A DEFORMING FINITE ELEMENT METHOD ANALYSIS OF INVERSE STEFAN PROBLEMS

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SUMMARY
A deforming FEM (DFEM) analysis of one-dimensional inverse Stefan problems is presented. Specifically, the problem of calculating the position and velocity of the moving interface from the temperature measurements of two or more sensors located inside the solid phase is addressed. Since the interface velocity is considered to be the primary variable of the problem, the DFEM formulation is found to have many advantages over other traditional front tracking methods. The present inverse formulation is based on a minimization of the error between the calculated and measured temperatures, utilizing future temperature data to calculate current values of the unknown parameters. Also, the use of regularization is found to be useful in obtaining more accurate results, especially when the interface is located far away from the sensors. The method is illustrated with several examples. The effects of the location of the sensors, of the error in the sensor measurements and of several computational parameters were examined.

INTRODUCTION
Heat transfer problems with phase changes are very common in physics and engineering. Typical examples include the melting, welding and casting processes of metals and alloys. All these nonlinear problems share the characteristic of an interface boundary which moves into the solid (melting) or into the liquid (solidification) region in accordance with the relative magnitudes of the temperature gradients on either side of the interface boundary. The flux discontinuity on the interface is related to its normal velocity by an equation balancing the rate of heat flow with the energy rate required to create a fresh amount of solid (or liquid) per unit time.

A heat transfer problem is considered to be a direct problem when the temperature or the flux histories at the boundary of a specified domain are prescribed as functions of time. In a typical inverse problem, the boundary heat flux and temperature histories must be determined from transient temperature measurements at one or more interior locations of the specified domain. Another case of inverse problems, which is the subject of this paper, includes Stefan problems where the interface velocity and location as well as the temperature field in the solid phase are predicted from the temperature history at specified sensor locations inside the solid phase. This problem, which has been previously examined by Katz and Rubinsky, can have many potential applications in the analysis and design of casting and welding processes. However, it is very difficult to experimentally measure the interface location or velocity. Also, the temperature measurements in the solid phase can be performed more easily and accurately than those in the liquid phase where convection effects may be significant.

Many numerical methods have been reported in the literature for the solution of direct phasechange problems. A short literature review is given by Zabaras and Mukherjee, and the excellent book by Crank is recommended. An extensive literature review of inverse heat transfer problems without phase changes is given in a recent book by Beck et al. Many different methods have been
applied to the area of heat transfer for the solution of such inverse problems. For example, least squares techniques have been extensively used.\textsuperscript{2,6-11} Also regularization techniques,\textsuperscript{12,13} and more recently, dynamic programming\textsuperscript{14,15} and filtering\textsuperscript{16} techniques are being used. Such techniques have been used in conjunction with the finite difference method,\textsuperscript{2} the finite element method\textsuperscript{17} and the boundary element method.\textsuperscript{18}

The limited literature on the subject of inverse heat transfer with a phase change includes Hsu \textit{et al.},\textsuperscript{19} Frederick and Greif,\textsuperscript{20} Katz and Rubinsky\textsuperscript{3} and Zabaras \textit{et al.}\textsuperscript{21} This last work refers to Stefan problems where the temperature, heat flux and front velocity are prescribed on the interface, while the temperature and the heat flux on the stationary boundary of the domain of interest are unknown and determined by the analysis. Such problems have potential applications in improving the cast structure. In this paper, the DFEM is used for the solution of one-dimensional inverse Stefan problems. Use of deforming finite element methods for the solution of moving boundary value problems is extensive.\textsuperscript{22-28} The advantage of the DFEM over other front tracking methods\textsuperscript{3} is that in the DFEM there is a systematic way to adopt the front motion. More specifically, the nodal points can move continuously according to the motion of the interface, while, for example, in the work reported by Katz and Rubinsky,\textsuperscript{3} only the node which coincides with the front moves. Their method requires adding or deleting nodes frequently to avoid large element aspect ratios and gives no special attention to the front motion.

In this paper, a method similar to that proposed by Beck \textit{et al.}\textsuperscript{2,6} for inverse heat conduction problems without phase changes is used in conjunction with a regularization technique. It will be demonstrated that the method is able to stabilize the inverse problem, and that it permits small time steps and experimental data with significant error. Extension to regular two-dimensional geometries is straightforward, while extension to complicated geometries and three dimensions is primarily connected with the currently difficult task of implementation of the DFEM\textsuperscript{27,28} for such problems. The motion of the front is treated as a primary variable, permitting accurate calculation of the front velocity and location. In the work of Katz and Rubinsky,\textsuperscript{3} there is no technique to account for the inverse nature of the problem, and the measured and the calculated temperatures at each time step are matched by trial and error. Their method is not advisable when error is introduced in the temperature data. This paper will start with a precise definition of the inverse problem and a brief review of a DFEM formulation for the direct problem. Then, the process of minimization, sensitivity analysis and the regularization technique will be given. Finally, the effectiveness of the method will be demonstrated with several examples.

