_i can be expressed in a matrix form as

$$[A_{ji}]\{\alpha_i\} = \{b_j\} \tag{5}$$

where the coefficients of matrix $[A_{ji}]$ are the known data composed by the values of fundamental solution for prescribed source and boundary or internal collocation points, and column matrix $\{b_j\}$ can be obtained from the boundary conditions or internal values. Therefore by applying Eq. (5), the coefficients α_i can be obtained, and the solution, $T(\mathbf{x})$ of Eq. (3), is solved. As we can collocate all the known value points either on the boundary or in the interested domain, the MFS has advantages over other numerical methods on processing all inverse problems since no iteration or regularization procedures are necessary if noise level is kept small.

4. Locations of source points and boundary collocation points

The distribution of source points and boundary collocation points is significant in the proposed numerical method. Fig. 1(a) describes a typical geometrical configuration of a Cauchy problem, in which Ω is the computational domain. Moreover, Γ' and Γ_0 are boundaries with and without boundary conditions respectively. We will then introduce a systematical procedure to locate source points and boundary collocation points:

Step 1. The boundary collocation points, $\mathbf{x}_f$, are uniformly distributed on the boundary Γ' with given boundary conditions (Fig. 1(b)).

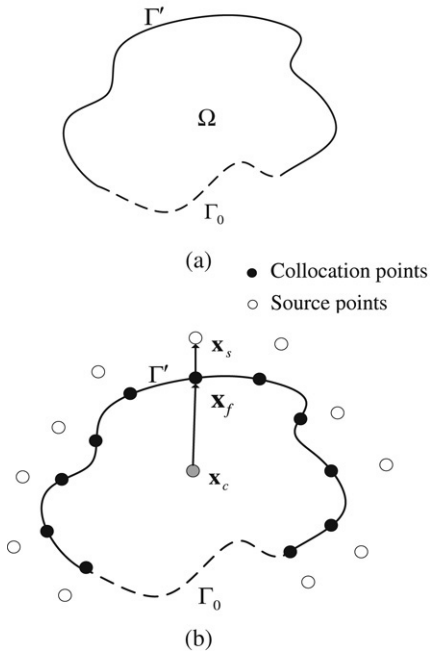

Fig. 1. (a) Typical geometrical configuration of the Cauchy problem (b) Schematic diagram for the distribution of collocation and source points.

Step 2. According to the boundaries of the physical domain, the geometric center, $\mathbf{x}_c$, can be obtained (Fig. 1(b)).

Step 3. The distributions of the source points, $\mathbf{x}_s$, are arranged by the following equation:

$$\mathbf{x}_s = \mathbf{x}_f + \lambda(\mathbf{x}_f - \mathbf{x}_c) \tag{6}$$

where $\mathbf{x}_s$ and $\mathbf{x}_f$ respectively are the spatial coordinates of the source and boundary points. Moreover, $\mathbf{x}_c$ is the center position of the computational domain and λ is a parameter of source location. Once the parameter of source location,λ, is allocated, the distributions of the source points can be obtained as depicted in Fig. 1(b).

Step 4. The source points are uniformly doubled for boundaries with over-specified boundary conditions since both Dirichlet and Neumann boundary conditions are given. Therefore, Eq. (5) has the same number of equations and unknowns for the Cauchy problems.

This procedure of locating source points and boundary collocation points for Cauchy problems can be easily extended to other inverse problems such as BVPs with internal points. For inverse problems with internal points, the same number of source points should be uniformly added.

5. Condition number and error analysis

We first define the condition number to analyze the accuracy of the MFS for inverse problems. The most popular measure of a matrix is its condition number, CDN, defined by

$$\text{CDN} = \text{max. singular value}/\text{min. singular value}. \tag{7}$$

The accurate computation of the singular values may be time and memory consuming since it requires singular value decomposition (SVD) technique [18]. However there are several algorithms to provide easy estimates of CDN without needing to obtain the exact singular values. In this paper, we adopted the LINPACK's Cholesky decomposition method [18] to obtain the relevant CDN.

