Enthalpy Methods for Moving Boundary Problems

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Institute of Applied Mathematics

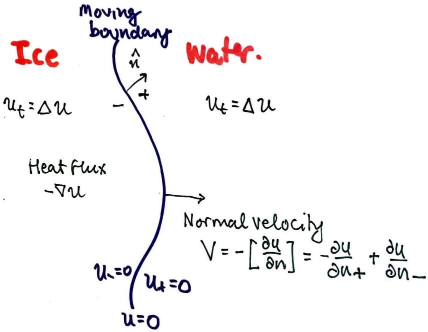
University of British Columbia

- Faculty participation from many departments.
- Interdisciplinary graduate programme.

Overview of the Talk

- Stefan Problem
- Oxygen Depletion Problem
- Two Phase Flow Model
- Generalized Problems
- Summary

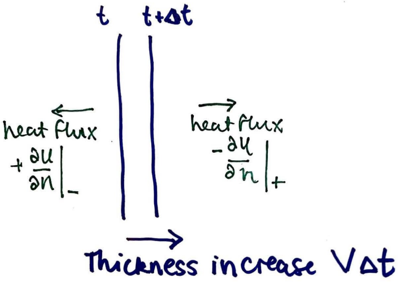
Stefan Problem



- Moving Boundary Value Problem in scaled temperature $u(\mathbf{x}, t)$
- Stefan: Annalen der Physik (1890)
- Crank: Free and Moving Boundary Problems (1984)
- Missing Physics: ice and water have different thermal properties and densities

Stefan Problem

Normal velocity derived from Enthalpy conservation



- Local volume of ice formed $AV\Delta t$.
- Heat removed $A\Delta t(\partial u/\partial n_{-} - \partial u/\partial n_{+})$
- Equating (Latent heat scaled to one) gives

$$V = -\left[\frac{\partial u}{\partial n}\right]$$

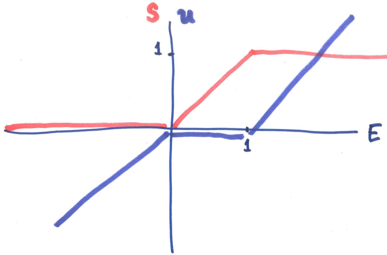
Stefan Problem

Enthapy

- Water fraction s ($s = 0$ ice, $s = 1$ water)
- Net heat flux changes Enthalpy $E = u + s$
- Thermal energy conservation in the whole domain

$$E_t = \Delta u$$

- (delta functions in the equations at the interface)
- Recover u and s from E (simple flash computation):



Stefan Problem

Enthapy Method I

- $E_t = u(E)_{xx}$
- FD discretization in space, explicit time stepping works! grid capturing method.
- Implicit time stepping:

$$E - k\Delta_h u(E) = E^n$$

  Three linear regimes for $u(E)$ at each grid point
- Convex optimization problem for E (unique discrete solution)
- $E = u + s$ and (u, s) minimizes

$$\sum \left(u^2 + us + k|Du|^2 - uE^n\right)$$

  with constraint $0 \leq s \leq 1$ at each grid point (Quadratic optimization with linear inequality constraints)

Other approaches: regularize $u(E)$ or introduce a freezing rate

Stefan Problem

Enthapy Method II

- Implicit time stepping:

$$E - k\Delta_h u(E) = E^n$$

  Three linear regimes for $u(E)$ at each grid point
- Iterative method based on simple regime flag updates
- In the context of (u, s) formulation, it is a (nonstandard) active set method
- This strategy works but no theory (that I know of)
- Advantages: Linear problems at every iteration, soft restart at next time step

Simulation Movies

Stefan Problem

Enthapy Method III

- Implicit time stepping:

$$u + s - k\Delta_h u(E) = E^n$$

- In commercial codes (FLUENT), phase change is treated as a source term in the implicit problem iteratively

$$u^{(m+1)} - kD_2 u^{(m+1)} = E^n - s^{(m)}$$

with $s^{(m)} = s(E^{(m)})$

- Proposed in Voller & Prakash Int J Heat Mass Transfer (1987)
- Evidence of linear convergence of iterations

