THE MOLLIFICATION METHOD AND THE NUMERICAL SOLUTION OF THE INVERSE HEAT CONDUCTION PROBLEM BY FINITE DIFFERENCES

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Abstract—The inverse heat conduction problem involves the calculation of surface heat flux and/or temperature histories from transient, measured temperatures inside solids. We consider the one dimensional semi-infinite linear case and present a new solution algorithm based on a data filtering interpretation of the mollification method that automatically determines the radius of mollification depending on the amount of noise in the data and finite differences. A fully explicit and stable space marching scheme is developed. We describe several numerical experiments of interest showing that the new procedure is accurate and stable with respect to perturbations in the data even for small dimensionless time steps.

1. INTRODUCTION

In several practical contexts, it is sometimes necessary to estimate the surface heat flux and/or temperature histories from transient, measured temperatures inside solids. This inverse heat conduction problem (IHCP) is frequently encountered, for example, in the determination of thermal constants in some quenching processes, the estimation of surface heat transfer measurements taken within the skin of a reentry vehicle, the determination of aerodynamic heating in wind tunnels and rocket nozzles, the design and development of calorimeter type instrumentation, the experimental determination of thermophysical properties of materials, and infrared computerized tomography.

The IHCP is a mathematically improperly posed problem because the solution does not depend continuously upon the data, that is, small errors in the interior data induce large errors in the surface heat flux or in the surface temperature solutions.

Several researchers have examined the IHCP and a number of different solution methods have been reported in the literature (see, for example, the comprehensive account given in Beck et al., [1] and the references therein). By attempting to reconstruct a slightly "mollified" or "filtered" image of the unknowns, Manselli and Miller [2] and Murio [3] have shown that it is possible to restore certain types of continuous dependence on the data. Beck [4] has attempted to stabilize the IHCP using several future-time temperatures with a least squares method to calculate components of the heat flux or temperature at a given time. A number of methods have been introduced based on deconvolution or regularization techniques [5-13]. In most cases, the problem is reformulated as a Volterra integral equation of the first kind.

Time marching finite difference algorithms for the approximate solution of the IHCP have been presented by Blackwell [14] and Beck et al. [15] without fully addressing the question of numerical stability. However, the use of finite differences—as opposed to the integral representation approach—allows for a straightforward discretization of the differential equation even for problems with non-constant coefficients or, more generally, for nonlinear problems. In this setting, maximum computational flexibility might be obtained by implementing space marching finite difference methods for the numerical solution of the IHCP. Such an approach was introduced by Weber [16], who replaced the heat equation with a closely related hyperbolic one. The numerical stability of this method can be greatly improved by judiciously "filtering" the noisy data [17]. Carasso [18] combined the regularization method with a space marching algorithm, restoring continuous dependence on the data up to, but not including, the boundary. Hensel and Hills [19] also developed a space marching finite difference procedure—the stability question remaining unanswered—based on a new interpretation of the mollification method originally presented by
Manselli and Miller [2]. In any case, it is not immediately obvious how to numerically implement these last two algorithms since no discussion on the choice of the regularization parameter or the radius of mollification, respectively, is given.

In this paper, a new fully explicit and stable space marching finite difference method is introduced, using the interpretation of the mollification method given by Hensel and Hills [19] and further developed by Murio [20]. Our approximation is generated initially by automatically filtering the noisy data by discrete convolution with a suitable averaging kernel and then using finite differences, marching in space, to numerically solve the associated well-posed problem.

In Section 2, the nondiscrete version of the semi-infinite one dimensional problem with constant thermal properties is presented. With data specified on a continuum of times and data error measured in the $L_2$ norm, we derive stability bounds for the IHCP. We examine only the linear problem of heat conduction for easy of presentation; the same technique may be applied to nonlinear problems with suitable modifications.

The discretized problem, involving data at only a discrete sampling of times, is studied in Section 3. We show that the finite difference scheme is stable and consistent with the stabilized version of the IHCP.

Section 4 describes the procedure that uniquely determines the radius of mollification as a function of the amount of noise in the data.

The efficiency of the method is demonstrated in Section 5, where, together with a detailed description of the algorithm we present the results of several numerical experiments of interest.

Section 6 gives a summary and some conclusions.

2. DESCRIPTION OF THE PROBLEM

We consider a one-dimensional semi-infinite slab. After measuring the transient history temperature $F(t)$ at the interior point $x = 1$, it is desired to recover the boundary temperature function $f(t)$ at $x = 0$. We assume linear heat conduction with constant coefficients and without loss of generality, the problem is normalized by using dimensionless quantities.