We alternatively adopt the root mean squared (r.m.s) error for the error analysis, which is defined as follows:

$$\text{r.m.s error} = \sqrt{\frac{\sum_{i=1}^{N}(T_{\text{numerical},i} - T_{\text{exact},i})^2}{N}} \tag{8}$$

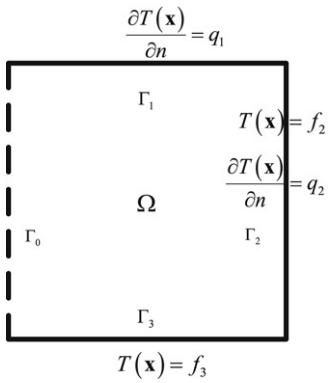

Fig. 2. Schematic diagram for the Cauchy problem.

where N is the number of total points considered, $T_{\text{numerical},i}$ is the numerical solution at point i and $T_{\text{exact},i}$ is the exact solution at point i.

6. Results and discussions

The capability of the MFS is first demonstrated by mathematically more rigorous Cauchy problem in example (Section 6.1). The proposed method is then applied to some practical inverse problems in engineering applications, and for example (Section 6.2) shape identification problem.

6.1. Cauchy problem

For validation purpose, the Cauchy problem of the Laplace equation in an isotropic material is solved for a square domain as discussed by Lesnic et al. [4]. The schematic diagram of the computational domain with the boundary conditions for the temperature is shown in Fig. 2, and the boundary conditions are given by

$$\begin{aligned}
&\partial_n T_{|\Gamma_1} = \frac{\partial T}{\partial y}(x, L) = q_1(x) = \cos(x)\sinh(L) + \sin(x)\cosh(L)\\
&T_{|\Gamma_2} = T(L, y) = f_2(y) = \cos(L)\cosh(y) + \sin(L)\sinh(y)\\
&\partial_n T_{|\Gamma_2} = \frac{\partial T}{\partial x}(L, y) = q_2(y) = -\sin(L)\cosh(y) + \cos(L)\sinh(y)\\
&T_{|\Gamma_3} = T(x, 0) = f_3(x) = \cos(x).
\end{aligned} \tag{9}$$

The analytical solution of the temperature for the problem is

$$T(x, y) = \cos(x)\cosh(y) + \sin(x)\sinh(y). \tag{10}$$

Fig. 3 depicts the distribution of source points for the square domain in this problem. Fig. 4 further demonstrates the relations among the parameter of source location, r.m.s error, and CDN for various number of source points. It is observed that when the source points move outward the solution accuracy improves while the condition number deteriorates. Quantitatively, as the parameter of source location increases, the r.m.s error reaches its smallest value (10^{-3}–10^{-2} for single precision and 10^{-6}–10^{-5} for double precision) once CDN approaches its highest value (10^8 for single precision and 10^{17} for double precision). The limits of equation solver, 10^8 for single precision and 10^{17} for double precision, are defined by FORTRAN 8-byte single precision and 16-byte double precision respectively, as well as the LINPACK's Cholesky decomposition [18]. This limit can be easily obtained by carrying out more numerical experiments. We also found that since we adopted the same equation solver and computational environments, the limit is the same in all the following numerical experiments. In Figs. 5(a) and (b) the analytical solutions are compared with the present numerical results of temperature and the heat flux distributions on the under-specified boundary. The results computed by the double precision MFS show very good agreement with the analytical solutions.

Furthermore, we consider noisy boundary data as follows:

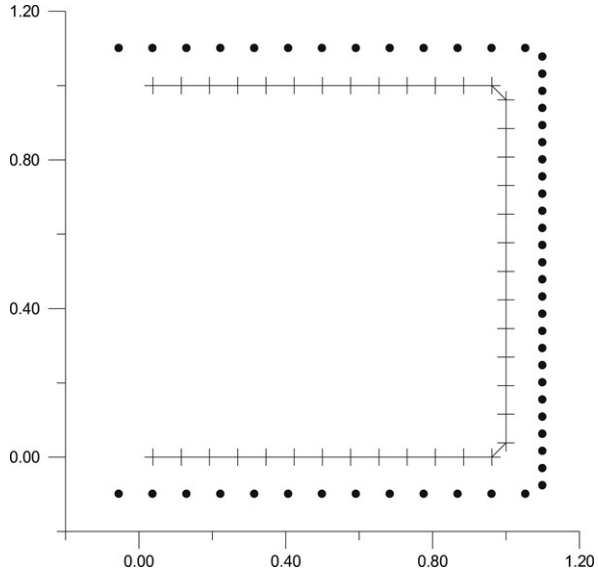

Fig. 3. The distribution of collocation and source points for the Cauchy problem.

