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# A comparison of different regularization methods for a Cauchy problem in anisotropic heat conduction

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***Abstract*** *In this paper, various regularization methods are numerically implemented using the boundary element method (BEM) in order to solve the Cauchy steady-state heat conduction problem in an anisotropic medium. The convergence and the stability of the numerical methods are investigated and compared. The numerical results obtained confirm that stable numerical results can be obtained by various regularization methods, but if high accuracy is required for the temperature, or if the heat flux is also required, then care must be taken when choosing the regularization method since the numerical results are substantially improved by choosing the appropriate method.*

## 1. Introduction

Many natural and man-made materials cannot be considered isotropic and the dependence of the thermal conductivity with direction has to be taken into account in the modelling of the heat transfer. For example, crystals, wood, sedimentary rocks, metals that have undergone heavy cold pressing, laminated sheets, composites, cables, heat shielding materials for space vehicles, fibre reinforced structures, and many others are examples of anisotropic materials. Composites are of special interest to the aerospace industry because of their strength and reduced weight. Therefore, heat conduction in anisotropic materials has numerous important applications in various branches of science and engineering and hence its understanding is of great importance.

If the temperature or the heat flux on the surface of a solid $\Omega$ is given, then the temperature distribution in the domain can be calculated, provided the temperature is specified at least at one point. However, in the direct problem, many experimental impediments may arise in measuring or in the enforcing of the given boundary conditions. There are many practical applications which arise in engineering where a part of the boundary is not accessible for temperature or heat flux measurements. For example, the temperature or the heat flux measurement may be seriously affected by the presence of the sensor and hence there is a loss of accuracy in the measurement, or, more simply, the surface of the body may be unsuitable for attaching a sensor to measure

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the temperature or the heat flux. The situation when neither the temperature nor the heat flux can be prescribed on a part of the boundary while both of them are known on the other part leads in the mathematical formulation to an ill-posed problem which is termed as "the Cauchy problem".

This problem is much more difficult to solve both numerically and analytically since its solution does not depend continuously on the prescribed boundary conditions. Violation of the stability of the solution creates serious numerical problems since the system of linear algebraic equations obtained by discretising the problem is ill-conditioned. Therefore, a direct method to solve this problem cannot be used since such an approach would produce a highly unstable solution. A remedy for this is the use of regularization methods which attempt to find the right compromise between accuracy and stability.

Currently, there are various methods to deal with ill-posed problems. However, their performance depends on the particular problem being solved. Therefore, it is the purpose of this paper to investigate and compare several regularization methods for a Cauchy anisotropic heat conduction problem. There are different methods to solve an ill-posed problem such as the Cauchy problem. One approach is to use the general regularization methods such as Tikhonov regularization, truncated singular value decomposition, conjugate gradient method, etc. On the other hand, specific regularization methods can be developed for particular problems in order to make use of the maximum amount of information available. The use of any extra information available for a specific problem is particularly important in choosing the regularization parameter of the method employed. Both general regularization and specific regularization methods developed for the Cauchy problems are considered in this paper.

These methods are investigated and compared in order to reveal their performance and limitation. All the methods employed are numerically implemented using the boundary element method (BEM) since it was found that this method performs better for linear partial differential equations with constant coefficients than other domain discretisation methods. Numerical results are given in order to illustrate and compare the convergence, accuracy and stability of the methods employed.

## 2. Mathematical formulation

Consider an anisotropic medium in an open bounded domain $\Omega \subset \mathbb{R}^2$ and assume that $\Omega$ is bounded by a curve $\Gamma$ which may consist of several segments, each being sufficiently smooth in the sense of Liapunov. We also assume that the boundary consists of two parts, $\partial\Omega = \Gamma = \Gamma_1 \cup \Gamma_2$, where $\Gamma_1, \Gamma_2 \neq \emptyset$ and $\Gamma_1 \cap \Gamma_2 = \emptyset$. In this study, we refer to steady heat conduction applications in anisotropic homogeneous media and we assume that heat generation is absent. Hence the function $T$, which denotes the temperature distribution in $\Omega$, satisfies the anisotropic steady-state heat conduction equation, namely,

$$LT = \sum_{i,j=1}^{2} k_{ij} \frac{\partial^2 T}{\partial x_i \, \partial x_j} = 0, \quad \underline{x} \in \Omega \tag{1}$$

where $k_{ij}$ is the constant thermal conductivity tensor which is assumed to be symmetric and positive-definite so that equation (1) is of the elliptic type. When $k_{ij} = \delta_{ij}$, where $\delta_{ij}$ is the Kronecker delta symbol, we obtain the isotropic case and $T$ satisfies the Laplace equation

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

In the direct problem formulation, if the temperature and/or heat flux on the boundary $\Gamma$ is given then the temperature distribution in the domain can be calculated, provided that the temperature is specified at least at one point. However, many experimental impediments may arise in measuring or enforcing a complete boundary specification over the whole boundary $\Gamma$. The situation when neither the temperature nor the heat flux can be prescribed on a part of the boundary while both of them are known on the other part leads to the mathematical formulation of an inverse problem consisting of equation (1) which has to be solved subject to the boundary conditions

$$T(\underline{x}) = f(\underline{x}) \quad \text{for } \underline{x} \in \Gamma_1 \tag{3}$$

$$\frac{\partial T}{\partial \nu^+}(\underline{x}) = q(\underline{x}) \quad \text{for } \underline{x} \in \Gamma_1 \tag{4}$$

where $f,q$ are prescribed functions, $\partial / \partial \nu^+$ is given by

$$\frac{\partial}{\partial \nu^+} = \sum_{i,j=1}^{2} k_{ij} \cos(\nu, x_i) \frac{\partial}{\partial x_j} \tag{5}$$

and cos $(\nu, x_i)$ are the direction cosines of the outward normal vector $\nu$ to the boundary $\Gamma$. In the above formulation of the boundary conditions (3) and (4) it can be seen that the boundary $\Gamma_1$ is overspecified by prescribing both the temperature $f$ and the heat flux $q$, whilst the boundary $\Gamma_2$ is underspecified since both the temperature $T|_{\Gamma_2}$ and the heat flux

$$\frac{\partial T}{\partial \nu^+}|_{\Gamma_2}$$

are unknown and have to be determined.