**PROBLEM DEFINITION**

Let us consider the melting of a pure substance which is initially (at time $t = 0$) in a solid state, and occupies the region $(0 < x < h)$ with the known temperature distribution $T_{in}(x)$ below the melting point $T_m$. It is assumed that at time $t = 0$, melting starts at $x = 0$. The position of the interface at time $t$ is denoted by $s(t) [s(0) = 0]$, while the interface velocity is $\dot{s}(t)$ (Figure 1).

The governing equations for the temperature field $T(x,t)$ are:\textsuperscript{1}

for the solid phase $(s(t) < x < h)$

$$\rho_slc_s \frac{\partial T_s(x,t)}{\partial t} = \chi^{-m} \frac{\partial}{\partial x} \left( K_s \chi^m \frac{\partial T_s(x,t)}{\partial x} \right) \quad (1)$$

for the liquid phase $(0 < x < s(t))$

$$\rho_lc_l \frac{\partial T_l(x,t)}{\partial t} = \chi^{-m} \frac{\partial}{\partial x} \left( K_l \chi^m \frac{\partial T_l(x,t)}{\partial x} \right) \quad (2)$$
with the following initial conditions:

\[ s(0) = 0 \]
\[ T_s(x, 0) = T_{in}(x) \quad 0 \leq x \leq h \]

where \( K, \rho \) and \( c \) denote the thermal conductivity, density and specific heat, and the subscripts \( S \) and \( L \) denote solid and liquid phases, respectively. The coefficient \( m \) defines the specific geometry of the problem (\( m = 0 \) planar, \( m = 1 \) cylindrical and \( m = 2 \) spherical).

The conditions at the isothermal moving interface are as follows:

\[ T(s(t), t) = T_m \]  \hspace{1cm} (5)

and

\[ \rho \mathcal{L} \dot{s}(t) = K_L \frac{\partial T_L(s(t), t)}{\partial x} - K_S \frac{\partial T_S(s(t), t)}{\partial x} \]  \hspace{1cm} (6)

where equation (6) is the energy balance equation at the interface. Here \( \mathcal{L} \) denotes the latent heat of fusion.

A direct problem can then be defined as follows.

Solve equations (1)–(6) with additional temperature or heat flux conditions at \( x = 0 \) and \( x = h \) (boundary conditions).

For more details on such direct problems, the reader should consult the book by Crank.\(^5\) Let us now consider that \((N + 1)\) sensors (thermocouples) are embedded inside the region \( 0 \leq x \leq h \). In this work, we are interested in using only the information given by sensors before the interface arrives in their locations. Mathematically, this means that the following information is available:

\[ T(\hat{x}_k(t), t) \cong Y_k(t) \quad \text{for} \quad t < t_k(\hat{x}_k), \quad k = 1, 2, \ldots, (N + 1) \]  \hspace{1cm} (7)

where the symbol \( \cong \) indicates the approximate nature of equation (7), \( \hat{x}_k \) is the position of the \( k \)-th sensor (without loss of generality, it is assumed that \( 0 < \hat{x}_1 < \hat{x}_2 < \ldots < \hat{x}_{N+1} = h \)), \( t_k(\hat{x}_k) \) is the arrival time of the interface at the \( k \)-th sensor location \( \hat{x}_k \) and \( Y_k(t) \) is the measured temperature history at \( \hat{x}_k \).

Now the inverse problem of interest can be defined as follows.

Given the thermocouple measurements (equation (7)) and the geometry as shown in Figure 1, solve the system of equations (1)–(6) to find the front velocity and position.
If two sensors \((N = 1)\) are available at the locations \(\hat{x}_1\) and \(\hat{x}_2 = h\), then from equation (7) one can conclude that the solution to the inverse problem is achievable only up to time \(t_*(\hat{x}_1)\). To proceed further in time, more sensors are necessary at the locations \(x > \hat{x}_1\). It is clear that the assumption of \(N = 1\) above defines the minimum required number of sensors in order that the solution can be obtained at the time interval referred to previously. With the solution to this inverse problem known, ideas similar to those previously developed by Zabaras et al.\(^2\) can be applied subsequently to calculate unknown parameters in the liquid phase.

In practice, one may be interested in the interface location rather than its velocity. Nevertheless, since the velocity is more sensitive to errors in the thermocouple measurements, the velocity has been selected to be the primary unknown variable of the problem in this work.