$$\begin{aligned} T &= (1+k\varepsilon)f(x) \\ \frac{\partial T}{\partial n} &= (1+k\varepsilon)q(x) \end{aligned} \quad -1 \le \varepsilon \le 1 \tag{11}$$

where $f(x)$ and $q(x)$ are boundary conditions defined in Eq. (9), ε is a uniformly distributed random number, and k is the amplitude of noise. These random numbers are generated by the FORTRAN subroutine RANDOM_SEED. Hon and Wu [19] tested the sensitivity of solution subject to noisy boundary data from $k = 10^{-5}$ to 10^{-4}. Cheng and Cabral [13] tested the much lager noise from $k = 10^{-5}$ to 10^{-2}. In our experiment, we also solve the large noise from $k = 10^{-5}$ to 10^{-2}. The numerical results are shown in Fig. 6 for different noises k. The results are also in good agreement with analytical solutions. However for larger values of k such as 1% noise level regularization is now necessary, since $k = 10^{-2}$ will not give very good flux result as shown in Fig. 6.

6.2. Shape identification problem

Hon and Wu [19] and Cheng and Cabral [13] investigated the following Cauchy problem of shape identification in practical engineering applications. This problem often arises in the industrial nondestructive testing or medical examinations. Let us assume the domain of interest to be a half plane and the inside domain is inaccessible for measurement. Observation can still be conducted on a finite segment of the boundary, with both the measured potential and the flux. The task is to search for an internal trajectory of the equal potential.

For the test problem, we assume that the Cauchy boundary condition is prescribed on the segment $\{-0.5 \le x \le 0.5;\ y = 0\}$ as described in Fig. 7(a), where

$$T(x, y) = f(x) = x^2 - 0.31x - 1.089 \tag{12a}$$

$$\frac{\partial T(x, y)}{\partial n} = g(x) = 0.1x + 2.19. \tag{12b}$$

The task is to find the locations of the internal shapes along which $T(x, y) = 0$ in exact solution. The above boundary conditions are evaluated from the following potential:

$$T(x, y) = (x - 0.1)^2 - (y - 1.1)^2 + 0.1(x - 0.1)(y - 1.1) + 0.1 \tag{13}$$

and we are planning to recover this solution. In other words, we search for two trajectories that satisfy the zero potential condition:

