An iterative MFS algorithm for the Cauchy problem associated with the Laplace equation

Liviu Marin¹

Abstract: We investigate the numerical implementation of the alternating iterative algorithm originally proposed by Kozlov, Maz'ya and Fomin (1991) in the case of the Cauchy problem for the two-dimensional Laplace equation using a meshless method. The two mixed, well-posed and direct problems corresponding to every iteration of the numerical procedure are solved using the method of fundamental solutions (MFS), in conjunction with the Tikhonov regularization method. For each direct problem considered, the optimal value of the regularization parameter is chosen according to the generalized cross-validation (GCV) criterion. An efficient regularizing stopping criterion which ceases the iterative procedure at the point where the accumulation of noise becomes dominant and the errors in predicting the exact solutions increase, is also presented. The iterative MFS algorithm is tested for Cauchy problems associated with the Laplace operator in various two-dimensional geometries to confirm the numerical convergence, stability and accuracy of the method.

Keywords: Laplace Equation; Inverse Problem; Cauchy Problem; Iterative Method of Fundamental Solutions (MFS); Regularization.

1 Introduction

In most boundary value problems in heat transfer, the thermal equilibrium equation, i.e. the Laplace equation, has to be solved with the appropriate initial and boundary conditions for the temperature and/or normal heat flux, i.e. Dirichlet, Neumann, Robin or mixed boundary conditions. These problems are called *direct problems* and their existence and uniqueness have been well established. However, there are other engineering problems which do not belong to this category. For example, the thermal conductivities and/or the heat sources are unknown, the geometry of a por-

¹ Institute of Solid Mechanics, Romanian Academy, 15 Constantin Mille, Sector 1, P.O. Box 1-863, 010141 Bucharest, Romania. Tel./Fax: +40-(0)21-3126736. E-mails: marin.liviu@gmail.com; liviu@imsar.bu.edu.ro

tion of the boundary is not determined or the boundary conditions are incomplete, either in the form of under- and over-specified boundary conditions on different parts of the boundary or the solution is prescribed at some internal points in the domain. These problems are referred to as *inverse problems*

A classical example of an inverse problem for the Laplace equation is the *Cauchy problem*. In this case, the boundary of the solution domain, the thermal conductivities and/or the heat sources are all known, while the boundary conditions are incomplete. More precisely, both Dirichlet and Neumann conditions are prescribed on a part of the boundary, while on the remaining portion of the boundary no boundary conditions are given. It is well known that Cauchy problems are generally illposed [Hadamard (1923)], in the sense that the existence, uniqueness and stability of their solutions are not always guaranteed. Consequently, a special numerical treatment of these problems is required.

There are numerous important contributions in the literature, as well as various approaches, to the theoretical and numerical solutions of the Cauchy problem associated with the Laplace equation. The method of quasi-reversibility, in conjunction with a finite-difference method (FDM) and Carleman-type estimates, were employed by Klibanov and Santosa (1991) to solve this inverse problem.

Kozlov, Maz'va and Fomin (1991) proposed an alternating iterative algorithm for the stable solution of this problem, which was implemented using the boundary element method (BEM) by Lesnic, Elliott and Ingham (1997). Ang, Nghia and Tam (1998) reformulated the Cauchy problem as an integral equation problem and solved the latter by using the Fourier transform, together with the Tikhonov regularization method. Reinhardt, Han and Hào (1999) proved that the standard five-point FDM approximation to the Cauchy problem for the Laplace equation satisfies some stability estimates and hence it turns out to be a well-posed problem, provided that a certain bounding requirement is fulfilled. As a result of a variational approach to the Cauchy problem, the conjugate gradient method, in conjunction with the BEM, was proposed by Hào and Lesnic (2000) in order to obtain a stable solution. On using Green's formula, Cheng, Hon, Wei and Yamamoto (2001) transformed the original problem into a moment problem and they also provided an error estimate for the numerical solution. Hon and Wei (2001) converted the Cauchy problem into a classical moment problem whose numerical approximation can be achieved and also provided a convergence proof based on Backus-Gilbert algorithm. Cimetière, Delvare, Jaoua and Pons (2001) reduced the Cauchy problem for the Laplace equation to solving a sequence of optimization problems under equality constraints using the finite element method (FEM). The minimization functional consists of two terms that measure the gap between the optimal element and the over-specified data and the gap between the optimal element and the previous optimal element (regularization term), respectively. This method was later implemented using the BEM by Delvare, Cimetière and Pons (2002). Cimetière, Delvare, Jaoua and Pons (2002) reduced the solution of harmonic Cauchy problems to the resolution of a fixed point process, while the authors implemented numerically the proposed method by employing both the BEM and the FEM. Jourhmane, Lesnic and Mera (2004) developed three relaxation procedures in order to increase the rate of convergence of the algorithm of Kozlov, Maz'ya and Fomin (1991), at the same time selection criteria for the variable relaxation factors having been provided. Bourgeois (2005) approached the Cauchy problem for the Laplace equation by the mixed formulation of the method of quasi-reversibility, which finally led to a \mathscr{C}^0 FEM. And rieux, Baranger and Ben Abda (2006) introduced an energy-like error functional and converted the inverse problem into an optimization problem. In order to improve the reconstruction of the normal derivatives, Delvare and Cimetière (2008) extended the method originally proposed by Cimetière, Delvare, Jaoua and Pons (2001) to a higher-order one, which was implemented using the BEM. On assuming the available data to have a Fourier expansion, Liu (2008f) applied a modified indirect Trefftz method to solve the Cauchy problem for the Laplace equation.

The method of fundamental solutions (MFS) is a simple but powerful technique that has been used to obtain highly accurate numerical approximations of solutions to linear partial differential equations. Like the BEM, the MFS is applicable when a fundamental solution of the governing PDE is explicitly known. Since its introduction as a numerical method by Mathon and Johnston (1977), it has been successfully applied to a large variety of physical problems, an account of which may be found in the survey papers [Fairweather and Karageorghis (1998); Golberg and Chen (1999); Fairweather, Karageorghis and Martin (2003); Cho, Golberg, Muleshkov and Li (2004)].

The ease of implementation of the MFS and its low computational cost make it an ideal candidate for inverse problems as well. For these reasons, the MFS, in conjunction with various regularization methods (e.g. the Tikhonov regularization method, Morozov's discrepancy principle, singular value decomposition), have been used increasingly over the last decade for the numerical solution of inverse problems. For example, the Cauchy problem associated with the heat conduction equation [Hon and Wei (2002); Hon and Wei (2003); Hon and Wei (2004); Hon and Wei (2005); Mera (2005); Dong, Sun and Meng (2007); Wei, Hon and Ling (2007); Ling and Takeuchi (2008); Marin (2008); Young, Tsai, Chen and Fan (2008); Shigeta and Young (2009); Wei and Li (2009); Wei and Zhou (2009)], linear elasticity [Marin and Lesnic (2004); Marin (2005a)], steady-state heat conduction in functionally graded materials (FGMs) [Marin (2005b)], Helmholtz-type equations [Marin (2005c); Marin and Lesnic (2005a); Jin and Zheng (2006)], Stokes problems [Chen, Young, Tsai and Murugesan (2005)], the biharmonic equation [Marin and Lesnic (2005b)] etc. have been successfully addressed by employing the MFS.

To the best of our knowledge, the MFS has not, as yet, been applied iteratively to the numerical solution of inverse problems. Therefore, we have decided to use the MFS in an iterative manner for solving stably the Cauchy problem in two-dimensional steady-state heat conduction (Laplace equation). More precisely, we investigate the numerical implementation of the alternating iterative algorithm originally proposed by Kozlov, Maz'ya and Fomin (1991) using the MFS. At every iteration, two mixed, well-posed and direct problems are solved using the MFS, in conjunction with the Tikhonov regularization method. For each of the aforementioned direct problems, the optimal value of the regularization parameter is chosen according to the generalized cross-validation (GCV) criterion. An efficient regularizing stopping criterion which ceases the iterative procedure at the point where the accumulation of noise becomes dominant and the errors in predicting the exact solutions increase, is also presented. The iterative MFS algorithm is then tested for Cauchy problems associated with the Laplace operator in simply and doubly connected, convex and concave domains, with smooth or piecewise smooth boundaries.