In the following formulation, attention is given only to the solid phase (equations (1), (3), (4), (5) and (7)), and the subscript \(S\) has been dropped for notational convenience.

**Deforming finite element method formulation of direct Stefan problems**

The basic characteristic of a DFEM formulation is the assumption that element nodes are moving with time and following the motion of the interface. This assumption\(^2\) makes the shape functions implicitly dependent on time through the nodal co-ordinates. For example, for each finite element \(e\), one can write the following equation:

\[
T(x, t) = T^*\eta(x, t) \Phi^e(x, t) \tag{8}
\]

where \(T^*\eta(x, t)\) are the nodal temperatures, \(\Phi^e(x, t)\) are the element shape functions, and \(x\) is a spatial point lying inside the element \(e\). In equation (8), summation on \(i\) is implied \((i = 1, 2, \ldots, M^e)\), where \(M^e\) is the number of nodes in the element \(e\). By assuming an isoparametric transformation of the space \(x\) to the time independent space \(\xi\), with \(-1 \leq \xi \leq +1\), one can write

\[
x = X_i(t) \Phi_i(\xi) \tag{9}
\]

Let us concentrate only on the space occupied by the solid phase and assume that it is divided into \(E\) elements with \(M\) nodes. Then, at each time \(t\), one can employ a weak Galerkin formulation using the above shape functions, and finally, after assembling, write the following discretized equations:\(^3\)

\[
C_{ij} \frac{\partial T^e}{\partial t} + (B_{ij} + K_{ij}) T^e = F^e, \quad i, j = 1, 2, \ldots, M \tag{10}
\]

where

\[
C_{ij} = \sum_e C_{ij}^e = \sum_e \int_{\Omega_e} \rho c \Phi_i^e(x, t) \Phi_j^e(x, t) \, dx \tag{11}
\]

\[
B_{ij} = \sum_e B_{ij}^e = -\sum_e \int_{\Omega_e} \rho c \frac{\partial \Phi_i^e(x, t)}{\partial t} \Phi_j^e(x, t) \frac{\partial \Phi_i^e(x, t)}{\partial x} \, dx \tag{12}
\]

\[
K_{ij} = \sum_e K_{ij}^e = \sum_e \int_{\Omega_e} K \frac{\partial \Phi_i^e(x, t)}{\partial x} \frac{\partial \Phi_j^e(x, t)}{\partial x} \, dx - \sum_e \int_{\Omega_e} \frac{Km}{x} \Phi_i^e(x, t) \frac{\partial \Phi_i^e(x, t)}{\partial x} \, dx \tag{13}
\]

\[
F_i = \sum_e F_i^e = \sum_e q(s(i), t) \Phi_i^e(s(i), t) - \sum_e q(h(t)) \Phi_i^e(h(t)) \tag{14}
\]
with the flux \( q(x, t) \) defined as

\[
q(x, t) = -K \frac{\partial T}{\partial x}(x, t) \tag{15}
\]

and the integrations performed over the length \( \Omega_e(t) \) of each element \( e \). Obviously, \( \sum e \Omega_e(t) \) is the space occupied at time \( t \) by the solid phase. The matrix \( [B] \) accounts for the motion of the nodes and the rest of the notation follows the familiar finite formulation.\(^{29}\)

The calculations indicated in equations (11)–(14) above are quite straightforward if one can specify the location and velocity of the element nodes at each time. It is important to note here that the finite element nodes are moving only artificially. (No actual material motion exists.) Therefore, a method for moving nodes must be chosen.\(^{24}\) For example, the nodes can move in such a way that a uniform mesh is always present, or in the way suggested by Miller and Miller,\(^{22}\) where the node locations are primary variables of the problem and can be calculated together with nodal temperatures.

Following Hughes\(^{30}\) and denoting with \( T^n, n = 1, 2, \ldots \), the nodal temperatures at time \( t = n\Delta t \), where \( \Delta t \) is a fixed time step, an unconditionally stable integration scheme for equation (10) is

\[
\left[ \frac{C_n^{n+1} + \epsilon}{\Delta t} + \gamma (B_n^{n+1} + K_n^{n+1}) \right] T^n = F_n^{n+1} + \left[ \frac{C_n^{n-1} + \epsilon}{\Delta t} + (1 - \gamma)(B_n^{n-1} + K_n^{n-1}) \right] T^{n-1} \tag{16}
\]

where the subscript \( (n - 1 + \gamma) \) indicates time of reference for the calculation of the temperatures, and the superscript \( (n - 1 + \epsilon) \) denotes the reference position and velocity of the interface used for the calculation of the integrals in equations (11)–(14). For example, to determine \( C_n^{n-1} + \epsilon \), one calculates the material properties and the temperature field at time \( \bar{t} \) and then performs the integration indicated in equation (10) assuming that the interface location is \( \bar{s} \), where