The problem can be described mathematically as follows:

The unknown temperature $u(x, t)$ satisfies

\[ u_{xx} = u, \quad x > 0, \quad t > 0, \]  
\[ u(1, t) = F(t), \quad t > 0, \quad \text{with corresponding approximate data function } F_m(t), \]  
\[ u(x, 0) = 0, \quad x > 0, \]  
\[ u(0, t) = f(t), \quad t > 0, \quad \text{the desired but unknown temperature function}, \]  
\[ u(x, t) \text{ bounded as } x \to \infty. \]

In order to use some results from Fourier integral analysis, we extend the functions $F(t)$, $F_m(t)$ and $f(t)$ to the whole real $t$-axis by defining them to be zero for $t < 0$. We assume that all the functions involved are $L_2$ functions in $(-\infty, \infty)$ and use the corresponding $L_2$ norm, as defined below, to measure errors:

\[ \| f \| \left[ \int_{-\infty}^{+\infty} \left| f(t) \right|^2 dt \right]^{1/2}. \]

In this setting, it is quite natural to also assume that the exact data function $F(t)$ and the measured data function $F_m(t)$ satisfy the $L_2$ data error bound

\[ \| F - F_m \| \leq \varepsilon. \]
If
\[ \hat{f}(w) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(t) \exp(iwt) \, dt, \quad -\infty < w < \infty, \] (4)
denotes the Fourier transform of \( f \), transforming equation (1a), we get
\[ \frac{\partial^2 \hat{u}}{\partial x^2}(x, w) = -iw \hat{u}(x, w), \quad x \geq 0, \quad -\infty < w < \infty, \quad i = \sqrt{-1}. \] (5)

Taking into account equations (1d) and (1e), the unique solution of equation (5) is given by
\[ \hat{u}(x, w) = \exp\left[ \frac{x}{w} \right] \hat{\alpha}(0, w), \] (6)
where \( \sigma = \text{sign}(w) \).

For the inverse problem, we have
\[ \hat{u}(0, w) = \exp\left[ \frac{x}{w} \right] \hat{\alpha}(x, w). \] (7)

In particular, for \( x = 1 \), we obtain
\[ \hat{f}(w) = \exp\left[ \frac{x}{w} \right] \hat{F}(w). \] (8)

Attempting to go from \( F(t) \) to \( f(t) \) magnifies an error in a high frequency component by the factor \( \exp\left( \frac{x}{w} \right) \), showing that the IHCP is greatly ill-posed in the high frequency components.

We notice that from Parseval’s equality, \( \| f \|_2 = 1/\sqrt{2\pi} \| \hat{f} \| \) and for this norm to be finite, equation (8) implies a very rapid decay of the high frequency components of the Fourier transform of the exact data function \( F(t) \). The situation is quite different for the measured data function \( F_m(t) \). A realization of this function can be obtained by adding a random perturbation to the exact data function \( F(t) \) so that \( F_m(t) \) is an \( L_\infty(\mathbb{R}) \) function, but there is no reason to expect for all the high frequency components of the Fourier transform of the random noise function to decay as rapidly as required by equation (8).

**Stabilized Problem**

The IHCP can be stabilized if, instead of attempting to find the point values of the temperature function \( f(t) \), we attempt to reconstruct the \( \delta \)-mollification of the function \( f \) at time \( t \), given by
\[ J_\delta f(t) = (p_\delta * f)(t), \] (9)
where
\[ p_\delta(t) = \frac{1}{\delta \sqrt{\pi}} \exp\left( -t^2/\delta^2 \right) \] (10)
is the Gaussian kernel of radius \( \delta > 0 \). We observe that \( p_\delta \) and \( J_\delta f \) are \( C^\infty \) (infinitely differentiable) functions in \( (-\infty, \infty) \), with \( p_\delta \geq 0 \) and \( \int_{-\infty}^{\infty} p_\delta(s) \, ds = 1 \). The function \( p_\delta \) falls to nearly zero outside a few radii from its center \( (\approx 3\delta) \). For any locally integrable function \( f \), \( \| J_\delta f - f \| \to 0 \) as \( \delta \to 0 \), the convergence being uniform on any compact set where \( f \) is continuous [21]. \( J_\delta f \) behaves much like \( f \), but it is very smooth. Moreover, the Fourier transform of \( J_\delta f \),
\[ \hat{J}_\delta f(w) = 2\pi \hat{p}_\delta(w) \hat{f}(w) = \exp\left( -w^2\delta^2/4 \right) \hat{f}(w), \] (11)
shows that the mollification in equation (9) damps those Fourier components of \( f \) with wavelength \( 2\pi/w \) much shorter than \( 2\pi\delta \); the longer wavelengths are damped hardly at all.

Mollifying equation (8), we get
\[ \hat{p}_\delta(w) \hat{f}(w) = \exp\left[ \sqrt{\frac{w}{2}} (1 - i\sigma) \right] \hat{p}_\delta(w) \hat{F}(w). \] (12)
The function

\[ M_\delta(w) = \exp[\sqrt{w/2}(1 - i\sigma)]\hat{\rho}_\delta(w) \]

\[ = \exp[\sqrt{w/2}(1 - i\sigma) - w\delta^2/4] \] (13)

is uniformly bounded for \(-\infty < w < \infty\). More precisely,

\[ \max_w |M(w)| = \exp[1/(2(2\delta^2)^{1/3})]. \] (14)

From equation (12), using equation (14), we obtain

\[ |\hat{\rho}_\delta(w)\hat{f}(w)| \leq \exp[1/(2(2\delta^2)^{1/3})]|\hat{F}(w)|. \] (15)

Squaring, integrating and using Parseval’s equality, it follows that

\[ \|J_\delta f\| \leq 2\pi \exp[1/(2(2\delta^2)^{1/3})] \|F\|. \] (16)