This problem, termed the Cauchy 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 (Hadamard, 1923) that this solution is unstable with respect to the small perturbations in the data on $\Gamma_1$. Thus, the problem is ill-posed and we cannot use a direct approach, e.g. Gaussian elimination method, to solve the system of linear equations which arise from discretising the partial differential equations (1) or (2) and the boundary conditions (3) and (4). Therefore, regularization methods are required in order to accurately solve this Cauchy problem.

## 3. Regularization methods

### *3.1 Truncated singular value decomposition*

Consider the ill-conditioned system of equations

$$\mathbb{C}\underline{X} = \underline{d} \tag{6}$$

where $C \in \mathbb{R}^{M\times N}$, $\underline{X} \in \mathbb{R}^N$, $\underline{d} \in \mathbb{R}^M$ and $M \geq N$.

The singular value decomposition (SVD) of the matrix $\mathbb{C} \in \mathbb{R}^{M\times N}$ is given by

$$\mathbb{C} = \mathbb{W}\mathbb{X}\mathbb{V}^{\mathrm{T}} = \sum_{i=1}^{N} \underline{w}_i \sigma_i \underline{v}_i^{\mathrm{T}} \tag{7}$$

where $\mathbb{W} = \mathrm{col}[\underline{w}_1, \ldots, \underline{w}_M] \in \mathbb{R}^{M\times M}$, and $\mathbb{V} = \mathrm{col}[\underline{v}_1, \ldots, \underline{v}_N] \in \mathbb{R}^{N\times N}$ are orthogonal matrices

$$\mathbb{X} = \begin{pmatrix} \mathbb{S} \\ 0_{M-N} \end{pmatrix} \quad \text{if } M > N$$

$$\mathbb{X} = \mathbb{S} \quad \text{if } M = N$$

and the diagonal matrix $\mathbb{S} = \mathrm{diag}[\sigma_1, \ldots, \sigma_N]$ has a non-negative diagonal elements ordered such that

$$\sigma_1 \geq \sigma_2 \geq \sigma_3 \geq \ldots \geq \sigma_N \geq 0 \tag{8}$$

The non-negative quantities $\sigma_i$ are called the *singular values of the matrix* $\mathbb{C}$. The number of positive singular values of $\mathbb{C}$ is equal to the rank of the matrix $\mathbb{C}$. In the ideal setting, without perturbation and rounding errors, the treatment of the ill-conditioned system of equation (6) is straightforward, namely, we simply ignore the SVD components associated with the zero singular values and compute the solution of the system by means of

$$\underline{X} = \sum_{i=1}^{\mathrm{rank}(\mathbb{C})} \frac{\underline{w}_i^{\mathrm{T}} \underline{d}}{\sigma_i} \underline{v}_i \tag{9}$$

In practice, noise is always present in the problem and the vector $\underline{d}$ and the matrix $\mathbb{C}$ are only known approximately. Therefore, if some of the singular values of $\mathbb{C}$ are non-zero, but very small, instability arises due to division by these small singular values in expression (9). One way to overcome this instability is to modify the inverses of the singular values in expression (9) by multiplying them by a *regularizing filter function* $f_\lambda(\sigma_i)$ for which the product $f_\lambda(\sigma)/\sigma \rightarrow 0$ as $\sigma \rightarrow 0$. This filters out the components of the sum (9) corresponding to small singular values and yields an approximation for the solution of the problem with the representation

$$\underline{X}_\lambda = \sum_{i=1}^{\mathrm{rank}(\mathbb{C})} \frac{f_\lambda(\sigma_i)}{\sigma_i} (\underline{w}_i^{\mathrm{T}} \underline{d}) \underline{v}_i \tag{10}$$

To obtain some degree of accuracy, one must retain singular components corresponding to large singular values. This is done by taking $f_\lambda(\sigma) \approx 1$ for large values of $\sigma$. An example of such a filter function is

$$f_\lambda(\sigma) = \begin{cases} 1 & \text{if } \sigma^2 > \lambda \\ 0 & \text{if } \sigma^2 \leq \lambda \end{cases} \tag{11}$$

The approximation (10) then takes the form

$$\underline{X}_\lambda = \sum_{\sigma_i^2 > \lambda} \frac{1}{\sigma_i} (\underline{w}_i^{\mathrm{T}} \underline{d}) \underline{v}_i \tag{12}$$

and it is known as the truncated singular value decomposition (TSVD) solution of the problem (6). For different filter functions, $f_\lambda$, different regularization methods are obtained, see Section 3.2. A stable and accurate solution is then obtained by matching the regularization parameter $\lambda$ to the level of the noise present in the problem to be solved.

### *3.2 Tikhonov regularization*

In this section, we give a brief description of the Tikhonov regularization method. For further details on this method, we refer the reader to Tikhonov and Arsenin (1977) and Tikhonov *et al.* (1995).

Again consider the ill-conditioned system of equation (6). The Tikhonov regularized solution of the ill-conditioned system (6) is given by

$$\underline{X}_\lambda : T_\lambda(\underline{X}_\lambda) = \min\{T_\lambda(\underline{X}) | \underline{X} \in \mathbb{R}^N\} \tag{13}$$

where $T_\lambda$ represents the Tikhonov functional given by

$$T_\lambda(\underline{X}) = \|\mathbb{C}\underline{X} - \underline{d}\|_2^2 + \lambda^2 \|\mathbb{L}\underline{X}\|_2^2 \tag{14}$$

and $\mathbb{L} \in \mathbb{R}^{N \times N}$ induces the smoothing norm $\|\mathbb{L}\underline{X}\|_2$ with $\lambda \in \mathbb{R}$, the regularization parameter to be chosen. The problem is in the standard form, also referred to as Tikhonov regularization of order zero, if the matrix $\mathbb{L}$ is the identity matrix $\mathbb{I}_N \in \mathbb{R}^{N\times N}$.