\[
\bar{t} = (1 - \gamma)t_{n-1} + \gamma t_n \tag{17}
\]

and

\[
\bar{s} = (1 - \epsilon)s(t_{n-1}) + \epsilon s(t_n) \quad \text{(18a)}
\]

\[
\bar{s} = (1 - \epsilon)\bar{s}(t_{n-1}) + \epsilon \bar{s}(t_n) \quad \text{(18b)}
\]

and the integration parameters \( \gamma \) and \( \epsilon \) are defined as \( 0 < \gamma < 1 \), and \( 0 \leq \epsilon \leq 1 \). These independent approximations for temperature and interface location have been found to add further stability to the integration scheme.\(^{23}\)

Let us now suppose that \( s(t_{n-1}), \bar{s}(t_{n-1}) \) and the temperature distribution at time \( t = t_{n-1} \) are known and that the temperature field at \( t = t_n \) is to be calculated. An iterative procedure must be followed. For example, one assumes \( \bar{s}(t_n) \) to start the calculation, and then equation (16) is applied with all the integrations indicated in equations (11)–(14) performed on the solid space \( \bar{s} \leq x \leq h \), where \( \bar{s} \) may be found from equation (18a) with \( s(t_n) \) calculated by numerical integration of the velocity profile. The velocity term in equation (12) is defined based on the interface velocity \( \bar{s} \) given by equation (18b). After calculating \( T^n \) in the solid phase and similarly in the liquid phase, one can either proceed on time or update \( \bar{s}(t_n) \) by using equation (6), depending on the tolerance allowed on the temperature field or the interface velocity at time \( t_n \).
STRATEGY FOR THE SOLUTION OF THE INVERSE PROBLEM

In this section, a scheme for calculating the interface velocity and location is proposed with the temperature history or an approximation of it at \((N + 1)\) sensor locations known (equation (7)). The region of interest at time \(t\) is \(s(t) \leq x \leq h\), and the temperature \(T(x = h) \geq Y_{N+1}(t)\) is treated as the boundary condition on \(x = h\) here, rather than a sensor measurement. Therefore, there are \(N\) remaining sensors in the region \(0 < x < h\).

Let us consider a time stepping process which proceeds from time \(t = t_{n-1}\) to time \(t = t_n = t_{n-1} + \Delta t\), \(n = 1, 2, \ldots\), with a fixed time step \(\Delta t\). It is assumed that all the information (such as interface location and velocity, temperature field in the solid phase, etc.) for \(t \leq t_{n-1}\) is known, and the solution at \(t = t_n\) (with \(t_n < t_{n+1}(\hat{x}_1)\)) is to be found. The region \([s(t), h]\) is divided into two subregions, \(s(t) \leq x \leq \hat{x}_1\) and \(\hat{x}_1 < x \leq h\), and in each of the subregions the number of finite elements is kept constant. The elements in \(s(t) \leq x \leq \hat{x}_1\) are allowed to deform (as discussed previously), while the rest of the elements are stationary. In this way, one is free to select any scheme for node motion and still keep the same number of elements and nodal locations in the domain where the sensors are located. In this work, the following equations are used to define the node motion:

\[
V_1 = \left[ 1 - \frac{x_1 - s(t)}{\hat{x}_1 - s(t)} \right] \delta(t) \quad \text{for} \quad s(t) \leq x_1 \leq \hat{x}_1
\]

and

\[
V_I = 0 \quad \text{for} \quad \hat{x}_1 < x_I \leq h
\]

where \(V_I\) denotes the velocity at the \(I\)th nodal location \(x = x_I\) \((I = 1, 2, \ldots, M)\).

The main unknown of the problem at \(t = t_n\) is considered to be the interface velocity \(\delta_n\). To calculate \(\delta_n\), the future time method\(^2\) is used. Let us denote \(T^{n+i-1}_k\) as the temperature in the location of the \(k\)th sensor \((k = 1, 2, \ldots, N)\) at time \(t_{n+i-1}\), \(i = 1, 2, \ldots, r\), with \(r\) being any positive integer. Then, with given boundary conditions at \(x = h\) \([T(h, t) = Y_{N+1}(t)]\) and interface temperature, \(T_m\), from equation (5), one can conclude that \(T^{n+i-1}_k\) is a function of \(\delta_n, \delta_{n+1}, \ldots, \delta_{n+i-1}\), where \(\delta_{n+i-1} = \delta(t_{n+i-1}), i = 1, 2, \ldots, r\). Note that the solution to the problem is known for \(t \leq t_{n-1}\).

