CONTROL OF THE FREEZING INTERFACE MOTION IN TWO-DIMENSIONAL SOLIDIFICATION PROCESSES USING THE ADJOINT METHOD

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SUMMARY
The aim of this work is to calculate the optimum history of boundary cooling conditions that, in two-dimensional conduction driven solidification processes, results in a desired history of the freezing interface location/motion. The freezing front velocity and heat flux on the solid side of the front, define the obtained solidification microstructure that can be selected such that desired macroscopic mechanical properties and soundness of the final cast product are achieved.

The so-called two-dimensional inverse Stefan design problem is formulated as an infinite-dimensional minimization problem. The adjoint method is developed in conjunction with the conjugate gradient method for the solution of this minimization problem. The sensitivity and adjoint equations are derived in a moving domain. The gradient of the cost functional is obtained by solving the adjoint equations backward in time. The sensitivity equations are solved forward in time to compute the optimal step size for the gradient method. Two-dimensional numerical examples are analysed to demonstrate the performance of the present method.

KEY WORDS Design solidification Inverse problems Adjoint method

INTRODUCTION
Inverse problems have been under intense research in engineering over the past decades. Inverse problems are ill-posed in the sense that their solutions do not necessarily satisfy conditions of existence, uniqueness, and stability in small changes to the given data.\(^1\) One example of inverse problems is the system input identification problem, where the system input is identified given the parameters of a known model (i.e. known governing equations representing the system and the known material properties) and its output. The given output can either be a measured response of the system (the inverse problem) or a desired response (the inverse design problem). The given output is compared with the computed response obtained from a numerical model of the actual process. Then, the unknown system input is corrected such that a given error criterion is minimized. The output least square is the most common error criterion and is adopted in the present work.

Here a methodology is developed for the design of solidification processes in the framework of inverse design problems. The crystallographic growth morphology, scale of microstructures, and grain orientation in a casting process are directly related with the macroscopic properties of the final product, and as such their control is of extreme importance. The freezing front motion and the interface heat flux on the solid side define the crystallographic growth morphology and scale of microstructures (References 2 and 3). It is the aim of this work to calculate the required history
of cooling boundary conditions that achieves a desired freezing front motion in a two-di-
ensional solidification of a pure material. This problem is classified as the Inverse Stefan Design
Problem (ISDP).

Among a few mathematicians who approached numerically the two-dimensional inverse Stefan
problem, we particularly mention the work of Colton and Reemtsen. They solved the single
phase inverse Stefan problem in two space variables by minimizing the maximal defect in the
initial-boundary data with regularization. Zabaras et al. analyzed two-dimensional design Stefan
processes using the future information method developed by Beck et al. The minimization
process was performed over a time interval which starts at the present time where the boundary
flux must be calculated and includes some future time steps. With the future information method,
the unknown boundary flux was effectively regularized in time during the above interval (for
time example taken temporarily constant). To further stabilize their solution algorithm, Zabaras et al. also
introduced spatial regularization in the sense of Tikhonov.

Alifanov and colleagues solved several two-dimensional inverse heat conduction problems
(IHCP) without phase change using the so-called iterative regularizing gradient algorithm. They
computed the gradient of the discrepancy functional by solving the adjoint problem.

Delaunay and co-workers solved the inverse solidification problem of calculating the
freezing front position from noisy temperature measurements in the solid phase using an
optimization method with adjoint equations. They also compared their results with experimental
data.

Dantzig et al. solved the solidification optimization problem of computing the furnace wall
temperatures in a Bridgman furnace to produce a specified temperature distribution, in the
solidifying crystal, corresponding to conditions known to produce a desirable microstructure.
They minimized the difference between the desired temperature distribution and the calculated
temperature distribution for a distinct set of process parameters. They used a sensitivity analysis
derived with the direct differentiation method.

In this work, the two-dimensional ISDP is analyzed using an infinite-dimensional function
minimization technique. The minimization process is performed over the whole time domain of
interest and the unknown heat flux function is discretized after the minimization process is
analytically performed in the $L_2$ space. Zabaras and Kang implemented this minimization
technique for one-dimensional inverse design solidification problems. The adjoint method, which
yields the sensitivity and adjoint equations, is developed in conjunction with the conjugate
gradient method. The conjugate gradient method was modified from the ones in References 15
and 16 where the functional is minimized in a finite vector space. The gradient of the cost
functional is obtained by solving the adjoint equations backward in time and the sensitivity
equations are solved forward in time to compute the optimal step size for the gradient method.
The preprocessing required for the design of predetermined freezing interface location is also
addressed. Two two-dimensional numerical examples are tested to demonstrate the performance of
the present method.