2 Mathematical formulation

Consider an open bounded domain $\Omega \subset \mathbb{R}^d$, where *d* is the dimension of the space where the problem is posed, usually $d \in \{1, 2, 3\}$, occupied by an isotropic medium and assume that Ω is bounded by a piecewise smooth curve $\partial\Omega$, such that $\partial\Omega =$ $\Gamma_1 \cup \Gamma_2$, where $\Gamma_1 \neq \emptyset$, $\Gamma_2 \neq \emptyset$ and $\Gamma_1 \cap \Gamma_2 = \emptyset$. In this paper, we refer to steady heat conduction applications in isotropic homogeneous media in the absence of heat sources. Hence the function $u(\mathbf{x})$ denotes the temperature at a point $\mathbf{x} \in \Omega$ and satisfies the equation

$$\nabla^2 \mathbf{u}(\mathbf{x}) \equiv \sum_{i=1}^d \partial_i \partial_i \mathbf{u}(\mathbf{x}) = 0, \quad \mathbf{x} = (\mathbf{x}_1, \dots, \mathbf{x}_d) \in \Omega, \tag{1}$$

where $\partial_i \equiv \partial/\partial x_i$. We now let $\mathbf{n}(\mathbf{x})$ be the unit outward normal vector at $\partial \Omega$ and $q(\mathbf{x})$ be the normal heat flux at a point $\mathbf{x} \in \partial \Omega$ defined by

$$\mathbf{q}(\mathbf{x}) \equiv -\nabla \mathbf{u}(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) = -\sum_{i=1}^{d} \partial_i \mathbf{u}(\mathbf{x}) \, \mathbf{n}_i(\mathbf{x}), \quad \mathbf{x} \in \partial \Omega.$$
(2)

In the direct problem formulation, the knowledge of the location, shape and size of the entire boundary $\partial \Omega$, the temperature and/or normal heat flux on the entire

boundary $\partial \Omega$ gives the corresponding Dirichlet, Neumann, or mixed boundary conditions which enable us to determine the unknown boundary conditions, as well as the temperature distribution in the solution domain. A different and more interesting situation occurs when both the temperature and normal heat flux are prescribed on a part of the boundary, say Γ_1 , whilst no boundary conditions are supplied on the remaining part of the boundary $\Gamma_2 = \partial \Omega \setminus \Gamma_1$. More precisely, we consider the following *Cauchy problem* for steady heat conduction in an isotropic homogeneous medium:

$$\nabla^2 \mathbf{u}(\mathbf{x}) = \mathbf{0}, \quad \mathbf{x} \in \Omega, \tag{3a}$$

$$\mathbf{u}(\mathbf{x}) = \widetilde{\mathbf{u}}(\mathbf{x}), \quad \mathbf{x} \in \Gamma_1,$$
(3b)

$$\mathbf{q}(\mathbf{x}) = \widetilde{\mathbf{q}}(\mathbf{x}), \quad \mathbf{x} \in \Gamma_1, \tag{3c}$$

where \widetilde{u} and \widetilde{q} are prescribed Dirichlet and Neumann boundary conditions, respectively.

A necessary condition for the Cauchy problem given by Eqs. (3a) - (3c) to be identifiable is that meas $(\Gamma_1) \ge \text{meas}(\Gamma_2)$. This inverse problem is much more difficult to solve both analytically and numerically than the direct problem, since the solution does not satisfy the general conditions of well-posedness. Although the problem may have a unique solution, it is well known that this solution is unstable with respect to small perturbations into the data on Γ_1 , see e.g. Hadamard (1923). Thus the problem is ill-posed and we cannot use a direct approach, such as the least-squares method, in order to solve the system of linear equations which arises from the discretization of the partial differential equations (3*a*) and the boundary conditions (3*b*) and (3*c*). Therefore, regularization methods are required in order to solve accurately the inverse problem (3*a*) – (3*c*) for the Laplace equation.

3 Description of the algorithm

Kozlov, Maz'ya and Fomin (1991) proposed the following iterative algorithm for the simultaneous reconstruction of the unknown temperature $u|_{\Gamma_2}$ and normal heat flux $q|_{\Gamma_2}$ on the under-specified boundary:

Step 1. (i) If k = 1 then specify an initial boundary temperature guess on Γ_2 , namely $u^{(2k-1)} \in H^{1/2}(\Gamma_2)$.

(ii) If k > 1 then solve the following mixed, well-posed, direct problem:

$$\nabla^2 \mathbf{u}^{(2k-1)}(\mathbf{x}) = 0, \quad \mathbf{x} \in \Omega, \tag{4a}$$

$$\mathbf{u}^{(2k-1)}(\mathbf{x}) = \widetilde{\mathbf{u}}(\mathbf{x}), \quad \mathbf{x} \in \Gamma_1, \tag{4b}$$

$$q^{(2k-1)}(\mathbf{x}) = q^{(2k-2)}(\mathbf{x}), \quad \mathbf{x} \in \Gamma_2,$$
 (4c)

to determine $u^{(2k-1)}(\mathbf{x})$ for $\mathbf{x} \in \Omega$ and $u^{(2k-1)}(\mathbf{x})$ for $\mathbf{x} \in \Gamma_2$.

Step 2. Having constructed the approximation $u^{(2k-1)}$, $k \ge 1$, the following mixed, well-posed, direct problem:

$$\nabla^2 \mathbf{u}^{(2k)}(\mathbf{x}) = \mathbf{0}, \quad \mathbf{x} \in \Omega, \tag{5a}$$

$$q^{(2k)}(\mathbf{x}) = \widetilde{q}(\mathbf{x}), \quad \mathbf{x} \in \Gamma_1,$$
(5b)

$$\mathbf{u}^{(2k)}(\mathbf{x}) = \mathbf{u}^{(2k-1)}(\mathbf{x}), \quad \mathbf{x} \in \Gamma_2,$$
 (5c)

is solved in order to determine $u^{(2k)}(\mathbf{x})$ for $\mathbf{x} \in \Omega$ and $q^{(2k)}(\mathbf{x}) \equiv \nabla u^{(2k)}(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x})$ for $\mathbf{x} \in \Gamma_2$.

Step 3. Repeat steps 1 and 2 until a prescribed stopping criterion is satisfied.

Let $H^1(\Omega)$ be the Sobolev space and $H^{1/2}(\partial\Omega)$ be the space of traces on $\partial\Omega$ corresponding to $H^1(\Omega)$, see e.g. Lions and Magenes (1972). We denote by $H^{1/2}(\Gamma_i)$ the space of functions from $H^{1/2}(\partial\Omega)$ that are bounded on Γ_i and by $(H^{1/2}(\Gamma_i))^*$ the dual space of $H^{1/2}(\Gamma_i)$, for i = 1, 2. Kozlov, Maz'ya and Fomin (1991) showed that if $\partial\Omega$ is smooth, $\widetilde{u} \in H^{1/2}(\Gamma_1)$ and $\widetilde{q} \in (H^{1/2}(\Gamma_1))^*$, then the alternating iterative algorithm based on steps 1-3 produces two sequences of approximate solutions $\{u^{(2k-1)}\}_{k\geq 1}$ and $\{u^{(2k)}\}_{k\geq 1}$ which both converge in $H^1(\Omega)$ to the solution u of the Cauchy problem (3a) - (3c) for any initial guess $u^{(1)} \in H^{1/2}(\Gamma_2)$, provided that a solution to this Cauchy problem exists. Furthermore, the alternating iterative algorithm has a regularizing character. Also, the same conclusion holds if at the step 1 one specifies an initial guess for the unknown normal heat flux on Γ_2 , i.e. $q^{(1)} \in (H^{1/2}(\Gamma_2))^*$, instead of an initial guess for the temperature, $u^{(1)} \in H^{1/2}(\Gamma_2)$, and we modify steps 1 and 2 accordingly.

It should be mentioned that, in general, this iterative method does not converge if in the steps 1 and 2 of the algorithm the mixed problems are replaced by Dirichlet or Neumann problems. In addition, the Neumann direct problem associated with the Laplace equation is ill-posed owing to the non-uniqueness or non-existence of solution with respect to whether the integral of the normal heat flux q over the boundary $\partial \Omega$ vanishes or not, respectively.

At this stage, it should be noted that the well-posed, mixed, direct problems (4a) - (4c) and (5a) - (5c) are boundary value problems and these are solved numerically using a meshless method, namely the MFS. In this case, neither a boundary nor a domain discretization is required, as one would employ if using either the BEM, or the FEM or a finite-difference method (FDM), respectively. Moreover, the MFS determines simultaneously the boundary temperature and the normal heat

flux, without the need of integrating or further finite differencing. Also, this meshless method determines explicitly the temperature solution inside the solution domain, without the need of performing numerical or exact integration as required by the BEM, or domain discretization or interpolation onto grid cells as required by the FDM or FEM.