Stefan Problem

1D moving grid formulation

- Domain $x \in [0, 1]$, conditions at $x = 0$ (ice) and $x = 1$ (water)
- Let $\alpha(t)$ be the moving boundary
- Use coordinate $y = x/\alpha(t)$ for ice $u(y, t)$ (y in [0,1])

$$u_t = u_{yy}/\alpha^2 + \dot{\alpha} y u_y/\alpha$$

- Similarly use coordinate $z = (x - \alpha(t))/(1 - \alpha(t))$ in water.
- Interface conditions $u(y = 1, t) = 0$, $u(z = 0, t) = 0$ and

$$\dot{\alpha} = V = u_y(y = 1)/\alpha - u_z(z = 0)/(1 - \alpha)$$

- FE, FV, or FD spatial discretization gives high accuracy
- Limited applicability in higher dimensions

Moving Boundary Value Problems are always nonlinear

Oxygen Depletion Problem

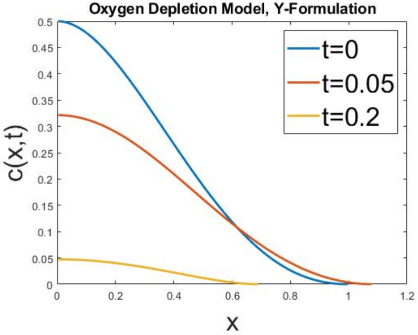
problem in 1D

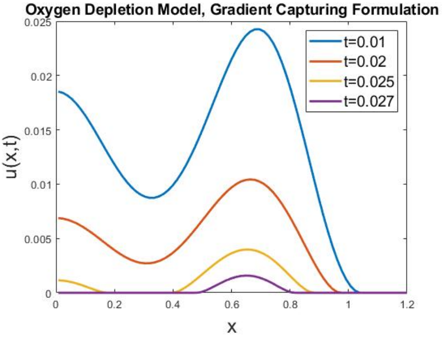
$$u_t = u_{xx} - 1$$

- Unknown $u(x,t)$ for $x \in [0, s(t)]$
- Free boundary $x = s(t)$ at which $u = 0$ and $u_x = 0$ (*implicit*)
- Consider the Cauchy problem or $u_x = 0$ at $x = 0$.
- Can derive an explicit velocity $V = -u_{xxx}$.
- The steady state problem is the *Elliptic Obstacle Problem*.

Oxygen Depletion Problem

1D results

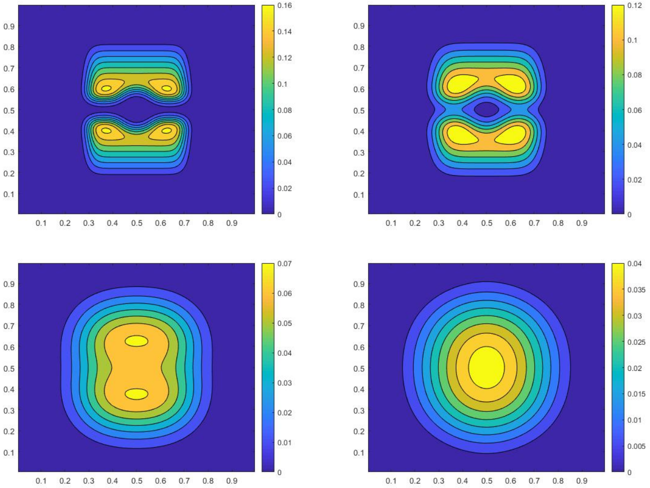




Open question: Generic limiting end state $u \to 0$?

Oxygen Depletion Problem

2D results



Oxygen Depletion Problem

Mapped Method

- Mapped coordinate $y = x/s(t)$, $y \in [0, 1]$
- $u_{yy} + \dot{s}syu_y - s^2u_t - s^2 = 0$, $u = 0$ and $u_y = 0$ at $y = 1$
- Numerical method using DAE time stepping
- No direct analysis for this formulation

The oxygen diffusion problem: Analysis and numerical solution, Mitchell and Vynnycky (2015)

Oxygen Depletion Problem

Gradient flow time stepping I

- Gradient flow of

$$\mathcal{E} = \int_\Omega \frac{1}{2}|\nabla u|^2 + u$$

  with $u \in H^1_+$.
- BE time step k from u^n to u minimizes

$$E[u] = \int_\Omega \frac{1}{2}|\nabla u|^2 + \frac{1}{2k}(u - u^n)^2 + u$$

- After spatial discretization, the problem for U is a quadratic minimization problem with linear inequality constraint
- Convergent strategy

Review of existing theory and extension to gradient flow formulation in Cheng and W, SIAP.