DEFINITION OF THE INVERSE STEFAN DESIGN PROBLEM

Governing equations of the direct Stefan problem

Consider solidification in a region $\Omega_0$ that is occupied with liquid of pure metal at temperature
$T_{in}$ (Figure 1). Solidification starts at time $t = 0$ and proceeds inward as the fixed boundary $\partial \Omega_0$ is
cooled down to a temperature lower than the melting temperature $T_m$. Let us denote $T(x, t)$ the
temperature at a position $x \in \Omega_0 ( = \Omega_L(t) \cup \Omega_S(t))$ and time $t$, $K$ the conductivity and $C = \rho c$ the
modified specific heat, where \( \rho \) is the density and \( c \) the specific heat. The thermal properties are assumed in general to be functions of temperature. The subscript \( S \) and \( L \) are used to denote solid and liquid phases, respectively. The governing equation defining the Stefan problem is as follows:

\[
C(T) \frac{\partial T}{\partial t}(x, t) = \nabla \cdot (K(T) \nabla T(x, t))
\]  

(1)

where

\[
C = C_S, \quad K = K_S, \quad T = T_S \quad \text{for} \quad x \in \Omega_S(t)
\]

\[
C = C_L, \quad K = K_L, \quad T = T_L \quad \text{for} \quad x \in \Omega_L(t)
\]

The initial/boundary conditions and the Stefan condition can be written as

\[
T(x, 0) = T_{in}, \quad x \in \Omega_0
\]  

(2)

\[
K_S(T(x, t)) \frac{\partial T(x, t)}{\partial n_o} = q(x, t), \quad x \in \partial \Omega_0
\]  

(3)

\[
T(x, t) = T_m, \quad x \in \partial \Omega_L(t)
\]  

(4)

\[
K_S(T_L(x, t)) \frac{\partial T_L(x, t)}{\partial n} - K_L(T_L(x, t)) \frac{\partial T_L(x, t)}{\partial n} = \rho H V \cdot n, \quad x \in \partial \Omega_L(t)
\]  

(5)

Equations (4) and (5) represent the isothermal freezing interface condition and the energy balance equation at \( \partial \Omega_L(t) \), respectively. \( n \) is a unit normal vector at a position on the interface boundary toward the liquid region, \( V \) is the freezing interface velocity vector at the same position, and \( H \) is the latent heat of fusion.

The direct Stefan problem is to find the history of temperature field in \( \Omega_0 \) as well as the motion/location of the freezing front at all times, given the material properties, initial temperature, melting temperature, and the proper history of boundary conditions on the fixed boundary \( \partial \Omega_0 \) (Figure 1).

**Definition of the inverse Stefan design problem**

The inverse Stefan design problem is defined as follows: Given the material properties, initial temperature, melting temperature, and the motion/location of the freezing front \( \partial \Omega_L(t) \) at all times, calculate the history of the flux and temperature on the fixed boundary \( \partial \Omega_0 \) and the history of temperature field in \( \Omega_0 \) (Figure 2).
Note that in the ISDP, unlike the conventional direct Stefan problem, the heat flux history $q$ at the fixed boundary in equation (3) is unknown. Instead, the history of motion of the freezing front, $\partial \Omega_s(t)$, is known at all times. The prescribed freezing front motion defines the flux discontinuity on $\partial \Omega_s(t)$ (equation (5)). In this sense, equations (4) and (5) constitute a set of overspecified boundary conditions on $\partial \Omega_s(t)$.

Mathematically the problem is formulated as an infinite-dimensional minimization problem: Given the material properties, initial temperature, melting temperature, and the motion of the freezing front at all times, find the optimal boundary heat flux $q^*(x,t)$, $(x,t) \in ([\partial \Omega_s(t)] \times [0,t_{\text{max}}])$ such that

$$S(q^*) \leq S(q), \quad q \in L_2([\partial \Omega_s(t)] \times [0,t_{\text{max}}]) \quad (6)$$

where

$$S(q) = \frac{1}{2} \| T_m - T(x,t;q) \|_{L_2([\partial \Omega_s(t)] \times [0,t_{\text{max}}])}^2 = \frac{1}{2} \int_0^{t_{\text{max}}} \int_{\partial \Omega_s(t)} \left( T_m - T(x,t;q) \right)^2 \, d\Gamma \, dt \quad (7)$$

The solution of the direct problem defined by equations (1)–(3) and equation (5) with known freezing front velocity is denoted as $T(x,t;q)$ to emphasize the functional dependence of the temperature field $T(x,t)$ on the boundary heat flux $q$. The cost functional in equation (7) is the $L_2$ norm of the error between the calculated temperature distribution $T(x,t;q)$ at the freezing front and the given melting temperature $T_m$ which, in the sense of inverse heat conduction problems, is used as a pseudo-temperature measurement at the freezing interface. The minimization process will be performed over the whole time domain of interest ($0 \leq t \leq t_{\text{max}}$) and the unknown heat flux function will be discretized after the minimization process is performed in the $L_2$ space.

**Preprocessing**

For the inverse design problem of concern here, certain preprocessing operations are necessary before the main solution algorithm is undertaken. At first, a time step $\Delta t = t^{n+1} - t^n$ is selected based on previous experiences with the FEM calculation of similar direct Stefan problems. Since the deforming FEM is used to analyze the problem, a finite element mesh must be introduced that at each time step conforms with the moving interface. Here, the mesh generation scheme developed by Ruan and Zabaras and McDaniel and Zabaras is followed. In their work, the whole region of solidification is divided into the solid and liquid regions. The solid region $\Omega_s(t)$ consists of a non-deforming subregion and a deforming subregion. Nodes are fixed in time in the non-deforming subregion. The deforming subregion consists of the elements of the solid phase.
next to the freezing front. These elements deform and change their sizes (grow) as \( \partial \Omega_i(t) \) moves inward. When the maximum size of these interface elements in a direction normal to \( \partial \Omega_i(t) \) reaches a maximum allowable prescribed size, new deforming elements are generated by splitting each of the previously deforming elements in two. Then, the new set of elements next to \( \partial \Omega_i(t) \) becomes the new deforming subregion, while the remaining element group of the previously deforming subregion becomes part of the non-deforming region. The number of elements in the liquid phase remains fixed in time and a remeshing scheme utilizing transfinite mapping is used. However, in the nearly unidirectional solidification processes, as new elements are added in the solid region the same number of elements are subtracted from the liquid region.