Formally, the Tikhonov regularized solution $\underline{X}_\lambda$ is given as the solution of the regularized equation

$$(\mathbb{C}^{\mathrm{T}}\mathbb{C} + \lambda^2\mathbb{L}^{\mathrm{T}}\mathbb{L})\underline{X} = \mathbb{C}^{\mathrm{T}}\underline{d} \tag{15}$$

However, the best way to solve equation (13) numerically is to treat it as a least squares problem of the form

$$\underline{X}_\lambda : T_\lambda(\underline{X}_\lambda) = \min_{\underline{X}\in\mathbb{R}^N}\left\| \begin{pmatrix} \mathbb{C} \\ \lambda\mathbb{L} \end{pmatrix}\underline{X} - \begin{pmatrix} \underline{d} \\ 0 \end{pmatrix} \right\|_2 \tag{16}$$

Regularization is necessary when solving inverse problems because the simple least squares solution obtained when $\lambda = 0$ is completely dominated by the contributions from the data and rounding errors. By adding regularization, we are able to damp out these contributions and maintain the norm $\|\mathbb{L}\underline{X}\|_2$ to be of reasonable size. If too much regularization, or smoothing, is imposed on the solution, then it will not fit the given data $\underline{d}$ and the residual norm $\|\mathbb{C}\underline{X} - \underline{d}\|_2$ will be too large. If too little regularization is imposed on the solution, then the fit will be good, but the solution will be dominated by the contributions from the data errors, and hence $\|\mathbb{L}\underline{X}\|_2$ will be too large. In this paper, we assume that $\mathbb{L} = \mathbb{I}_N$, i.e. we consider Tikhonov regularization of order zero.

If we insert the SVD (7) into the least squares formulation (15), then we obtain

$$\mathbb{V}(\mathbb{X}^2 + \lambda^2\mathbb{I})\mathbb{V}^{\mathrm{T}}\underline{X}_\lambda = \mathbb{V}\mathbb{X}^{\mathrm{T}}\mathbb{W}^{\mathrm{T}}\underline{d} \tag{17}$$

Solving equation (17) for $\underline{X}_\lambda$, we obtain

$$\underline{X}_\lambda = \left[\mathbb{V}(\mathbb{X}^2 + \lambda^2\mathbb{I})\mathbb{V}^{\mathrm{T}}\right]^{+}\mathbb{V}\mathbb{X}\mathbb{W}^{\mathrm{T}}\underline{d} = \mathbb{V}(\mathbb{X}^2 + \lambda^2\mathbb{I})^{+}\mathbb{X}\mathbb{W}^{\mathrm{T}}\underline{d} \tag{18}$$

where $^+$ denotes the Moore-Penrose pseudo inverse of a matrix. On substituting the matrices $\mathbb{W}$, $\mathbb{V}$ and $\mathbb{X}$ into equation (18), we obtain the regularized solution, as a function of the left and right singular vectors and the singular values, as follows:

$$\underline{X}_\lambda = \sum_{i=1}^{N}\frac{f_\lambda(\sigma_i)}{\sigma_i}(\underline{w}_i^{\mathrm{T}}\underline{d})\underline{v}_i \tag{19}$$

where $f_\lambda$ are the Tikhonov filter factors given by

$$f_\lambda(\sigma_i) = \frac{\sigma_i^2}{\sigma_i^2 + \lambda^2} \tag{20}$$

It should be noted that the Tikhonov filter factors, as defined earlier, depend on both the singular values $\sigma_i$ and the regularization parameter $\lambda$, and $f_i \approx 1$, if $\sigma_i \gg \lambda$, and $f_i \approx \sigma_i^2/\lambda^2$, if $\sigma_i \ll \lambda$. In particular, the basic least squares solution $X_{LS}$ is given by equation (19) with the regularization parameter $\lambda = 0$ and the Tikhonov filter factors $f_i = 1$ for $i = 1, \ldots, M$. Hence, comparing the regularized solution $\underline{X}_\lambda$ with the least squares solution $\underline{X}_{LS}$, we see that the filter factors practically filter out the contributions to the solution corresponding to small singular values, whilst they leave the SVD components corresponding to large singular values almost unaffected. Moreover, damping sets in for $\sigma_i \approx \lambda$.

### *3.3 Conjugate gradient method*

In this section, we describe a variational method that can be applied to solve the Cauchy problem. Since the boundary condition at $\Gamma_2$ is to be determined, we consider it as a control $v \in L^2(\Gamma_2)$ in a direct problem formulation to fit the Cauchy data $f \in L^2(\Gamma_1)$. Thus, we consider the direct problem

$$LT = 0 \tag{21}$$

$$T_{|\Gamma_2} = v \tag{22}$$

$$\frac{\partial T}{\partial \nu^+}|_{\Gamma_1} = q \tag{23}$$

with $q \in L^2(\Gamma_1)$. Assuming that $\Gamma$ is a Lipschitzian boundary consisting of two non-intersecting closed curves, $\Gamma_1$ and $\Gamma_2$, we note that since $q \in L^2(\Gamma_1)$ and $v \in L^2(\Gamma_2)$, there is a unique solution $T(q,v)$ of the direct problems (21)-(23) (Lions and Magenes, 1972). Then we aim to find $v$ such that

$$Av := T(q,v)_{|\Gamma_1} = f \tag{24}$$

In doing so, we try to minimise the functional

$$J(v) = \frac{1}{2}\|Av - f\|^2_{L^2(\Gamma_1)} \tag{25}$$

It has been established (Hao and Lesnic, 2000), that this functional is twice Frechet differentiable and its gradient can be calculated as

$$J'(v) = -\frac{\partial \psi}{\partial \nu^+}_{|\Gamma_2} \tag{26}$$

where $\psi$ is the solution of the adjoint problem

$$L\psi = 0 \tag{27}$$

$$\psi_{|\Gamma_2} = 0 \tag{28}$$

$$\frac{\partial \psi}{\partial \nu^+}|_{\Gamma_1} = T(q, v)_{|\Gamma_1} - f \tag{29}$$

Thus, the conjugate gradient method applied to our problem has the form of the following algorithm.

