

# The PCGM for Cauchy inverse problems in 3D potential

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## Abstract

The preconditioned conjugate gradient method (PCGM) in combination with the boundary element method (BEM) is developed for reconstructing the boundary conditions in 3-D potential. Morozov's discrepancy principle is employed to select the iteration step. The semi-analytical integral algorithm is proposed to treat the nearly singular integrals when the interior points are very close to the boundary. The numerical results confirm that the PCGM produces convergent and stable numerical solutions with respect to decreasing the amount of noise added into the input data. The numerical solutions are sensitive to the locations of the interior points when these points are distributed near the boundary without boundary conditions. The results are more accurate when these points are closer to the boundary.

*Keywords: BEM, inverse problems, Cauchy problems, potential, preconditioned conjugate gradient method.*

## 1 Introduction

Inverse problems are very important in engineering and science. Many unmeasurable physical quantities need to be determined from known data. There are different kinds of inverse problems. 1) Reconstruction inverse problem: the boundary conditions are unknown on all or part of the boundary. 2) Identification inverse problem: part of the domain or its boundary is unknown, such as the problems with crack, flaw, defect, cavity, erosion, etc. 3) Material property inverse problem: the properties of the material, such as Young's modulus, Poisson's ratio, the linear coefficient of thermal expansion, are not known. 4) External source inverse problem: the loads or sources are unknown. 5) Modelization inverse problem: the differential equation is not known. The



boundary element method is becoming more and more important as a classic numerical method to solve different inverse problems [1]. Inverse problems are in general unstable in the sense that small noise in the input data may amplify significantly the errors in the solution. So the regularization techniques are very critic to the inverse numerical analysis [2].

It is often encountered that all the potentials and potential gradients are known on a part of the boundary and no boundary data can be directly measured on the rest of the boundary in engineering for potential problems, which is the reconstruction inverse problem, also named as Cauchy problems. The measurable information of internal points is helpful to obtain all unknown boundary conditions.

The function specification method and the zeroth-order regularization procedure were employed by Kurpisz and Nowak [3] to solve the inverse transient heat conduction problems. The mathematical mechanism of the ill-posed Cauchy problem for Laplace equation was analyzed by Chen and Chen [5]. An iterative method was applied to solve Cauchy inverse problem for the Laplace equation by Lesnic *et al.* [4]. The sequential function specification method was used by Chantasiriwan to determine the unknown time-dependent boundary heat flux from temperature measurements inside a body or on its boundary [6]. The dual reciprocity boundary element method in conjunction with iterative regularization methods of conjugate gradient type was discussed by Singh *et al.* [7] for the solution of time-dependent inverse heat conduction problems. The influence of measurement location, measurement error and element option were investigated. An inverse problem for Laplace equations was recast into primary and adjoint boundary value problems by Hayashi *et al.* [8, 9]. The Dirichlet and Neumann data were specified on respective part of the boundary, while no data on the second part of the boundary were given and Robin condition was prescribed on the third part of the boundary. An iterative approach was introduced by Delvare *et al.* [10]. The Cauchy inverse problem for Laplace equation was reduced to a sequence of well-posed optimization problems under equality constraints. The desingularized meshless method was used to solve boundary-value problems with specified boundary conditions. The accompanied ill-posed problem in the inverse problem was remedied by using the Tikhonov regularization method and the truncated singular value decomposition method (TSVD) [11]. Mera *et al.* [12] proposed an iterative boundary element for singular Cauchy problems in anisotropic heat conduction with an abrupt change in the boundary conditions and with a sharp re-entrant corner. Onyango *et al.* [13–17] investigated the determination of the boundary conditions and time-dependent heat transfer coefficient in transient heat conduction using the BEM. Simoes *et al.* [18] developed an experimental validation of 2D and 2.5D BEM solutions for transient heat conduction in systems containing heterogeneities. They also presented an experimental validation of a semi-analytical solution for transient heat conduction in multilayer systems [19]. Alifanov and Nenarokomov [20] described an algorithm to process the data of unsteady-state thermal experiments and find the surface heat flux and temperature as functions of spatial coordinates and time. Gao and



He [20] and Cui *et al.* [22] proposed the complex-variable differentiation method to identify thermal properties for heat conduction problems.