$$y = 1.095 + 0.05x - 1.001\sqrt{0.1098 - 0.2x + x^2} \tag{14a}$$

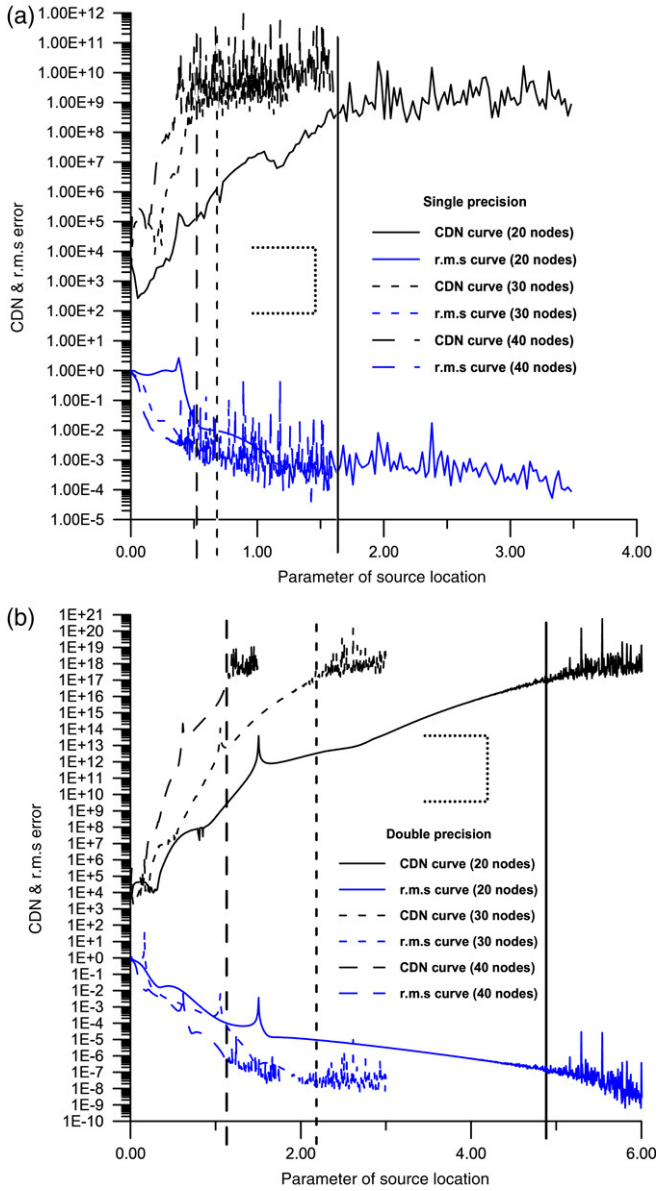

Fig. 4. The CDN and r.m.s error (a) single precision and (b) double precision for different parameters of source location for the Cauchy problem.

$$y = 1.095 + 0.05x + 1.001\sqrt{0.1098 - 0.2x + x^2}. \tag{14b}$$

Hence the problem is solved in a finite domain $[-2, 2] \times [0, 2]$ due to the constraint of finite range of available data and the instability of Cauchy condition.

In the MFS, we collocate for the Dirichlet and the Neumann conditions at 6 points on the Cauchy boundary as depicted in Fig. 7(b). Fig. 8 displays the resulted relation of CDN and r.m.s error for different parameters of source location. It is also observed that r.m.s error reaches its best value once CDN approaches the order of 10^{17}. After obtaining the solutions of 30×30 points in the computational domain $[-2, 2] \times [0, 2]$ through Eq. (3), we then are able to search the locations of the almost zero potential trajectories in which $-10^{-3} \leq T(x, y) \leq 10^{-3}$. The locations of almost zero potential results shown in Fig. 9 are compared with the analytical solutions and also Cheng and Cabral numerical results [13], in order to test the accuracy of the MFS. The zero potential results are further compared with Hon and Wu [19] numerical results as shown in Fig. 10. Better performances than those of Cheng and Cabral, as well