If the approximations \(\delta^{\ast}_{n+i-1}\) of \(\delta_{n+i-1}, i = 1, 2, \ldots, r\) are available, a truncated Taylor’s series expansion gives

\[
T^{n+i-1}_k = \ast T^{n+i-1}_k + \sum_{j=1}^{i} \frac{\partial T^{n+i-1}_k}{\partial \delta_{n+j-1}} (\delta_{n+j-1} - \delta^{\ast}_{n+j-1})
\]

where \(\ast T^{n+i-1}_k\) is the temperature at \(x = \hat{x}_k\) at time \(t_{n+i-1}\) calculated with the approximate velocities \(\delta^{\ast}_n, \delta^{\ast}_{n+1}, \ldots, \delta^{\ast}_{n+i-1}\). The goal of this analysis is to calculate the optimum velocities \(\delta^{\ast}_{n+i-1}, i = 1, 2, \ldots, r\), such that the error between the calculated (equation (20)) and measured temperatures \(Y^{n+i-1}_k [Y^{n+i-1}_k = Y_k(t_{n+i-1})]\) at the sensor locations is minimum:

\[
\min_{\delta_{n+i-1}} \left\{ \sum_{i=1}^{r} w_i \sum_{k=1}^{N} (Y^{n+i-1}_k - T^{n+i-1}_k)^2 + \sum_{i=1}^{r} \alpha_i (\delta^{n+i-1}_i)^2 \right\}
\]

Here, \(w_i, i = 1, 2, \ldots, r\) represent optimization weights and \(\alpha_i > 0, i = 1, 2, \ldots, r\) are regularization parameters corresponding to each future time step \(i\). In this work \(\alpha_i = i^2, i = 1, 2, \ldots, r\). The last regularization term\(^3\) has been added to keep the velocities at finite values. It is clear that equation (21) expresses minimization of the error between measured
and calculated temperatures, not just at time \( t_n \) but in the time interval \( t_n \leq t \leq t_{n+r-1} \). Equation (21) has \( r \) unknown velocities \( \dot{s}_{n+i-1} \), \( i = 1, 2, \ldots, r \), and this necessitates the minimization process computationally. For this reason, and to add additional stability,\(^2\) we temporarily restrict the velocities \( \dot{s}_{n+i-1} \), \( i = 1, 2, \ldots, r \) to behave in a specified way. For example, one can assume that the velocities are equal, or that \( \dot{s}(t) \) is a linear function of time for \( t_n < t < t_{n+r-1} \), etc. In this work, for each \( i, i = 1, 2, \ldots, r \), we assume the following:

\[
\dot{s}_{n+i-1} = \frac{\dot{s}_n}{b_i}
\]

where

\[
b_i = \sqrt{1 + (i - 1) \frac{\Delta t}{t_n}}
\]

This behaviour is very common for many phase change problems\(^1\) and a similar idea has been used previously for the solution of direct solidification problems.\(^1\) With the assumption of equation (22) valid for both \( \dot{s}_{n+i-1} \) and \( \dot{s}^*_n+i-1 \), \( i = 1, 2, \ldots, r \), equation (20) and (21) can be simplified as follows:

\[
T^{n+i-1}_k = T^{n+i-1}_k + S^{n+i-1}_k (\dot{s}_n - \dot{s}^*_n)
\]

and

\[
\min_{\dot{s}_n} \left\{ \sum_{i=1}^{r} w_i \sum_{k=1}^{N} \left( Y^{n+i-1}_k - T^{n+i-1}_k \right)^2 + \alpha(\dot{s}_n)^2 \right\}
\]

where the sensitivity coefficients \( S^{n+i-1}_k \), \( k = 1, 2, \ldots, N, i = 1, 2, \ldots, r \), are defined as

\[
S^{n+i-1}_k = \frac{\partial T^{n+i-1}_k}{\partial \dot{s}_n}
\]

These sensitivity coefficients express the change of temperature at each sensor location for a unit change of the velocity \( \dot{s}_n \). The calculation of these sensitivity coefficients will be discussed in more detail later in this paper. Here, the regularization parameter \( \alpha \) is a combination of the \( \alpha_i \)'s defined in equation (21) and the \( b_i \)'s given by equation (23). With the assumption of equation (22), \( \dot{s}_n \) is the only independent unknown variable left in the minimization process.