In this paper, the boundary potentials and potential gradients on a part of boundary are identified using the over-specified boundary conditions on the remaining boundary and the information of interior points in the BEM for 3-D Cauchy potential inverse problems. The PCGM in combination with the BEM is developed to regularize the Cauchy inverse problem. Morozov's discrepancy principle is employed to select the iteration step. The semi-analytical integral algorithm is proposed to treat the nearly singular integrals when the interior points are very close to the boundary.

## 2 Boundary integral equations

Consider three-dimensional potential problem. For an interior point  $\mathbf{y}$ , the boundary integral equation can be given as

$$u(\mathbf{y}) = \int_{\Gamma} u^*(\mathbf{x}, \mathbf{y}) q(\mathbf{x}) d\Gamma - \int_{\Gamma} q^*(\mathbf{x}, \mathbf{y}) u(\mathbf{x}) d\Gamma \quad (1)$$

When the source point  $\mathbf{y}$  locates on the boundary  $\Gamma$ , the boundary integral equation can be written as

$$C(\mathbf{y})u(\mathbf{y}) = \int_{\Gamma} u^*(\mathbf{x}, \mathbf{y}) q(\mathbf{x}) d\Gamma - \int_{\Gamma} q^*(\mathbf{x}, \mathbf{y}) u(\mathbf{x}) d\Gamma \quad (2)$$

where  $u^*(\mathbf{x}, \mathbf{y})$  is the fundamental solution of potential problems, and  $q^*(\mathbf{x}, \mathbf{y})$  is the gradient of potential with respect to an outward normal to the boundary.  $C(\mathbf{y})$  is the boundary singular coefficient, which is determined by the boundary geometry characterization.

The potential gradients  $q_k$  at the interior point  $\mathbf{y}$  with respect to directions  $x_k$  can be obtained by differentiating Eq. (1)

$$q_k(\mathbf{y}) = \int_{\Gamma} \frac{\partial u^*(\mathbf{x}, \mathbf{y})}{\partial y_k} q(\mathbf{x}) d\Gamma - \int_{\Gamma} \frac{\partial q^*(\mathbf{x}, \mathbf{y})}{\partial y_k} u(\mathbf{x}) d\Gamma \quad (k=1,2,3) \quad (3)$$

The integral kernel functions in Eqs (1)–(3) are given as follows

$$u^*(\mathbf{x}, \mathbf{y}) = \frac{1}{4\pi r} \quad (4)$$

$$q^*(\mathbf{x}, \mathbf{y}) = -\frac{1}{4\pi} \frac{r_n}{r^3} \quad (5)$$

$$\frac{\partial u^*(\mathbf{x}, \mathbf{y})}{\partial y_k} = \frac{1}{4\pi} \frac{r_k}{r^3}, \quad k=1,2,3 \quad (6)$$

$$\frac{\partial q^*(\mathbf{x}, \mathbf{y})}{\partial y_k} = -\frac{1}{4\pi} \left( -\frac{n_k}{r^3} + \frac{3r_k r_n}{r^5} \right), \quad k=1,2,3 \quad (7)$$

where  $r$  is the distance between the source point  $\mathbf{y}$  and arbitrary field point  $\mathbf{x}$  on the boundary.



After the boundary integral equations (1)–(3) are discretized by a set of boundary elements, and both the known boundary conditions and interior points' information are introduced in, the system equation can be written as

$$Ax = b \tag{8}$$

Next, the iterative regularization method is proposed to treat the boundary condition inverse problems with respect to Eq. (8).