4 Method of fundamental solutions

4.1 MFS approximation

The fundamental solution G of the heat balance equation (1) or (3a) for twodimensional steady heat conduction in isotropic homogeneous media, i.e. the Laplace equation, is given by, see e.g. Fairweather and Karageorghis (1998)

$$G(\mathbf{x},\boldsymbol{\xi}) = \frac{1}{2\pi} \log \frac{1}{\|\mathbf{x} - \boldsymbol{\xi}\|}, \quad \mathbf{x} \in \overline{\Omega}, \quad \boldsymbol{\xi} \in \mathbb{R}^2 \setminus \overline{\Omega}, \tag{6}$$

where ξ is a singularity or source point. The main idea of the MFS consists of approximating the temperature in the solution domain by a linear combination of fundamental solutions with respect to *M* singularities $\xi^{(j)}$, j = 1, ..., M, in the form

$$\mathbf{u}(\mathbf{x}) \approx \mathbf{u}_M(\mathbf{c}, \boldsymbol{\xi}; \mathbf{x}) = \sum_{j=1}^M \mathbf{c}_j \, G(\mathbf{x}, \boldsymbol{\xi}^{(j)}), \quad \mathbf{x} \in \overline{\Omega},$$
(7)

where $\mathbf{c} = [\mathbf{c}_1, \dots, \mathbf{c}_M]^\mathsf{T}$ and $\boldsymbol{\xi} \in \mathbb{R}^{2M}$ is a vector containing the coordinates of the singularities $\boldsymbol{\xi}^{(j)}$, $j = 1, \dots, M$. On taking into account the definitions of the normal heat flux (2) and the fundamental solution for the two-dimensional Laplace equation (6) then the normal heat flux, through a curve defined by the outward unit normal vector $\mathbf{n}(\mathbf{x})$, can be approximated on the boundary $\partial \Omega$ by

$$\mathbf{q}(\mathbf{x}) \approx \mathbf{q}_M(\mathbf{c}, \boldsymbol{\xi}; \mathbf{x}) = \sum_{j=1}^M \mathbf{c}_j H(\mathbf{x}, \boldsymbol{\xi}^{(j)}), \quad \mathbf{x} \in \partial \Omega,$$
(8)

where

$$H(\mathbf{x},\boldsymbol{\xi}) = -\nabla_{\mathbf{x}} G(\mathbf{x},\boldsymbol{\xi}) \cdot \mathbf{n}(\mathbf{x}) = \frac{1}{2\pi} \frac{(\mathbf{x}-\boldsymbol{\xi}) \cdot \mathbf{n}(\mathbf{x})}{\|\mathbf{x}-\boldsymbol{\xi}\|^2}, \quad \mathbf{x} \in \partial\Omega, \quad \boldsymbol{\xi} \in \mathbb{R}^2 \setminus \overline{\Omega}.$$
(9)

Next, we select the N_1 MFS collocation points $\{\mathbf{x}^{(i)}\}_{i=1}^{N_1}$ on the boundary Γ_1 and the N_2 MFS collocation points $\{\mathbf{x}^{(i)}\}_{i=N_1+1}^{N_1+N_2}$ on the boundary Γ_2 , such that the total number of MFS collocation points used to discretize the boundary $\partial \Omega$ of the solution domain Ω is given by $N = N_1 + N_2$.

According to the MFS approximations (7) and (8), the discretized versions of the the boundary value problems (4a) - (4c) and (5a) - (5c) recast as

$$\mathbf{A}^{(1)} \mathbf{c}^{(2k-1)} = \mathbf{b}^{(2k-1)}, \quad k > 1,$$
(10)

and

$$\mathbf{A}^{(2)} \mathbf{c}^{(2k)} = \mathbf{b}^{(2k)}, \quad k \ge 1,$$
(11)

respectively. Here the components of the MFS matrices and right-hand side vectors corresponding to Eqs. (10) and (11) are given by

$$\mathbf{A}_{ij}^{(1)} = \begin{cases} G(\mathbf{x}^{(i)}, \boldsymbol{\xi}^{(j)}), & i = 1, \dots, N_1, & j = 1, \dots, M, \\ H(\mathbf{x}^{(i)}, \boldsymbol{\xi}^{(j)}), & i = N_1 + 1, \dots, N_1 + N_2, & j = 1, \dots, M, \end{cases}$$
(12a)

$$\mathbf{b}_{i}^{(2k-1)} = \begin{cases} \widetilde{\mathbf{u}}(\mathbf{x}^{(i)}), & i = 1, \dots, N_{1}, \\ \mathbf{q}^{(2k-2)}(\mathbf{x}^{(i)}), & i = N_{1} + 1, \dots, N_{1} + N_{2}, \end{cases}$$
(12b)

and

$$\mathbf{A}_{ij}^{(2)} = \begin{cases} H(\mathbf{x}^{(i)}, \boldsymbol{\xi}^{(j)}), & i = 1, \dots, N_1, \\ G(\mathbf{x}^{(i)}, \boldsymbol{\xi}^{(j)}), & i = N_1 + 1, \dots, N_1 + N_2, \\ j = 1, \dots, M, \end{cases}$$
(13a)

$$\mathbf{b}_{i}^{(2k)} = \begin{cases} \widetilde{\mathbf{q}}(\mathbf{x}^{(i)}), & i = 1, \dots, N_{1}, \\ \mathbf{u}^{(2k-1)}(\mathbf{x}^{(i)}), & i = N_{1} + 1, \dots, N_{1} + N_{2}, \end{cases}$$
(13b)

respectively.

Each of Eqs. (10) and (11) represents a system of *N* linear algebraic equations with *M* unknowns, namely the MFS coefficients $\mathbf{c}^{(2k-1)} = \left[\mathbf{c}_1^{(2k-1)}, \dots, \mathbf{c}_M^{(2k-1)}\right]^{\mathsf{T}}$ and $\mathbf{c}^{(2k)} = \left[\mathbf{c}_1^{(2k)}, \dots, \mathbf{c}_M^{(2k)}\right]^{\mathsf{T}}$, respectively. It should be noted that in order to uniquely determine the solutions $\mathbf{c}^{(2k-1)} \in \mathbb{R}^M$ and $\mathbf{c}^{(2k)} \in \mathbb{R}^M$ to the systems of linear algebraic equations (10) and (11), respectively, the number *N* of MFS boundary collocation points on the boundary $\partial \Omega$ and the number *M* of singularities must satisfy the inequality $M \leq N$. However, the systems of linear algebraic equations (10) and (11) cannot be solved by direct methods, such as the least-squares method, since such an approach would produce a highly unstable solution in the case of noisy Cauchy data on Γ_1 .

4.2 MFS boundary collocation points and singularities

In order to implement the MFS, the location of the singularities has to be determined and this is usually achieved by considering either the static or the dynamic approach. In the static approach, the singularities are pre-assigned and kept fixed throughout the solution process, whilst in the dynamic approach, the singularities and the unknown coefficients are determined simultaneously during the solution process, see Fairweather and Karageorghis (1998). Thus the dynamic approach transforms the inverse problem into a more difficult nonlinear ill-posed problem which is also computationally much more expensive. The advantages and disadvantages of the MFS with respect to the location of the fictitious sources are described at length in Heise (1978) and Burgess and Maharejin (1984).

Recently, Gorzelańczyk and Kołodziej (2008) thoroughly investigated the performance of the MFS with respect to the shape of the pseudo-boundary on which the source points are situated, proving that, for the same number of boundary collocation points and sources, more accurate results are obtained if the shape of the pseudo-boundary is similar to that of the boundary of the solution domain. Therefore, we have decided to employ the static approach in our computations, at the same time accounting for the findings of Gorzelańczyk and Kołodziej (2008).

5 Regularization

It is well-known that the MFS discretisation matrices $A^{(i)}$, i = 1, 2, are severely ill-conditioned. The accurate and stable solutions of Eqs. (10) and (11) are very important for obtaining physically meaningful numerical results. It is the purpose of this section to present a classical regularization procedure for obtaining stable solutions to the systems of linear algebraic equations (10) and (11), as well as details regarding the optimal choice of the regularization parameter.

5.1 Tikhonov regularization method

Several regularization techniques used for the stable solution of systems of linear and nonlinear algebraic equations are available in the literature, such as the singular value decomposition [Hansen (1998)], the Tikhonov regularization method [Tikhonov and Arsenin (1986)] and various iterative methods [Kunisch and Zou (1998)]. Recently, Liu (2008a) proposed a new and robust numerical technique for the stable solution of ill-posed systems of linear algebraic equations, namely the Fictitious Time Integration Method (FTIM). This method consists of introducing a fictitious time variable that plays the role of a regularization parameter, while its filtering effect is better than that of the Tikhonov and exponential filters. The FTIM was successfully applied to solving inverse vibration problems [Liu (2008b); Liu (2008c); Liu, Chang, Chang and Chen (2008)], nonlinear complementarity problems [Liu (2008d)], large systems of nonlinear algebraic equations [Liu and Atluri (2008a)], boundary value problems for elliptic partial differential equations [Liu (2008e)] and inverse Sturm-Liouville problems [Liu and Atluri (2008b)]. Liu and Atluri (2009) have recently shown that, when applied to solving an ill-posed system of linear equations, the general FTIM may be viewed a special case of the Tiknonov regularization method.

