A rescaling scheme for computing moving boundary problems

Shuwang Li
sli@math.iit.edu
Department of Applied Mathematics
Illinois Institute of Technology, Chicago

Joint with: Meng Zhao (IIT), Amlan Barua (IIT), X. Li (IIT), John
Lowengrub (UC-Irvine), Martin Glicksman (FIT), Perry Leo (UMN),
Peter Palffy-Muhoray (Kent State U.), Andrew Belmonte (Penn State),
Wenjun Ying (Shanghai Jiaotong U.)

NUS—IMS: Workshop on High Performance and Parallel Computing
Methods and Algorithms for Materials Defects, Singapore, Feb. 2015
Outline

• Moving boundary problems and classical examples.
• The idea of the rescaling scheme.
• The growing Hele-Shaw problem with (elastic membrane)
• The shrinking Hele-Shaw problem.

Acknowledgement: NSF supports
Introduction -- Moving Boundary Problems

• Definition: boundary value problems defined in a domain whose boundary is
  – a priori unknown
  – evolving with time

• Classical examples
  – Fluid: multiphase flow (Hele-Shaw problem)
  – Material: crystal/epitaxial growth problem (phase change) and grain boundaries
  – Biosystem: bio-membrane, tumor, and pattern formation

• Characteristics
  – solve a moving boundary problem:
    identify the boundary, solve the PDE and evolve the boundary
  – interface stability
    stable (simple/compact shape)
    unstable (evolves to complex shape)

• Significance
  – improve the secondary and tertiary oil recovery in the petroleum industry
  – design high quality crystals for Nanotech and semiconductor fabrication
  – understand the bio-mechanisms of diseases such as cancer

Goal: understand the dynamics → understand the instability → control the shape
Computational challenges besides solving PDEs


\[ \frac{d(\text{Bubble volume}: 4\pi R^3(t)/3)}{dt} = J, \quad \text{i.e. velocity} = \frac{dR}{dt} \sim \frac{J}{R^2} \]

– slow dynamics for the growth problem (R increase); need to increase resolution.
– fast dynamics for the shrinking problem (R decrease); need to reduce resolution.

• From a computational point of view, we would like to

– speed up the dynamics for the slow growth problem;
– slow down the dynamics for the fast shrinking problem;
– without changing the physics.

• Rescaling scheme, a long story…
Experiments: two parallel, closely spaced plates sandwich a viscous fluid; another less viscous fluid is injected into the system; the interface experiences Saffman-Taylor instability.

open non-equilibrium system: no conserved geometric quantities.

Example: Hele-Shaw problem (crystal growth)

Governing equations: Laplace equation for the pressure

\[
\nabla^2 P = 0
\]

Darcy's law: \( \mathbf{u} = -\frac{b^2}{12\mu} \nabla p \)

Incompressibility: \( \nabla \cdot \mathbf{u} = 0 \)

Laplace-Young boundary condition

\[
[P] = \tau \kappa
\]
Non-dimensional equations of the Hele-Shaw problem

- Governing equations

\[
\nabla^2 P = 0 \quad \text{in} \quad \Omega_L \\
V = -\nabla P \cdot \mathbf{n} \quad \text{on} \quad \Sigma(t)
\]

- Boundary conditions

\[
P_{in} - P_{out} = \tau(n)\kappa \quad \text{on} \quad \Sigma(t) \\
J(t) = \frac{1}{2\pi} \int_{\Sigma(t)} V \, d\Sigma
\]

- Fredholm boundary integral equation for \( \mu(x) \):

\[
\tau(n)\kappa(x) = -\frac{1}{2} \mu(x) + \int_{\Sigma} \mu(x') \frac{\partial G(|x - x'|)}{\partial n(x')} \, d\Sigma(x') + \frac{J}{2\pi} \log |x|
\]

\[
V(x) = (-\nabla \int_{\Sigma} \mu(x') \frac{\partial G(|x - x'|)}{\partial n(x')} \, d\Sigma(x')) + J\nabla \log |x| \cdot \mathbf{n}(x)
\]

- Interface evolution:

\[
\frac{d}{dt} x \cdot \mathbf{n} = V(x), \quad x \in \Sigma(t)
\]

\( \kappa \): curvature

\( \tau(n) \): surface tension; in 2D \( \tau(\theta) = 1 - (m^2 - 1)v\cos(m\theta) \)

\( G(x) \) is the Green’s function

2D: \( G(x) = \frac{1}{2\pi} \log |x| \)
Linear stability theory (Mullins-Sekerka)

Single mode perturbation: \[ r_\Sigma (\theta,t) = R(t) + \delta(t) \cdot \cos(k\theta) \]

Growth: \[ J(t) = R \frac{dR}{dt} + O(\delta/R)^2, \quad R(t) \sim t^{1/2} \text{ for const. } J; \quad R(t) \sim t^{1/3} \text{ for } J=1/R(t); \]