### 3 The preconditioned conjugate gradient method (PCGM)

The PCGM is an iterative regularization method to solve the linear algebraic equation, and it is one of the most effective methods [23, 24]. For the ill-posed linear algebraic equation  $Ax = b$ , we have the computation procedure as follows

1). Compute  $x^{(0)} = W(AW^+)b$

2). Initialization:  $r^{(0)} = b - Ax^{(0)}$ ,  $s^{(0)} = A^T r^{(0)}$

$$q_1^{(0)} = (L_{11}^{-1})^T s^{(0)}, Q_1^{(0)} = q_1^{(0)} / \|q_1^{(0)}\|$$

$$q^{(0)} = \begin{pmatrix} L_{11}^{-1} q_1^{(0)} \\ 0 \end{pmatrix} - WT_{11} L_{11}^{-1} q_1^{(0)}$$

$$p^{(1)} = q^{(0)}$$

3). For the  $k$ th ( $k = 1, 2, 3, \dots$ ) step, the iteration is given as

$$A_p^{(k)} = Ap^{(k)}$$

$$\alpha^{(k)} = \frac{(s^{(k)}, q^{(k-1)})}{(A_p^{(k)}, A_p^{(k)})}$$

$$x^{(k)} = x^{(k-1)} + \alpha^{(k)} p^{(k)}$$

$$r^{(k)} = r^{(k-1)} - \alpha^{(k)} A_p^{(k)}$$

$$s^{(k)} = A^T r^{(k)}$$

$$\hat{q}_1^{(k)} = (L_{11}^{-1})^T s^{(k)}$$

$$q_1^{(k)} = \hat{q}_1^{(k)} - (Q_1^{(k-1)}, \hat{q}_1^{(k)}) Q_1^{(k-1)} - \dots - (Q_1^{(0)}, \hat{q}_1^{(k)}) Q_1^{(0)}$$

$$Q_1^{(k)} = q_1^{(k)} / \|q_1^{(k)}\|$$

$$q^{(k)} = \begin{pmatrix} L_{11}^{-1} q_1^{(k)} \\ 0 \end{pmatrix} - WT_{11} L_{11}^{-1} q_1^{(k)}$$

$$\beta^{(k)} = \frac{(s^{(k)}, q^{(k)})}{(s^{(k-1)}, q^{(k-1)})}$$

$$p^{(k)} = q^{(k)} + \beta^{(k)} p^{(k)}$$



where the matrix  $A \in \mathbb{R}^{m \times n}$ , the matrix  $L \in \mathbb{R}^{d \times n}$  is a  $d \times n$  ( $d \leq n$ ) discrete approximation of a derivative operator.  $L$  is the identity matrix when  $d = n$ , and  $L$  has the following form

$$L = \begin{pmatrix} 1 & -1 & & & & \\ & 1 & -1 & & & \\ & & \ddots & \ddots & & \\ & & & \ddots & \ddots & \\ & & & & 1 & -1 \\ & & & & & 1 & -1 \end{pmatrix}_{(n-1) \times n}$$

when  $d = n - 1$ , the matrix  $W$  holds a basis for the null space of  $L$ .

$T = (AW)^+$   $A \in \mathbb{R}^{(n-d) \times n}$ . The matrix  $T$ ,  $L$  and the vector  $x$  can be partitioned

as  $L = (L_{11}, L_{12})$ ,  $T = (T_{11}, T_{12})$ ,  $x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$ , where  $L_{11} \in \mathbb{R}^{d \times d}$ ,  $T_{11} \in \mathbb{R}^{(n-d) \times d}$ ,  $x_1 \in \mathbb{R}^d$ .