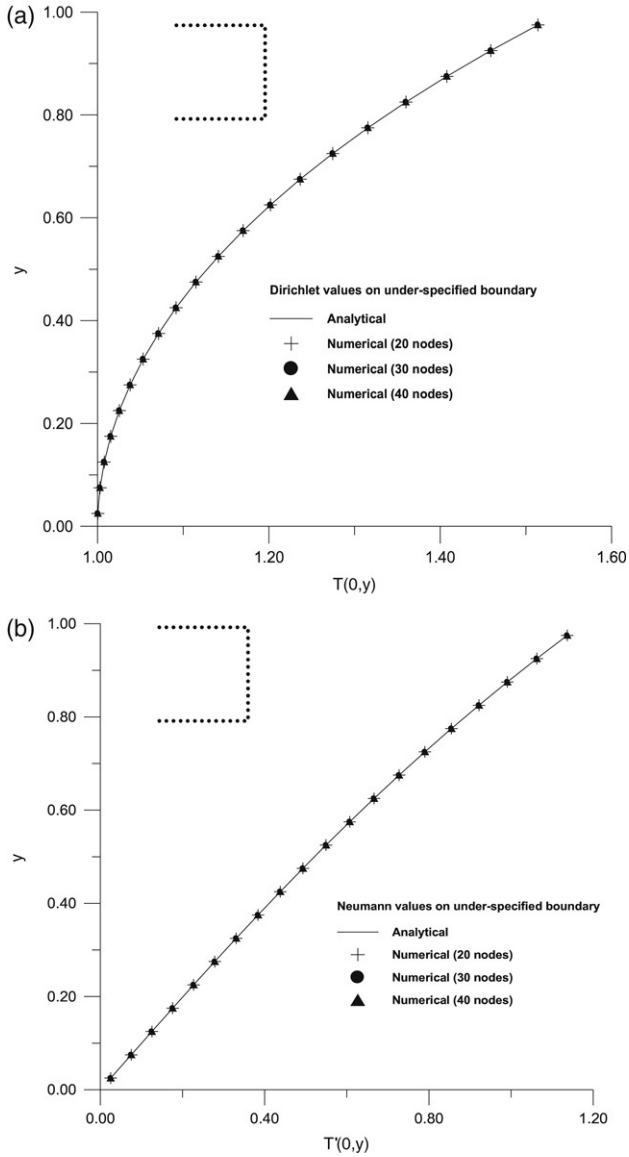

Fig. 5. The comparisons of (a) temperature and (b) heat flux distributions on the under-specified boundary with the analytical solutions for the Cauchy problem.

as Hon and Wu are observed as far as the present proposed method is concerned. Furthermore, to test the sensitivity of the solution subject to noisy boundary data, a larger noise level, from $k = 10^{-5}$ to 10^{-2} are tested. The zero potential results also show good accuracy when low noise ranges ($k = 10^{-5}$–10^{-3}) are considered as depicted in Fig. 11. However for larger values of k such as 1% noise level regularization is still necessary since $k = 10^{-2}$ will not give promising result in the upper branch but acceptable result in the lower branch as shown in Fig. 11. Nevertheless, for such a high noise of $k = 10^{-2}$, Cheng and Cabral [13] RBFCM model will fail unless auxiliary information is used.

6.3. Discussions

From these two numerical experiments, it is found that there is a definite relation among the parameter of source location, r.m.s error, and CDN. As stated in the works of Bogomolny [11] and Tsai et al. [20], when the source points move outward the solution accuracy improves and the condition number deteriorates. Our numerical experiments are carried out by FORTRAN single and double precisions and LINPACK's Cholesky decomposition method [18]. It is

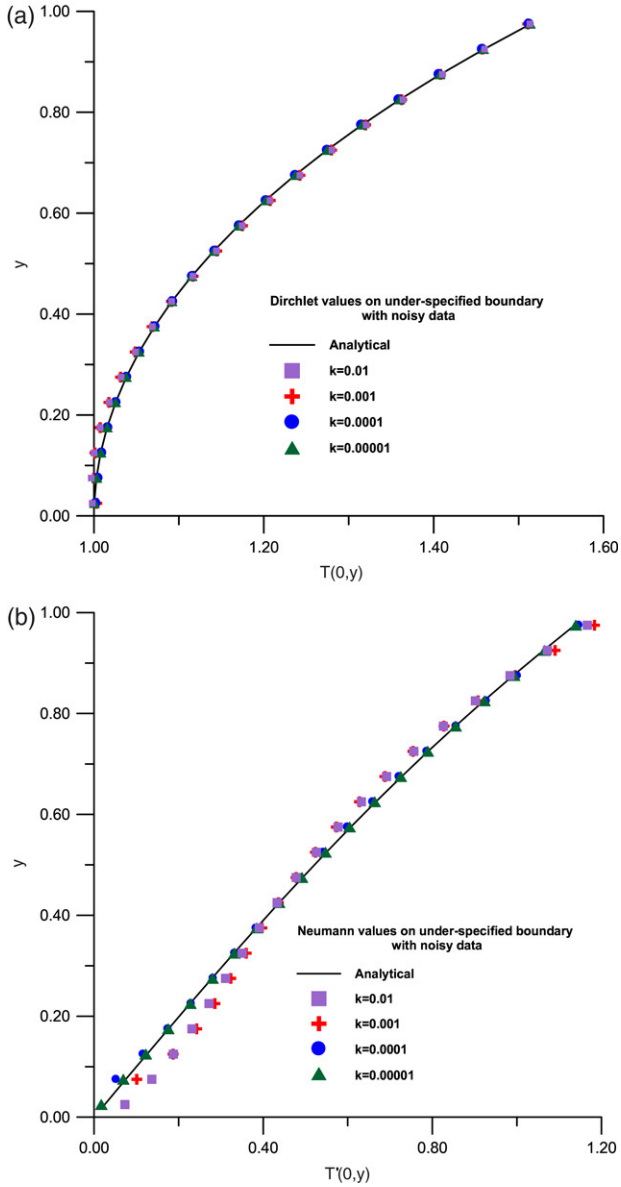

Fig. 6. The distributions of (a) temperature and (b) heat flux on the under-specified boundary with noisy data for the Cauchy problem.