If \( \hat{J}_\delta f_m(w) = 2\pi\hat{\rho}_\delta(w)\hat{F}_m(w) \) indicates the Fourier transform of the mollified boundary transient temperature history obtained using equation (12) with \( \hat{F}_m(w) \) instead of \( \hat{F}(w) \), we get

\[ \hat{\rho}_\delta(w)\hat{F}_m(w) = \exp[\sqrt{w/2}(1 - i\sigma)]\hat{\rho}_\delta(w)\hat{F}_m(w). \] (17)

Subtracting equation (17) from equation (12) and repeating the same procedure as for obtaining equation (16), we get

\[ \|J_\delta f - J_\delta f_m\| \leq 2\pi \exp[1/(2(2\delta^2)^{1/3})] \|F - F_m\|. \] (18)

Finally, using equation (3),

\[ \|J_\delta f - J_\delta f_m\| \leq \epsilon 2\pi \exp[1/(2(2\delta^2)^{1/3})]. \] (19)

This shows that attempting to reconstruct \( J_\delta f \) at some times \( t \) of interest and for some radius \( \delta > 0 \), is a formally stable problem with respect to perturbations in the data. The error is guaranteed to go to zero as \( \epsilon \to 0 \) for fixed \( \delta \). Alternatively, the stability analysis also shows that the high frequency components of the function \( \hat{\rho}_\delta(w)\hat{F}_m(w) \) in equation (17) must decay as rapidly as the high frequency components of the Fourier transform of the exact data function \( F(t) \) in equation (8). This observation allows for a new interpretation of the mollified method, suggested by Hensel and Hills [19]: The function \( \hat{\rho}_\delta(w)\hat{F}_m(w) \) in Fourier space, can be thought, in real space, as a suitable filtered data function \( J_\delta f_m(t) = (\hat{\rho}_\delta\ast\hat{F}_m)(t) \) that transforms the evaluation of \( J_\delta f_m \) into a mathematically stable problem.

We thus have the following stabilized problem: Attempt to find the linear functional \( J_\delta f_m(t) = J_\delta u(0, t) \) at some times \( t \) of interest and for some blurring radius \( \delta \), given that \( J_\delta u(x, t) \) satisfies

\[ (J_\delta u)_{xx}(x, t) = (J_\delta u)(x, t), \quad x > 0, \quad t > 0, \] (20a)

\[ J_\delta u(x, 0) = 0, \quad x > 0, \] (20b)

\[ J_\delta u(1, t) = J_\delta F_1(t), \quad t \geq 0, \] (20c)

However, due to technical reasons to be fully explained in Section 3, we consider a slightly further modified well-posed problem: Attempt to find the linear functional \( J_\delta z_m(t) = J_\delta z(0, t) \) at some times \( t \) of interest and for some blurring radius \( \delta \), given that \( J_\delta z(x, t) \) satisfies

\[ (J_\delta z)_{xx}(x, t) = (J_\delta z)(x, t) - \gamma J_\delta z(x, t), \quad x > 0, \quad t > 0, \] (21a)

\[ J_\delta z(x, t) = 0, \quad x > 0, \] (21b)

\[ J_\delta z(1, t) = J_\delta F_1(t), \quad t > 0, \] (21c)

where \( \gamma \) is a “small” positive constant.
The unique solutions of problems (20) and (21), $J_\delta u$ and $J_\delta z$ respectively, are related by

$$J_\delta z(x, t) = e^{\delta t} J_\delta u(x, t), \quad x \geq 0, \quad t > 0,$$

and, in particular,

$$J_\delta z_m(t) = e^{\delta t} J_\delta f_m(t), \quad t > 0.$$  (23)

To estimate the $L_2$ norm of the error between the exact boundary temperature history $f(t)$ and the approximate boundary temperature function $J_\delta z_m(t)$, on any finite interval of interest $T = \{ t: 0 \leq t \leq t_T \}$, we can proceed as follows: From

$$f(t) - J_\delta z_m(t) = f(t) - J_\delta f(t) + J_\delta f(t) - J_\delta f_m(t) + J_\delta f_m(t) - J_\delta z_m(t),$$

taking norms,

$$\| f - J_\delta z_m \|_T \leq \| f - J_\delta f \|_T + \| J_\delta f - J_\delta f_m \|_T + \| J_\delta f_m - J_\delta z_m \|_T$$  (24)

It is well known that $\| f - J_\delta f \|_T \to 0$ as $\delta \to 0$, but without further hypothesis on $f$, it is difficult to estimate the rate of convergence as a function of the radius of mollification. On the other hand, if we assume, for example, that $\| df/dt \|_T \leq M_1$, then we immediately get

$$\| f - J_\delta f \|_T \leq C_1 M_1 \delta = 0(\delta),$$  (25)

where $C_1$ is a constant independent of $\delta$ [21].

Using equation (23), we have

$$J_\delta z_m(t) - J_\delta f_m(t) = J_\delta f_m(1 - e^{\delta t}),$$  (26)

and recalling that $\| J_\delta f_m \|_T \leq M_2$ for some constant $M_2 > 0$, we obtain

$$\| J_\delta z_m - J_\delta f_m \|_T \leq M_2 T \gamma = 0(\gamma).$$  (27)

From equation (19), it follows that

$$\| J_\delta f - J_\delta f_m \|_T \leq \epsilon 2\pi \exp[1/(2(2\delta^2)^{1/3})].$$  (28)

Using inequalities (25), (27) and (28) in equation (24), we get the estimate

$$\| f - J_\delta z_m \|_T \leq 0(\delta) + \epsilon \exp[1/(2(2\delta^2)^{1/3})] + 0(\gamma).$$  (29)

In Section 3 we analyze a finite difference approximation that converges, as the mesh parameters tend to zero, to $J_\delta z_m$, the solution of the stabilized IHCP (21). The discrete error estimate is obtained, essentially, by adding the corresponding truncation error associated with equation (27) to the estimate (29).