(i) Specify an initial guess $v_0$ for the temperature on $\Gamma_2$ and set $k = 0$.

(ii) Solve the direct problems (21)-(23) with $v = v_k$ and determine the *residual*

$$\tilde{r}_k := Av_k - f \tag{30}$$

(iii) Determine the gradient $r_k$ by solving the adjoint problems (27)-(29) with

$$\frac{\partial \psi_k}{\partial \nu^+_{|\Gamma_1}} = \tilde{r}_k \tag{31}$$

then calculate $d_k = -r_k + \beta_{k-1} d_{k-1}$, with the convention that $\beta_{-1} = 0$ and

$$\beta_{k-1} = \frac{\|r_k\|^2}{\|r_{k-1}\|^2} \tag{32}$$

(iv) Determine $A_0 d_k = T(0, d_k)_{|\Gamma_1}$ by solving the problems (21)-(23) with $q = 0$ and $v = d_k$,

$$v_{k+1} = v_k + \xi_k d_k, \tag{33}$$

$$\xi_k = \frac{\|r_k\|^2}{\|A_0 d_k\|^2} = \frac{\|r_k\|^2}{\|T(0, d_k)_{|\Gamma_1}\|^2} \tag{34}$$

(v) Increase $k$ by one and go to (ii) until a prescribed stopping criterion is satisfied.

It is known that, in general, the conjugate gradient method produces a stable solution for ill-posed problems, provided that a regularizing stopping criterion is used. The performance of this method for the Cauchy problem for anisotropic heat conduction is investigated and compared with other regularization methods in Section 5.

### *3.4 An alternating iterative algorithm*

Apart from general regularization methods, which can be applied for solving any ill-posed problems, typical solution methods may be developed for particular ill-posed problems. In this section, we describe such a particular regularization algorithm developed for Cauchy problems. The algorithm uses the fact that a part of the boundary is overspecified and the remainder is unspecified in order to reduce the ill-posed problem to a sequence of well-posed problems by alternating the given data on the overspecified part of the boundary. This iterative algorithm was first proposed by Kozlov and Mazya (1990) and consists of the following steps.

(i) Specify an initial boundary temperature guess $u_0$ on $\Gamma_2$.

(ii) Solve the mixed well-posed direct problem

$$\sum_{i,j=1}^{2} k_{ij} \frac{\partial^2 T^{(0)}}{\partial x_i \, \partial x_j} = 0 \tag{35}$$

$$T^{(0)}_{|\Gamma_2} = u_0; \quad \frac{\partial T^{(0)}}{\partial \nu^+}|_{\Gamma_1} = q \tag{36}$$

to determine $T^{(0)}(\underline{x})$ for $\underline{x} \in \Omega$ and $\nu_0 = \frac{\partial T^{(0)}}{\partial \nu^+}|_{\Gamma_2}$.

(iii) (a) If the approximation $T^{(2k)}$ is constructed, solve the mixed well-posed direct problem

$$\sum_{i,j=1}^{2} k_{ij} \frac{\partial^2 T^{(2k+1)}}{\partial x_i \, \partial x_j} = 0 \tag{37}$$

$$T^{(2k+1)}_{|\Gamma_1} = f; \quad \frac{\partial T^{(2k+1)}}{\partial \nu^+}|_{\Gamma_2} = \nu_k \tag{38}$$

to determine $T^{(2k+1)}(\underline{x})$ for $\underline{x} \in \Omega$ and $u_{k+1} = T^{(2k+1)}|_{\Gamma_0}$.

(b) Having constructed $T^{(2k+1)}$, solve the mixed well-posed direct problem

$$\sum_{i,j=1}^{2} k_{ij} \frac{\partial^2 T^{(2k+2)}}{\partial x_i \, \partial x_j} = 0 \tag{39}$$

$$T^{(2k+2)}_{|\Gamma_2} = u_{k+1}; \quad \frac{\partial T^{(2k+2)}}{\partial \nu^+}|_{\Gamma_1} = q \tag{40}$$

to determine $T^{(2k+2)}(\underline{x})$ for $\underline{x} \in \Omega$ and

$$\nu_{k+1} = \frac{\partial T^{(2k+2)}}{\partial \nu^+}|_{\Gamma_2}$$

(iv) Repeat step (iii) for $k \geq 0$ until a prescribed stopping criterion is satisfied.

According to Kozlov and Mazya (1990), the above algorithm produces two sequences of approximate solutions, namely $\{T^{(2k)}(x)\}_{k\geq 0}$ and $\{T^{(2k+1)}(x)\}_{k\geq 0}$, which both converge in $H^1(\Omega)$ to the solution $T$ of the Cauchy problem given by equations (1), (3) and (4) for any initial guess $u_0 \in H^{1/2}(\Gamma_2)$.

We note that, provided the initial guess $u_0$ is in $H^{1/2}(\Gamma_2)$ and the boundary data $f$ and $q$ are in $H^{1/2}(\Gamma_1)$ and $H^{1/2}(\Gamma_1)^*$, respectively, the problems given at step (iii) of the algorithm are both well-posed and uniquely solvable in $H^1(\Omega)$ (Lions and Magenes, 1972). These intermediate mixed well-posed problems are solved using the BEM described in Section 4.

