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N.B.: When citing this work, cite the original publication.

Berntsson, F., Chen, L., Xu, T., Wokiyi, D., (2017), An efficient regularization method for a large scale ill-posed geothermal problem, *Computers & Geosciences*, 105, 1-9.
<https://dx.doi.org/10.1016/j.cageo.2017.04.010>

Original publication available at:

<https://dx.doi.org/10.1016/j.cageo.2017.04.010>

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An efficient regularization method for a large scale ill-posed geothermal problem

Fredrik Berntsson*, Chen Lin[†], Tao Xu[‡] and Dennis Wokiyi*

May 5, 2017

Abstract

The inverse geothermal problem consists of estimating the temperature distribution below the earth's surface using measurements on the surface. The problem is important since temperature governs a variety of geologic processes, including the generation of magmas and the deformation style of rocks. Since the thermal properties of rocks depend strongly on temperature the problem is non-linear.

The problem is formulated as an ill-posed operator equation, where the righthand side is the heat-flux at the surface level. Since the problem is ill-posed regularization is needed. In this study we demonstrate that Tikhonov regularization can be implemented efficiently for solving the operator equation. The algorithm is based on having a code for solving a well-posed problem related to the above mentioned operator. The algorithm is designed in such a way that it can deal with both $2D$ and $3D$ calculations.

Numerical results, for $2D$ domains, show that the algorithm works well and the inverse problem can be solved accurately with a realistic noise level in the surface data.

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1 Introduction

Temperature controls many physical properties of rocks and governs a variety of geologic processes, including the generation of magmas and the deformation style of rocks [1, 3, 20, 26], see also [9, 10, 23]. Thus, knowledge of the thermal structure of the lithosphere is essential for understanding geophysical observations and dynamic processes in the deep interior. However, temperature cannot be directly measured beyond a few kilometers depth, in deep mines or drill holes [12, 21]. To obtain the information about the temperature distribution in the lithosphere, the surface observations, e.g. surface heat flux, are extrapolated to the lithosphere base using a heat conduction model [5, 8]. Since the thermal conductivity of rocks are temperature and pressure dependent [11] the problem is non-linear. For the one-dimensional case an analytical solution can be found [7, 14] but for the two or three-dimensional case numerical modeling is required. Several previous studies investigated this type of problems using the least squares approach, see [32, 29], and also [19, 9], but these authors did not strictly treat the nonlinear aspect resulting from the temperature-dependent thermal properties of rocks.

The inverse geothermal problem can be formulated as a boundary value problem for the stationary heat equation in a domain, but where the temperature and heat-flux data are only known on a part of the boundary. This is often referred to as the Cauchy problem for the heat equation [2, 15], see also [4] and [5]. The problem is ill-posed and a regularization technique is needed to stabilize the computations, see [35] for a good overview of regularization techniques used in geophysics.

We reformulate the problem as a non-linear operator equation; where the operator maps the heat-flux at the lower boundary to the heat-flux at the surface level. The operator can thus be evaluated by solving a well-posed boundary value problem for the temperature distribution inside the domain under consideration. The inverse problem is solved by using Tikhonov regularization. In our implementation we solve the normal equations, that correspond to the minimization of the Tikhonov functional, using the conjugate gradient method. The bulk of the computational work in the algorithm consists of solving several linear systems of equations originating from a finite difference discretization of the underlying well-posed boundary value problem. We also show how to treat the non-linearity of the problem. An important feature of the algorithm is that it can be generalized to the case surface data is available on a $2D$ area and the temperature distribution for a $3D$ region below the surface is desired.

The outline of this paper is as follows: In Section 2 we introduce a well-posed boundary value problem for the heat-equation that allows us to reformulate the inverse geothermal problem as a non-linear operator equation. We also give the details of our thermal model. In Section 3 we start by investigating

the inverse geothermal problem for the case of a constant thermal conductivity and heat production. For this case we can use the singular value decomposition and demonstrate the ill-posedness of the problem. Also we apply Tikhonov regularization and give numerical results. The non-linear case is treated in Section 4. We show how to implement Tikhonov regularization efficiently by using the conjugate gradient method. Finally, we give numerical results in Section 4.2 and present conclusions in Section 5.

2 The Direct Problem

For geothermal calculations the goal is to estimate the temperature distribution in the lithosphere [9]. The model is two dimensional and confined to the domain $(x, z) \in \Omega = (0, L_x) \times (0, L_z)$, where x is the lateral coordinate, and z is the depth.