Using equation (24) one can finally derive from equation (25) the following equation:

\[
\dot{s}_n = \frac{\sum_{i=1}^{r} w_i \sum_{k=1}^{N} (S^{n+i-1}_k)^2}{\sum_{i=1}^{r} w_i \sum_{k=1}^{N} S^{n+i-1}_k (Y^{n+i-1}_k - T^{n+i-1}_k)} - \frac{\sum_{i=1}^{r} w_i \sum_{k=1}^{N} S^{n+i-1}_k (Y^{n+i-1}_k - T^{n+i-1}_k)}{\sum_{i=1}^{r} w_i \sum_{k=1}^{N} (S^{n+i-1}_k)^2 + \alpha}
\]

Equation (27) gives an updated value of the interface velocity at time \( t_n \). In order for equation (27) to be effective, one should provide a way to calculate the starred temperatures \( *T^{n+i-1}_k \) and the sensitivity coefficients \( S^{n+i-1}_k \). This subject is undertaken in detail in the next two paragraphs. As the first approximation of the starred velocity in each time step, one can take the following, based on equations (22) and (23):

\[
\dot{s}^*_n = \frac{\dot{s}_{n-1}}{\frac{t_n}{t_{n-1}}}
\]
The velocity calculated using equation (27) is considered to be acceptable when the following condition is satisfied:

\[
\frac{|\hat{s}_n - \hat{s}^*_n|}{\hat{s}^*_n} < \delta \tag{29}
\]

where \( \delta \) is a prescribed tolerance. If this condition is not satisfied, the calculation is repeated with \( \hat{s}^*_n \leftarrow \hat{s}_n \). At the end of a successful iteration, one can calculate \( s_n \) as

\[
s_n = s(t_n) = s(t_{n-1}) + \hat{s}_n \Delta t \tag{30}
\]

and then proceed to time \( t_{n+1} \). The temperature field can be found as part of the solution process.

**Calculation of the starred temperatures**

With the approximated velocities \( \hat{s}^*_{n+i-1}, i = 1, 2, \ldots, r \) given (equations (22) and (23)), one can specify the nodal velocities (equation (19)) and find the positions of the front node using the following approximated equation based on the temporary assumption given by equation (22):

\[
s^*_{n+i-1} = s^*_{n+i-2} + 2s^*_{n+i-1} \sqrt{t_{n+i-1} - \sqrt{t_{n+i-1} - t_{n+i-2}}} \tag{31}
\]

Then, with given temperature conditions at \( x = s(t) \) and \( x = h \) at time \( t_{n+i-1} \), a direct problem (equation (16)) must be solved to obtain the starred temperature nodal field \( T^*_{n+i-1} \).

**Calculation of the sensitivity coefficients**

The first approximation of \( \hat{s}_n \) at each time step, i.e., \( \hat{s}^*_n \), is given by equation (28) for \( t > \Delta t \). Then, assuming a velocity constraint such as those in equations (22)–(23), one can find the approximations \( \hat{s}^*_{n+i-1} \) for each \( \hat{s}_{n+i-1}, i = 1, 2, \ldots, r \). With these velocities known, the temperature on \( s(t) < x < h \) can be calculated by solving a direct boundary value problem. Therefore, the temperatures \( * T^*_{k+i-1} \) at the sensor locations can also be found. Let us now perturb \( \hat{s}^*_n \) to a nearby value \( (1 + \lambda) \hat{s}^*_n \) for a number (here \( \lambda = 0.001 \)). Repeating the above approach, one calculates the new values \( ** T^*_{k+i-1} \) of the temperature at the sensor locations. Then, using a finite difference method, the sensitivity coefficients can be approximated as

\[
S^*_{k+i-1} \approx \frac{** T^*_{k+i-1} - * T^*_{k+i-1}}{\lambda \hat{s}^*_n} \tag{32}
\]

The above calculation of the sensitivity coefficients must be repeated at each new iteration of each time step. At this point, one should appreciate the computational savings associated with the velocity constraint. Note that the above definition is theoretically dependent on \( \hat{s}^*_n \) and on the current geometry, temperature boundary conditions at \( x = s(t) \) and \( x = h \), as well as on the constraint of equations (22) and (23).

**Summary of the solution algorithm**

It is assumed that all the parameters of the problem are known at \( t \leq t_{n-1} \), the following steps are required to find the velocity and position of the melting front at time \( t = t_n \).

1. Calculate velocity \( \hat{s}^*_n \) using equation (28).
2. Use the velocity constraint (equations (22) and (23)) to calculate \( \hat{s}^*_{n+i-1}, i = 1, 2, \ldots, r \), and use equation (31) to find \( s^*_{n+i-1}, i = 1, 2, \ldots, r \).
3. With these approximate front velocities and front positions, as well as the given temperature conditions at \( x = s(t) \) \( T = T_m \) and \( x = h \) \( T = Y_{N+1}(t) \), solve the direct problem (equation (16)) and find the starred temperatures \( T^{n+1}_{k+1-i} \), \( i = 1, 2, \ldots, r \) at the \( N \) sensor locations \((k = 1, 2, \ldots, N)\).