The same conclusions about the convergence and the regularizing character are obtained, if at the step (i) we specify an initial guess for the heat flux $\nu_0 \in H^{1/2}(\Gamma_2)^*$, instead of an initial guess for the temperature $u_0 \in H^{1/2}(\Gamma_2)$, and we modify accordingly the steps (ii) and (iii) such that the mixed problems are solved. The algorithm did not converge, if in the steps (ii) and (iii) the mixed problems were replaced by Dirichlet or Neumann problems. In addition, the Neumann direct problem itself is ill-posed due to the non-uniqueness or non-existence of the solution, if the integral of the heat flux $q$ over the boundary $\Gamma$ vanishes or not, respectively.

A detailed numerical implementation of this algorithm may be found in Mera *et al.* (2000), where it was shown that, if a regularizing stopping criterion is used, then the iterative algorithm produces a convergent and stable numerical solution for the Cauchy problem considered. Therefore, only those features necessary to compare this iterative algorithm with other regularization methods are presented in this paper.

## 4. The BEM

BEM (Chang *et al.*, 1973; Wrobel, 2002) is used to discretise the Cauchy problem considered. One way of dealing with the anisotropicity is to transform the governing partial differential equation (1) into its canonical form by changing the spatial coordinates. However, after the transformation, the domain deforms and rotates and the boundary conditions become, in general, more complicated than the original ones. Therefore, rather than adopt this approach, we use the fundamental solution for the differential operator $L$ of the equation (1) in its original form. By using the fundamental solution of the heat equation and Green's identities, the governing partial differential equation (1) is transformed into the following integral equation (Chang *et al.*, 1973)

$$\eta(\underline{x})T(\underline{x}) = \int_\Gamma \left[ G(\underline{x},\underline{x}') \frac{\partial T}{\partial \nu^+}(\underline{x}') - T(\underline{x}') \frac{\partial G}{\partial \nu^+}(\underline{x},\underline{x}') \right] \mathrm{d}\Gamma_{\underline{x}'} \qquad (41)$$

where

(1) $\underline{x} \in \bar{\Omega}$, $\underline{x}' \in \Gamma$,

(2) $\eta(\underline{x}) = 1$, if $\underline{x} \in \Omega$ and $\eta(\underline{x}) = \frac{1}{2}$, if $\underline{x} \in \Gamma$ (smooth),

(3) $d\Gamma_{\underline{x}'}$ denotes the differential increment of $\Gamma$ at $\underline{x}'$

(4) $G$ is the fundamental solution of equation (1), namely,

$$G(\underline{x}, \underline{x}') = -\frac{|k^{ij}|^{\frac{1}{2}}}{2\pi} \ln(R) \tag{42}$$

where $k^{ij}$ is the inverse matrix to the matrix $k_{ij}$ and the geodesic distance $R$ is defined by

$$R^2 = \sum_{i,j=1}^{2} k^{ij}(x_i - x_i')(x_j - x_j'). \tag{43}$$

In practice, the boundary integral equation (41) may rarely be solved analytically and thus some form of numerical approximation is necessary. Generically, if the boundaries $\Gamma_1$ and $\Gamma_2$ are discretised into $N_1$ and $N_2$ boundary elements, then equation (41) reduces to solving the following system of linear algebraic equations

$$\mathbb{A}\underline{T}' - \mathbb{B}\underline{T} = 0 \tag{44}$$

where $\mathbb{A}$ and $\mathbb{B}$ are matrices which depend solely on the geometry of the boundary $\Gamma$ and can be calculated analytically. The vectors $\underline{T}$ and $\underline{T}'$ are the discretised values of the temperature and heat flux, respectively, which are assumed to be constant over each boundary element and take their values at the midpoint of each element. Equation (44) represents a system of $N$ linear algebraic equations with $2N$ unknowns, where $N = N_1 + N_2$. The discretisation of the boundary conditions given by equations (3) and (4) provides the values of $2N_1$ of the unknowns and the problem reduces to solving a system of $N_1 + N_2$ equations with $2N_2$ unknowns, which generically can be written as

$$\mathbb{C}\underline{X} = \underline{d} \tag{45}$$

where $\underline{d}$ is computed using the boundary conditions (3) and (4), the matrix $\mathbb{C}$ depends solely on the geometry of the boundary $\Gamma$ and the unknown vector $\underline{X}$ contains the values of the temperature and the heat flux on the boundary $\Gamma_1$. In order to determine the system of equation (45), we need to have $N_1 \geq N_2$ or $\text{meas}(\Gamma_1) \geq \text{meas}(\Gamma_2)$, which is in fact a necessary condition for the Cauchy problem to be numerically identifiable, when the mesh discretisation is uniform.

## 5. Numerical results and discussion

In order to illustrate the performance of the numerical method proposed, we solve a Cauchy problem in a two-dimensional smooth geometry such as the unit disc $\Omega = \{(x, y) | \quad x^2 + y^2 < 1\}$. We assume that the boundary $\Gamma = \{(x, y) | \quad x^2 + y^2 = 1\}$ of the solution domain is divided into two disjoint parts, namely, $\Gamma_1 = \{\underline{x} = (x, y) | \quad \underline{x} \in \Gamma, \theta(\underline{x}) \leq \alpha\}$ and $\Gamma_2 = \{\underline{x} = (x, y) | \underline{x} \in \Gamma, \theta(\underline{x}) > \alpha\}$ and where $\theta(\underline{x})$ is the angular polar coordinate of $\underline{x}$ and $\alpha$ is a specified angle in the interval $(0, 2\pi)$. In order to illustrate the typical numerical results, we have taken $\alpha = 3\pi/2$. Various values may be prescribed for $\alpha$, but a necessary condition for the inverse Cauchy problem to be numerically identifiable when a uniform mesh discretisation is adopted is that $\text{meas}(\Gamma_1) \geq \text{meas}(\Gamma_2)$, i.e. $\alpha \geq \pi$.