The boundary of the domain Ω consists of the *surface* where measurements are available, the *base* where we specify the heat flux, and the *sides* where we assume a zero flux. Thus the thermal model is the following: The temperature $T(x, z) \in C^2(\Omega) \cap C^1(\bar{\Omega})$ satisfies,

$$\begin{cases} (\kappa T_x)_x + (\kappa T_z)_z + A_p = 0, & 0 < x < L_x, \quad 0 < z < L_z, \\ T_x(0, z) = T_x(L_x, z) = 0, & 0 < z < L_z, \\ T(x, 0) = T_0(x), & 0 < x < L_x, \\ \kappa T_z(x, L_z) = Q_m(x), & 0 < x < L_x, \end{cases} \quad (2.1)$$

where $\kappa := \kappa(x, z, T)$ is the thermal conductivity and $A_p := A_p(x, z, T)$, or more commonly $A_p := A_p(x, z)$, is the heat production. The above problem is *well-posed* [13] and provided that we have access to the heat-flow Q_m and the surface temperature T_0 we can compute the temperature distribution $T(x, z)$ in the domain Ω . This allows us to define a non-linear operator as follows: In (2.1) we consider the surface temperature T_0 to be fixed. If, in addition, we specify the heat-flux Q_m then we have a well-posed problem that we can solve for the temperature distribution $T(x, z)$ in the domain. Having obtained $T(x, z)$ we can compute the surface heat-flux Q_0 . This means that we can introduce a mapping from Q_m to Q_0 that we denote by

$$Q_0 = \kappa T_z(x, 0) = \mathcal{K}(\kappa, A_p, T_0)Q_m, \quad (2.2)$$

In order to simplify the notation in the paper we also introduce a function

$$[T, Q_0] = \mathcal{F}(\kappa, A_p, T_0, Q_m), \quad Q_0 = \kappa T_z|_{z=0}. \quad (2.3)$$

Note that since the model is non-linear an iterative procedure is required for evaluating the operator $\mathcal{K}$ or the function $\mathcal{F}$. We refer to evaluating the operator

93 $\mathcal{K}$, for a given heat-flux Q_m , i.e. solving (2.1), as the *direct problem*. In contrast
 94 solving operator equation (2.2), for a given surface heat-flux Q_0 , is referred to
 95 as the *inverse problem*, see Section 3.

96 2.1 Numerical Solution of the Direct Problem

97 If the thermal conductivity and the heat production are independent of the
 98 temperature, i.e. $\kappa := \kappa(x, z)$ and $A_p := A_p(x, z)$, then solving (2.1) is a
 99 standard problem.

100 By introducing a computational grid (x_i, z_j) , $i = 1, \dots, N$ and $j = 1, \dots, M$, on
 101 the domain Ω , we represent the function $T(x, z)$ by its values at the grid points,
 102 i.e. the unknowns are $T = (T_{i,j}) = (T(x_i, z_j))$. Similarly the boundary data T_0
 103 and Q_m are represented by vectors, e.g. $Q_m = (Q_m(x_i))$. Thus, having a code
 104 for solving (2.1) effectively means that we have have a functional relation

$$[T, Q_0] = FDM(\kappa, A_p, T_0, Q_m), \quad (2.4)$$

105 where T , κ , and A_p are matrices, and T_0 , Q_0 and Q_m are vectors. The above
 106 function represents a discrete approximation of the function $\mathcal{F}$, see (2.3), and
 107 can be used to approximate the operator $\mathcal{K}$, introduced in (2.2).

108 In our work we use finite differences [31] to discretize the differential equation.
 109 The details of our code are described briefly. At interior points we discretize
 110 the governing equation using a symmetric difference approximation,

$$(\kappa T_x)_x(x_i, z_j) = \frac{1}{\Delta x^2} \left(\kappa_{i-\frac{1}{2},j} T_{i-1,j} - (\kappa_{i-\frac{1}{2},j} + \kappa_{i+\frac{1}{2},j}) T_{i,j} + \kappa_{i+\frac{1}{2},j} T_{i+1,j} \right), \quad (2.5)$$

111 where the values of $\kappa(x, z)$ at half-index points are evaluated using linear in-
 112 terpolation. Neumann-type boundary conditions, e.g. $\kappa T_z(x, L_z) = Q_m(x)$ or
 113 $T_z(0, z) = 0$, are implemented using one-sided finite differences. The finite dif-
 114 ference approximation leads to a linear system of equations $Au = b$, where u is
 115 a vector that contains the temperature values at the grid points. Having solved
 116 for u we can compute the surface heat flux using a one sided difference quotient.

117 We remark that the linear system $Au = b$ is large and sparse but can be solved
 118 effectively using either direct or iterative methods. Also, the matrix A only
 119 depends on the thermal conductivity κ . The righthand side b contains the
 120 boundary data, i.e. T_0 and Q_m , and also the heat production values A_p at
 121 interior points.

Layer	κ_0 ($W/m^\circ C$)	c ($1/^\circ C$)	A_p (W/m^3)
Sediment	3.0	0	$1.5 \cdot 10^{-6}$
Upper Crust	3.0	$1.5 \cdot 10^{-3}$	$2.0 \cdot 10^{-6}$
Lower Crust	2.6	$1.0 \cdot 10^{-4}$	$0.45 \cdot 10^{-6}$
Mantle	2.5	$-2.5 \cdot 10^{-4}$	$0.02 \cdot 10^{-6}$

Table 1: The parameters used in our model of the thermal conductivity κ and heat production A_p in the different lithosphere layers, see [6, 11, 14].

2.2 A Numerical Example with Artificial Data

In order to illustrate the geothermal problem we give numerical results for case where we picked a realistic heat-flux Q_m at the base of the model and solved the problem (2.1) using finite differences. Note that this is an artificially generated test problem with a known solution. For the actual application the heat-flux at the base of the model, i.e. Q_m , would be unknown. Having a test problem with a known heat flux Q_m is convenient for testing purposes.