For the present design problem, the location of the interface \( \partial \Omega_i(t) \) is considered prescribed at all times. The position \((x_i^{n+1}, y_i^{n+1})\) of the \(i\)th interface node at time \(t^{n+1}\) is selected such that the interface elements have favourable element shapes that provide a well-conditioned finite element system. Once the interface nodal positions are designed, the components of the interface nodal velocities are obtained using finite difference approximations (Figure 3):

\[
V_{ix}^{n+1} = \frac{x_i^{n+1} - x_i^n}{t^{n+1} - t^n}, \quad V_{iy}^{n+1} = \frac{y_i^{n+1} - y_i^n}{t^{n+1} - t^n}
\]

(8)

where \((x_i^{n+1}, y_i^{n+1}) \in \partial \Omega_i(t^{n+1})\) and \((x_i^n, y_i^n) \in \partial \Omega_i(t^n)\). These approximations of interface nodal velocity components at all discrete times are kept in memory and used for the mesh generation required in the deforming FEM solution of the direct, adjoint, and sensitivity problems. They are also used for evaluating the interface flux jump.

**Calculation of the flux discontinuity at the freezing interface**

Since the melting temperature condition in equation (4) is used as a pseudo-measurement at the interface in the ISDP, the heat flux jump condition in equation (5) is used as the interface boundary condition. In a Galerkin finite element formulation context, the force vector at the interface has the form:15

\[
F_i = \sum_{b=1}^{E_i} \sum_{k=1}^{F_k^b} \int_{\partial \Omega_i^k} \left[ K_S \nabla T_S - K_L \nabla T_L \right] \cdot \mathbf{n} \Psi_i^b(x, y, t) \, d\Gamma
\]

\[
= \sum_{b=1}^{E_i} \int_{\partial \Omega_i^k} \left[ \rho \mathbf{H} \mathbf{V} \cdot \mathbf{n} \right] \Psi_i^b(x, y, t) \, d\Gamma
\]

(9)

![Figure 3. Discretization of the freezing interface based on its desired motion](image-url)
where $\partial \Omega_{b}^{f}$ is the $b$th interface segment ($b = 1, 2, \ldots, E_{f}$). Here, the velocity can be approximated as follows:

$$\mathbf{v} = \sum_{i} \mathbf{v}_{b}^{i} \Psi_{i}^{b}(x, y, t)$$

(10)

where $\mathbf{v}_{b}^{i}$ is the nodal velocity at the interface defined through equation (8), $\Psi_{i}^{b}(x, y, t)$ is the one-dimensional shape functions defined at the interface boundary segments, and the normal $n$ becomes $\mathbf{N}_{b}^{i}$ defined at the interface boundary segment $b$ through the interface nodal coordinates. Then, we have

$$F_{i} = \sum_{b=1}^{E_{f}} \int_{\partial \Omega_{b}^{f}} \rho H \mathbf{v}_{b}^{i} \mathbf{N}_{b}^{i} \cdot \sum_{h} \Psi_{h}^{b} \mathbf{v}_{h}^{b} \mathrm{d} \Gamma$$

(11)

where $F_{i}$ is the component of the force vector at the interface.

It is clear that once the directional cosines of the unit normal $\mathbf{N}_{b}^{i}$ to the interface segment $b$ are defined, then the term $F_{i}$ can be evaluated without any difficulty because the Cartesian components $V_{bx}^{b}$ and $V_{by}^{b}$ of the interface nodal velocities $\mathbf{v}_{h}^{b}$ along with the interface nodal coordinates are provided from the previously reported preprocessing procedure.

THE ADJOINT METHOD

Definition of the sensitivity and adjoint problems

The adjoint method is used in conjunction with the conjugate gradient method. The conjugate gradient method (Reference 19) consists of constructing the minimizing sequence $q^{0}, q^{1}, \ldots, q^{k}, \ldots$

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

(12)

where $q^{k}$ is the minimizer of the cost functional, $\alpha^{k}$ is the step size, and $p^{k}$ is the conjugate search direction.

Calculation of $p^{k}$ requires the gradient of the cost functional defined in equation (7). At first the sensitivity problem has to be derived by means of a perturbation to the unknown heat flux $q$. Let us define the sensitivity function $\theta(x, t; q, \Delta q)$ as the directional derivative of the temperature field $T(x, t; q)$ in the direction of the function increment $\Delta q$, i.e.

$$\theta(x, t; q, \Delta q) \equiv T_{q}(x, t; q) \cdot (\Delta q) \equiv D_{\Delta q} T(x, t; q)$$

(13)

The sensitivity problem can be derived by considering the governing equations (1)–(3) and (5) corresponding to the direct problems defining the fields $T(x, t; q)$ and $T(x, t; q + \Delta q)$. A linearization of the field $T(x, t; q + \Delta q)$ and of the material properties $C(T(x, t; q + \Delta q))$ and $K(T(x, t; q + \Delta q))$ is performed as follows:

$$T(x, t; q + \Delta q) = T(x, t; q) + \theta(x, t; q, \Delta q) + O(\| \Delta q \|^2)$$