The determination of the radius of mollification, $\delta$, as a function of the amount of noise in the data, $\epsilon$, is discussed in Section 4.

3. DISCRETIZED PROBLEM

Given a fixed radius of mollification $\delta$, in this section we consider the approximate solution of the mollified problem (21) by means of finite difference equations (FDE). Without loss of generality, we attempt to reconstruct the unknown mollified boundary temperature function $J_\delta z_m$ at the sample points of the time interval $I = [0, 1]$. We introduce a uniform grid by defining the following discrete set of points in the $x, t$ plane:

$$x_n = nh, \quad n = 0, 1, \ldots, N - 1, N; \quad Nh = 1,$$  (30)

and

$$t_j = jk, \quad j = 0, 1, \ldots, M - 1, M; \quad Ml = L, L > 1.$$
If the grid function \( v \) in our finite difference approximation is denoted by \( v^j = v(x_n, t_s) \), then the discrete convolution of the Gaussian kernel \( p_\delta(t) \) (restricted to the grid points) and the grid function \( v \) at the grid point \((x_n, t_s)\) is denoted by \( \tilde{V}^j = (p_\delta * v)(x_n, t_s) \). Notice that \( \tilde{V}^j = F^j_m(t_s) \) and \( V^j_0 = 0 \).

We approximate the partial differential equation (21a) by the finite difference quotients

\[
\frac{1}{h^2} [V^j_{n+1} - 2V^j_n + V^j_{n-1}] = \frac{1}{2k} [V^j_{n+1} - V^j_{n-1} - \gamma V^j_n],
\]

\( n = N - 1, N - 2, \ldots, 2, 1; \quad 1 < j \leq M - 1. \) (31)

The exact solution of the differential equation (21a), \( \partial \varphi / \partial \tau \), when restricted to the grid points, fails to satisfy the FDE (31) at the grid point \((x_n, t_s)\) by the amount

\[
- \frac{h^2}{12} \frac{\delta^4}{\delta x^4} (p_\delta * z)(\bar{x}, \bar{t}) + \frac{k^2}{6} \frac{\partial^3}{\partial t^3} (p_\delta * z)(\bar{x}, \bar{t}),
\]

\((n - 1)h < \bar{x} < (n + 1)h, \quad (j - 1)k < \bar{t} < (j + 1)k.\) Assuming \( |\delta^4/\delta x^4(p_\delta * z)(x, t)| < \infty, x \geq 0, t > 0,\) the FDE (31) is a second order approximation in space and time, i.e. the local (global) truncation error behaves as \( O(h^2 + k^2) \) as \( h, k \rightarrow 0 \). The FDE (31) is consistent with the partial differential equation (21a). For computational purposes, the system of equations (31) should be rewritten

\[
V^j_n = \frac{h^2}{2k} [V^j_{n+1} - V^j_{n-1}] + (2 - \gamma) V^j_{n+1} - V^j_{n+2},
\]

\( n = N - 2, N - 3, \ldots, 1, 0; \quad j = 0, 1, \ldots, M - N + n + 1. \) (32)

Equation (32) shows that two initial conditions are necessary to determine a solution. This is in complete agreement with the fact that equation (21a) is being treated as a second order ordinary differential equation when marching in space. Physically, this means that an extra thermocouple should be implanted at location \( x = 1 - \frac{h}{2} \) to obtain the measured data function \( F^j_m(t_j) \). Thus, we assume that \( V^j_0 = (p_\delta * F^j_m)(t_j) \) and \( V^j_{N-1} = (p_\delta * p^j_{\delta})(t_j), j = 0, 1, \ldots, M - 1, M \) are given with \( F^j_m \) satisfying the data error bound \( \| F^j_m - F^j_{m-1} \| \leq \epsilon \), similar to equation (3). As we march backward in space, at each step we must drop the evaluation of the interior temperature at the highest previous point in time. Since at the end of the \( N \)th iteration in space, we want to evaluate \( V^j_N \) at the grid points of \( I = [0, 1] \), we need to determine the minimum initial length, \( L = Mk \), of the data sample interval. \( L \) depends on the ratio \( h/k \) and might be obtained by imposing the condition \( Mk - (N - 1)k = 1 \). This leads to

\[
L = Mk = 1 - k + k/h.
\]

For \( 0 \leq n \leq N - 2 \), the corresponding maximum of the time index is \( j = M - N + n + 1 \).