In our previous paper [9] we used actual measured data at the surface to estimate Q_m for the eastern Tibetan margin. In this work we use the same model for the thermal conductivity and the heat production. The thermal conductivity, at crustal conditions, is assumed to vary inversely with temperature [7, 8], i.e.

$$\kappa = \frac{\kappa_0}{1 + cT}, \quad (2.6)$$

where κ_0 is the thermal conductivity at surface conditions and c is an experimentally determined constant. At low temperatures the thermal conductivity generally decreases with increasing temperature, i.e. $c > 0$, while in the range $300 - 500^\circ C$ the conductivity varies very little with temperature. At temperatures above $500^\circ C$ the conductivity instead increases with temperature, i.e. $c < 0$ [30]. Further we assume that the heat production, i.e. A_p in (2.1), is constant in each lithosphere layer. For discussions of more detailed heat production models see [27, 18]. The specific values used in our simulations are listed in Table 1, see also Figure 1. Note that the heat production is not temperature dependent.

For the numerical simulations, with the above thermal model, we picked a computational grid (x_i, z_j) , with $N = 300$ equidistant grid points in the x -direction, and $M = 250$ grid points in the z -direction. The physical size of the computational domain was where $L_x = 560 km$ and $L_z = 80 km$. At the surface we used a constant temperature $T_0 = 10^\circ C$. The heat-flux Q_m is seen in Figure 1.

Starting from the initial guess $T^{(0)}(x, z) = 0$ we used our finite difference code

149 to solve (2.1) iteratively,

$$[T^{(k+1)}, Q_0^{(k+1)}] = FDM(\kappa(T^{(k)}), A_p(T^{(k)}), T_0, Q_m);$$

150 until the update $\|T^{(k+1)} - T^{(k)}\|_F$ is sufficiently small. At each step we solve a
151 sparse linear system of size 75000×75000 , with 371412 non-zero elements.

152 The convergence is rather fast, see Figure 1. The final temperature distribution
153 $T(x, z)$, after convergence, is also displayed. We emphasize that the choice of
154 the initial approximation $T^{(0)}(x, z) = 0$ is not very good and thus we start with
155 a large error. Still only about five iterations are needed to reach a sufficiently
156 small error.

157 It is interesting to note that the temperature in the mantle layer varies in the
158 interval $500 < T < 1150^\circ C$. This means that the thermal conductivity changes
159 significantly, $5.1 < \kappa < 6.3 W/m^\circ C$ [34], within the mantle layer. Thus a
160 constant value for the thermal conductivity in the whole mantle layer would not
161 give an accurate solution.

162 3 The Linear Inverse Problem and Regulariza- 163 tion

164 In the previous section we presented the thermal model that is used for our
165 test simulations. Provided that we have access to the heat-flow Q_m at the base
166 of the model and the surface temperature T_0 we can solve (2.1) and obtain
167 the temperature distribution $T(x, z)$. In practice we cannot measure the heat-
168 flux Q_m . Instead we measure both the temperature T_0 and the heat-flux Q_0
169 at surface level; i.e. we have *Cauchy data* $[T_0, Q_0]$ and want to compute the
170 corresponding heat-flux Q_m . Thus we consider (2.2) as a non-linear operator
171 equation,

$$\mathcal{K}Q_m = Q_0, \quad \mathcal{K} := \mathcal{K}(\kappa, A_p, T_0), \quad (3.7)$$

172 that can be solved for the desired heat-flux Q_m .

173 In our model the thermal conductivity and heat production are temperature de-
174 pendent. Even though we are interested in solving the non-linear equation (3.7)
175 we begin by studying the case where the coefficients κ and A_p are independent
176 of the temperature. We assume that an approximate temperature distribution
177 $T^{(0)}$ is available and use the notation

$$\kappa := \kappa(x, z) := \kappa(x, z, T^{(0)}), \quad \text{and,} \quad A_p := A_p(x, z) := A_p(x, z, T^{(0)}),$$

178 in the remainder of this section.

Figure 1: For the test problem we illustrate the heat-flux Q_m at the base of the model (top,left), and the convergence history $\|T^{(k)} - T^{(k-1)}\|_F$, measured in the Frobenius norm (top,right). The temperature distribution $T(x, z)$ in the lithosphere (bottom,left) and the thermal conductivity $\kappa(x, z, T)$ (bottom,right) are also displayed.

179 In the case where the thermal conductivity κ and heat production A_p are both
 180 independent of the temperature we can transform the operator (2.2) into a linear
 181 operator. The procedure is as follows: First, find a function $V(x, z)$ that satisfies
 182 (2.1) with the heat-flux $T_z(L_z, x) = 0$ at the base of the model, i.e.

$$[V, Q_1] = \mathcal{F}(\kappa, A_p, T_0, 0). \quad (3.8)$$

183 Second, set the surface temperature and the heat production to zero, so that
 184 W is defined by

$$[W, Q_2] = \mathcal{F}(\kappa, 0, 0, Q_m), \quad (3.9)$$

185 Then $T = V + W$ and we have $Q_0 = Q_1 + Q_2$. We conclude that

$$\tilde{\mathcal{K}}Q_m = Q_2 = Q_0 - Q_1, \quad \tilde{\mathcal{K}} = \mathcal{K}(\kappa, 0, 0), \quad (3.10)$$

186 and that $\tilde{\mathcal{K}}$ is a *linear* operator.