(14a)

$$C(T(x, t; q + \Delta q)) = C(T(x, t; q)) + \frac{dC(T(x, t; q))}{dT} \theta(x, t; q + \Delta q) + O(\| \Delta q \|^2)$$

(14b)

$$K(T(x, t; q + \Delta q)) = K(T(x, t; q)) + \frac{dK(T(x, t; q))}{dT} \theta(x, t; q + \Delta q) + O(\| \Delta q \|^2)$$

(14c)

Substitution of equations (14a)–(14c) to the governing equations (1)–(3) and (5) corresponding to $T(x, t; q + \Delta q)$ and subtracting the corresponding governing equations (1)–(3) and (5) for $T(x, t; q)$, leads to the following sensitivity problem:

$$\frac{\partial}{\partial t} \left[ C(T) \theta(x, t; q, \Delta q) \right] = \nabla^{2} \left[ K(T) \theta(x, t; q, \Delta q) \right], \quad x \in \Omega_{b}(t) \cup \Omega_{L}(t)$$

(15)
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\[ \theta(x, 0; q, \Delta q) = 0, \quad x \in \Omega_0 \]  
\tag{16} \]

\[ \frac{\partial}{\partial n_0} [K_S(T_S) \theta_S] = \Delta q(x, t), \quad x \in \partial \Omega_0 \]  
\tag{17} \]

\[ \frac{\partial}{\partial n} [K_S(T_S) \theta_S] - \frac{\partial}{\partial n} [K_L(T_L) \theta_L] = 0, \quad x \in \partial \Omega_i(t) \]  
\tag{18} \]

where the material properties are defined as in equation (1).

The gradient \( S'(q) \) of the cost functional \( S(q) \) is obtained from the directional derivative \( D_{\Delta q} S(q) \) of \( S(q) \) at \( q \) in the direction of the increment \( \Delta q \), where \( q \) and \( \Delta q \in L_2([\Omega_0] \times [0, t_{\text{max}}]) \):

\[ D_{\Delta q} S(q) \equiv (S'(q), \Delta q)_{L_2([\Omega_0] \times [0, t_{\text{max}}])} \]

\[ = -(T_m - T(x, t; q), \theta(x, t; q, \Delta q))_{L_2([\Omega_i(t)] \times [0, t_{\text{max}}])} \]  
\tag{19} \]

Here, the last term of equation (19) is derived using equation (7). The inner products used in the equation above are defined as follows:

\[ (f, g)_{L_2([\Omega_0] \times [0, t_{\text{max}}])} = \int_0^{t_{\text{max}}} \int_{\Omega_0} f g \, d\Gamma \, dt \]  
\tag{20a} \]

\[ (f, g)_{L_2([\Omega_i(t)] \times [0, t_{\text{max}}])} = \int_0^{t_{\text{max}}} \int_{\Omega_i(t)} f g \, d\Gamma \, dt \]  
\tag{20b} \]

Let us now introduce a linear operator \( L \) from the sensitivity problem (equations (15)–(18)):

\[ L(\theta) = \frac{\partial}{\partial t} [C(T) \theta(x, t; q, \Delta q)] - \nabla^2 [K(T) \theta(x, t; q, \Delta q)], \quad (x, t) \in ([\Omega_0] \times [0, t_{\text{max}}]) \]  
\tag{21} \]

where \( C(T) \) and \( K(T) \) are defined as before. The adjoint operator \( L^*(\Psi) \) of \( L(\theta) \) is defined such that

\[ \int_0^{t_{\text{max}}} \int_{\Omega_0} \Psi L(\theta) \, d\Omega \, dt = \int_0^{t_{\text{max}}} \int_{\Omega_0} L^*(\Psi) \theta \, d\Omega \, dt \]  
\tag{22} \]

where \( \Psi \) is the so-called adjoint function.

With multiple integration by parts of the left-hand side of the above equation we can show that:

\[ \int_0^{t_{\text{max}}} \int_{\Omega_0} \Psi L(\theta) \, d\Omega \, dt = \int_0^{t_{\text{max}}} \int_{\Omega_0} \Psi \frac{\partial}{\partial t} (C \theta) - \nabla^2 (K \theta) \, d\Omega \, dt \]

\[ = \int_{\Omega_0} \Psi C \theta \, d\Omega |_{t=_{\text{max}}} - \int_{\Omega_0} \Psi C \theta \, d\Omega |_{t=0} \]

\[ - \int_0^{t_{\text{max}}} \int_{\Omega_0} \frac{\partial \Psi}{\partial t} (C \theta) \, d\Omega \, dt \]

\[ + \int_0^{t_{\text{max}}} \int_{\Omega_0} \nabla \Psi \cdot \nabla (K \theta) \, d\Omega \, dt \]

\[ - \int_0^{t_{\text{max}}} \int_{\Omega_0} \Psi \frac{\partial}{\partial n_0} (K \theta) \, d\Gamma \, dt \]

\[ - \int_0^{t_{\text{max}}} \int_{\Omega_i(t)} \Psi \frac{\partial}{\partial n} [K \theta] \, d\Gamma \, dt \]  
\tag{23} \]
where the direction of the normal \( \mathbf{n} \) is inward at the interface \( \partial \Omega_0(t) \) and the discontinuity term, 
\[ (\partial/\partial \mathbf{n}) \left[ |K\theta| \right]_{\partial \Omega_0(t)} \] (left-hand side of equation (18)), comes from the divergence theorem with discontinuity in the domain \( \Omega_0 \). The adjoint function \( \Psi \) was assumed to be continuous at \( \partial \Omega_0(t) \).