In order to analyze the numerical value stability of our method, we recall that given a function \( g_j = g(jk), j \text{ integer}, \) defined on the whole discrete line, we can define the discrete Fourier transform of \( g, \hat{g} \), by

\[
\hat{g}(w) = \sum_j g_j \exp(ikw), \quad 0 \leq |w| \leq \pi/k, \quad i = \sqrt{-1}.
\]

Applying the discrete Fourier transform to the system (31), imagining the equations to hold on the entire discretized line, we get

\[
\hat{\varphi}^n(w) = \frac{h^2}{2k} [\exp(-ikw) - \exp(ikw)] \hat{\varphi}_{n+1}^n(w) + (2 - \gamma) \hat{\varphi}_{n+1}^n(w) - \hat{\varphi}_{n+2}^n(w),
\]

\( n = N - 2, N - 3, \ldots, 1, 0; \quad 0 \leq |w| \leq \pi/k, \) (35)

\[
\hat{\varphi}^N(w) = 2\pi \hat{\varphi}_0(w) \hat{F}_m^1(w) \text{ and } \hat{\varphi}^{N-1}(w) = 2\pi \hat{\varphi}_0(w) \hat{F}_m^2(w) \text{ given.}
\]

Equivalently,

\[
\begin{bmatrix}
\hat{\varphi}^n(w) \\
\hat{\varphi}_{n+1}^n(w)
\end{bmatrix} =
\begin{bmatrix}
2 - \gamma - i \frac{h^2}{k} \sin(wk) & -1 \\
0 & 1
\end{bmatrix}
\begin{bmatrix}
\hat{\varphi}^{n+1}(w) \\
\hat{\varphi}_{n+2}^{n+1}(w)
\end{bmatrix}, \quad 0 \leq |w| \leq \pi/k.
\]

(36)
The mollification method and the numerical solution

Thus,

\[
\begin{bmatrix}
\hat{\varphi}_0(w) \\
\hat{\varphi}_1(w)
\end{bmatrix} = \begin{bmatrix}
2 - \gamma - i \frac{h^2}{k} \sin(wk) - 1 \\
1
\end{bmatrix}^{-1} \begin{bmatrix}
\hat{\varphi}_{N-1}(w) \\
\hat{\varphi}_N(w)
\end{bmatrix}, \quad 0 \leq |w| \leq \pi/k.
\] (37)

Using the initial conditions, we get

\[
\begin{bmatrix}
\hat{\varphi}_0(w) \\
\hat{\varphi}_1(w)
\end{bmatrix} = \begin{bmatrix}
2 - \gamma - i \frac{h^2}{k} \sin(wk) - 1 \\
1
\end{bmatrix}^{-1} 2\pi \hat{\varphi}_2(w) \begin{bmatrix}
\hat{F}_0(w) \\
\hat{F}_1(w)
\end{bmatrix}, \quad 0 \leq |w| \leq \pi/k.
\] (38)

The eigenvalues \( \lambda_1 \) and \( \lambda_2 \) of the iteration matrix

\[
G_{\omega,k}(w) = \begin{bmatrix}
2 - \gamma - i \frac{h^2}{k} \sin(wk) - 1 \\
1
\end{bmatrix}
\] (39)

are given by

\[
\lambda_{1,2} = \frac{1}{2} \left\{ 2 - \gamma - i \frac{h^2}{k} \sin(wk) \pm \left[ \left(2 - \gamma - i \frac{h^2}{k} \sin(wk)\right)^2 - 4 \right]^{1/2}\right\},
\]

\[
0 \leq |w| \leq \pi/k.
\]

We notice that \( \lambda_1 \cdot \lambda_2 = 1 \).

For \( |w| = 0 \) or \( \pi/k \), with \( 0 < \gamma < 1 \), the eigenvalues of \( G_{\omega,k} \) are

\[
\lambda_{1,2} = 1 - \frac{\gamma}{2} \pm i \sqrt{\gamma \sqrt{1 - \gamma/4}}
\] (40)

and \( |\lambda_1| = |\lambda_2| = 1 \).

For \( 0 < |w| < \pi/k \) and \( h \) sufficiently small, a short calculation shows that

\[
|\lambda_1| = 1 + C_1 \frac{h}{\sqrt{k}} \sqrt{\sin |wk|},
\]

and

\[
|\lambda_2| < 1,
\] (41)

\( C_1 > 0 \), independent of \( h, k \) and \( w \). In all cases, the eigenvalues of the iteration matrix are distinct.

Thus, there exist a nonsingular matrix \( P \), having as columns the two linearly independent eigenvectors of \( G_{\omega,k}(w) \), and a constant \( C_2 \) such that

\[
P^{-1}G_{\omega,k}(w)P = \begin{bmatrix}
\lambda_1(w) & 0 \\
0 & \lambda_2(w)
\end{bmatrix}
\]

and \( \|P\|_2 \|P^{-1}\|_2 \leq C_2 \). Here \( \|A\|_2 = \sqrt{\lambda} \) denotes the \( l_2 \) norm of the matrix \( A \) (\( \lambda \) is the maximum eigenvalue of \( A^*A \) and \( A^* \) stands for the transpose conjugate of the matrix \( A \)). It follows that

\[
\begin{bmatrix}
\hat{\varphi}_0(w) \\
\hat{\varphi}_1(w)
\end{bmatrix} = P \begin{bmatrix}
\lambda_1^{N-1} & 0 \\
0 & \lambda_2^{N-1}
\end{bmatrix} P^{-1} 2\pi \hat{\varphi}_2(w) \begin{bmatrix}
\hat{F}_0(w) \\
\hat{F}_1(w)
\end{bmatrix}, \quad 0 \leq |w| \leq \pi/k,
\] (42)