187 3.1 Analysis of the Linear Problem

188 In this section we study the linear operator $\tilde{\mathcal{K}}$ analytically. In order to be able
189 to carry out the analysis we simplify the model and assume that the thermal
190 conductivity κ is a constant.

191 Taking $A_p=0, T_0=0$ and κ a constant, the problem (2.1) transforms into

$$\begin{cases} T_{xx} + T_{zz} = 0, & 0 < x < L_x, \quad 0 < z < L_z, \\ T_x(0, z) = T_x(L_x, z) = 0, & 0 < z < L_z, \\ T(x, 0) = 0, & 0 < x < L_x, \\ \kappa T_z(x, L_z) = Q_m(x), & 0 < x < L_x. \end{cases} \quad (3.11)$$

192 By separation of variables, we can write the solution as

$$T(x, z) = \sum_{n=0}^{\infty} a_n \cos\left(\frac{n\pi x}{L_x}\right) \left(-e^{-\frac{n\pi z}{L_x}} + e^{\frac{n\pi z}{L_x}}\right). \quad (3.12)$$

193 The condition $\kappa T_z(x, L_z) = Q_m(x)$ can also be written as

$$\kappa T_z(x, L_z) = \sum_{n=1}^{\infty} \kappa a_n \cos\left(\frac{n\pi x}{L_x}\right) \left(\frac{n\pi}{L_x} e^{-\frac{n\pi L_z}{L_x}} + \frac{n\pi}{L_x} e^{\frac{n\pi L_z}{L_x}}\right) = Q_m(x),$$

194 If we then write $Q_m(x)$ as a Fourier cosine series,

$$Q_m(x) = \sum_{n=1}^{\infty} A_n \cos\left(\frac{n\pi x}{L_x}\right), \text{ where } A_n = \frac{2}{L_x} \int_0^{L_x} Q_m(x) \cos\left(\frac{n\pi x}{L_x}\right) dx, \quad (3.13)$$

195 and compare the two expressions we find that the constants a_n can be written
196 as

$$a_n = \frac{2\kappa^{-1}}{n\pi \left(e^{-\frac{n\pi L_z}{L_x}} + e^{\frac{n\pi L_z}{L_x}}\right)} \int_0^{L_x} Q_m(x) \cos\left(\frac{n\pi x}{L_x}\right) dx. \quad (3.14)$$

197 At the earth's surface the heat flux $\kappa T_z(x, 0) = Q_0$ is then given by

$$\kappa T_z(x, 0) = \sum_{n=1}^{\infty} \kappa \frac{2n\pi a_n}{L_x} \cos\left(\frac{n\pi x}{L_x}\right) = Q_0(x),$$

198 substituting for a_n and reorganizing the expression gives the result

$$\int_0^{L_x} \sum_{n=0}^{\infty} \frac{4}{L_x \left(e^{-\frac{n\pi L_z}{L_x}} + e^{\frac{n\pi L_z}{L_x}}\right)} \cos\left(\frac{n\pi x'}{L_x}\right) \cos\left(\frac{n\pi x}{L_x}\right) Q_m(x') dx' = Q_0(x).$$

199 The above solution formula can be interpreted as follows: If proper function
200 spaces are introduced the operator $\tilde{\mathcal{K}}$ is compact and its singular system [13] is

201 given by

$$\{\sigma_n, u_n, v_n\} = \left\{ \frac{1}{e^{-n\pi\frac{L_z}{L_x}} + e^{n\pi\frac{L_z}{L_x}}}, \frac{2}{\sqrt{L_x}} \cos\left(\frac{n\pi}{L_x}x\right), \frac{2}{\sqrt{L_x}} \cos\left(\frac{n\pi}{L_x}x\right) \right\}. \quad (3.15)$$

202 The degree of ill-posedness for an operator equation, e.g. (3.10), is defined in
 203 terms of its singular values [13, p. 40]. If the singular values decay as $\mathcal{O}(n^{-\alpha})$,
 204 for some $\alpha > 0$, then the problem is *mildly ill-posed*. If on the other hand the
 205 singular values decay exponentially, i.e. as $\mathcal{O}(e^{-n\alpha})$, then the operator equation
 206 is *severely ill-posed*. In our case the singular values decays exponentially, which
 207 indicates that the operator equation $\tilde{\mathcal{K}}Q_m = Q_0$ is severely ill-posed.