The most significant quantity to characterize the anisotropy of a medium is the determinant of the conductivity coefficients, i.e. $|k_{ij}| = k_{11}k_{22} - k_{12}^2$. The smaller the value of $|k_{ij}|$, the more asymmetric are the temperature fields and the heat flux vectors and the more difficult is the numerical calculation (Chang *et al.*, 1973). We consider a typical benchmark example which governs the steady heat conduction in a two-dimensional anisotropic medium with the thermal conductivity tensor $k_{ij}$ given by $k_{11} = 1.0$, $k_{12} = k_{21} = 0.5$ and $k_{22} = 1.0$, and the analytical temperature distribution to be retrieved, given by $T(x, y) = x^2 - 4xy + y^2$.

### *5.1 Direct approach*

The system of linear equation (45) cannot be solved by a direct approach, such as a Gaussian elimination method, since the sensitivity matrix $\mathbb{C}$ is ill-conditioned. The condition number $\text{cond}(\mathbb{C}) = \det(\mathbb{C}\mathbb{C}^{\mathrm{T}})$ of the sensitivity matrix $\mathbb{C}$ was calculated using the NAG subroutine F03AAF (NAG Fortran Library Manual, 1991), which evaluates the determinant of a matrix using the Crout factorisation method with partial pivoting. The condition number of the system of equation (45) was found to be $O(10^{-86})$ and $O(10^{-251})$ for $N = 40$ and 80 boundary elements while for numbers of boundary elements exceeding $N = 160$, the matrix $(\mathbb{C}\mathbb{C}^{\mathrm{T}})$ was found to be approximately singular, the value of its determinant becoming uncomputable, thus revealing the high degree of ill-posedness of the Cauchy problem being investigated. Thus, a direct approach to the problem produces a highly unstable solution and that is why regularization methods, such as those presented here, must be used.

### *5.2 Discrepancy principle*

The accuracy of the numerical solution $\underline{X}_\lambda$ obtained by using the regularization methods based on the singular value decomposition of the problem clearly depends on the choice of the parameter $\lambda$ which is known as the *regularization parameter*. Therefore, in order to obtain an accurate solution for an ill-conditioned problem, it is important to choose the regularization parameter that gives the right balance between the accuracy and the stability of the numerical solution. Currently, there are various criteria available for choosing the regularization parameter, but the most widely used is the *discrepancy principle* of Morozov (1966).

According to this principle, the regularization parameter should be chosen such that

$$\|\mathbb{C}\underline{X}_{\lambda} - \underline{d}\| \approx \delta \tag{46}$$

where $\delta$ is an estimate of the level of noise present in the problem, i.e.

$$\delta = \|\underline{d} - \underline{d}^{\in}\| \tag{47}$$

where $\underline{d}^{\in}$ is the perturbed value of the right hand side of the system of equation (6).

For the iterative regularization methods, the stability is ensured by stopping the iterative process at the point where the errors in predicting the exact solution start increasing. Thus, regularization is achieved by truncating the iterative process after a specific number of iterations and the number of iterations performed acts as a regularization parameter. Also for these iterative algorithms the discrepancy principle may be used for choosing the regularization parameter by stopping the iterative process when

$$\|\mathbb{C}\underline{X}_{k} - \underline{d}\| \approx \delta \tag{48}$$

where $\underline{X}_k$ is the numerical solution obtained for the discrete problem (45) by substituting in the vector $\underline{X}$ the boundary values of the heat flux and of the temperature calculated by the iterative method considered after $k$ iterations. Thus, for the iterative methods regularization is achieved by matching the number of iterations to the level of noise in the problem. For all the regularization methods considered in this paper, the regularization parameter was chosen using the discrepancy principle.

*5.3 Comparison of the numerical results*

It is the purpose of this section to present and compare the numerical results for the Cauchy problem, obtained using the four regularization methods mentioned earlier. In order to investigate the stability and the regularization properties of the methods considered, the boundary data $f = T|_{\Gamma_1}$ was perturbed as follows:

$$\tilde{f} = f + \tau \tag{49}$$

where $\tau$ is a Gaussian random variable with mean zero and standard deviation $\zeta = (s/100)\max|f|$ generated by the NAG routine G05DDF (NAG Fortran Library Manual, 1991) and $s$ is the percentage of additive noise included in the input data $T|_{\Gamma_1}$ in order to simulate the inherent measurement errors.

The numerical results presented in this section were obtained using $N = 160$ boundary elements. Various number of boundary elements were tested, but it was found that no substantial improvement in the numerical solution is obtained, if the number of boundary elements is increased above $N = 160$.

The TSVD and Tikhonov regularization methods were applied to the overdetermined system of linear equation (45) in order to simultaneously retrieve the temperature and the heat flux on the boundary $\Gamma_2$. Figure 1(a) and (b) shows the numerical solution obtained by using the TSVD and the Tikhonov