and recalling that the discrete Fourier transform of the mollifier is given by

\[
2\pi \hat{\varphi}_2(w) = \exp(-w^2 \delta^2/4) + \sum_{\frac{j\pi}{n} = 0}^{\infty} \exp[-(2 + j\pi/k)^2 \delta^2/4],
\]

using \( |\hat{\varphi}_2| \leq 4 \exp(-w^2 \delta^2/4) \), we have

\[
\left\| \begin{bmatrix}
\hat{V}_0 \\
\hat{V}_1
\end{bmatrix}
\right\|_2 \leq \|P\|_2 \|P^{-1}\|_2 \max_{0 \leq |w| \leq \pi/k} \left(1 + C_1 \frac{h}{\sqrt{k}} \sqrt{\sin |wk|}\right)^{N-1} \sqrt{4/\pi} \exp(-w^2 \delta^2/4) \left\| \begin{bmatrix}
\hat{F}_0 \\
\hat{F}_1
\end{bmatrix}
\right\|_1.
\] (43)
Thus,

\[ \| V^0 \|_2 \leq 4\sqrt{2\pi} C_2 \max_{0 \leq |w| \leq \pi/k} \left( 1 + C_r \frac{h}{\sqrt{k}} \sqrt{\sin |wk|} \right)^{N-1} \exp(-w^2 \delta^2/4) \| F_m^2 \|_2 \]  \tag{44}

Here we have used the \( l_1 \) norm of a discrete vector function defined by

\[ \| V, V' \|_2 = \left\{ \sum_j [(V_j)^2 + (V_j')^2] \right\}^{1/2} \]

and the fact that

\[ \| V \|_2 = 1/\sqrt{2\pi} \| \tilde{V} \| [22]. \]

Recalling that \( Nh = 1 \) and using the inequality \( \sin |wk| \leq k |w| \), we have

\[ \left( 1 + C_r \frac{h}{\sqrt{k}} \sqrt{\sin |wk|} \right)^{N-1} \exp(-w^2 \delta^2/4) \leq (1 + C_r h \sqrt{|w|})^{N-1} \exp(-w^2 \delta^2/4) \]

\[ \leq \exp(C_r(Nh)\sqrt{|w|}) \exp(-w^2 \delta^2/4) = \exp(C_r \sqrt{|w|} - w^2 \delta^2/4) \]

\[ \leq \exp(\frac{1}{4} C_4 \delta^{-2/3}). \]  \tag{45}

Finally, using inequality (45) in (44), we obtain

\[ \| V^0 \| \leq 4\sqrt{2\pi} C_2 \exp(\frac{1}{4} C_4 \delta^{-2/3}) \| F_m^2 \|_2 \]  \tag{46}

showing that the fully explicit finite difference scheme is unconditionally stable. By the equivalence theorem [22], the consistent and stable finite difference approximation converges to the solution of the mollified (well-posed) problem (21).

Remark. If \( \gamma = 0 \), for \( |w| = 0 \) or \( \pi/k \), the iteration matrix \( G_{kk} \) becomes

\[ \begin{bmatrix} 2 & -1 \\ 1 & 0 \end{bmatrix} \]

with \( \lambda_1 = \lambda_2 = 1 \). Moreover,

\[ \begin{bmatrix} 2 & -1 \\ 1 & 0 \end{bmatrix}^{N-1} = \begin{bmatrix} N & -N+1 \\ N-1 & -N+2 \end{bmatrix} \]

and \( \| G_{kk} \|_2 \to \infty \) as \( N \to \infty \). The introduction of the \( \gamma \) parameter makes it possible to "separate" the eigenvalues of the iteration matrix for \( 0 \leq |w| \leq \pi/k \). The numerical solution of several examples using the algorithm described by equation (32) is illustrated in Section 5. In the next section we briefly discuss the automatic selection of the radius of mollification, an important practical detail for the successful implementation of the method.

4. AUTOMATIC SELECTION OF THE RADII OF MOLLIFICATION

In this section we indicate a procedure to determine the radii of mollification based on properties of the filtered data functions \( J \phi F_m^i, i = 1, 2 \).

Our selection criterion is founded in the following monotonicity property: If \( \delta_1 > \delta_2 > 0 \), then \( \| J \phi F_m^1 - F_m^2 \| \geq \| J \phi F_m^1 - F_m^2 \|, i = 1, 2 \). For a proof of this proposition and some related discussions, the reader is referred to Murio [20]. This shows that the mollification of the data functions \( F_m^i, i = 1, 2 \), by convolution against the Gaussian kernel \( p_\delta \) is an averaging process such that the equations

\[ \| J \phi F_m^i - F_m^i \| = \epsilon \]  \tag{47}

have unique solutions \( \delta^i, i = 1, 2 \).

