Parabolic Free Boundary Problems: Method of Invariant Imbedding

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Outline

1. Introduction
2. Solution technique
   - Step 1: Line discretization (MOL)
   - Step 2: Invariant imbedding
3. Implementation details
4. Numerical experiment

Abstract

Parabolic Free Boundary Problems: Method of Invariant Imbedding

Free boundary problems often arise in the modeling of physical processes. One typical example is ice melting (Stefan problem). In this talk, the method of invariant imbedding for solving one-dimensional parabolic problems will be presented. The idea of the method is to convert the BVP with an unknown boundary to a set of easy-to-solve well-posed IVPs. Algorithmic implementation of the method will be explained and results of numerical experiments will be discussed.

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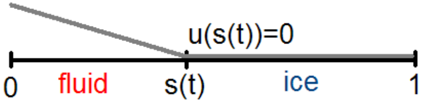
Melting ice

1D Stefan problem



Mathematical model

PDE: $u_{xx} - cu_t = 0, \quad t \in \mathbb{R}^+, x \in [0, s(t)].$

ICs: $u(x, 0) = 0, \quad s(0) = 0.$

BCs: $u(0, t) = \alpha(t), \quad u(s(t), t) = 0, \quad u_x(s(t), t) = -\lambda \frac{ds}{dt}.$

$u(x, t)$ - temperature, $s(t)$ - position of the unknown moving boundary

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Generalized problem

Mathematical model

PDE:
$$\left(\frac{\partial}{\partial x}\left(k\frac{\partial}{\partial x}\right)+a\frac{\partial}{\partial x}+b-c\frac{\partial}{\partial t}\right)u=f,$$
u, k, a, b, c, f depend on x and t, $\quad t \in \mathbb{R}^+,\ x \in [0, s(t)]$.

ICs: $u(x,0)=u_0(x), \quad s(0)=s_0.$

BCs:
$$\alpha_1(t)u(0,t)+\alpha_2(t)u_x(0,t)=\alpha(t),\ t>0,\ \alpha_1^2+\alpha_2^2\neq 0,$$
$$H(u(s,t),u_x(s,t),u_t(s,t),s(t),s'(t),t)=0, \quad t\in\mathbb{R}^+.$$

$H=(H_1,H_2)^T\in\mathbb{R}^2$ - given function, incorporates BCs at the moving interface.

Particular free boundary problems

Stefan problem

$$H = \begin{pmatrix} u \\ u_x + \lambda s' \end{pmatrix}$$

Generalized Stefan problem

$$H = \begin{pmatrix} u + \mu_1(s,t) \\ u_x + \lambda s' + \mu_2(s,t) \end{pmatrix}$$

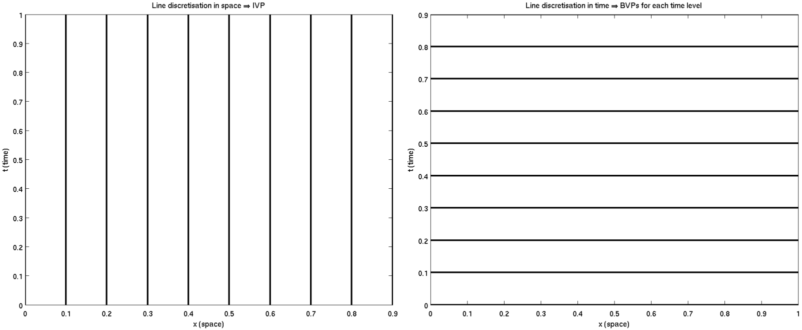
Optimal stopping

$$H = \begin{pmatrix} u \\ u_x \end{pmatrix}$$

Bubble growth

$$H = \begin{pmatrix} u - \mu_1 e^{\mu_2/s} \\ u_x - (\mu_3 - u)s' \end{pmatrix}$$

The Method of lines for IBVPs



Discretization in time

Equidistant grid:

$0 = t_0 < t_1 < \ldots < t_N = T, \quad \Delta t = t_i - t_{i-1}, i = 1, \ldots, N.$

$$u_t(x, t_n) \approx \frac{u(x, t_n) - u(x, t_{n-1})}{\Delta t}, \quad s'(t_n) \approx \frac{s(t_n) - s(t_{n-1})}{\Delta t}$$

BVP with a free boundary, to be solved at each time level

$$(k u_n')' + a u_n' + b u_n - c \frac{u_n - u_{n-1}}{\Delta t} = f,$$

$$\alpha_1(t_n) u_n(0) + \alpha_2(t_n) u_n'(0) = \alpha(t_n),$$
$$H\left(u_n(s_n), u_n'(s_n), \frac{u_n(s_n) - u_{n-1}(s_{n-1})}{\Delta t}, s_n, \frac{s_n - s_{n-1}}{\Delta t}, t_n\right) = 0.$$

Invariant imbedding (2a: convert to 1st order)

2nd order ODE ⇒ System of 1st order ODEs, set $\alpha_2 = 1$.