#### 4 Numerical example

Example 1: Heat conduction in a cube. The side length of the cube is 2m, as shown in Fig. 1. The temperature and flux conditions on the 4 lateral surfaces and the upper surface are specified. All boundary conditions on the bottom surface are unknown. The exact temperature solution for the problem is  $u(x_1, x_2, x_3) = 300 - 50x_1 - 50x_2 - 50x_3$ . In the BEM model, the boundary is discretized by 24 8-node quadratic elements.

In order to investigate the accuracy of numerical solutions, we evaluate the relative errors defined by

$$e_u = \frac{\|u^{\text{num}} - u^{\text{exa}}\|}{\|u^{\text{exa}}\|}, \quad e_q = \frac{\|q^{\text{num}} - q^{\text{exa}}\|}{\|q^{\text{exa}}\|} \quad (9)$$

where  $u^{\text{num}}$  and  $q^{\text{num}}$  represent the numerical solutions of the potentials and the gradients, respectively, whilst  $u^{\text{exa}}$  and  $q^{\text{exa}}$  are exact values.

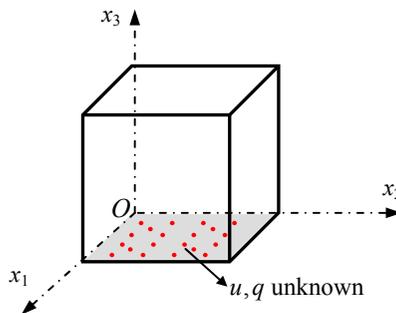


Figure 1: Heat conduction in a cube.

Numerical experiments show that we cannot obtain accurate results if without information at sufficient internal points. So we add 20 internal points on the surface  $x_3 = 1\text{cm}$  to discuss the influence of the random perturbations. The fluxes of these interior points are given. The exact and numerical solutions of potentials  $u$  and gradients  $q$  at the nodes on the bottom surface of the cube, respectively, are shown in Figs 2 and 3 for different random perturbations. The relative errors  $e_u$  and  $e_q$  for each case are listed in Tab. 1. From Figs 2 and 3, it can be seen that numerical solutions are in good agreement with exact solutions. Furthermore, the numerical solutions converge to the exact ones as the random perturbations decrease. From Tab. 1, it can be seen that the relative errors decrease as the random perturbations decrease from 1% to 0%. Numerical experiments show that the results of the gradients will be inaccurate if the perturbation increase to 2%, so the results are omitted to plot in Figs 2 and 3.

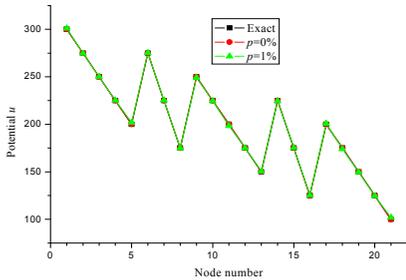


Figure 2: Potentials at nodes on the bottom surface for different perturbations.

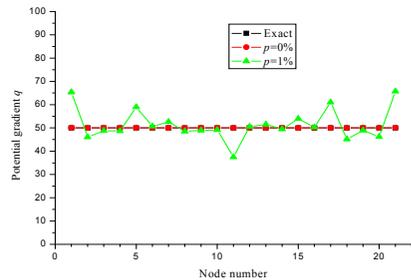


Figure 3: Potential gradients at nodes on the bottom surface for different perturbations.

Table 1: The relative error for different perturbations.

$P / \%$	0	1
$e_u$	0.0e0	1.6e-5
$e_q$	9.6e-8	1.8e-2

Table 2: The relative error for different positions with perturbation  $p=1\%$ .

Position	1 on Surface $x_3 = 1\text{cm}$	2 on Surface $x_3 = 2\text{cm}$	3 on Surface $x_3 = 3\text{cm}$
$e_u$	1.6e-5	1.8e-5	2.0e-5
$e_q$	1.8e-2	2.2e-2	2.5e-2



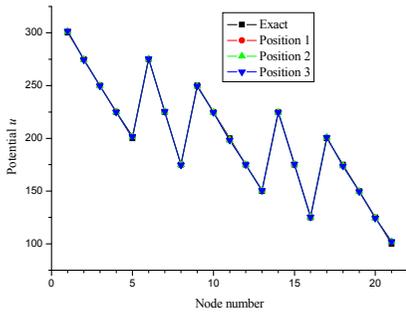


Figure 4: Potentials at nodes on the bottom surface for different positions.