The parameter selection criteria introduced by equation (47) determines \( \delta^1 \) and \( \delta^2 \) in a manner which is consistent with the amount of noise in the data. Furthermore, the bisection method can easily be implemented to numerically estimate \( \delta^1 \) and \( \delta^2 \).
In actual computations, according to equation (13), once \( h \) and \( k \) are selected, the data functions \( F'_m, \ i = 1, 2, \) are required to be known only on the finite data record interval \( D = [0, L], \ L = 1 - k + k/h. \) However, due to the nature of the convolution procedure, if we wish to compute \( J_\delta F'_m(t), \ i = 1, 2, \) for all \( t \) in \( D, \) the data interval should be extended to \( D_a = [-a, L + a], \) where \( 2a = 6d_{\text{max}} \) indicates the largest "support" of the \( p_s \) kernels needed to determine \( \delta^1 \) and \( \delta^2. \) In practice, this means that we consider the data to be zero for \(-a \leq t < 0\) and that the data functions \( F'_m \) and \( F'_m \) are recorded for \( 0 \leq t \leq L + a \) instead of \( 0 \leq t \leq L. \) The radii of mollification \( \delta^1 \) and \( \delta^2 \) are now estimated by solving the equations

\[
\| J_\delta F'_m - F'_m \|_D = \epsilon, \quad i = 1, 2. \tag{48}
\]

The computational details are presented in the next section.

5. NUMERICAL PROCEDURE

Since in practice only a discrete set of points is generally available, we assume that the data functions \( F'_m \) and \( F'_m \) are discrete functions measured at equally spaced sample points in the interval \( D_a = [-a, L + a], \) where \( L = 1 - k + k/h, Nh = 1 \) and \( k < a = 3d_{\text{max}} \leq \frac{1}{2}. \) The data functions are defined to be zero in the subinterval \([-a, 0]\) and the \( M + 1 \) sample points in the interval \( D = [0, L] \) are denoted by \( t_j = jk, j = 0, 1, \ldots, M; Mk = L. \)

The parameter selection criteria is implemented by solving the discrete versions of equations (48) using the bisection method. The following steps, applied first to \( F_m = F'_m \) and then to \( F_m = F'_m, \) summarized the algorithm. Notice that in order to compute \( J_\delta F_m(t_j) \) for all \( t \) in \( D, \) in Step 2 of the procedure, we need \( F_m \) in \( D_a. \)

**Step 1:** Let \( \delta_{\text{min}} = k, \delta_{\text{max}} = 10k < \frac{1}{k} \) and choose an initial value of \( \delta \) between \( \delta_{\text{min}} \) and \( \delta_{\text{max}}. \)

**Step 2:** Compute \( J_\delta F_m(t_j) = (p_s * F_m)(t_j) \) by discrete convolution, \( j = 0, 1, \ldots, M. \)

**Step 3:** If

\[
F(\delta) = \left( \frac{1}{M + 1} \sum_{j=0}^{M} [J_\delta F_m(t_j) - F_m(t_j)]^2 \right)^{1/2} = \epsilon \pm \eta,
\]

where \( \eta \) is a given tolerance, exit.

**Step 4:** If \( F(\delta) - \epsilon < -\eta, \) set \( \delta_{\text{min}} = \delta. \) If \( F(\delta) - \epsilon > \eta, \) set \( \delta_{\text{max}} = \delta. \) The updated value of \( \delta \) is always given by \( (\delta_{\text{min}} + \delta_{\text{max}})/2. \)

**Step 5:** Return to Step 2.

Once the radii of mollification \( \delta^1, \delta^2 \) and the discrete filtered data functions \( J_\delta F'_m(t_j) = V'_j, J_\delta F'_m(t_j) = V''_j, j = 0, 1, \ldots, M \) are determined, we apply the finite difference algorithm described in Section 3, marching backward in space

\[
V'_j = \frac{h^2}{2k} (V'_{j+1}^n - V'_{j-1}^n) + (2-\gamma)V'_{j}^{n+1} - V'_{j+2}^n, \quad n = N - 2, N - 3, \ldots, 1, 0; \quad j = 1, \ldots, M - N + n + 1;
\]

\[
V''_0 = 0, \quad n = N, N - 1, \ldots, 1, 0. \quad (49)
\]

The solution \( V'_j, j = 0, 1, \ldots, M - N + 1 \) is then taken as the accepted value for the approximate boundary temperature history.

**Numerical results**

In order to test the accuracy of our method, in Problem 1, the approximate reconstruction of a surface heat temperature \( f(t) \) is investigated for a semi-infinite body exposed to a temperature of value 1 between \( t = 0.2 \) and \( t = 0.4 \) and of value 0 at other times. Such a curve has the difficult characteristics of an abrupt rise and an equality abrupt drop and constitutes a severe test because the algorithm anticipates changes in the solution temperature and gives delayed values. In Problem 2, we also investigate the approximate reconstruction of a very smooth surface temperature that rises as the square root of its time argument.
In all our examples, we use \( h = k = 0.01 \). Thus, \( N = 100, \delta_{\text{max}} = 10k = 0.1, a = 3\delta_{\text{max}} = 0.3, L = 1 - k + k/h = 1.99, M = 199, D = [0, 1.99] \) and \( D_o = [-0.3, 2.29] \). The exact data temperature is denoted by \( F(t) \) and the noisy data, \( F'_m(t) \), is obtained by adding a random error to \( F(t) \). Thus, for every grid point \( t_j \) in \( D_o \),

\[
F'_m(t_j) = F(t_j) + \epsilon_j, \quad i = 1, 2,
\]

where \( \epsilon_j \) is a Gaussian random variable of variance \( \sigma^2 = \epsilon^2 \). The exact data temperatures for Problem 1 are

\[
F^i(t) = \phi(1, t - 0.2) - \phi(1, t - 0.6)
\]

and

\[
F^2(t) = \phi(0.99, t - 0.2) - \phi(0.99, t - 0.6),
\]

where

\[
\phi(x, t) = \begin{cases} \text{erfc}(x/\sqrt{t}), & t > 0 \\ 0, & t \leq 0. \end{cases}
\]