Consider the following system of linear algebraic equations

$$\mathbf{A}\,\mathbf{c}=\mathbf{b},\tag{14}$$

where $N \ge M$, $\mathbf{A} \in \mathbb{R}^{N \times M}$, $\mathbf{c} \in \mathbb{R}^M$ and $\mathbf{b} \in \mathbb{R}^N$. Note that Eq. (14) may describe each of the MFS systems of linear equations (10) and (11), provided that

$$\mathbf{A} = \mathbf{A}^{(1)}, \quad \mathbf{c} = \mathbf{c}^{(2k-1)}, \quad \mathbf{b} = \mathbf{b}^{(2k-1)}, \quad k > 1,$$
 (15)

and

$$\mathbf{A} = \mathbf{A}^{(2)}, \qquad \mathbf{c} = \mathbf{c}^{(2k)}, \qquad \mathbf{b} = \mathbf{b}^{(2k)}, \qquad k \ge 1,$$
(16)

respectively. The Tikhonov zeroth-order regularized solution to the generically written system of linear algebraic equations (14) is sought as, see Tikhonov and Arsenin (1986)

$$\mathbf{c}_{\lambda}: \quad \mathscr{F}_{\lambda}\left(\mathbf{c}_{\lambda}\right) = \min_{\mathbf{c} \in \mathbb{R}^{M}} \mathscr{F}_{\lambda}\left(\mathbf{c}\right), \tag{17}$$

where \mathscr{F}_{λ} represents the Tikhonov zeroth-order regularization functional given by, see Tikhonov and Arsenin (1986)

$$\mathscr{F}_{\lambda}(\cdot) : \mathbb{R}^{M} \longrightarrow [0,\infty), \quad \mathscr{F}_{\lambda}(\mathbf{c}) = \left\| \mathbf{A} \, \mathbf{c} - \mathbf{b} \right\|^{2} + \lambda^{2} \left\| \mathbf{c} \right\|^{2},$$
(18)

and $\lambda > 0$ is the regularization parameter to be prescribed. Formally, the Tikhonov regularized solution c_{λ} of the problem (14) is given as the solution of the normal equation

$$\left(\mathbf{A}^{\mathsf{T}}\mathbf{A} + \lambda^{2}\mathbf{I}_{M}\right)\mathbf{c} = \mathbf{A}^{\mathsf{T}}\mathbf{b},\tag{19}$$

where $\mathbf{I}_M \in \mathbb{R}^{M \times M}$ is the identity matrix. If the Cauchy data on the over-specified boundary Γ_1 are noisy and hence the right-hand side of Eq. (14) is corrupted by noise, i.e.

$$\left\|\mathbf{b}^{\epsilon} - \mathbf{b}\right\| \le \epsilon,\tag{20}$$

then the following stability estimate holds, see Engl, Hanke and Neubauer (2000),

$$\|\mathbf{c}_{\lambda}^{\epsilon} - \mathbf{c}_{\lambda}\| \leq \frac{\epsilon}{\lambda},\tag{21}$$

where

$$\mathbf{c}_{\lambda} = \mathbf{A}^{\dagger} \mathbf{b}, \quad \mathbf{A}^{\dagger} \equiv \left(\mathbf{A}^{\mathsf{T}} \mathbf{A} + \lambda^{2} \mathbf{I}_{M}\right)^{-1} \mathbf{A}^{\mathsf{T}}.$$
 (22)

To summarize, the Tikhonov regularization method solves a constrained minimization problem using a smoothness norm in order to provide a stable solution which fits the data and also has a minimum structure.

5.2 Selection of the optimal regularization parameter

The performance of regularization methods depends crucially on the suitable choice of the regularization parameter. One extensively studied criterion is the discrepancy principle, see e.g. Morozov (1966). Although this criterion is mathematically rigorous, it requires a reliable estimation of the amount of noise added into the data which may not be available in practical problems. Heuristical approaches are preferable in the case when no *a priori* information about the noise is available. For the Tikhonov zeroth-order regularization method, several heuristical approaches have been proposed, including the L-curve criterion, see Hansen (1998), and the generalized cross-validation (GCV), see Wahba (1977). In this paper, we employ the GCV criterion to determine the optimal regularization parameter, λ_{opt} , for the Tikhonov zeroth-order regularization method, namely

$$\lambda_{\text{opt}}: \quad \mathscr{G}\left(\lambda_{\text{opt}}\right) = \min_{\lambda > 0} \mathscr{G}\left(\lambda\right). \tag{23}$$

Here

$$\mathscr{G}(\cdot):(0,\infty)\longrightarrow[0,\infty),\quad \mathscr{G}(\lambda)=\frac{\left\|\mathbf{A}\mathbf{c}_{\lambda}-\mathbf{b}^{\varepsilon}\right\|^{2}}{\left[\operatorname{trace}\left(\mathbf{I}_{N}-\mathbf{A}\mathbf{A}^{\dagger}\right)\right]^{2}},$$
(24)

where \mathbf{c}_{λ} is given by Eq. (21) with $\mathbf{b} = \mathbf{b}^{\epsilon}$.

6 Numerical results and discussion

In this section, we present the performance of the proposed numerical method, namely the alternating iterative MFS described in Sections 3 and 4. To do so, we solve numerically the Cauchy geometric problem given by Eqs. (3a) - (3c) for the two-dimensional Laplace equation in the geometries described below.

6.1 Examples

Example 1. (Simply connected convex domain with a piecewise smooth boundary) We consider the following analytical solutions for the temperature and the normal heat flux

$$\mathbf{u}^{(\mathrm{an})}(\mathbf{x}) = \cos(\mathbf{x}_1)\cosh(\mathbf{x}_2) + \sin(\mathbf{x}_1)\sinh(\mathbf{x}_2), \quad \mathbf{x} = (\mathbf{x}_1, \mathbf{x}_2) \in \overline{\Omega},$$
(25a)

and

$$\begin{aligned} q^{(an)}(\mathbf{x}) &= \left[-\sin(x_1)\cosh(x_2) + \cos(x_1)\sinh(x_2)\right]n_1(\mathbf{x}) \\ &+ \left[\cos(x_1)\sinh(x_2) + \sin(x_1)\cosh(x_2)\right]n_2(\mathbf{x}), \quad \mathbf{x} = (x_1, x_2) \in \partial\Omega, \end{aligned} \tag{25b}$$

respectively, in the rectangle $\Omega = (-r,r) \times (-r/2,r/2)$, where r = 1.0. Here $\Gamma_1 = \{r\} \times (-r/2,r/2) \cup [-r,r] \times \{\pm r/2\}$ and $\Gamma_2 = \{-r\} \times (-r/2,r/2)$.

Example 2. (Simply connected convex domain with a smooth boundary) We consider the following analytical solution for the temperature

$$\mathbf{u}^{(an)}(\mathbf{x}) = \mathbf{x}_1^2 - \mathbf{x}_2^2, \quad \mathbf{x} = (\mathbf{x}_1, \mathbf{x}_2) \in \overline{\Omega},$$
 (26a)

and the corresponding analytical normal heat flux

$$q^{(an)}(\mathbf{x}) = 2 [x_1 n_1(\mathbf{x}) - x_2 n_2(\mathbf{x})], \quad \mathbf{x} = (x_1, x_2) \in \partial\Omega,$$
(26b)

in the unit disk $\Omega = \{ \mathbf{x} = (x_1, x_2) | \rho(\mathbf{x}) < r \}$, where $\rho(\mathbf{x}) = \sqrt{x_1^2 + x_2^2}$ is the radial polar coordinate of \mathbf{x} and r = 1.0. Here $\Gamma_1 = \{ \mathbf{x} \in \partial \Omega | 0 \le \theta(\mathbf{x}) \le 3\pi/2 \}$ and $\Gamma_2 = \{ \mathbf{x} \in \partial \Omega | 3\pi/2 < \theta(\mathbf{x}) < 2\pi \}$, where $\theta(\mathbf{x})$ is the angular polar coordinate of \mathbf{x} .

Example 3. (Doubly connected concave domain with a smooth boundary) We consider the following analytical solutions for the temperature and the normal heat flux

$$\mathbf{u}^{(\mathrm{an})}(\mathbf{x}) = \mathbf{x}_1 \, \mathbf{x}_2, \quad \mathbf{x} = (\mathbf{x}_1, \mathbf{x}_2) \in \overline{\Omega}, \tag{27a}$$

and

$$q^{(an)}(\mathbf{x}) = x_2 n_1(\mathbf{x}) + x_1 n_2(\mathbf{x}), \quad \mathbf{x} = (x_1, x_2) \in \partial\Omega,$$
(27b)

respectively, in the annular domain $\Omega = \{\mathbf{x} = (x_1, x_2) | r_{int} < \rho(\mathbf{x}) < r_{out}\}$, where $r_{int} = 2.0$ and $r_{out} = 3.0$. Here $\Gamma_1 = \{\mathbf{x} \in \partial \Omega | \rho(\mathbf{x}) = r_{out}\}$ and $\Gamma_2 = \{\mathbf{x} \in \partial \Omega | \rho(\mathbf{x}) = r_{int}\}$.

Example 4. (Simply connected concave domain with a smooth boundary) We consider the analytical solutions for the temperature and normal heat flux given by Eqs. (26a) and (26b), respectively, in the epitrochoid, see e.g. Liu (2008f),

$$\Omega = \left\{ \mathbf{x} = (x_1, x_2) \ \left| \ 0 \le \rho(\mathbf{x}) < \sqrt{(a+b)^2 - 2h(a+b)\cos\left(a\theta/b\right) + h^2}, \ \theta \in [0, 2\pi) \right. \right\},$$

where a = 4.0 and b = h = 1.0. Here $\Gamma_1 = \left\{ \mathbf{x} \in \partial \Omega \, \middle| \, 0 \le \theta(\mathbf{x}) \le 3\pi/2 \right\}$ and $\Gamma_2 = \left\{ \mathbf{x} \in \partial \Omega \, \middle| \, 3\pi/2 < \theta(\mathbf{x}) < 2\pi \right\}$.