208 3.2 Numerical Solution of the Linear Inverse Problem

209 After having introduced a computational grid (x_i, z_j) the functions T , κ , and
 210 A_p are represented by matrices, and Q_0 , T_0 , and Q_m are vectors. The linear
 211 operator $\tilde{\mathcal{K}}$, see (3.10), is approximated by a matrix-relation

$$\tilde{K}Q_m := FDM(\kappa, 0, 0, Q_m). \quad (3.16)$$

212 The product of the matrix $\tilde{K}$ and a vector Q_m can be computed by solving a
 213 well-posed boundary value problem using our code. Let $\{e_i\}$ be the standard
 214 basis on $\mathbb{R}^N$. Since the above relation is linear we can compute the matrix $\tilde{K}$
 215 explicitly by,

$$\tilde{K}(:, i) = \tilde{K}e_i = FDM(\kappa, 0, 0, e_i), \quad i = 1, \dots, N. \quad (3.17)$$

216 In the remainder of this section we are concerned with solving the ill-conditioned
 217 linear system of equations,

$$\tilde{K}Q_m = \tilde{Q}_0, \quad (3.18)$$

218 where the vector $\tilde{Q}_0$ is computed as, see (3.10),

$$[V, Q_1] = FDM(\kappa, A_p, T_0, 0), \quad \text{and} \quad \tilde{Q}_0 = Q_0 - Q_1. \quad (3.19)$$

219 The linear system (3.18) is ill-conditioned and regularization is needed[13, 16].
 220 We use Tikhonov regularization[25, 33]; i.e. the regularized solution is computed
 221 by minimizing the Tikhonov functional,

$$\|\tilde{K}Q_m^\lambda - \tilde{Q}_0\|_2^2 + \lambda^2 \|Q_m^\lambda\|_2^2, \quad (3.20)$$

222 where $\lambda > 0$ is a regularization parameter. If the matrix $\tilde{K}$ is explicitly known
 223 then the solution can be computed efficiently using the singular value decom-
 224 position [16].

225 The above techniques can be summarized as follows: For the case of temperature
 226 independent coefficients the inverse problem (3.7) can be solved using Tikhonov
 227 regularization. We obtain a functional relation,

$$Q_m^\lambda := LT(\kappa, A_p, T_0, Q_0, \lambda). \quad (3.21)$$

228 where, as previously, κ and A_p are matrices, and Q_0^λ , T_0 , and Q_0 are vectors,
 229 and λ is a scalar.

230 The regularization parameter λ controls the weight given to the regularization
 231 term, $\lambda^2 \|Q_m^\lambda\|_2$, relative to the residual $\|\tilde{K}Q_m^\lambda - \tilde{Q}_0\|_2$. If only a little regular-
 232 ization is used, i.e. if λ is small, then the noise can be magnified during the
 233 computations and destroy the solution. If more regularization is used, i.e. a
 234 larger λ , then the noise is effectively filtered out but the solution may be too
 235 smooth and the residual might be large.

236 The appropriate choice of the parameter λ represents a compromise between
 237 accuracy, i.e. keeping the residual small, and stability, i.e. preventing the
 238 noise from being magnified too much. There are several standard methods for
 239 selecting a good regularization parameter for a concrete problem. Two of the
 240 most widely used are the *Discrepancy principle* and the *L-curve*.

241 The Discrepancy principle, attributed to Morozov[24], can be used if the noise
 242 level in the data is available. The regularization parameter λ is then defined as

$$\lambda := \sup\{\lambda > 0 \mid \|KQ_m^\lambda - \tilde{Q}_0^\delta\| \leq \tau\delta\}, \quad (3.22)$$

243 where δ is the noise level, and $\tau \geq 1$ is a suitable constant. This means that the
 244 method finds a solution where the residual is of the same order of magnitude
 245 as the noise level in the data. The discrepancy principle is known to work
 246 well under very general assumptions regarding the ill-posed problem its applied
 247 to[13].

248 The L-curve, originally introduced in [22], see also [17], which is a plot of the
 249 residual norm $\|KQ_m^\lambda - \tilde{Q}_0^\delta\|_2$ versus $\|Q_m^\lambda\|_2$ for different values of λ , is a con-
 250 venient graphical tool for analysis of ill-posed problems. The L-curve displays
 251 the compromise between the minimization of the two quantities. For discrete
 252 ill-posed problems, the L-curve, when plotted in a log-log scale, often has a char-
 253 acteristic L-shaped appearance with a distinct corner separating the vertical and
 254 horizontal parts of the curve. Less regularization corresponds to the uppermost
 255 part of the curve and more regularization corresponds to the rightmost of the
 256 curve. The optimal regularization parameter, that ensures a solution with a
 257 good balance between the noise magnification and the approximation error is
 258 the value λ that corresponds to the corner[16].

Figure 2: The singular values $\{\sigma_k\}$ for the computed matrix $\tilde{K}$. The singular values decay exponentially, illustrating that the operator equation $\tilde{K}Q_m = \tilde{Q}_0$ is severely ill-posed. Only about 60 of the values σ_k are above the machine precision.

259 3.3 A Numerical Example

260 In order to illustrate the ill-posedness of the operator $\tilde{K}$, and also the effects of
 261 applying Tikhonov regularization we solve a numerically generated test problem
 262 and present the results. The test problem is the one presented in Section 2.2,
 263 i.e. the grid (x_i, z_j) consists of $N = 300$ points in the x -direction and $M = 250$
 264 points in the z -direction.