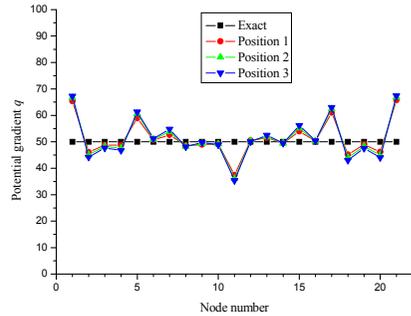


Figure 5: Potential gradients at nodes on the bottom surface for different positions.

It should be noted that the interior points located on the three different surfaces are very close to the boundary, the discretized boundary integrals are nearly singular. The boundary condition solutions will oscillate if the boundary integrals are calculated by the conventional Gaussian quadrature, even the PCGM for the inverse problem is normally carried out. In this instance, the semi-analytical integral algorithms [25, 26] are employed to tackle the nearly singular integrals. Therefore the accurate numerical solutions can be obtained by the PCGM.

## 5 Conclusions

Three-dimensional Cauchy inverse problems for the Laplace equation are solved by using the boundary element method in conjunction with the PCGM. The boundary element method has a great advantage on solving this kind of inverse problems, because only the contour of the considered domain is divided into meshes and the unknown boundary conditions can be identified based on the given boundary data and internal information. The PCGM is a stable method to regularize the inverse problem. Morozov's discrepancy principle is effective to select the iteration step. The semi-analytical integral algorithm is accurate to treat the nearly singular integrals when the interior points are very close to the boundary. The numerical results confirm that the PCGM produces convergent and stable numerical solutions with respect to decreasing the amount of noise added into the input data. The numerical solutions are sensitive to the locations of the interior points when these points are located near the boundary without known boundary conditions. The results are more accurate when these points are closer to the boundary.

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## References

- [1] Ingham DB, Wrobel LC (eds). *Boundary integral formulations for inverse analysis*. Southampton, UK: Computational Mechanics Publications, 1997.
- [2] Engl HW, Hanke M, Neubauer A. *Regularization of inverse problems*. Dordrecht: Kluwer Academic Publishers, 2000.
- [3] Kurpisz K, Nowak AJ. BEM approach to inverse heat conduction problems. *Engineering Analysis with Boundary Elements*, 1992, 10(4): 291–297.
- [4] Lesnic D, Elliott L, Ingham DB. An iterative boundary element method for solving numerically the Cauchy problem for the Laplace equation. *Engineering Analysis with Boundary Elements*, 1997, 20(2): 123–133.
- [5] Chen JT, Chen KH. Analytical study and numerical experiments for Laplace equation with overspecified boundary conditions, *Applied Mathematical Modelling*, 1998, 22(9): 703–725.
- [6] Chantasiriwan S. An algorithm for solving multidimensional inverse heat conduction problem. *International Journal of Heat and Mass Transfer*, 2001, 44(20): 3823–3832.
- [7] Singh KM, Tanaka M. Dual reciprocity boundary element analysis of inverse heat conduction problems. *Comput Methods Appl Mech Engrg*, 2001, 190(40-41): 5283–5295.
- [8] Hayashi K, Ohura Y, Onishi K. Direct method of solution for general boundary value problem of the Laplace equation. *Engineering Analysis with Boundary Elements*, 2002, 26(9): 763–771.
- [9] Hayashi K, Onishi K, Ohura Y. Direct numerical identification of boundary values in the Laplace equation. *Journal of Computational and Applied Mathematics*, 2003, 152(1-2): 161–174.
- [10] Delvare F, Climetiere A, Pons F. An iterative boundary element method for Cauchy inverse problems. *Computational Mechanics*, 2002, 28(3-4): 291–302.
- [11] Chen KH, Wu KL, Kao JH, Chen JT. Desingularized meshless method for solving Laplace equation with over-specified boundary conditions using regularization techniques. *Computational Mechanics* 2009; 43(6): 827–837.
- [12] Mera NS, Elliott L, Ingham DB, Lesnic D. An iterative algorithm for singular Cauchy problems for the steady state anisotropic heat conduction equation. *Engineering Analysis with Boundary Elements* 2002; 26(2): 157–168.
- [13] Onyango TTM, Ingham DB, Lesnic D. Restoring boundary conditions in heat conduction, *J Eng Math*, 2008, 62(1): 85–101.