The inverse problems investigated in this paper have been solved using the uniform distribution of both the MFS boundary collocation points $\mathbf{x}^{(i)}$, i = 1, ..., N, and the singularities $\boldsymbol{\xi}^{(j)}$, j = 1, ..., M. Furthermore, the numbers of MFS boundary collocation points N_1 and N_2 corresponding to the over- and under-specified boundaries Γ_1 and Γ_2 , respectively, as well as the distance d_S between the physical boundary $\partial \Omega$ and the pseudo-boundary $\partial \Omega_S$ on which the singularities are situated, were set to:

- (i) $N_1 = 97$, $N_2 = 19$ and $d_S = 2.0$ in the case of Example 1;
- (ii) $N_1 = 60$, $N_2 = 20$ and $d_S = 3.0$ for Example 2;
- (iii) $N_1 = 60$, $N_2 = 40$, and $d_S = 1.0$ and $d_S = 3.0$ for the inner and outer boundaries, respectively, in the case of Example 3;
- (iv) $N_1 = N_2 = 40$ and $d_S = 4.0$ for Example 4.

In addition, for Examples 1-3 the number of singularities was taken to be equal to that of the MFS boundary collocation points, i.e. $M = N = N_1 + N_2$, while for Example 4 the number of singularities was taken to be M = N/2 = 40.

6.2 Initial guess

An arbitrary real valued function $u^{(1)} \in H^{1/2}(\Gamma_2)$ may be specified as an initial guess for the unknown temperature on the under-specified boundary Γ_2 . In order to improve the rate of convergence of the iterative algorithm, one may choose a real valued function which ensures the continuity of the boundary temperature at the common endpoints of the over- and under-specified boundaries Γ_1 and Γ_2 , respectively, and which is also linear with respect to either the Cartesian x_2 -coordinate in the case of Example 1, or the angular polar coordinate θ for Examples 2 and 4, see e.g. Lesnic, Elliott and Ingham (1997), Mera, Elliott, Ingham and Lesnic (2000), Marin, Elliott, Ingham and Lesnic (2001), Marin, Elliott, Heggs, Ingham,

Lesnic and Wen (2003). More precisely, for Example 1 and Examples 2 and 4 the following initial guesses for the unknown temperature on Γ_2 may be chosen:

$$\mathbf{u}^{(1)}(\mathbf{x}) = \frac{\mathbf{x}_2^{(2)} - \mathbf{x}_2}{\mathbf{x}_2^{(2)} - \mathbf{x}_2^{(1)}} \mathbf{u}^{(an)}(\mathbf{x}^{(1)}) + \frac{\mathbf{x}_2 - \mathbf{x}_2^{(1)}}{\mathbf{x}_2^{(2)} - \mathbf{x}_2^{(1)}} \mathbf{u}^{(an)}(\mathbf{x}^{(2)}), \quad \mathbf{x} \in \Gamma_2,$$
(28a)

and

$$\begin{aligned} \mathbf{u}^{(1)}(\mathbf{x}) &= \frac{\theta(\mathbf{x}^{(2)}) - \theta(\mathbf{x})}{\theta(\mathbf{x}^{(2)}) - \theta(\mathbf{x}^{(1)})} \mathbf{u}^{(an)}(\mathbf{x}^{(1)}) + \frac{\theta(\mathbf{x}) - \theta(\mathbf{x}^{(1)})}{\theta(\mathbf{x}^{(2)}) - \theta(\mathbf{x}^{(1)})} \mathbf{u}^{(an)}(\mathbf{x}^{(2)}), \\ \mathbf{x} \in \Gamma_2, \end{aligned}$$
(28b)

respectively, where $\mathbf{x}^{(1)}$ and $\mathbf{x}^{(2)}$ are the common endpoints of the over- and underspecified boundaries, i.e. $\overline{\Gamma}_1 \cap \overline{\Gamma}_2 = \{\mathbf{x}^{(1)}, \mathbf{x}^{(2)}\}.$

However, in the general situation when the over- and under-specified boundaries have no common points, as is the case of Example 3, one cannot use the procedure described above. Therefore, in this case, the initial guess for the unknown temperature on the under-specified boundary Γ_2 is chosen as

$$\mathbf{u}^{(1)}(\mathbf{x}) = 0, \quad \mathbf{x} \in \Gamma_2.$$

In this study, we have decided to use the initial guess (29). In this way, the most general situations regarding the geometry of the solution domain are accounted for and the robustness of the alternating iterative algorithm with respect to the initial guess for the unknown temperature on Γ_2 is also tested.

6.3 Convergence of the algorithm

If N_i MFS collocation points, $\{\mathbf{x}^{(\ell)}\}_{\ell=1}^{N_i}$, are considered on the boundary $\Gamma_i \subset \partial \Omega$ then the *root mean square error* (RMS error) associated with the real valued function $f(\cdot) : \Gamma_i \longrightarrow \mathbb{R}$ on Γ_i is defined by

$$\operatorname{RMS}_{\Gamma_{i}}(f) = \sqrt{\frac{1}{N_{i}} \sum_{\ell=1}^{N_{i}} f(\mathbf{x}^{(\ell)})^{2}},$$
(30)

In order to investigate the convergence of the algorithm, at every iteration, $k \ge 1$, we evaluate the following accuracy errors corresponding to the temperature and normal heat flux on the under-specified boundary, Γ_2 , which are defined as *relative RMS errors*, i.e.

$$\mathbf{e}_{\mathbf{u}}(k) = \frac{\mathbf{RMS}_{\Gamma_{2}}(\mathbf{u}^{(2k-1)} - \mathbf{u}^{(an)})}{\mathbf{RMS}_{\Gamma_{2}}(\mathbf{u}^{(an)})} = \frac{\|\mathbf{u}^{(2k-1)}\|_{\Gamma_{2}} - \mathbf{u}^{(an)}\|_{\Gamma_{2}}\|_{2}}{\|\mathbf{u}^{(an)}\|_{\Gamma_{2}}\|_{2}}, \quad k \ge 1,$$
(31a)

and

$$\mathbf{e}_{\mathbf{q}}(k) = \frac{\mathbf{RMS}_{\Gamma_{2}}(\mathbf{q}^{(2k)} - \mathbf{q}^{(an)})}{\mathbf{RMS}_{\Gamma_{2}}(\mathbf{q}^{(an)})} = \frac{\|\mathbf{q}^{(2k)}\|_{\Gamma_{2}} - \mathbf{q}^{(an)}\|_{\Gamma_{2}}\|_{2}}{\|\mathbf{q}^{(an)}\|_{\Gamma_{2}}\|_{2}}, \quad k \ge 1,$$
(31b)



Figure 1: The accuracy errors, e_u and e_q , as functions of the number of iterations, k, obtained using exact Cauchy data on Γ_1 and various numbers of MFS boundary collocation points, namely $N \in \{56, 116, 176\}$, for Example 1.

where $u^{(2k-1)}$ and $q^{(2k)}$ are the temperature and normal heat flux on the boundary Γ_2 retrieved after k iterations by solving the well-posed, mixed, direct, boundary value problems (4a) - (4c) and (5a) - (5c), respectively. The error in predicting the temperature inside the solution domain, Ω , may also be evaluated, but it has an evolution similar to that of the errors e_u and e_q given by Eqs. (31a) and (31b), respectively, and hence this is not pursued herein.

Fig. 1 shows the accuracy errors e_u and e_q as functions of the number of iterations, k, obtained using exact Cauchy data on the over-specified boundary, Γ_1 , and various numbers of MFS collocation points, i.e. $N \in \{56, 116, 176\}$, for the inverse problem given by Example 1. It can be seen from this figure that both errors e_u and e_q decrease even after a large numbers of iterations, e.g. k = 300, and as expected $e_u < e_q$ for all MFS discretizations employed, i.e. normal heat fluxes are





Figure 2: The analytical and numerical (a) temperatures u, and (b) normal heat fluxes q, on the under-specified boundary Γ_2 , obtained using exact Cauchy data on Γ_1 , k = 300 iterations and various numbers of MFS boundary collocation points, namely $N \in \{56, 116, 176\}$, for Example 1.

more inaccurate than temperatures. Furthermore, as N increases, the errors e_u and e_q decrease showing that in the case of Example 1, $N \ge 116$ ensures a sufficient discretisation for the accuracy to be achieved.