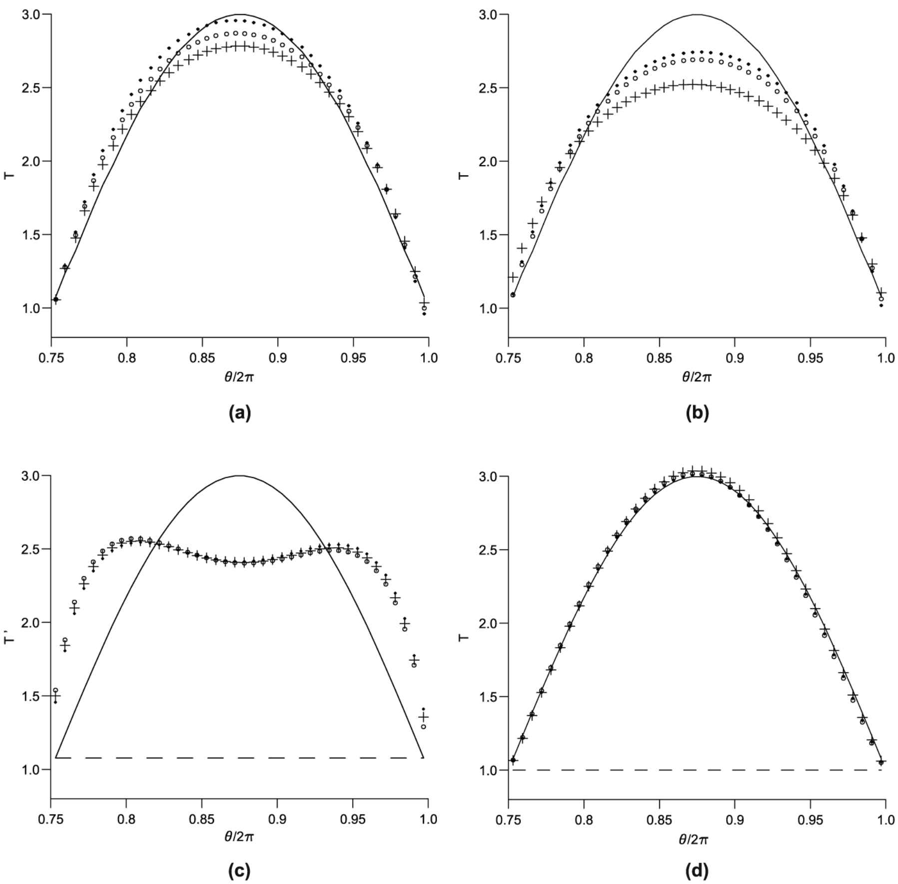



**Figure 1.**
The numerical solution for the temperature on the boundary $\Gamma_2$ obtained by using (a) the SVD method, (b) the Tikhonov regularization method, (c) the conjugate gradient method and (d) the iterative alternating algorithm described in Section 3.4 for $N=160$ boundary elements and various levels of noise, namely, $s = 1$ per cent (•), $s = 3$ per cent (○) and $s = 5$ per cent (+), in comparison with the exact solution (–)

regularization method, respectively, for the temperature on boundary $\Gamma_2$ for various levels of noise $s \in \{1, 3, 5\}$. It can be seen that as $s$ decreases, the numerical solution approximates better than the exact solution while remaining stable. If the level of noise is not too big, then the numerical solution obtained by TSVD is a good approximation for the exact solution.

We note that the numerical solution obtained by the Tikhonov regularization method is less accurate than the numerical solution obtained by the TSVD method, but it is still a reasonably good approximation to the exact solution of the problem since we have solved a highly ill-posed problem.

Although, not presented here, it is reported that for both the TSVD and the Tikhonov regularization methods, the discrepancy principle was found to be very efficient in choosing the optimum value of the regularization parameter, i.e. the level of truncation for the singular values of the matrix $\mathbb{C}$ and the parameter $\lambda$. Numerous other test examples have been investigated and it was found that both the TSVD and the Tikhonov regularization methods produce a convergent and stable solution with respect to decreasing the amount of noise. However, the TSVD was found to produce in general more accurate results than the Tikhonov regularization method.

The conjugate gradient method and the alternating iterative algorithm described in Section 3.4 both require an initial guess to be specified for the temperature on the boundary $\Gamma_2$. This initial guess is improved at every iteration and approaches the exact solution. Therefore, the rate of convergence and the accuracy of these methods clearly depend on how close to the exact solution is the initial guess specified. Since the temperature at the end-points of the boundary $\Gamma_2$ is known, the most natural initial guess is a function, which ensures the continuity of the temperature at these points and is a linear function with respect to the angular polar coordinate $\theta$. For the test example considered in this paper, the initial guess is given by the constant function $u_0 = v_0 = 1$.

The numerical results for the temperature on the boundary $\Gamma_2$ obtained by the conjugate gradient method for various levels of noise are presented in Figure 1(c) in comparison with the exact solution and the initial guess specified. It can be seen that the numerical solution is not accurate even for small levels of noise. We note that the test example considered here is a very severe test example for iterative methods since the exact solution is very far from the most natural initial guess available. Numerous test example have been investigated and it was found that the conjugate gradient method produces good results for simple test examples for which the initial guess is not very far from the exact solution. However, for more difficult test examples, as the one presented in this paper, the method failed to produce accurate results for the unspecified boundary data.

A detailed BEM numerical implementation of the alternating iterative algorithm presented in Section 3.4 was given in Mera *et al.* (2000). It was shown that a substantial improvement in the rate of convergence is obtained by relaxing the marching condition

$$u_{k+1} = T^{(2k+1)}|_{\Gamma_2}$$

through

$$u_{k+1} = \varphi T^{(2k+1)}|_{\Gamma_2} + (1 - \varphi)u_k$$

when passing from step iii(a) to iii(b), where $\varphi$ is a variable relaxation factor with respect to the angular polar coordinate given by

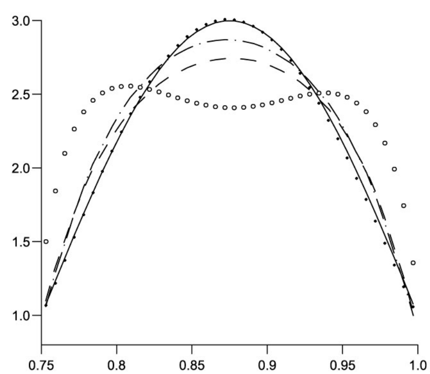
$$\varphi(\theta) = A\sin\left[\pi\left(\frac{\theta - \alpha}{2\pi - \alpha}\right)\right] \tag{50}$$

and $A \in [0, 2]$ is a positive constant. This relaxation procedure was found not only to reduce the number of iterations necessary to obtain the convergence but also to substantially increase the accuracy of the numerical solution. We note that the same relaxation procedure was found to be very efficient in increasing the rate of convergence also for the conjugate gradient method.