BVP with a free boundary, to be solved at each time level

$$
\begin{aligned}
v_n' &= \frac{c}{\Delta t}u_n - \frac{a}{k}v_n - bu_n + f - \frac{c}{\Delta t}u_{n-1}(x),\\
u_n' &= v_n/k,
\end{aligned}
$$

$$
\begin{aligned}
&v_n(0) = (\alpha(t_n) - \alpha_1(t_n)u_n(0))k,\\
&H\left(u_n(s_n), \frac{v_n(s_n)}{k(s_n,t_n)}, \frac{u_n(s_n)-u_{n-1}(s_n)}{\Delta t}, s_n, \frac{s_n - s_{n-1}}{\Delta t}, t_n\right) = 0.
\end{aligned}
$$

Invariant imbedding (2b: remove right BC)

- Remove the BC at the moving interface
- Make $u_n(0) = r$ a free parameter

IVP with a free parameter

$$\begin{pmatrix} v_n \\ u_n \end{pmatrix}' = \begin{pmatrix} -\frac{a}{k} & \frac{c}{\Delta t} - b \\ \frac{1}{k} & 1 \end{pmatrix} \begin{pmatrix} v_n \\ u_n \end{pmatrix} + \begin{pmatrix} f - \frac{cu_{n-1}(x)}{\Delta t} \\ 0 \end{pmatrix},$$

$$\begin{pmatrix} v_n \\ u_n \end{pmatrix}(0) = \begin{pmatrix} (\alpha(t_n) - \alpha_1(t_n)r)k \\ r \end{pmatrix}.$$

$$\mathbf{y}' = A(x)\mathbf{y}+\mathbf{b}, \quad \Rightarrow \quad \mathbf{y}(x) = \Phi(x,0)\left[\mathbf{y}(0) + \int_0^x \Phi^{-1}(x,\tau)\mathbf{b}(\tau)\,d\tau\right]$$

Invariant imbedding (2c: relate u_n and v_n)

$$\begin{pmatrix} v_n \\ u_n \end{pmatrix} = \Phi_n(x,0)\begin{pmatrix} (\alpha(t_n)-\alpha_1(t_n)r)k \\ r \end{pmatrix} + \Phi_n(x,0)\int_0^x \Phi_n^{-1}(x,\tau)\begin{pmatrix} f-\frac{cu_{n-1}(x)}{\Delta t} \\ 0 \end{pmatrix} d\tau$$

- Solve 2nd eq. for r: $r = u_n/\Phi_n(x,0)$
- Subst. in the 1st eq.:

$$v_n = -\alpha_1 k u_n + \Phi_n(x,0)\left(\alpha k + \int_0^x ...d\tau\right) = R_n(x)u_n(x,r) + z_n(x)$$

- Compare with $v_n(0) = -\alpha_1(t_n)ku_n(0) + \alpha(t_n)k$ (left BC) to determine the ICs for R_n and z_n

$$R_n(0) = -\alpha_1(t_n)k(0,t_n), \quad z_n(0) = \alpha(t_n)k(0,t_n).$$

Invariant imbedding (2d: eqn. for u_n)

- Differentiate the expression $v_n = R_n u_n + z_n$

$$v_n' \quad = \quad R_n' u_n + R_n u_n' + z_n' = R_n' u_n + R_n \frac{v_n}{k} + z_n'$$

- Use the ODE for v_n'

$$v_n' = \frac{c}{\Delta t} u_n - \frac{a}{k} v_n - b u_n + f - \frac{c}{\Delta t} u_{n-1}(x)$$

- Equate the right hand sides

$$\left[R_n' + \frac{1}{k} R_n^2 + \frac{a}{k} R_n - \frac{c}{\Delta t} - b \right] u_n(x,r)$$
$$= \left[-z_n' - \frac{R_n z_n}{k} - \frac{a}{k} z_n + f(x,t_n) - \frac{c}{\Delta t} u_{n-1}(x) \right]$$

Invariant imbedding (2e: well-defined IVP)

Well-defined IVP (invariant imbedding equations)

$$\begin{aligned} R_n' &= -\frac{1}{k}R_n^2 - \frac{a}{k}R_n + \frac{c}{\Delta t} - b, \qquad & R_n(0) = -\alpha_1(t_n)k(0,t_n) \\ z_n' &= -\left[\frac{R_n}{k} + \frac{a}{k}\right] z_n + f - \frac{c}{\Delta t}u_{n-1}(x), & z_n(0) = \alpha(t_n)k(0,t_n) \end{aligned}$$