4. Find the sensitivity coefficients \( S_i^{n+1} \) using equation (32).

5. Obtain a better estimate of \( s(t) \) from equation (27).

6. Check the tolerance using equation (29). If equation (29) is not satisfied, update the velocities and continue with step 2. If equation (29) is satisfied, calculate \( s(t) \) using equation (30) and solve equation (16) for the temperature field. Finally, update the interface velocity, temperature field, etc., and continue with step 1 for the next time step.

**NUMERICAL EXAMPLES**

To demonstrate the validity of the inverse technique discussed in this paper, several numerical tests have been performed. The melting of a one-dimensional semi-infinite domain of ice is studied with the temperature at two specified locations inside the solid phase (sensor locations) calculated from a given analytical solution. The parameter \( m \) in the governing equations (1) and (2) is 0 (planar) in this one-dimensional melting problem. In all the cases, the temperature data in the solid phase are used to predict the interface position and velocity.

The initial and boundary conditions for the example are as follows:

\[
T_{in} = -5^\circ C, \quad T(0,t) = 5^\circ C, \quad T(\infty, t) = -5^\circ C, \quad T_m = 0^\circ C
\]

The thermophysical properties of ice and water are that: for ice, \( K_s = 0.022185 \text{ J/s cm}^\circ C, \quad \kappa_s = 0.0115 \text{ cm}^2/\text{s}, \quad c_s = 1.9088 \text{ J/g}^\circ C, \) and for water, \( K_L = 0.0060278 \text{ J/s cm}^\circ C, \quad \kappa_L = 0.00144 \text{ cm}^2/\text{s}, c_L = 4.186 \text{ J/g}^\circ C, \) where \( \kappa \) is the thermal diffusivity. The analytical solution for the temperature distribution in the solid phase (i.e. in ice) is given as

\[
T = T_{in} - \frac{T_{in} - T_m}{\text{erfc}(\beta \sqrt{K_L/K_s})} \frac{x}{2 \sqrt{\kappa_s} t}
\]

The front position and velocity are

\[
s = 2 \beta \sqrt{K_L} t
\]

and

\[
\dot{s} = \frac{\beta \sqrt{K_L}}{\sqrt{t}}
\]

respectively, with \( \beta = 0.115 \), where \( \text{erfc} \) is the complementary error function.

The numerical results for this example are given in Figures 2–15, using different time steps, future time steps, regularization parameter, sensor locations (here \( N = 1, h = \hat{x}_2 \)) and errors in the internal temperature data. In these tests, equation (33) is used to generate the internal temperature data. In some of the cases below, these internal data were multiplied by \( (1 + 0.02 \tau) \), where \( \tau \) is a random variable on \([-1, +1]\), in order to simulate more realistic experimental cases. For all the cases reported below, five linear elements were used in the region \( s(t) \leq x \leq \hat{x}_1 \), and five linear elements in the region \( \hat{x}_1 \leq x \leq \hat{x}_2 \). The integration parameters \( \gamma \) and \( \varepsilon \) used in equations (17), (18a) and (18b) are 0.85. The maximum number of iterations was 20 (for early time with small time steps and internal data with error), and the minimum was 2 (for later time and exact internal data), with a tolerance \( \delta = 0.005 \) in front velocity \( \dot{s}(t) \) (in equation (29)) used. To start the algorithm at time \( t = 0 \), an arbitrary initial front velocity was assumed.
Figure 2. Velocity of the melting front

Figure 3. Position of the melting front
Figure 4. Velocity of the melting front

Figure 5. Position of the melting front
Figure 6. Velocity of the melting front

Figure 7. Position of the melting front
Figure 8. Velocity of the melting front

Figure 9. Position of the melting front
Figure 10. Velocity of the melting front

Figure 11. Position of the melting front
Figure 12. Velocity of the melting front

Figure 13. Position of the melting front
Figures 2 and 3 show the effect of the number of future times $r$ to the solution, with fixed sensor locations and time steps, and without regularization. The thermocouple measurements are assumed to be without error. It can be seen that, by increasing $r$, a significant improvement in the front velocity and location can be achieved.

The same case is repeated with a smaller time step. The interface velocity (Figure 4) and position (Figure 5) appear to oscillate in the beginning, but later the results are better than those in Figures 2 and 3.

Figure 2–5 also demonstrate that, when the time step is decreased, the stability of the solution decreases and when future time steps are increased, the stability increases.