For Problem 2, the exact data temperatures corresponding to the surface temperature \( f(t) = \sqrt{t} \) are given by

\[
F^1(t) = g(1, t) \quad \text{and} \quad F^2(t) = g(0.99, t),
\]

where

\[
g(x, t) = \begin{cases} \sqrt{t} \left( \exp(-x^2/4t) - \sqrt{\pi} \frac{x}{2\sqrt{t}} \text{erfc}(x/2\sqrt{t}) \right), & t > 0 \\ 0, & t \leq 0. \end{cases}
\]

To study the numerical stability of our algorithm, we use different average perturbations for \( \epsilon = 0, 0.001, 0.002, 0.003, 0.004 \) and \( 0.005 \) respectively. The parameter selection criteria was implemented with the tolerance \( \eta \), used in Step 3 of the procedure, set to reflect a 5\% error in the satisfaction of the constraint, except for \( \epsilon = 0 \), where we used \( \delta^1 = \delta^2 = k = 0.01 \). If the discretized computed boundary temperature component is denoted by \( V^o_j \) and the true component is \( f_j = f(t_j) \), we use the sample root mean square norm to measure the error in the discretized interval \( I = [0, 1] \).

The solution error is then given by

\[
\| V^o - f \|_1 = \left( \frac{1}{M - n + 1} \sum_{j=1}^{M-n+1} (V^o_j - f_j)^2 \right)^{1/2}.
\]

The stability analysis of the previous sections indicates that the \( \gamma \)-parameter should be chosen as small as possible. In fact, all our numerical experiments have shown that the algorithm is almost totally insensitive to values of \( \gamma \) between 0 and approx. \( 10^{-6} \). This strongly suggests that the stability requirement \( \gamma > 0 \) for \( |w| = 0 \) or \( \pi/k \) has, if violated, no computational consequences. Accordingly, we implemented the algorithm with the choice \( \gamma = 0 \).

Tables 1 and 2 show the results associated with Problems 1 and 2 respectively.

In all cases, the stability of the method with respect to perturbations in the data is readily confirmed. The uniformly smaller error norms for Problem 2 are expected since we use the same amount of noise in both problems and the same data interval length, but the maximum data temperature value of Problem 1 is about 0.2 while for Problem 2 is about 0.7. Moreover, the boundary temperature solution in Problem 2 is \( f(t) = \sqrt{t} \), a very smooth function, much easier to approximate by our numerical convolutions (with fixed radius of mollification) than

<table>
<thead>
<tr>
<th>Table 1. Error norm as a function of the amount of noise in the data</th>
<th>Table 2. Error norm as a function of the amount of noise in the data</th>
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</thead>
<tbody>
<tr>
<td>( \epsilon )</td>
<td>( \delta^1 )</td>
</tr>
<tr>
<td>0.000</td>
<td>0.01</td>
</tr>
<tr>
<td>0.001</td>
<td>0.03</td>
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<tr>
<td>0.002</td>
<td>0.04</td>
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<td>0.003</td>
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discontinuous solution of Problem 1. In the absence of noise or for small level of noise ($\epsilon = 0, 0.001, 0.002$), the approximated solution is better for Problem 2 than for Problem 1. However, as the amount of noise in the data increases, the numerical solution in Problem 1 is relatively less sensitive (more stable) than the numerical solution of Problem 2.

The qualitative behavior of the reconstructed surface temperatures for Problem 1 is illustrated in Fig. 1 where the numerical solutions for $\epsilon = 0.003$ (unbroken line) and $\epsilon = 0.005$ (broken line) are plotted. Figures 2 and 3 show the reconstructed surface temperatures (broken lines) and true solutions (unbroken lines) for Problem 2 corresponding to noise levels $\epsilon = 0.003$ and $\epsilon = 0.005$ respectively.
6. CONCLUSIONS

A new interpretation of the mollification method that leads very naturally to a discrete convolution filtering technique that automatically adjusts the radii of mollification to the amount of noise in the data is successfully combined with a finite difference approximation. The fully explicit, space marching algorithm is second order in space and time and converges to the mollified version of the surface temperature history. Great computational flexibility is gained by using finite differences marching in space. It is possible to discretize the differential equation directly and the method can be used, with suitable modifications, to approximately solve the nonlinear inverse heat conduction problem. Also, the temperature profiles are computed for all values of \( x \), providing any necessary intermediate information. In particular, knowing the approximate temperature histories at \( x = 0 \) and \( x = h \) (immediately close to the surface), it is feasible to estimate the surface heat flux, if desired.

Two examples are investigated. One corresponds to a discontinuous unit step surface temperature and the other to a very smooth surface temperature. In both cases, the sample mean square norm of the error is studied as a function of the amount of noise in the data. The numerical examples do verify the numerical stability of the method. Furthermore, the accuracy of the procedure is quite acceptable, even when a relative high noise level in the data is used.

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REFERENCES