found that the limit of equation solver is about CDN $\sim 10^8$ for single precision and CDN $\sim 10^{17}$ for double precision. Therefore it has been numerically proved that r.m.s error reaches its best value (10^{-3}–10^{-2} for single precision and 10^{-6}–10^{-5} for double precision) once CDN approaches the limit of equation solver. Accordingly, it is suggested that the following procedures should be carried out for inverse problems without exact solutions:

Step 1: Solve the desired problem by the MFS and draw the figure of parameter of source location v.s. CDN.

Step 2: Select the parameter of source location for which CDN is near the limit of equation solver from the figure of *Step* 1. Therefore, the source points are selected at the same time.

Step 3: Solve the problem by the source points determined from *Step* 2.

7. Conclusions

The MFS together with the condition number analysis is used to solve the inverse problems associated with the 2D Laplace equation. The present method is used to validate the steady-state Cauchy heat conduction problems in a

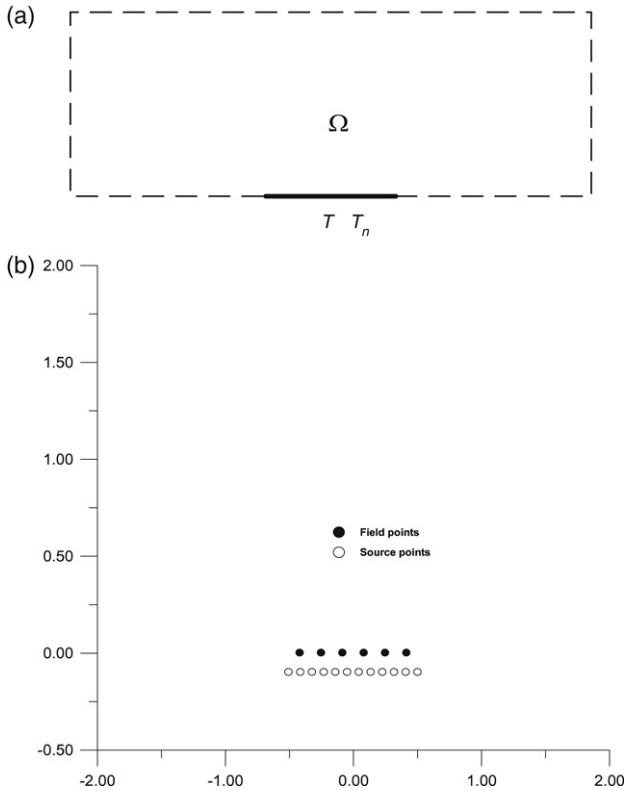

Fig. 7. Shape identification problem (a) geometrical configuration (b) source and collocation points.

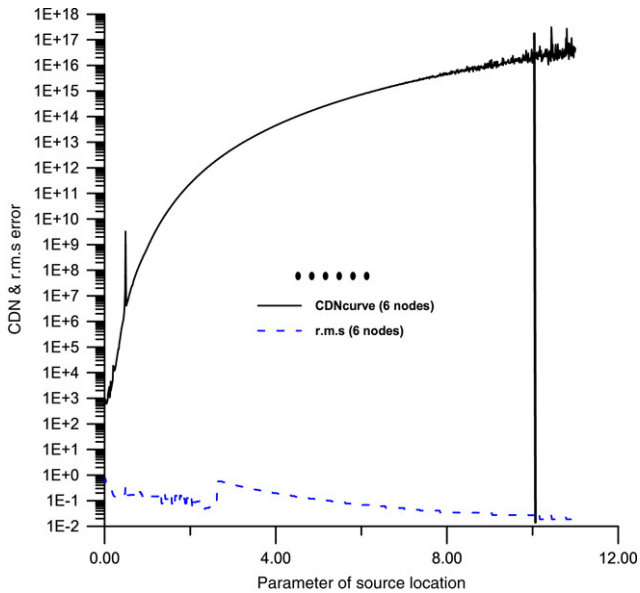

Fig. 8. The CDN and r.m.s error (6 nodes) for different parameters of source location for the shape identification problem.