265 By selecting a vector Q_m , representing the exact heat flux at the base of the
 266 model, and solving the direct problem repeatedly until convergence, we obtain
 267 Cauchy data $[T_0, Q_0]$, at the surface level, matrices κ and A_p representing the
 268 thermal conductivity and heat production on the grid.

269 First, using the technique described in Section 3, we compute the matrix $\tilde{K}$, of
 270 size 300×300 , representing the linear operator. Since the matrix is relatively
 271 small we can compute its singular value decomposition. The results are dis-
 272 played in Figure 2. The results clearly demonstrate that the problem is severely
 273 ill-posed.

274 Secondly we add artificially generated noise to the Cauchy data $[T_0, Q_0]$. For
 275 this test we use normally distributed noise of variance $\epsilon_1 = 5 \cdot 10^{-3} \text{ } ^\circ\text{C}$ and
 276 $\epsilon_2 = 5 \cdot 10^{-5} \text{ W/m}^\circ\text{C}$ to obtain the simulated measurements $[T_0^{\epsilon_1}, Q_0^{\epsilon_2}]$. The
 277 simulated data vectors are illustrated in Figure 3. The noise is of a realistic order
 278 of magnitude. In order to find a good value of the regularization parameter we
 279 use the L -curve, and minimize the Tikhonov functional for a range of parameter
 280 values λ . The method predicts that $\lambda = 6.3 \cdot 10^{-3}$ is an appropriate value for the

Figure 3: We display the data vectors $Q_0^{\epsilon_2}$ (top,left) and $T_0^{\epsilon_1}$ (top,right). In both cases we display the noisy data (black curve) and the exact data (blue curve). The L -curve technique is used to identify a suitable value for λ (bottom,left). The corner point (red,ring) corresponds to $\lambda = 6.3 \cdot 10^{-3}$. The results obtained using $\lambda = 6.3 \cdot 10^{-3}$ (bottom,left) are also displayed. The Tikhonov solution Q_m^λ (blue curve) and the exact solution Q_m (black dashed curve) are presented.

281 regularization parameter. Even though the data contains significant amounts
 282 of noise the reconstruction of the heat flux at the base of the model is very
 283 successful.

284 In order to illustrate the ill-posedness of the problem we also solve the equation
 285 using less regularization. The solution Q_m^λ computed using $\lambda = 7 \cdot 10^{-4}$ is
 286 displayed in Figure 4. Clearly the solution is highly oscillating as a result
 287 of noise magnification during the computations. Also we present a solution
 288 computed using $\lambda = 9 \cdot 10^{-2}$. In this case too much regularization results in a
 289 too smooth solution and features from the exact solution are not reconstructed
 290 accurately.

Figure 4: We display the Tikhonov solutions Q_m^λ , using $\lambda = 7 \cdot 10^{-4}$ (left, blue curve) and $\lambda = 9 \cdot 10^{-2}$ (right, blue curve). In the first case the not enough regularization has been applied and in the second case we have too much regularization. The exact solution Q_m (black dashed curve) is also presented.

291 4 The Non-linear Problem

292 We recall that our goal is to solve the non-linear case, where both the thermal
 293 conductivity κ and the heat production A_p depend on the temperature. Our
 294 idea is to solve a sequence of linear problems using Tikhonov regularization. Let
 295 $T^{(0)}$ be an approximate temperature distribution. The algorithm is as follows:
 296 First solve the linearized problem using Tikhonov regularization to obtain

$$Q_m^{(k+1),\lambda} := LT(\kappa(T^{(k)}), A_p(T^{(k)}), T_0, Q_0, \lambda). \quad (4.23)$$

297 The new approximate heat-flux $Q_m^{(k+1),\lambda}$, at the base of the model, is then used
 298 to compute the next temperature distribution

$$T^{(k+1)} := FDM(\kappa(T^{(k)}), A_p(T^{(k)}), T_0, Q_m^{(k+1),\lambda}). \quad (4.24)$$

299 The process is repeated until the update $\|T^{(k+1)} - T^{(k)}\|_F$ is sufficiently small.

300 The algorithm works well, provided that a sufficiently large regularization pa-
 301 rameter λ is used, but is computationally demanding. At each step we need to
 302 form a linear system of equations $Au = b$, see Section 2.1. For relatively small
 303 grid sizes, i.e. 2D calculations, it is feasible to solve the linear system using
 304 Gaussian elimination. If the matrix $\tilde{K}$, see (3.17), is desired then we make use
 305 of the observation that the matrix A only depends on the thermal conductivity
 306 $\kappa(T^{(k)})$. Thus we can compute the LU decomposition of the sparse matrix A
 307 and reuse it when evaluating $\tilde{K}e_i$, for all the basis vectors e_i . After having
 308 computed the matrix $\tilde{K}$ explicitly we can easily find the regularized solution of
 309 the inverse problem by solving the least squares problem (3.20).