The numerical solutions for the temperature $u|_{\Gamma_2}$ and the normal heat flux $q|_{\Gamma_2}$ obtained after k = 300 iterations for the Cauchy problem given by Example 1 are presented in Figs. 2(a) and 2(b), respectively. From these figures, it can be seen that the accuracy in predicting both the temperature distribution and normal heat flux on the boundary Γ_2 is very good. As expected, the errors in predicting the normal heat flux $q|_{\Gamma_2}$ are larger than the errors in predicting the temperature $u|_{\Gamma_2}$ since the normal heat flux contains higher-order derivatives of the latter. Similar results have also been obtained for the other examples investigated in this study, as well as for the Cauchy problem with perturbed Neumann data on the over-specified boundary Γ_1 , and therefore these are not presented herein.

From Figs. 1 and 2, it can be concluded that the MFS-based alternating iterative algorithm described in Sections 3 and 4 produces an accurate and convergent numerical solution for both the missing boundary temperature and normal heat flux with respect to increasing the number of iterations, k, and the number of MFS boundary collocation points, N, provided that exact input Cauchy data are used. However, exact data are seldom available in practice since measurement errors always include noise in the prescribed boundary conditions and this is investigated next.

6.4 Stopping criterion

Once the convergence with respect to increasing N of the numerical solution to the exact solution has been established, we fix N = M = 116 and investigate the stability of the numerical solution for Example 1. In what follows, the temperature, $u|_{\Gamma_1} = u^{(an)}|_{\Gamma_1}$, and/or the normal heat flux, $q|_{\Gamma_1} = q^{(an)}|_{\Gamma_1}$, on the over-specified boundary have been perturbed as

$$\widetilde{u}^{\epsilon}|_{\Gamma_1} = u|_{\Gamma_1} + \delta u, \quad \delta u = \text{GO5DDF}(0, \sigma_u), \quad \sigma_u = \max_{\Gamma_1} |u| \times (p_u/100),$$
(32)

and

$$\widetilde{q}^{\epsilon}|_{\Gamma_{1}} = q|_{\Gamma_{1}} + \delta q, \quad \delta q = \texttt{GO5DDF}(0, \sigma_{q}), \quad \sigma_{q} = \max_{\Gamma_{1}} |q| \times \left(p_{q}/100\right), \tag{33}$$

respectively. Here δu and δq are Gaussian random variables with mean zero and standard deviations σ_u and σ_q , respectively, generated by the NAG subroutine G05DDF [NAG Library Mark 21 (2007)], while p_u % and p_q % are the percentages





Figure 3: The accuracy errors (a) e_u , and (b) e_q , as function of the number of iterations, *k*, obtained using N = 116 MFS boundary collocation points and various levels of noise added into the Dirichlet data on Γ_1 , namely $p_u \in \{1\%, 3\%, 5\%\}$, for Example 1.

of additive noise included into the input boundary temperature, $u|_{\Gamma_1}$, and normal heat flux, $q|_{\Gamma_1}$, respectively, in order to simulate the inherent measurement errors. Figs. 3(a) and 3(b) present the accuracy errors e_u and e_q , respectively, for various levels of Gaussian random noise $p_u \in \{1\%, 3\%, 5\%\}$ added into the temperature data $u|_{\Gamma_1}$. From these figures it can be seen that as p_u decreases then e_u and e_q decrease. However, the errors in predicting the temperature and the normal heat flux on the under-specified boundary Γ_2 decrease up to a certain iteration number and after that they start increasing. If the iterative process is continued beyond this point then the numerical solutions lose their smoothness and become highly oscillatory and unbounded, i.e. unstable. Therefore, a regularizing stopping criterion must be used in order to terminate the iterative process at the point where the errors in the numerical solutions start increasing.

After each iteration, k, we evaluate the following convergence error which is associated with the temperature on the over-specified boundary, Γ_1 , namely

$$\mathbf{E}_{\mathbf{u}}(k) = \frac{\mathbf{RMS}_{\Gamma_{1}}\left(\mathbf{u}^{(2k)} - \widetilde{\mathbf{u}}^{\epsilon}\right)}{\mathbf{RMS}_{\Gamma_{1}}\left(\widetilde{\mathbf{u}}^{\epsilon}\right)} = \frac{\left\|\mathbf{u}^{(2k)}\right\|_{\Gamma_{1}} - \widetilde{\mathbf{u}}^{\epsilon}\right\|_{\Gamma_{1}}}{\left\|\widetilde{\mathbf{u}}^{\epsilon}\right\|_{\Gamma_{1}}}, \quad k \ge 1,$$
(34)

where $u^{(2k)}$ is the temperature on the boundary Γ_1 retrieved numerically after k iterations by solving the well-posed, mixed, direct, boundary value problem (5a) - (5c). This error E_u should tend to zero as the sequences $\{u^{(2k-1)}\}_{k\geq 1}$ and $\{u^{(2k)}\}_{k\geq 1}$ tend to the analytical solution, $u^{(an)}$, in the space $H^1(\Omega)$ and hence they are expected to provide an appropriate stopping criterion. Indeed, if we investigate the error E_u obtained at every iteration for Example 1 for various levels of Gaussian random noise added into the input temperature data $u|_{\Gamma_1}$, we obtain the curves graphically represented in Fig. 4. By comparing Figs. 3 and 4, it can be noticed that the convergence error E_u , as well as the accuracy errors e_u and e_q , attain their corresponding minimum at around the same number iterations. Therefore, for noisy Cauchy data a natural stopping criterion ceases the MFS alternating iterative algorithm at the optimal number of iterations, k_{opt} , given by:

$$k_{\text{opt}}: \quad \mathbf{E}_{\mathbf{u}}(k_{\text{opt}}) = \min_{k \ge 1} \mathbf{E}_{\mathbf{u}}(k). \tag{35}$$

As mentioned in the previous section, for exact data the iterative process is convergent with respect to increasing the number of iterations, k, since the accuracy errors e_u and e_q keep decreasing even after a large number of iterations, see Fig. 1. It should be noted in this case that a stopping criterion is not necessary since the numerical solution is convergent with respect to increasing the number of iterations. However, even in this case the errors E_u , e_u and e_q have a similar behaviour



Figure 4: The convergence error, E_u , as a function of the number of iterations, k, obtained using N = 116 MFS boundary collocation points and various levels of noise added into the Dirichlet data on Γ_1 , namely $p_u \in \{1\%, 3\%, 5\%\}$, for Example 1.

and the error E_u may be used to stop the iterative process at the point where the rate of convergence is very small and no substantial improvement in the numerical solution is obtained even if the iterative process is continued. Therefore, it can be concluded that the regularizing stopping criterion proposed is very efficient in locating the point where the errors start increasing and the iterative process should be ceased.

6.5 Stability of the algorithm

Based on the stopping criterion described in Section 6.4, the analytical and numerical values for the temperature, u, and normal heat flux, q, on the under-specified boundary Γ_2 , obtained using various levels of noise added into the temperature data on the over-specified boundary Γ_1 for Example 1, are illustrated in Figs. 5(a) and 5(b), respectively. From these figures it can be seen that the numerical solution is a stable approximation for the exact solution, free of unbounded and rapid oscillations. It should also be noted from Figs. 5(a) and 5(b) that the numerical solution converges to the exact solution as the level of noise, p_u , added into the input Dirichlet data decreases.





Figure 5: The analytical and numerical (a) temperatures u, and (b) normal heat fluxes q, on the under-specified boundary Γ_2 , obtained using N = 116 MFS boundary collocation points and various levels of noise added into the Dirichlet data on Γ_1 , namely $p_u \in \{1\%, 3\%, 5\%\}$, for Example 1.





Figure 6: The analytical and numerical (a) temperatures u, and (b) normal heat fluxes q, on the under-specified boundary Γ_2 , obtained using N = 80 MFS boundary collocation points and various levels of noise added into the Dirichlet data on Γ_1 , namely $p_u \in \{1\%, 3\%, 5\%\}$, for Example 2.





Figure 7: The analytical and numerical (a) temperatures u, and (b) normal heat fluxes q, on the under-specified boundary Γ_2 , obtained using N = 100 MFS boundary collocation points and various levels of noise added into the Neumann data on Γ_1 , namely $p_q \in \{1\%, 3\%, 5\%\}$, for Example 2.





Figure 8: The analytical and numerical (a) temperatures u, and (b) normal heat fluxes q, on the under-specified boundary Γ_2 , obtained using N = 100 MFS boundary collocation points and various levels of noise added into the Dirichlet data on $Γ_1$, namely $p_u ∈ \{1\%, 3\%, 5\%\}$, for Example 3.





Figure 9: The analytical and numerical (a) temperatures u, and (b) normal heat fluxes q, on the under-specified boundary Γ_2 , obtained using N = 80 MFS boundary collocation points and various levels of noise added into the Dirichlet data on Γ_1 , namely $p_u \in \{1\%, 3\%, 5\%\}$, for Example 4.

The proposed MFS-alternating iterative algorithm, in conjunction with the stopping criterion (35), works equally well also for the Cauchy problem (3a) - (3c) associated with the Laplace equation in a simply connected convex domain with a smooth boundary, such as the disk investigated in Example 2. Figs. 6(a) and 6(b) show the numerical results for the temperature and normal heat flux on the boundary Γ_2 , obtained using the stopping criterion (35), M = N = 80 and various amounts of noise added into the Dirichlet data, namely $p_u \in \{1\%, 3\%, 5\%\}$, in comparison with their corresponding analytical values, in the case of Example 2.