Shape evolution: \[ (\delta/R)^{-1} \left( \frac{\delta}{R} \right)^* = \frac{(k-2)}{R^d} (J-J_k) \] Critical flux: \[ J_k = \frac{C_k}{R(t)}, \quad C_k \sim \frac{k^3}{k-2} \]

- \( J > J_k \) unstable evolution, e.g. Saffman-Taylor instability
- \( J = J_k \) mode unchanged \( \frac{\delta(t)}{R(t)} = \frac{\delta(0)}{R(0)} = \text{const.} \)
- \( J < J_k \) stable evolution, perturbation decays

• J=Constant gives unstable growth; J=Const/R(t) may give self-similar growth.

• If the initial shape is a mode mixture, in 2D, the flux for the fastest growth mode (say mode k) is \[ J^*_k = \frac{3k^2 - 1}{R(t)}. \] Mode k dominates the shape.
Understanding self-similarity

- **Physics**: mode unchanged evolution behaves like the self-similar evolution for a single mode, indicating the competition between stabilizing factors (e.g., surface tension) and destabilizing factors (e.g., flux) is balanced.

- **Mathematics**: self-similar evolution is the repetition of a base shape on different size scale, i.e.,

\[ X(s, t) = R(t) \tilde{X}(s) \]

**Motivation for the rescaling scheme**

- **Rescaling scheme**:

\[ X(s, t) = \tilde{R}(t(\tilde{t}))\tilde{X}(s, \tilde{t}) \]
Nonlinear numerical method

• Solve field equations and compute the normal velocity $V(x)$

• Interface evolution: $\frac{d}{dt} \sum x \bullet n = V(x)$
  
  - use arclength and tangent angle to represent the interface
  
  - equal arclength scheme to avoid points clustering using a special tangent velocity
  
  - 2nd order Adam-Bashforth to solve for arclength and tangent angle by an integrating factor method in Fourier space


• Two issues: resolution and slow growth/fast shrinking when $R$ is large/small (Recall Srolovitz’s public lecture on Monday).

  - complicated morphology requires more mesh points to resolve
  
  - the growth process slows down as, $\frac{dA}{dt} = J(t)$, i.e. $\frac{dR}{dt} = \frac{J}{R} = \begin{cases} \frac{\text{Const.}}{R} & \text{if } J=\text{const.} \\ \frac{\text{Const.}}{R^2} & \text{if } J=\text{const} \end{cases}$
A time-space rescaling scheme

- **Idea**: isolate morphological change from overall growth by mapping onto a new time and space: \((x,t) \rightarrow (\tilde{x},\tilde{t})\) i.e. scale out the growth: \(R(t(\tilde{t})) = \tilde{R}(\tilde{t})\)

\[
x(\alpha,t) = \tilde{R}(\tilde{t})\tilde{x}(\alpha,\tilde{t})
\]

\[
\tilde{t} = \int_0^t \frac{1}{\rho(t')} \, dt'
\]

- Variables in the new frame
  - flux \(J(t(\tilde{t})) = \tilde{J}(\tilde{t})\)
  - normal velocity \(V(\alpha,t) = \frac{dx(\alpha,t)}{dt} \cdot n \Rightarrow \tilde{V}(\alpha,\tilde{t}) = \tilde{\rho} \tilde{V}(t(\tilde{t})) - \tilde{\dot{x}} \cdot n \, d\tilde{R} / \tilde{R} / d\tilde{t}\)

- Choose \(R(t(\tilde{t}))\) such that \(\int_0^{2\pi} \tilde{V}(\alpha,\tilde{t}) \, d\alpha = 0\) i.e. \(A(\tilde{t}) = A(0) = \tilde{A}(0), \quad \tilde{\dot{\rho}}(\tilde{t}) = \frac{\tilde{R}^2 \tilde{A}}{\bar{J} \pi}\)

\[
R(t) = \tilde{R}(\tilde{t}) = \exp(\tilde{t})
\]

- New interface evolves:
  \[
  \frac{d\tilde{x}(\alpha,\tilde{t})}{d\tilde{t}} \cdot n = \tilde{V}(\alpha,\tilde{t})
  \]

- Makes **accurate, efficient, long-time** simulations possible

Ref: S. Li, J. Lowengrub, P. Leo, Journal of Computational Physics, 2007.
Results for viscous fingering

A benchmark problem: Hele-Shaw bubble simulation  \( r(\alpha, 0) = 1.0 + 0.1(\cos 3\alpha + \sin 2\alpha) \)
\( \tau = 0.001; \quad J = 1.0 \)

mesh points, N=8,192
Computer used in 1993
run 50 days, T=45, max(r)=12
rescaling scheme: 10 hours
Hou, Lowengrub, Shelley

mesh points, N=32,768
P4, CPU 2.2GHz, 2005
run 50 days, T=500, max(r)=45
rescaling scheme: 6 days
Fast, Shelley
JCP 212, 2006.