- [14] Onyango TTM, Ingham DB, Lesnic D. Reconstruction of heat transfer coefficients using the boundary element method, *Computers and Mathematics with Applications*, 2008, 56(1): 114–126.
- [15] Onyango TTM, Ingham DB, Lesnic D, Slodicka M. Determination of a time-dependent heat transfer coefficient from non-standard boundary measurements, *Mathematics and Computers in Simulation*, 2009, 79(5): 1577–1584.
- [16] Onyango TTM, Ingham DB, Lesnic D. Inverse reconstruction of boundary condition coefficients in one-dimensional transient heat conduction, *Applied Mathematics and Computation*, 2009, 207(2): 569–575.
- [17] Onyango TTM, Ingham DB, Lesnic D. Reconstruction of boundary condition laws in heat conduction using the boundary element method, *Computers and Mathematics with Applications*, 2009, 57(1): 153–168.
- [18] Simoes I, Simoes N, Tadeu A, Reis M, Vasconcellos CAB, Mansur WJ. Experimental validation of a frequency domain BEM model to study 2D and 3D heat transfer by conduction, *Engineering Analysis with Boundary Elements*, 2012, 36(11): 1686–1698.
- [19] Simoes N, Simoes I, Tadeu A, Vasconcellos CAB, Mansur WJ. 3D transient heat conduction in multilayer systems - Experimental validation of semi-analytical solution, *International Journal of Thermal Sciences*, 2012, 57: 192–203.
- [20] Alifanov OM, Nenarokomov AV. Three dimensional boundary inverse heat conduction problem for regular coordinate systems, *Inverse Problems in Engineering*, 1999, 7(4): 335–362.
- [21] Gao XW, He MC. A new inverse analysis approach for multi-region heat conduction BEM using complex-variable-differentiation method, *Engineering Analysis with Boundary Elements*, 2005, 29(8): 788–795.
- [22] Cui M, Gao XW, Zhang JB. A new approach for the estimation of temperature-dependent thermal properties by solving transient inverse heat conduction problems, *International Journal of Thermal Sciences*, 2012, 58: 113–119
- [23] Hansen PC. Rank-Deficient and Discrete Ill-posed Problems: Numerical Aspects of Linear Inversion, SIAM, Philadelphia, 1998.
- [24] Zhou HL, Jiang W, Hu H, Niu ZR. Boundary element methods for boundary condition inverse problems in elasticity using PCGM and CGM regularization, *Engineering Analysis with Boundary Elements*, 2013, 37(11): 1471–1482
- [25] Niu ZR, Wendland WL, Wang XX, Zhou HL. A semi-analytical algorithm for the evaluation of the nearly singular integrals in three-dimensional boundary element methods. *Computer Methods in Applied Mechanics and Engineering* 2005, 194(9-11): 1057–1074.
- [26] Zhou HL, Niu ZR. Regularization of nearly singular integrals in the boundary element method for 3-D potential problems. *Chinese Journal of Computational Physics* 2005, 22(6): 501–506 (in Chinese).