Use of Green's theorem with discontinuity in the domain \( \Omega_0 \), gives that:

\[
\int_0^{t_{\text{max}}} \int_{\Omega_0} \nabla \Psi \cdot \nabla (K\theta) \, d\Omega \, dt = -\int_0^{t_{\text{max}}} \int_{\Omega_0} K\theta \nabla^2 \Psi \, d\Omega \, dt \\
+ \int_0^{t_{\text{max}}} \int_{\partial \Omega_0} K\theta \frac{\partial \Psi}{\partial \mathbf{n}} \, d\Gamma \, dt \\
+ \int_0^{t_{\text{max}}} \int_{\partial \Omega_0(t)} \theta \left[ K \frac{\partial \Psi}{\partial \mathbf{n}} \right]_{\partial \Omega_0(t)} \, d\Gamma \, dt \tag{24a}
\]

where

\[
\left[ K \frac{\partial \Psi}{\partial \mathbf{n}} \right]_{\partial \Omega_0(t)} = K_S \frac{\partial \Psi_S}{\partial \mathbf{n}} - K_L \frac{\partial \Psi_L}{\partial \mathbf{n}}, \quad \mathbf{x} \in \partial \Omega_0(t) \tag{24b}
\]

and \( \theta \) is taken to be continuous at \( \partial \Omega_0(t) \).

Therefore, using equations (24a) and (24b), equation (23) can be simplified as follows:

\[
\int_0^{t_{\text{max}}} \int_{\Omega_0} \Psi L(\theta) \, d\Omega \, dt = \int_{\Omega_0} \Psi C \theta |_{t=t_{\text{max}}} \, d\Omega - \int_{\Omega_0} \Psi C \theta |_{t=0} \, d\Omega \\
- \int_0^{t_{\text{max}}} \int_{\Omega_0} \theta \left[ C \frac{\partial \Psi}{\partial t} + K \nabla^2 \Psi \right] \, d\Omega \, dt \\
- \int_0^{t_{\text{max}}} \int_{\partial \Omega_0} \Psi \frac{\partial}{\partial \mathbf{n}} (K\theta) \, d\Gamma \, dt \\
- \int_0^{t_{\text{max}}} \int_{\partial \Omega_0(t)} \Psi \frac{\partial}{\partial \mathbf{n}} \left[ |K\theta| \right]_{\partial \Omega_0(t)} \, d\Gamma \, dt \\
+ \int_0^{t_{\text{max}}} \int_{\partial \Omega_0(t)} K \frac{\partial \Psi}{\partial \mathbf{n}} \, d\Gamma \, dt \\
+ \int_0^{t_{\text{max}}} \int_{\partial \Omega_0(t)} \theta \left[ K \frac{\partial \Psi}{\partial \mathbf{n}} \right]_{\partial \Omega_0(t)} \, d\Gamma \, dt \tag{25}
\]

Note that \( \theta \) is the solution of the sensitivity equations (15)–(18). By defining the adjoint operator \( L^* \) as,

\[
L^*(\Psi) \equiv C(T) \frac{\partial \Psi}{\partial t}(x, t; q) + K(T) \nabla^2 \Psi(x, t; q) = 0, \quad x \in \Omega_S(t) \cup \Omega_L(t) \tag{26a}
\]

and by imposing the following constraints to the adjoint function \( \Psi(x, t; q) \)

\[
\Psi(x, t_{\text{max}}; q) = 0, \quad x \in \Omega_S(t_{\text{max}}) \cup \Omega_L(t_{\text{max}}) \tag{26b}
\]

\[
- \left[ K \frac{\partial \Psi}{\partial \mathbf{n}} \right]_{\partial \Omega_0(t)} = \left( K_S \frac{\partial \Psi_S}{\partial \mathbf{n}} - K_L \frac{\partial \Psi_L}{\partial \mathbf{n}} \right) = T_m - T(x, t; q), \quad x \in \partial \Omega_0 \tag{26c}
\]

\[
K \frac{\partial \Psi(x, t; q)}{\partial \mathbf{n}_0} = 0, \quad x \in \partial \Omega_0 \tag{26d}
\]
one can obtain from equation (25) the following:

\[ - \int_0^{t_{\text{max}}} \int_{\partial \Omega_0} \Psi \Delta q \, d\Gamma \, dt - \int_0^{t_{\text{max}}} \int_{\partial \Omega(t)} \theta (T_m - T(x, t; q)) \, d\Gamma \, dt = 0 \]  

(27)

or

\[ (\Psi(x, t; q), \Delta q)_{L_2([\partial \Omega_0] \times [0, t_{\text{max}}])} = -(T_m - T(x, t; q), D_{\Delta q} T(x, t; q))_{L_2([\partial \Omega_0(t)] \times [0, t_{\text{max}}])} \]  

(28)

From equations (19) and (28), one can finally conclude that

\[ S\prime(x, t; q) = \Psi(x, t; q), \quad (x, t) \in ([\partial \Omega_0] \times [0, t_{\text{max}}]) \]  

(29)

i.e. the gradient of the cost functional is the solution of the adjoint function \( \Psi(x, t; q) \) defined from equations (26a)-(26d) at the fixed boundary. The system of equations (26a)-(26d) is the so-called adjoint problem to the sensitivity problem defined by equations (15)-(18).