Oxygen Depletion Problem

Gradient flow time stepping II

- Index iteration strategy on

$$Q(\mathbf{U}) = \sum_j k(U_j - U_{j-1})^2/(2h^2) - U_j V_j + kU_j + U_j^2/2$$

- Boolean index $I_j^{(m)}$ ($U_j = 0$ or $U_j > 0$).
- Solve for $\mathbf{U}^{(m)}$, linear system

$$U_j^{(m)} = 0 \quad \text{or} \quad -kD_2 U_j^{(m)} + U_j^{(m)} + k - V_j = 0$$

- If $I^{(m)} = 1$ and $U_j^{(m)} < 0$, set $I_j^{(m+1)} = 0$
- If $I^{(m)} = 0$, $V_j - k - k(U_{j-1}^{(m)} + U_{j+1}^{(m)})/h^2 > 0$ set $I_j^{(m+1)} = 1$
- missing theory to this strategy

Motivating Problem: Two Phase Flow

cartoon model equations

Heat and water transport in a porous medium:

u: temperature

v: water vapour

w: water liquid

Γ: condensation rate

$S(u)$: vapour saturation (we take $S(u) = e^u$).

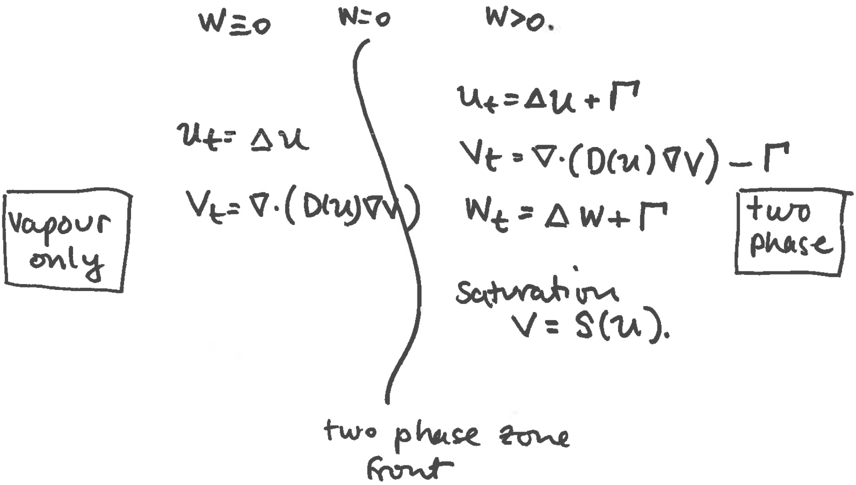
Equations:

$$
\begin{aligned}
u_t &= \Delta u + \Gamma \\
v_t &= \nabla \cdot (D(u)\nabla v) - \Gamma \quad \text{(we take } D(u) = 2(1+u)^2\text{)}. \\
w_t &= \Delta w + \Gamma
\end{aligned}
$$

Motivation: transport in fuel cell electrodes and baking bread

Two Phase Flow

cartoon model picture



Two Phase Flow

two zone formulation

Vapour only region ($w \equiv 0$):

$$\begin{aligned} u_t &= \Delta u \\ v_t &= \nabla \cdot (D(u)\nabla v) \end{aligned}$$

Two phase zone region ($v = S(u)$):

$$\begin{aligned} S'(u)u_t + w_t &= \nabla \cdot (S'(u)D(u)\nabla u) + \Delta w \\ (1 + S'(u))u_t &= \nabla \cdot ((1 + S'(u)D(u))\nabla u) \end{aligned}$$

Interface conditions:

1. $w = 0$ (two phase)
2. $[u] = 0$
3. $v = S(u)$ (vapour)
4. $[\partial u/\partial n] = \partial w/\partial n$ (heat flux evaporates water flux)
5. $[D(u)\partial v/\partial n] = \partial w/\partial n$ (water conserved)