The same cases as shown in Figures 2–5 were repeated with a $\pm 2$ per cent random error applied to the internal temperature data. In these cases, the internal temperatures are calculated by multiplying equation (33) by $(1 + 0.02x)$. As shown in Figures 6–9, the future data algorithm is able to handle the internal data with error. If the time step is decreased, the number of future time steps $r$ must be increased to obtain an acceptable accuracy (Figures 8 and 9). Calculations have been repeated with different error in the internal data, and as expected, the larger the error in the internal data, the more future time steps (bigger $r$) are needed for accuracy comparable to the previous cases.

The effect of regularization is shown in Figures 10 and 11, where the exact internal temperature data are used with a fixed future time step and sensor locations. It is illustrated that the large values of $\alpha$ (with moderate $r$) help to stabilize the velocity (Figure 10) and front position (Figure 11) at early times when the interface is far away from the sensors.

The cases shown in Figures 12, 13 and Figures 14, 15 demonstrate the effect of the sensor location $\hat{x}_1$ on the prediction of the melting front, and they also illustrate the effect of the future time steps and regularization parameter on the numerical solution. In these cases, the first sensor location $\hat{x}_1$ is far away from the origin ($x = 0$) compared with the previous cases, and the time
steps are also very small. This means that these cases are much more unstable than previous cases. To improve the stability, one can use the future time method with more future time steps, or use the regularization method with a relatively large regularization parameter, or combine the future time method and regularization method with the proper number of future time steps and regularization parameter. In Figures 12 and 13, only the future time method is used, and as expected, one needs a bigger $r$ with increased $\dot{x}_1$ and decreased $\Delta t$ to maintain accuracy. In Figures 14 and 15, the combination of future time method and regularization method is applied. In this case, only two future time steps are used, but the result with $\alpha=0.5$ is much more stable than that with $\alpha = 0$. The scale of the last two graphs is exaggerated to demonstrate the effect of the slight regularization.

Comparing all the cases, one can conclude that more future times, large time steps and a large regularization parameter will increase the stability, and one can also conclude that the further the sensor location $\dot{x}_1$ is from the origin, the less stable the solution will be. Therefore, in order to obtain stable and accurate results, it is necessary to properly choose the time step, the number of future time steps and regularization parameter according to the sensor locations and random errors in the internal temperature data.

Also, the cases where the front velocity decays exponentially in time rather than in the form of equation (35) have been examined. The present method is found to work very well for all these problems with (the examples reported here) or without infinite initial front velocity.

**DISCUSSION AND CONCLUSIONS**

In this paper, a combination of Beck's future time method$^2$ and the regularization method, using the DFEM, have been shown to be effective tools for handling the inverse Stefan problem accurately, and can be used to calculate the interface velocity, interface location and the
temperature field in the solid phase using temperature measurements with random error at
discrete points inside the solid phase. It was demonstrated that a combination of small time steps
and a moderate regularization parameter leads to very accurate results even when the interface is
located far away from the sensors. As expected, small time steps are more accurate but less stable
than bigger time steps. This means that if a time interval (i.e. the future time interval) is used
for future calculations at each time step, one will have better accuracy by dividing the interval into
more time steps (bigger \( r \)). Also, the fact that the algorithm may work with very small time steps
provides the possibility of using the experimental data more effectively (note that the acquisition
time step is usually very small).

The algorithm works very well without regularization. Nevertheless, moderate regularization
will increase stability and accuracy as well as convergence rate (less iterations are required in the
case with regularization). The calculated values of the velocity are very close to the analytical
solution with or without regularization, but, since small errors in the velocity will be carried to the
interface position during integration (equations (30) and (31)), it is recommended that a moderate
regularization always be used. Also note that, since the future temperature calculations require an
extensive computational effort, one can save computational time by introducing a small regular-
ization parameter.

There are four main parameters that affect the stability of the inverse problem: (1) the number
of future time steps \( r \), (2) time step \( \Delta t \), (3) regularization parameter \( \alpha \) and (4) sensor location \( \hat{x}_1 \).
For \( \Delta t \), \( \alpha \), and \( \hat{x}_1 \) fixed, if \( r \) is increased, the stability and accuracy will increase; for \( r \), \( \alpha \), and \( \hat{x}_1 \)
fixed, if \( \Delta t \) is increased, the stability will increase and the accuracy will decrease; for \( r \), \( \Delta t \) and \( \hat{x}_1 \)
fixed, if \( \alpha \) is increased, the stability will increase, but the accuracy will decrease if very large \( \alpha \) is
used; and finally, for \( r \), \( \Delta t \) and \( \alpha \) fixed, if \( \hat{x}_1 \) is increased, the stability and accuracy will decrease.

The work presented here is being extended to two-dimensional problems and to cases with real
experimental temperature data.

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