The optimal step size \( \alpha^k \) is obtained by minimizing the cost functional \( S(q^{k+1}) = S(q^k + \alpha p^k) \) at each iteration step, i.e.

\[ \frac{d}{dx} S(q^k + \alpha p^k) = \frac{d}{dx} \| T(x, t; q^k + \alpha p^k) - T_m \|_{L_2([\partial \Omega_0(t)] \times [0, t_{\text{max}}])^2} = 0 \]  

(30)

Table I. The conjugate gradient algorithm

---

**Step 1:** Pick an initial guess \( q^0(x, t) \) in \( L_2([\partial \Omega_0] \times [0, t_{\text{max}}]) \). Set \( k = 0 \).

**Step 2:** Calculation of conjugate search direction \( p^k(x, t) \)

a. Define the scalar \( \gamma^k \).

a1. Solve the direct Stefan problem forward in time for \( T(x, t; q^k(x, t)) \)

a2. Compute the residual \( T_m - T(x, t; q^k(x, t)) \) in \( L_2([\partial \Omega_0(t)] \times [0, t_{\text{max}}]) \)

a3. Solve the adjoint equations backward in time for \( \Psi(x, t; q^k(x, t)) \).

Evaluate \( S\prime(q^k(x, t))(x, t) = \Psi(x, t; q^k(x, t)) \) in \( L_2([\partial \Omega_0(t)] \times [0, t_{\text{max}}]) \)

b. Define the direction \( p^k(x, t) \).

If \( k = 0 \), set \( p^0(x, t) = -S\prime(q^k)(x, t) \),

otherwise, \( p^k(x, t) = -S\prime(q^k)(x, t) + \gamma^k p^{k-1}(x, t) \)

**Step 3:** Calculate the optimal step size \( \alpha^k \)

a. Solve the sensitivity equations to calculate \( \theta(x, t; p^k) \)

b. Set optimal step size

\[ \alpha^k = \frac{(S\prime(q^k)(x, t), p^k(x, t))_{L_2([\partial \Omega_0] \times [0, t_{\text{max}}])}}{\| S\prime(q^k)(x, t; p^k) \|_{L_2([\partial \Omega_0] \times [0, t_{\text{max}}])}^2} \]

**Step 4:** Update \( q^{k+1}(x, t) = q^k(x, t) + \alpha^k p^k(x, t) \)

**Step 5:**

If \( \| q^{k+1}(x, t) - q^k(x, t) \|_{L_2([\partial \Omega_0] \times [0, t_{\text{max}}])} < \varepsilon \) (specified tolerance), stop

Otherwise set \( k = k + 1 \) and go to step 2.
from which using equations (13) and (28) it can be shown that
\[
\phi^k = \frac{-\langle S'(q^k), p^k \rangle_{L_2([\partial \Omega_0] \times [0,t_{\text{max}}])}}{\| \theta(x, t; q^k, p^k) \|_{L_2([\partial \Omega(t)\times [0,t_{\text{max}}])}^2}
\]
(31)

The conjugate gradient algorithm

The CGM algorithm is summarized in Table I. The calculation of the optimal step requires the values of the sensitivity function at the freezing front (equation (31)). Several inner products and norms have to be calculated in the spaces \( L_2([\partial \Omega_0] \times [0,t_{\text{max}}]) \) and \( L_2([\partial \Omega(t)] \times [0,t_{\text{max}}]) \). At \( \partial \Omega_0 \) the lengths of the boundary segments are fixed in time. As such, the corresponding inner product is computed using the following approximation:
\[
(f, g)_{L_2([\partial \Omega_0] \times [0,t_{\text{max}}])} = \int_0^{t_{\text{max}}} \int_{\partial \Omega_0} fg \, d\Gamma \, dt = \sum_{j=1}^{N-1} \sum_{i=1}^{E_0} f_{i+1/2,j+1/2} g_{i+1/2,j+1/2} \Delta S_i \Delta t_j
\]
(32a)
where
\[
f_{i+1/2,j+1/2} = \frac{1}{2} (f_{i,j} + f_{i+1,j} + f_{i+1,j+1} + f_{i,j+1}),
\]
(32b)
\[
g_{i+1/2,j+1/2} = \frac{1}{2} (g_{i,j} + g_{i+1,j} + g_{i+1,j+1} + g_{i,j+1}),
\]
(32c)
and the temporal step size \( \Delta t_j = t_{j+1} - t_j \). \( N \) is the total number of temporal points, \( E_0 \) is the total number of line segments in the discretization of the fixed boundary \( \partial \Omega_0 \), and \( \Delta S_i \) is the length of the \( i \)th boundary segment.