In the case of Example 2, very good results have also been retrieved for both the unknown temperature, $u|_{\Gamma_2}$, and normal heat flux, $q|_{\Gamma_2}$, when using the stopping criterion (35), M = N = 80 and various levels of noise added into the Neumann data on Γ_1 , namely $p_q \in \{1\%, 3\%, 5\%\}$, and these are presented in Figs. 7(*a*) and 7(*b*), respectively. By comparing Figs. 6 and 7 we can conclude that, as expected, the numerical results obtained using the proposed MFS alternating iterative algorithm, in conjunction with the stopping criterion (35), are more sensitive to perturbations in the normal heat flux on the over-specified boundary than to noisy boundary temperature on Γ_1 .

Similar stable numerical results for both the unknown temperature, $\mathbf{u}|_{\Gamma_2}$, and normal heat flux, $\mathbf{q}|_{\Gamma_2}$, which are at the same time free of unbounded and rapid oscillations, have been obtained for the Cauchy problem (3a) - (3c) corresponding to the Laplace equation in a doubly connected concave domain with a smooth boundary, namely the annular domain considered in Example 3, and these are illustrated in Figs. 8(a) and 8(b), respectively. The same conclusions have been obtained when solving the Cauchy problem (3a) - (3c) corresponding to the Laplace equation in a simply connected concave domain with a smooth boundary, such as the epitrochoid considered in Example 4, and the analytical and numerical results for the unknown temperature, $\mathbf{u}|_{\Gamma_2}$, and normal heat flux, $\mathbf{q}|_{\Gamma_2}$, are displayed in Figs. 9(a) and 9(b), respectively.

From the numerical results presented in this section, it can be concluded that the stopping criterion developed in Section 6.4 has a regularizing effect and the numerical solution obtained by the iterative MFS described in this paper is convergent and stable with respect to increasing the number of MFS boundary collocation points and decreasing the level of noise added into the Cauchy input data, respectively.

7 Conclusions

In this paper, the alternating iterative algorithm of Kozlov, Maz'ya and Fomin (1991) was implemented, for the Cauchy problem associated with the two-dimensional Laplace equation, using a meshless method. The two mixed, well-posed and direct

problems corresponding to every iteration of the numerical procedure were solved using the MFS, in conjunction with the Tikhonov regularization method. For each direct problem considered, the optimal value of the regularization parameter was selected according to the GCV criterion. An efficient regularizing stopping criterion which ceases the iterative procedure at the point where the accumulation of noise becomes dominant and the errors in predicting the exact solutions increase, was also presented. The MFS-based iterative algorithm was tested for Cauchy problems associated with the Laplace operator in simply and doubly connected, convex and concave domains, with smooth or piecewise smooth boundaries.

From the numerical results presented in this study, it can be concluded that the proposed method is consistent, accurate, convergent with respect to increasing the number of MFS boundary collocation points and stable with respect to decreasing the amount of noise added into the Cauchy data. One possible disadvantage of the MFS-based iterative algorithm is related to the optimal choice of the regularization parameter associated with the Tikhonov regularization method which requires, at each step of the alternating iterative algorithm of Kozlov, Maz'ya and Fomin (1991), additional iterations with respect to the regularization parameter. However, this inconvenience can be overcome by introducing relaxation procedures in the MFS iterative algorithm and this is currently being under investigation.

The implementation of the MFS in an iterative manner can be extended to the alternating iterative method of Kozlov, Maz'ya and Fomin (1991) applied to twodimensional Cauchy problems associated with elliptic partial differential operators whose fundamental solutions are available, such as the Navier-Lamé system of linear elasticity, the modified Helmholtz equation and steady-state anisotropic heat conduction, as well as other iterative algorithms and similar three-dimensional inverse problems, but these are deferred as future work.

Acknowledgement: The financial support received from the Romanian Ministry of Education, Research and Innovation through IDEI Programme, Exploratory Research Projects, Grant PN II–ID–PCE–1248/2008, is gratefully acknowledged.

References

Andrieux, S.; Baranger, T.; Ben Abda, A. (2006): Solving Cauchy problems by minimizing an energy-like functional. *Inverse Problems*, vol. 22, pp. 115–133.

Ang, D. D.; Nghia, H.; Tam, N. C. (1998): Regularized solutions of a Cauchy problem for the Laplace equation in an irregular layer: A three-dimensional model. *Acta Mathematica Vietnamica*, vol. 23, pp. 65–74.

Bourgeois, L. (2005): A mixed formulation of quasi-reversibility to solve the Cauchy problem for Laplace's equation. *Inverse Problems*, vol. 21, pp. 1087–1104.

Burgess, G.; Maharejin, E. (1984): A comparison of the boundary element and superposition methods. *Computers & Structures*, vol. 19, pp. 697–705

Chen, C. W.; Young, D. L.; Tsai, C. C.; Murugesan, K. (2005): The method of fundamental solutions for inverse 2D Stokes problems. *Computational Mechanics*, vol. 37, pp. 2–14.

Cheng, J.; Hon, Y. C.; Wei, T.; Yamamoto, M. (2001): Numerical computation of a Cauchy problem for Laplace's equation. *ZAMM - Zeitschrift für Angewandte Mathematik und Mechanik*, vol. 81, pp. 665–674.

Cho, H. A.; Golberg, M. A.; Muleshkov, A. S.; Li, X. (2004): Trefftz methods for time dependent partial differential equations. *CMC: Computers, Materials, and Continua*, vol. 1, pp. 1–37.

Cimetière, A,; Delvare, F.; Jaoua, M.; Pons, F. (2001): Solution of the Cauchy problem using iterated Tikhonov regularization. *Inverse Problems*, vol. 17, pp. 553–570.

Cimetière, A,; Delvare, F.; Jaoua, M.; Pons, F. (2002): An inversion method for harmonic functions reconstruction. *International Journal of Thermal Sciences*, vol. 41, pp. 509–516.

Delvare, F.; Cimetière, A. (2008): A first order method for the Cauchy problem for the Laplace equation using BEM. *Computational Mechanics*, vol. 41, pp. 789–796.

Delvare, F.; Cimetière, A.; Pons, F. (2002): An iterative boundary element method for Cauchy inverse problems. *Computational Mechanics*, vol. 28, pp. 291–302.

Dong, C. F.; Sun, F. Y.; Meng, B. Q. (2007): A method of fundamental solutions for inverse heat conduction problems in an anisotropic medium. *Engineering Analysis with Boundary Elements*, vol. 31, pp. 75–82.

Engl, H. W.; Hanke, M.; Neubauer, A. (2000): *Regularization of Inverse Problems*. Kluwer Academic, Dordrecht.

Fairweather, G.; Karageorghis, A. (1998): The method of fundamental solutions for elliptic boundary value problems. *Advances in Computational Mathematics*, vol. 9, pp. 69–95.

Fairweather, G.; Karageorghis, A.; Martin, P. A. (2003): The method of fundamental solutions for scattering and radiation problems. *Engineering Analysis with Boundary Elements*, vol. 27, pp. 759–769.

Golberg, M. A.; Chen, C. S. (1999): The method of fundamental solutions for potential, Helmholtz and diffusion problems. In: M. A. Golberg (ed.) *Boundary Integral Methods: Numerical and Mathematical Aspects*, WIT Press and Computational Mechanics Publications, Boston, pp. 105–176.

Gorzelańczyk, P.; Kołodziej, A. (2008): Some remarks concerning the shape of the shape contour with application of the method of fundamental solutions to elastic torsion of prismatic rods. *Engineering Analysis with Boundary Elements*, vol. 32, pp. 64–75.

Hadamard, J. (1923): Lectures on Cauchy Problem in Linear Partial Differential Equations. Yale University Press, New Haven.

Hansen, P. C. (1998): Rank-Deficient and Discrete Ill-Posed Problems: Numerical Aspects of Linear Inversion. SIAM, Philadelphia.

Hào, D. N.; Lesnic, D. (2000): The Cauchy problem for Laplace's equation via the conjugate gradient method. *IMA Journal of Applied Mathematics*, vol. 65, pp. 199–217.

Heise, U. (1978): Numerical properties of integral equations in which the given boundary values and the sought solutions are defined on different curves. *Computers & Structures*, vol. 8, pp. 199–205.

Hon, Y. C.; Wei, T. (2001): Backus-Gilbert algorithm for the Cauchy problem of the Laplace equation. *Inverse Problems*, vol. 17, pp. 261–271.

Hon, Y. C.; Wei, T. (2002): A meshless computational method for solving inverse heat conduction problem. *International Series on Advances in Boundary Elements*, vol. 13, pp. 135–144.

Hon, Y. C.; Wei, T. (2003): A meshless scheme for solving inverse problems of Laplace equation. In: Y. C. Hon, M. Yamamoto, J. Cheng and J. L. Lee (eds.) *Recent Developments in Theories and Numerics. International Conference on Inverse Problems*, World Scientific, Hong Kong, pp. 291–300.