- Solve for $\bar{u}$, $\bar{x}$ to determine position/value for the free boundary

$$H\left(\bar{u}, \frac{R_n(\bar{x})\bar{u} + z_n(\bar{x})}{k(\bar{x},t_n)}, \frac{\bar{u} - u_{n-1}(s_{n-1})}{\Delta t}, \bar{x}, \frac{\bar{x} - s_{n-1}}{\Delta t}, t_n\right) = 0$$

- To determine u_n, integrate the R/z-representation of v

$$v_n = ku_n' = R_n(x)u_n + z_n(x), \quad u_n(s_n = \bar{x}) = \bar{u}.$$

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Finding roots of H(.)

$$H\left(\bar{u}, \frac{R_n(\bar{x})\bar{u} + z_n(\bar{x})}{k(\bar{x}, t_n)}, \frac{\bar{u} - u_{n-1}(s_{n-1})}{\Delta t}, \bar{x}, \frac{\bar{x} - s_{n-1}}{\Delta t}, t_n\right) = 0$$

Eliminate u or u_x to reduce to a scalar equation: $\boxed{\phi(x) = 0}$

Stefan problem:

$$\phi_n(x) = z_n(x) + \lambda \frac{x - s_{n-1}}{\Delta t} k(x, t_n) = 0$$

Optimal stopping:

$$\phi_n(x) = z_n(x) = 0$$

Backward integration

"Final" value problem

$$u'(x) = A(x)u(x) + b(x), \quad x \in [0, s], \quad u(s) = \bar{u}$$

New coordinates: $y = s - x$

New unknown: $v(y) = u(x)$

$$\frac{dv(y)}{dy} = \frac{du(x)}{d(s-x)} = -\frac{du(x)}{dx} \quad \Rightarrow \quad u'(x) = -v'(y)$$

Standard IVP

$$-v'(y) = A(s-y)v(y) + b(s-y), \quad y \in [0, s], \quad v(0) = \bar{u}$$

Step-by-step procedure

For each time level do the following:

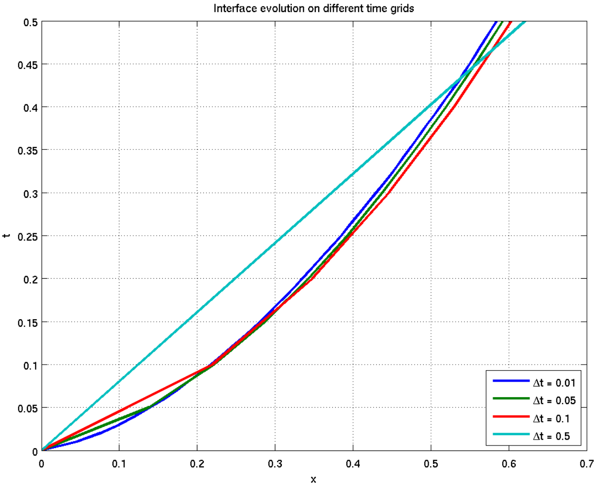
- Integrate the nonlinear ODEs for R_n, z_n
- After each integration step evaluate $\phi_n(x_i)$
- If $\phi_n(x_{i-1}) < 0$ and $\phi_n(x_i) > 0$, then place the boundary at x_i, i.e. $s_n = x_i$
- Compute the solution u by integrating backward the R/z-representation of v (starting from s_n, $u(s_n) = \bar{u}$)

One time step in detail

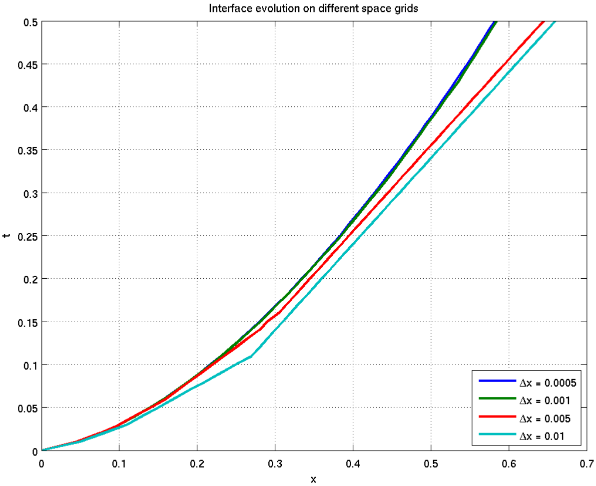
Outline

Example of a numerical solution

Interface evolution on different time grids



Interface evolution on different space grids



Last

Thank You!

Questions?