square domain. Numerical results obtained by the proposed analysis are in very close agreement with the analytical solutions for the temperature and the heat flux distributions over the under-specified boundaries. They outperform other numerical methods including even the existence of small noise levels. Good performance is observed when

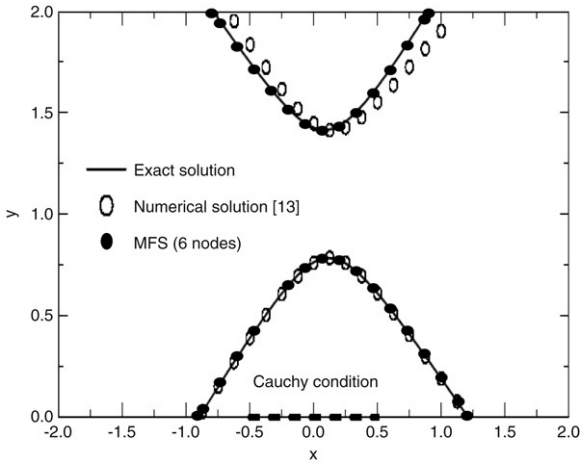

Fig. 9. The comparisons of the two trajectories with the analytical and Cheng and Cabral [13] numerical solutions.

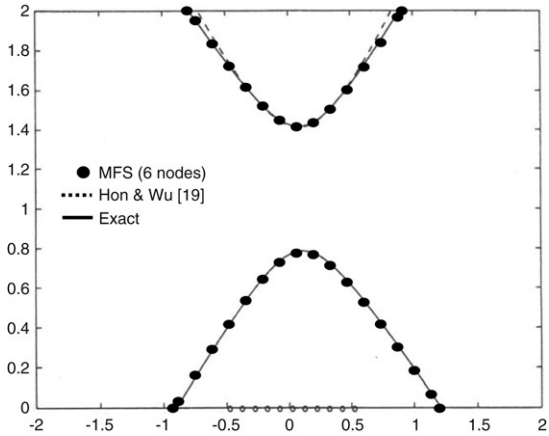

Fig. 10. The comparisons of the two trajectories with the analytical and Hon and Wu [19] numerical solutions.

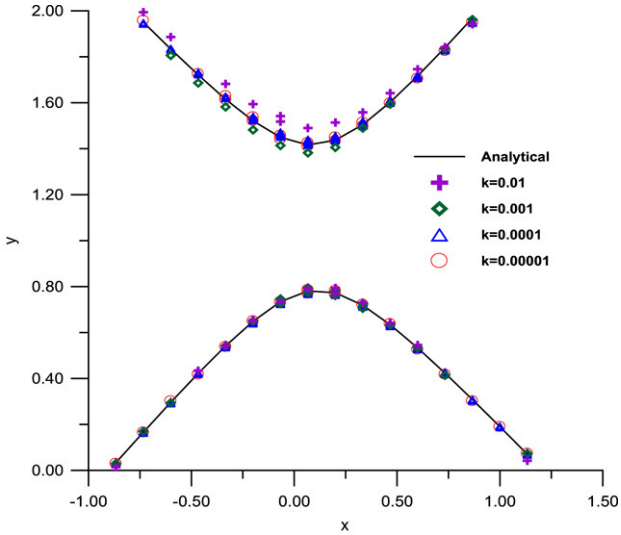

Fig. 11. The comparisons of the two trajectories with the analytical solution for noisy boundary data.

the proposed method is applied to some practical inverse problems in engineering applications, including shape identification problem with or without noisy boundary data. The proposed numerical method has proved the capability of the MFS together with the condition number analysis to easily handle the 2D inverse Laplace problems with small noise levels. However for larger values of noise ranges such as 1% perturbation regularization becomes necessary in order to obtain better results.

The capability of equation solver has been significantly improved with the advances of computer science. Many problems traditionally considered to be ill-conditioned, now can be accurately calculated without difficulty by using the proposed MFS together with the analysis of condition number. A more systematic study on the accuracy and condition number for the MFS deserves further investigation.

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