310 4.1 Modified Normal Equations and an Iterative Method

311 For large grid sizes, e.g. 3D calculations, it is necessary to avoid forming $\tilde{K}$,
 312 see (3.17), explicitly. Instead we note that the minimization problem (3.20) is
 313 equivalent to solving the *modified normal equations*,

$$(\tilde{K}^T \tilde{K} + \lambda^2 I) Q_m^\lambda = \tilde{K}^T \tilde{Q}_0. \quad (4.25)$$

314 Instead of forming the matrix $\tilde{K}$ explicitly we solve the normal equations using
 315 the conjugate gradient method[28]. The matrix-vector product $\tilde{K} Q_m$ can be
 316 evaluated by solving the direct problem using finite differences, i.e.

$$\tilde{K} Q_m := FDM(\kappa, 0, 0, Q_m). \quad (4.26)$$

317 The core of the finite difference code is a linear system of equations $Au = b$,
 318 where $u_k = T(x_i, z_j)$, $k = (i-1)n+j$. The right hand side b is zero except for a
 319 block that contains the vector Q_m . In matrix form this can be written as

$$b = W_2 Q_m, \quad W_2 \in \mathbb{R}^{NM \times N},$$

320 where W_2 is a matrix that places the values in Q_m at the correct locations in
 321 the vector b . After having computed the temperatures T_{ij} at the grid points a
 322 finite difference formula is used to obtain the heat-flux at the surface level. This
 323 can also be represented in matrix form as

$$\tilde{Q}_0 = W_1 u, \quad W_1 \in \mathbb{R}^{N \times NM},$$

324 where W_1 is a matrix that computes a finite difference approximation of the
 325 surface heat flux given the temperature values stored in the vector u . The
 326 matrix $\tilde{K}$ can be written in factorized form as,

$$\tilde{Q}_0 = W_1 u = W_1 A^{-1} b = W_1 A^{-1} W_2 Q_m = \tilde{K} Q_m, \quad (4.27)$$

327 and its transpose can be written as,

$$\tilde{K}^T = W_2^T (A^T)^{-1} W_1^T. \quad (4.28)$$

328 In order to evaluate a matrix-vector product $\tilde{K}^T Q$ we need to solve a system
 329 of equations involving the matrix A^T . Our finite difference code is written so
 330 it can compute matrix-vector products involving both $\tilde{K}$ and $\tilde{K}^T$. In order to
 331 evaluate the product,

$$(\tilde{K}^T \tilde{K} + \lambda^2 I) Q_m$$

332 we need to form the matrix A once and we need to solve two linear systems of
 333 equations (one with A and one with A^T). Note that if the LU decomposition
 334 of A is computed then the relation $A^T P^T = U^T L^T$ can be used to solve the
 335 system involving A^T efficiently. If the matrix A is too large, e.g. the 3D case,
 336 then instead we use an iterative method, e.g. CG or GMRES[28].

Thus in the implementation of (4.23) the minimization problem (3.20) is solved by finding the solution $Q^{(k+1),\lambda}$ of the linear system of equations,

$$((\tilde{K}^{(k)})^T \tilde{K}^{(k)} + \lambda^2 I) Q_m^{(k+1),\lambda} = (\tilde{K}^{(k)})^T \tilde{Q}_0, \quad (4.29)$$

where $\tilde{K}^{(k)}$ is the matrix defined by the relation (4.26) above; with $\kappa := \kappa(T^{(k)})$. The previous solution $Q_m^{(k),\lambda}$ can be used as an initial guess to start the CG iterations.

4.2 Numerical Tests for the Non-Linear Problem

Here we present the results from the numerical testing of the methods. For all tests we use the numerically constructed example from Section 2.2. The grid (x_i, z_j) consists of $N = 300$ points in the x -direction and $M = 250$ points in the z -direction. For the tests a vector Q_m , representing the exact heat-flux at the base of the model, was selected and the direct problem solved repeatedly until convergence. In all cases the direct problems were solved with sufficient accuracy that the generated Cauchy data $[T_0, Q_0]$ can be considered exact.

To the generated Cauchy data we add normally distributed noise of variance ϵ_1 and ϵ_2 to obtain the simulated measurements $[T_0^{\epsilon_1}, Q_0^{\epsilon_2}]$. The vectors T_0 and Q_0 are of different orders of magnitude so it is important to use different noise levels for the temperature and heat-flux vectors respectively. For our tests we used the noise levels $\epsilon_1 = 5 \cdot 10^{-3} {}^\circ C$ and $\epsilon_2 = 5 \cdot 10^{-5} W/m {}^\circ C$. The simulated data vectors are illustrated in Figure 5. The noise levels are realistic. The same data vectors and noise are used for all tests presented in the text below.

The purpose of the tests is to illustrate how the algorithm for solving the non-

Figure 5: The simulated Cauchy data at the surface level. We display the heat-flux Q_0 (left) and the temperature T_0 . In both cases we display both the exact function (blue,dashed curve) and the noisy function (black, solid curve).

Figure 6: Results for non-linear Tikhonov regularization. We display the heat-flux Q_m at the base of the model (right, dashed blue curve) the approximation $Q_m^{(10),\lambda}$ (right, black curve), and the convergence history $\|T^{(k),\lambda} - T^{(k-1),\lambda}\|_F$, measured in the Frobenius norm (left).

linear problem, i.e. the steps (4.24) and (4.24), works in practice. For the Tikhonov regularization to work well a good regularization parameter is needed. We suggest that the L -curve is used and in our tests we use the value $\lambda = 6.3 \cdot 10^{-3}$ that was obtained by the L -curve for the constant coefficient case, see Section 3.2.