Figure 1(d) presents the numerical solution for the temperature on the boundary $\Gamma_2$ obtained using the iterative alternating algorithm presented in Section 3.4 coupled with the relaxation procedure (50) in comparison with the exact solution and the initial guess. It can be seen that even for large amounts of noise added into the input data, there is a very good agreement between the numerical and the exact solution for the problem. Therefore, it can be concluded that this alternating iterative algorithm is very efficient in regularizing the Cauchy problem considered.

We note that for both the conjugate gradient method and for the iterative alternating algorithm presented in Section 3.4, the regularization is achieved by truncating the iterative process at the point where the errors in predicting the exact solution start increasing. Thus, a stable solution is achieved by matching the number of iterations to the level of noise present in the data. Although not presented here, it is reported that the discrepancy principle was found to be efficient in choosing the regularization parameter also for these iterative methods. However, it was found to be more robust for the iterative alternating algorithm than for the conjugate gradient method.

In order to compare the four regularization method considered, Figure 2 graphically shows the numerical solution for the temperature on the boundary obtained with each of these methods for $N = 160$ boundary elements and $s = 3$ per cent noise.




**Note:** Obtained by using various regularization methods, namely, the iterative alternating algorithm described in Section 3.4 (•), the SVD method (– · – · –), the Tikhonov regularization method (- - -) and the conjugate gradient method (o) for $N = 160$ boundary elements and $s = 3\%$ noise in comparison with the exact solution (——)

**Figure 2.**
The numerical solution for the temperature on the boundary $\Gamma_2$

It can be seen that the most accurate solution is the one given by the iterative alternating algorithm of Kozlov and Mazya (1990). The TSVD and the Tikhonov regularization methods both give a reasonably good approximation for the temperature on the boundary, but TSVD was in general found to produce more accurate results. The numerical solution obtained by the conjugate gradient method is very poor in comparison with the numerical solutions obtained by the other methods. However, for less severe test examples, it was found that also the conjugate gradient method produces numerical solutions almost as accurate as the numerical solution obtained by the Tikhonov regularization method. The differences between the regularization methods considered are even large, if the numerical solution for the heat flux is sought. Figure 3 presents the numerical solution for the heat flux on the boundary $\Gamma_2$ obtained with regularization methods for $N = 160$ boundary elements and $s = 3$ per cent noise.

Again it can be seen that the TSVD method outperforms the Tikhonov regularization method while both of them produce more accurate results than the conjugate gradient method. However, for all these three methods, the numerical solution for the heat flux is far from the exact solution. In the case of the heat flux, the iterative alternating algorithm of Kozlov and Mazya (1990) was the only method that produced accurate results. It can be seen in Figure 3 that the numerical solution for the heat flux obtained by this algorithm is in a very good agreement with the exact solution while the other methods considered fail to produce accurate results. Numerous other test examples have been investigated and similar conclusions have been drawn.

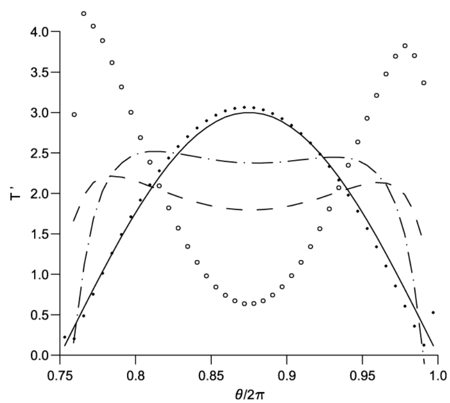



**Figure 3.**
The numerical solution for the heat flux on the boundary $\Gamma_2$

**Note:** Obtained by using various regularization methods, namely, the iterative alternating algorithm described in Section 3.4 (•), the SVD method (– · – · –), the Tikhonov regularization method (- - -) and the conjugate gradient method (o) for $N = 160$ boundary elements and $s = 3\%$ noise in comparison with the exact solution (——)

## 6. Conclusions

In this paper, four regularization methods were investigated and compared for a Cauchy problem in the steady-state anisotropic heat conduction. Three of the methods considered were general regularization methods while the fourth one was an alternating iterative algorithm developed for the Cauchy problems. It was found that the Cauchy problem can be regularized by any of the regularization methods considered since all of them produced a stable numerical solution.

However, the numerical solutions obtained by these methods differ in terms of accuracy. It was found that the TSVD method outperforms the Tikhonov regularization method while the latter outperforms the conjugate gradient method. All these three general regularization methods were outperformed by the iterative alternating algorithm described in Section 3.4. We note that for the severe test example considered, the conjugate gradient method failed to produce an accurate solution both for the temperature and the heat flux. A possible reason for this is that in the conjugate gradient method described in Section 3.3, the boundaries $\Gamma_1$ and $\Gamma_2$ should be disjoint non-intersecting closed curves which is not the case for our test example considered. The TSVD method and Tikhonov regularization methods were found to produce reasonably accurate results for the temperature, but they were both found to be less accurate for the heat flux. The iterative alternating algorithm of Kozlov and Mazya (1990) was found to be the only method to produce a good approximation for both the temperature and the heat flux.

Overall, it may be concluded that the Cauchy problem for the anisotropic steady-state heat conduction may be regularized by various methods such as the general regularization methods presented in this paper, but more accurate results are obtained by particular methods such as the iterative alternating algorithm investigated in this paper, which takes into account the particular structure of the problem.

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## Further reading

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