In the moving interface the spatial step size (the length of the interface line segment) changes with time. Therefore, the inner product at the moving boundary is evaluated in the same manner as that at the fixed boundary except from the evaluation of the spatial step size:
\[
(f, g)_{L_2([\partial \Omega(t)] \times [0,t_{\text{max}}])} = \int_0^{t_{\text{max}}} \int_{\partial \Omega(t)} fg \, d\Gamma \, dt = \sum_{j=1}^{N-1} \sum_{i=1}^{E_t} f_{i+1/2,j+1/2} g_{i+1/2,j+1/2} \Delta S_{i,j+1/2} \Delta t_j
\]
(33a)
where
\[
\Delta S_{i,j+1/2} = \frac{1}{2} (\Delta S_{i,j} + \Delta S_{i,j+1})
\]
(33b)
with \( \Delta S_{i,j} \) the length of the \( i \)th boundary segment at time \( t_j \), and \( E_t \) the total number of line segments in the discretization of the moving boundary \( \partial \Omega(t) \).

The required norms in Table I are computed in the same manner as the inner products discussed above. In this paper only solidification examples with temperature-independent thermal properties are considered.

**NUMERICAL EXAMPLES**

**Example A**

The first example is a nearly unidirectional problem introduced earlier by Zabaras et al.\(^5\) (Figure 4). The material properties used for this problem are summarized in Table II. A sinusoidal
heat flux $q$ is applied to the bottom of a rectangular casting ($y = 0$, $0 \leq x \leq 1.2$ m), where

$$q(x, y, t) = 5 \{1 + 2 \sin[(\pi/1.2)x]\} \text{ W/m}^2$$ \hspace{1cm} (34)

as shown in Figure 5. The desired interface location was obtained by solving the corresponding direct problem. The calculated front position will now be used as the desired freezing interface location and our task is to identify the applied boundary flux condition given by equation (34). The present example is ill-posed in nature in the sense that the shape of the interface becomes flatter as the freezing front moves further away from the fixed boundary as shown in Figure 6, and therefore after some time the front motion does not realize the spatial variation of the boundary flux $q$.

For the solution of the direct, adjoint and sensitivity problems, a deforming finite element analysis was used with 72 bilinear quadrilateral elements. Initially, seven elements were used to model the solid region. The total number of elements (solid and liquid) was preserved at all times. The maximum allowable size of the interface elements was taken as 0.1 m and seven nodes were placed at the interface. The time step used for the time integration scheme was $10^{-3}$ s and the total number of time steps was 300.

The conjugate gradient method as shown in Table I was implemented. Zabarás and Kang\textsuperscript{14} previously emphasized that the selection of the initial guess is extremely important since it affects the rate of convergence. Figure 7(a) shows the initial guess taken for this specific test ($q^0(x, y, t) = 10$ W/m$^2$), while Figures 7(b)–(d) show the space-time behaviour of the calculated boundary heat flux at several iteration steps. Note that the calculated solution stays practically unchanged in the vicinity of the final time $t_{\text{max}} (= 0.3$ s) due to final condition in the adjoint problem (equation (26b)). However, it converged to the exact solution in the time interval of $[0, 0.2]$ s. Zabarás and co-workers\textsuperscript{5} solved the same test problem using the future information method and spatial regularization. Their solution converged up to 0.07 s without future time or regularization, 0.12 s with future time, and 0.16 s with future time and regularization.

Table III shows the values of the calculated cost functional at several iteration steps. It can be seen that for a value of the cost functional equal to $10^{-7}$, one will need more than 100 iterations.
The accuracy and rate of convergence of the solution tremendously deteriorated due to the final condition in the adjoint problem. In other words, the unknown function $q^{k+1}(x, t)$, where $x \in \partial\Omega_0$ and $k$ is the iteration step, is updated such that

$$q^{k+1}(x, t_{\text{max}}) = q^k(x, t_{\text{max}})$$

because the search direction $p^k(x, t_{\text{max}}) = 0$ for all iteration steps. Some preliminary ideas for correcting the problem induced by the final condition in the adjoint problem are discussed by Zabaras and Kang.\(^{14}\)

**Example B**

The second example is concerned with solidification in an infinite corner region (Figure 8). The material properties used in this example can be found in Table IV. The initial temperature of the liquid is set to 0-3°C and constant temperature of $-1$°C was applied to the fixed boundary. However, the corresponding boundary heat flux varies both spatially in $\partial\Omega_0$ as well as in time. The analytical solution for the interface position was obtained by Rathjen and Jiji\(^{20}\) and is shown
in Table V. This analytical interface position in time shown in Table V and Figure 8 is used as the desired freezing front history.

One-hundred ninety two (192) quadrilateral elements (with 24 elements in the solid region) and bilinear shape functions were used for the initial finite element mesh in solving the direct, adjoint, and sensitivity problems. The maximum allowable size of the interface elements was taken as 0.3 m and 25 nodes were placed at the interface. The time step used for the time integration scheme was $10^{-3}$ s and the total number of time steps was 500.