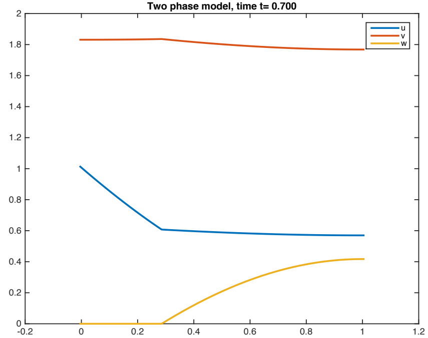
Two Phase Flow

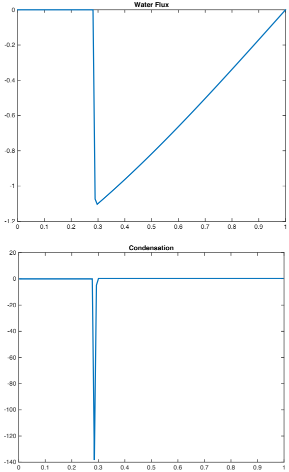
two zone formulation: discussion

- Count check: four component second order parabolic equations, five mixed Dirichlet/Neumann conditions
- This is an implicit moving boundary value problem
- There can be a condensation delta function at the free boundary
- Motivates the investigation of general implicit moving boundary problems

Model Problem

1D computation (using the M2 method)





Movie

Two Phase Flow

M2 capturing method

$$
\begin{aligned}
u_t &= \Delta u + \Gamma \\
v_t &= \nabla \cdot (D(u) \nabla v) - \Gamma \\
w_t &= \Delta w + \Gamma \\
v &= S(u) \quad \text{when } w > 0
\end{aligned}
$$

Introduce total water $\rho = v + w$ and "Enthalpy" $Q = u + v$:

$$
\begin{aligned}
\rho_t &= \nabla \cdot (D(u) \nabla v) + \Delta w \\
Q_t &= \nabla \cdot (D(u) \nabla v) + \Delta u
\end{aligned}
$$

Recover u, v and w from the "M2 map":

- if $\rho < S(Q - \rho)$, all vapour $w = 0$, $v = \rho$, $u = Q - \rho$.
- otherwise solve $Q = u + S(u)$ for u, $v = S(u)$, $w = \rho - v$.

Two Phase Flow

scheme one: M2 method (discussion)

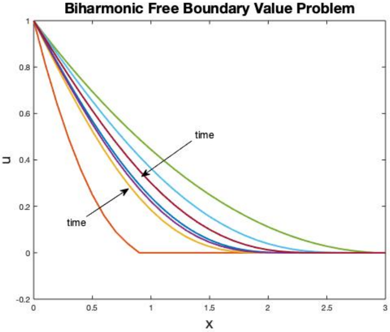
- M2 map approach proposed by Wang and Beckermann, IJHMT, 1993.
- M2 map is continuous with derivative discontinuities.
- Computational convergence study Bridge and W, JCP, 2007, on a more physical model with degenerate water diffusion. No theory.
- Implemented on a fixed grid with Backward Euler time stepping and the status flag approach.
- Status flag change at each Newton iteration. Status flag iterations always converge. No theory.
- $O(k) + O(h^q)$ $(1 < q < 2)$ convergence observed in $\|\cdot\|_1$ on the current model.

Biharmonic Problem

- Scaled, linear, viscoelastic motion of a beam over a flat surface:

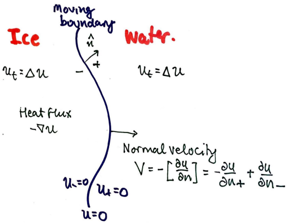
$$\begin{aligned} u_t &= -u_{xxxx} - 1 \text{ subject to } u \geq 0 \\ & u = 0, u_x = 0, u_{xxx} = 0 \text{ (moving boundary)} \end{aligned}$$

- Gradient flow structure
- Successful index iteration strategy



Explicit Interface Motion

to steady state



- At steady state $u_- = u_+ = [\partial u / \partial n] = 0$
- Solving with $u_- = u_+ = 0$ and using explicit time stepping with $V = -[\partial u / \partial n]$ requires times steps $k = O(h)$
- Solving with $[\partial u / \partial n] = [u] = 0$ and using explicit time stepping with $V = u$ allows time steps independent of h

Donaldson and W: IMAMAT (2006)

Summary

- Presented a collection of methods for moving boundary value problems with numerical evidence of convergence.
- Lots of missing theory:
  - Existence and regularity theory for the underlying problems
  - Convergence of discretizations
  - Generalized problems: What moving boundary value problems be written in a convergent status flag formulation? Which have gradient flow structure?
  - Convergence of the discrete status iterations

Students

Roger Donaldson: MSc 2003, CTO Avigilon Technologies

Lloyd Bridge: PhD 2007, Senior Lecturer UWE

Xinyu Cheng: PhD 2017, PDF Fudan

Honorable Mention:

Iain Moyles: PhD 2015, Faculty York (Canada)

Huaxiong Huang: "It's a 1D problem, how hard can it be?"