For the first test we use the simplest implementation of Tikhonov regularization, i.e. in each step the matrix $\tilde{K}^{(k)}$, defined by the relation (3.18), is computed explicitly and the minimization problem (3.20) is solved by computing the SVD of the matrix. It is also assumed that the linear systems of equations that arise due to the finite difference discretizations are solved using a sparse LU decomposition.

The results are presented in Figure 6. The convergence is rapid and only 3 iterations is enough to reach a level where the first decimal digits of the temperatures $T^{(k)}$ stops changing. The large initial error is due to the poor starting guess $T^{(0)} = 0$.

We remark that this is a very inefficient approach. At each step of the algorithm we need to solve two different types of finite difference equations. First, the functional relation (3.19) is implemented by first forming the matrix in the finite difference equations and computing its LU decomposition. Second, we need to form the finite difference equations defined by the relation (3.16), compute its LU decomposition and solve $2N$ triangular linear systems to obtain the matrix $\tilde{K}^{(k)}$. Minimizing the small Tikhonov functional, e.g. (3.20), is cheap by comparison and the cost can be neglected.

In our second test we solve the same problem again using the iterative implemen-

Figure 7: Results obtained using the iterative implementation of Tikhonov regularization. We display the convergence history $\|T^{(k),\lambda} - T^{(k-1),\lambda}\|_F$, measured in the Frobenius norm (left) and also the number of CG iterations needed to reach the stopping criteria at each step of the algorithm (right). The stopping criteria for the CG iterations were set at either 10^{-9} (blue curves) and 10^{-5} (red curves).

382 tation of Tikhonov regularization, see Section 4.1. The starting guess $T^{(0)} = 0$
383 was used and the stopping criteria for the CG iterations was a relative resid-
384 ual of magnitude less than 10^{-9} . The results are illustrated in Figure 7. Note
385 that after iteration 8 the solution from the previous step already satisfies the
386 stopping criteria and the algorithm can be said to have converged to desired
387 precision, also as the quality of the solution improves fewer CG iterations are
388 needed. The obtained solution $Q_m^{(8),\lambda}$ is presented in Figure 8. The quality of
389 the obtained solution is the same as the one seen previously in Figure 6. Note
390 that even $Q^{(k),\lambda}$ has converged the temperature $T^{(k),\lambda}$ can still change due to
391 the fact that the problem is non-linear and $\kappa(T^{(k),\lambda})$ is recomputed in each step.

392 The computational work for the second test is as follows. For each step of the
393 algorithm we need to form two linear systems corresponding to (3.19) and (3.16).
394 The first system is solved once and the second needs to be solved twice during
395 each step in the CG algorithm. The amount of work required is significantly
396 less than for the first test above.

397 In order to further reduce the amount of computational work we stop the CG
398 iterations when the relative residual is less than 10^{-5} . This means the linear
399 systems are solved less accurately. The results are also displayed in Figure 7.
400 Here it is enough to perform 5 iterations to reach convergence. A total 10
401 systems of finite difference equations needs to be formed, and 58 linear system
402 solves are needed. The obtained solution $Q_m^{(5),\lambda}$, after 5 steps of the algorithm,
403 is displayed in Figure 8.

Figure 8: Results for the iterative implementation of Tikhonov regularization. We display the heat-flux Q_m at the base of the model (dashed blue curves) and the computed approximations $Q_m^{(8),\lambda}$ (left, black curve), for the case then the stopping in the CG algorithm criteria was set to 10^{-9} and also the solution $Q_m^{(5),\lambda}$ (right, black curve) for the case when the stopping criteria were 10^{-5} . The two solutions are of equally good quality.

5 Concluding Remarks

In this paper we have presented the inverse geothermal problem. The application is important since many geophysical process are influenced by the temperature. The physical properties of rocks depend strongly on the temperature and the problem is non-linear.

We have demonstrated that the problem is severely ill-posed and regularization is needed. One of the most popular regularization techniques is Tikhonovs method. The method requires that we rewrite the geothermal problem as an operator equation, and minimize a related least squares problem. The tests in the paper demonstrates that this approach works well. Though the results may be sensitive with respect to the thermal model used the influence from random measurement errors is relatively small and the computations are numerically stable.

Our implementation is based on having a finite difference solver for a related, well-posed, direct problem. We show how to use software for the direct problem when implementing Tikhonov regularization for the inverse problem. Our algorithm is iterative and the conjugate gradient method is used for solving the normal equations that appear due to the Tikhonov regularization. The method is efficient and solving the inverse problem requires only about an order of magnitude additional work compared to solving only the direct problem. It is worth noting that instead starting from a finite element solver for the direct problem would work equally well.

426 In our work we consider only $2D$ models however the algorithm can be expected
 427 to work well for $3D$ calculations as well. As long as the corresponding direct
 428 problem can be solved we can also solve the inverse problem. Calculations on a
 429 realistic full $3D$ model is something we intend to do in the future.

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