Hon, Y. C.; Wei, T. (2004): A fundamental solution method for inverse heat conduction problems. *Engineering Analysis with Boundary Elements*, vol. 28, pp. 489–495.

Hon, Y. C.; Wei, T. (2005): The method of fundamental solutions for solving multidimensional heat conduction problems. *CMES: Computer Modeling in Engineering & Sciences*, vol. 13, pp. 219–228.

Jin, B. T.; Zheng, Y. (2006): A meshless method for some inverse problems associated with the Helmholtz equation. *Computer Methods in Applied Mechanics and Engineering*, vol. 195, pp. 2270–2280.

Jourhmane, M.; Lesnic, D.; Mera, N. S. (2004): Relaxation procedures for an iterative algorithm for solving the Cauchy problem for the Laplace equation. *Engineering Analysis with Boundary Elements*, vol. 28, pp. 655–665.

Klibanov, M.; Santosa, F. (1991): A computational quasi-reversibility method for Cauchy problems for Laplace's equation. *SIAM Journal on Applied Mathematics*, vol. 51, pp. 1653–1675.

Kozlov, V. A.; Maz'ya, V. G.; Fomin, A. V. (1991): An iterative method for solving the Cauchy problem for elliptic equations. *Computational Mathematics and Mathematical Physics*, vol. 31, pp. 45–52.

Kunisch, K.; Zou, J. (1998): Iterative choices of regularization parameters in linear inverse problems. *Inverse Problems*, vol. 14, pp. 1247–1264.

Lesnic, D.; Elliott, L.; Ingham, D. B. (1997): An iterative boundary element method for solving numerically the Cauchy problem for the Lapace equation. *Engineering Analysis with Boundary Elements*, vol. 20, pp. 123–133.

Ling, L.; Takeuchi, T. (2008): Boundary control for inverse Cauchy problems of the Laplace equations. *CMES: Computer Modeling in Engineering & Sciences*, vol. 29, pp. 45–54.

Lions, J.-L.; Magenes, E. (1972): Non-Homogeneous Boundary Value Problems and Their Applications. Springer Verlag, Heidelberg.

Liu, C.–S. (2008a): Solving an inverse Sturm-Liouville problem by a Lie-group method. *Boundary Value Problems*, vol. 2008, Article ID 749865.

Liu, C.–S. (2008b): Identifying time-dependent damping and stiffness functions by a simple and yet accurate method. *Journal of Sound and Vibration*, vol. 318, pp. 148–165.

Liu, C.–S. (2008c): A Lie-group shooting method for simultaneously estimating the time-dependent damping and stiffness coefficients. *CMES: Computer Modeling in Engineering & Sciences*, vol. 27, pp. 137–149.

Liu, C.–S. (2008d): A time-marching algorithm for solving non-linear obstacle problems with the aid of an NCP-function. *CMC: Computers, Materials & Continua*, vol. 8, pp. 53–65.

Liu, C.–S. (2008e): A fictitious time integration method for two-dimensional quasilinear elliptic boundary value problems. *CMES: Computer Modeling in Engineering & Sciences*, vol. 33, pp. 179–198.

Liu, C.–S. (2008f): A modified collocation Trefftz method for the inverse Cauchy problem of Laplace equation. *Engineering Analysis with Boundary Elements*, vol. 32, pp. 778–785.

Liu, C. -S.; Atluri, S. N. (2008a): A novel time integration method for solving a large system of non-linear algebraic equations. *CMES: Computer Modeling in Engineering & Sciences*, vol. 31, pp. 71–83.

Liu, C.–S.; Atluri, S. N. (2008b): A novel fictitious time integration method for solving the discretized inverse Sturm-Liouville problems, for specified eigenvalues. *CMES: Computer Modeling in Engineering & Sciences*, vol. 36, pp. 261–285.

Liu, C.–S.; Atluri, S. N. (2009): A fictitious time integration method for the numerical solution of the Fredholm integral equation and for numerical differentiation of noisy data, and its relation with the filter theory. *CMES: Computer Modeling in Engineering & Sciences*, vol. 41, pp. 243–261.

Liu, C.–S.; Chang, J. R.; Chang, K. H.; Chen, Y. W. (2008): Simultaneously estimating the time-dependent damping and stiffness coefficients with the aid of vibrational data. *CMC: Computers, Materials & Continua*, vol. 7, pp. 97–107.

Marin, L. (2005a): A meshless method for solving the Cauchy problem in threedimensional elastostatics. *Computers & Mathematics with Applications*, vol. 50, pp. 73–92.

Marin, L. (2005b): Numerical solutions of the Cauchy problem for steady-state heat transfer in two-dimensional functionally graded materials. *International Journal of Solids and Structures*, vol. 42, pp. 4338–4351.

Marin, L. (2005c): A meshless method for the numerical solution of the Cauchy problem associated with three-dimensional Helmholtz-type equations. *Applied Mathematics and Computation*, vol. 165, pp. 355–374.

Marin, L. (2008): The method of fundamental solutions for inverse problems associated with the steady-state heat conduction in the presence of sources. *CMES: Computer Modeling in Engineering & Sciences*, vol. 30, pp. 99–122.

Marin, L.; Lesnic, D. (2004): The method of fundamental solutions for the Cauchy problem in two-dimensional linear elasticity. *International Journal of Solids and Structures*, vol. 41, pp. 3425–3438.

Marin, L.; Lesnic, D. (2005a): The method of fundamental solutions for the Cauchy problem associated with two-dimensional Helmholtz-type equations. *Computers & Structures*, vol. 83, pp. 267–278.

Marin, L.; Lesnic, D. (2005b): The method of fundamental solutions for inverse boundary value problems associated with the two-dimentional biharmonic equation. *Mathematical and Computers in Modelling*, vol. 42, pp. 261–278.

Marin, L.; Elliott, L.; Ingham, D. B.; Lesnic; D. (2001): Boundary element method for the Cauchy problem in linear elasticity. *Engineering Analysis with Boundary Elements*, vol. 25, pp. 783–793.

Marin, L.; Elliott, L.; Heggs, P. J.; Ingham, D. B.; Lesnic; D.; Wen, X. (2003): An alternating iterative algorithm for the Cauchy problem associated to the Helmholtz equation. *Computer Methods in Applied Mechanics and Engineering*, vol. 192, pp. 709–722.

Mathon, R.; Johnston, R. L. (1977): The approximate solution of elliptic boundary value problems by fundamental solutions. *SIAM Journal on Numerical Analysis*, vol. 14, pp. 638–650.

Mera, N. S. (2005): The method of fundamental solutions for the backward heat conduction problem. *Inverse Problems in Science and Engineering*, vol. 13, pp. 79–98.

Mera, N. S.; Elliott, L.; Ingham, D. B.; Lesnic; D. (2000): The boundary element solution of the Cauchy steady heat conduction problem in an anisotropic medium. *International Journal for Numerical Methods in Engineering*, vol. 49, pp. 481–499.

Morozov, V. A. (1966): On the solution of functional equations by the method of regularization. *Doklady Mathematics*, vol. 7, pp. 414–417.

Numerical Algorithms Group Library Mark 21 (2007). NAG(UK) Ltd, Wilkinson House, Jordan Hill Road, Oxford, UK.

Reinhardt, H. J.; Han, H.; Hào, D. N. (1999): Stability and regularization of a discrete approximation to the Cauchy problem for Laplace's equation. *SIAM Journal on Numerical Analysis*, vol. 36, pp. 890–905.

Shigeta, T.; Young, D. L. (2009): Method of fundamental solutions with optimal regularization techniques for the Cauchy problem of the Laplace equation with singular points. *Journal of Computational Physics*, vol. 228, pp. 1903–1915.

Tikhonov, A. N.; Arsenin, V. Y. (1986): *Methods for Solving Ill-Posed Problems*. Nauka, Moscow.

Wahba, G. (1977): Practical approximate solutions to linear operator equations when the data are noisy. *SIAM Journal on Numerical Analysis*, vol. 14, pp. 651–667.

Wei, T.; Hon, Y. C.; Ling, L. (2007): Method of fundamental solutions with regularization techniques for Cauchy problems of elliptic operators. *Engineering Analysis with Boundary Elements*, vol. 31, 373–385.

Wei, T.; Li, Y. S. (2009): An inverse boundary problem for one-dimensional heat equation with a multilayer domain. *Engineering Analysis with Boundary Elements*, vol. 33, pp. 225–232.

Wei, T.; Zhou, D. Y. (2009): Convergence analysis for the Cauchy problem of Laplace's equation by a regularized method of fundamental solutions. *Advances in Computational Mathematics*, in press, DOI 10.1007/s10444-009-9134-7.

Young, D. L.; Tsai, C. C.; Chen, C. W.; Fan, C. M. (2008): The method of fundamental solutions and condition number analysis for inverse problems of Laplace equation. *Computers and Mathematics with Applications*, vol. 55, pp. 1189–1200.