The goal in this example is also to identify the applied cooling boundary conditions. Figure 9 shows the space-time behaviour of the exact boundary heat flux at one side of the corner region ($0 \leq x \leq 3$ m). Note that for plotting reasons, in this and the following figures, the time axis was selected as (0.5-time) s.
Figure 8. Solidification in a corner region with the exact freezing interface position (Example B)

Table IV. Material properties for Example B

\[ K_S = K_L = 1 \text{ W/m}^\circ\text{C} \quad c_S = c_L = 1 \text{ J/kg}^\circ\text{C} \quad H = 0.25 \text{ J/kg} \]
\[ \rho = 1 \text{ kg/m}^3 \quad T_m = 0^\circ\text{C} \]

Table V. Exact freezing front location for Example B
(Reference 20)

\[ y = \left( \lambda^* + \frac{C}{x^* - \lambda^*} \right)^{\frac{1}{2}} \sqrt{4at} \]
\[ C = 0.159 \quad u = 5.02 \quad \lambda = 0.70766 \quad x^* = x / \sqrt{4at} \]
\[ a = 1 \text{ m}^2/\text{s} \text{ (thermal diffusivity)} \]

Two different initial guesses were used to observe the behaviour of the present design algorithm. In the first case, the initial guess function was taken as \( q^0(x, t) = 1.0 \text{ W/m}^2 \), \( 0 \leq t \leq 0.5 \text{ s} \), as shown in Figure 10(a). It was selected such that its value at \( t_{\text{max}} \) is close to that of the exact solution at \( t_{\text{max}} \), i.e. \( q^0(x, t_{\text{max}}) \approx q^{\text{exact}}(x, t_{\text{max}}) \).

Figures 10(b)–(d) show the space time behaviour of the unknown boundary heat flux at several iteration steps. The stopping criterion was taken as the combination of the \( L_2 \) norm of the change of the unknown function during two successive iterations (i.e. refer to Step 5 in Table I) and the value of the cost functional (i.e. error norm in equation (7)). This was mainly because the first criterion alone cannot guarantee the convergence on the solution. In this case, the tolerance for the first criterion was specified as \( 0.5 \times 10^{-2} \), while for the second \( 0.1 \times 10^{-3} \). The solution converged at iteration 13. The obtained solution shown in Figure 10(d) is, therefore, an optimal one for the given tolerances. To demonstrate the accuracy of the present algorithm, the converged solution was compared with the exact one, and the spatial variation of the boundary heat flux is shown in Figure 11. At early time, the solution shows an oscillatory behaviour in the vicinity of the corner region. However, it becomes stable as the freezing front moves away from the corner.

As a second test case, an initial guess function \( q^0(x, t) = 4.0 \text{ W/m}^2 \), \( 0 \leq t \leq 0.5 \text{ s} \) was taken such that its value at \( t_{\text{max}} \) is far from the exact solution as shown in Figure 12(a). Figures 12(b)–(d)
Figure 9. The space-time history of the exact boundary heat flux function (Example B)

Figure 10. (a) The initial guess of the boundary heat flux function (Example B, test case \#1); (b) The boundary heat flux at the 1st iteration (Example B, test case \#1); (c) the 2nd iteration (Example B, test case \#1) and (d) The optimal boundary heat flux function (iteration \#13 for Example B, test case \#1)

show the space-time behaviour of the calculated boundary heat flux at several iteration steps. The solution converged at iteration \#14 with the same tolerances as above. One can notice that the solution remains unchanged near the final time $t_{\text{max}}$ due to the final condition of the adjoint problem as explained in example A. This has resulted in deterioration of the solution accuracy.
Figure 11. Spatial variation of the optimal boundary heat flux at various times (Example B, test case #1)

Figure 12. (a) The initial guess of boundary heat flux function (Example B, test case #2); (b) The boundary heat flux at the 1st iteration (Example B, test case #2); (c) the 5th iteration (Example B, test case #2) and (d) The optimal boundary heat flux (iteration #14 for Example B, test case #2)
Note that this end condition problem could not be seen clearly in the first trial case due to the choice of the initial guess function. When the initial guess was further away from the exact solution, the final condition affected the solution accuracy and also slowed down the rate of convergence. For instance, the case of initial guess function equal to 100 W/m² converged in 23 iteration steps with the tolerances given earlier.

CONCLUSIONS

The adjoint method was developed as part of the infinite-dimensional minimization technique in conjunction with the conjugate gradient method to obtain the optimum history of boundary cooling condition that results in a desired location/motion of the freezing front in two-dimensional conduction driven solidification processes. The present method is a valuable tool that can be used for a better design of casting processes because the freezing front motion together with the thermal gradient at the freezing interface define the solidification microstructures. The control of freezing front motion can also be used to prevent partial solidification.

Two two-dimensional solidification examples were solved to demonstrate the performance of the present methodology. The present method gave a convergent solution in a longer time interval than the sequential method (i.e. future information technique with spatial regularization). When the value of the initial guess function was far from that of the true solution at the final time, the accuracy and rate of convergence of the solution deteriorated due to the final condition in the adjoint problem. Modifications to account for this end condition can lead to more accurate and faster algorithm.

In one-dimensional inverse Stefan design problems with two fixed boundaries, both interface velocity and interface thermal gradient to the solid side could be independently prescribed. However, in two-dimensional problems with one fixed boundary where the unknown cooling function is applied, only the interface location could be controlled via the cooling function at the fixed boundary. Therefore, one should introduce an additional independent function to control the thermal gradient at the solid side of the interface. Such a controller can be a heat source in the liquid region related to the liquid feeding to the contracting freezing front or an electromagnetic force which is used to stir the liquid region (one should incorporate melt convection in this case). The design and modelling of casting processes incorporating such additional control functions is extremely challenging and of practical importance.

ACKNOWLEDGEMENTS

This work was funded by NSF grant CTS-9115438 to Cornell University. The computing for this project was supported by the Cornell National Supercomputer facility, which receives major funding by the NSF and IBM Corporation, with additional support from the New York State.

REFERENCES