mesh points, N=65,536
P4, CPU 2.2GHz, 2006
run 21 days, T=2400, max(r)=110
Li, Lowengrub, Leo
A large Hele-Shaw bubble simulation

\[ r(\alpha,0) = 1.0 + 0.1(\cos 3\alpha + \sin 2\alpha) \]
\[ \tau = 0.001; \quad J = 1.0, \quad N=64k \]
\[ J = 1.0; \quad R(t) \sim t^{1/2} \]

Isotropic surface tension: repeated tip-splitting

Area is conserved
\[ A(\tilde{t}) = A(0) \]

movie: \( \tilde{x}(\alpha, \tilde{t}) \)
real shape:
\[ x(\alpha, t) = \tilde{R}(\tilde{t})\tilde{x}(\alpha, \tilde{t}) \]
\[ \tilde{R} = 1 \sim 68 \]

Ref: S. Li, J. Lowengrub, P. Leo, JCP, 2007.
Same perturbations with different flux

\[ J(t) \sim \frac{1}{R(t)} \]

\[ J(t) = \frac{96}{R} \]

\[ J(t) = \frac{74}{R} \quad \text{reduce flux} \]

\[ J(t) = \frac{150}{R} \quad \text{increase flux} \]
Generic perturbations: 6-fold case

Universal limiting shapes depend on the applied flux only.
A morphology diagram for the Hele-Shaw problem

Linear theory: zero growth rate
$C = k(k^2-1)/(k-2)$

Linear theory: max. growth rate
$C = 3k^2-1$

Experiment result #1: a 5-fold shape

Experimental demonstration that the symmetry of an expanding bubble in castor oil can be selected using the flux $J(t) = \frac{C \sigma b^2 2\pi b}{12\mu R(t)}$

($\tau = 0.048 N/m$, $\mu = 1 Pa.s$, $b = 0.5 mm$, the size of the cell $R_* \approx 10 cm$)

$C = 74$, theory predicts a 5-fold shape
Experiment result #2: an 8-fold shape

For \( C=191 \), theory predicts an 8-fold shape. Experiments agree with the theory.
An interesting experiment: new patterns

• Chemical reaction change the property of the interface, e.g. CTAB into NaSal

• The interface is gel-like and increase the membrane elasticity and resistance. Non-fingering morphologies.

• How to model the interface?

A. Belmonte et al. Fingering instabilities of a reactive micellar interface, PRE, 76, 016202 (2007)
Elastic boundary condition

• Model interface by an elastic membrane: \( E_b = \frac{1}{2} \int_{\Sigma(t)} \sigma \, ds \)
  
  -- if \( \omega = \sigma \), a constant/anisotropy, we get the classical Young-Laplace condition.
  
  -- if \( \sigma = \nu(\kappa)\kappa^2 \) where \( \nu \) is a rigidity function. For the case of \( \nu \) = constant, we get the Helfrich energy for cell membrane.

• The curvature weakening: high curvature region has small bending stiffness.
  \( \nu(\kappa) = \nu_0(Ce^{-\lambda^2\kappa^2} + 1 - C) \), \( C \) is the rigidity fraction

\[
\frac{d}{dt} E_b = \int_{\Sigma(t)} [p]_t \, V \, ds
\]

\[
[P]_t = -\frac{1}{2} \nu''' \kappa^2 \kappa_s^2 - \nu''(3\kappa \kappa_s^2 + \frac{1}{2}\kappa^2 \kappa_{ss}) - \nu'(\frac{1}{2}\kappa^4 + 3\kappa_s^2 + 2\kappa \kappa_{ss}) - \nu(\frac{1}{2}\kappa^3 + \kappa_{ss})
\]

= \[ -(\frac{1}{2}\nu'' \kappa^2 + 2\nu' \kappa + \nu)\kappa_{ss} - (\frac{1}{2}\nu''' \kappa^2 + 3\nu'' \kappa + 3\nu')\kappa_s^2 - (\frac{1}{2}\nu' \kappa + \frac{1}{2}\nu)\kappa^3 \]
Linear stability analysis #1

- Perturbed interface: \( r_{\Sigma}(\theta, t) = R(t) + \delta(t) \cdot \cos(n \theta) \)
- Do a perturbation analysis and find the first order solution
- Shape evolution
  \[
  \left( \frac{\delta}{R} \right)^{-1} \left( \frac{\delta}{R} \right)^* = \frac{\eta}{\lambda^5} S_n(C, \eta, J, \Psi, \lambda) \Rightarrow \begin{cases} \text{stable if } S_n < 0 \\ \text{unstable if } S_n > 0 \\ \text{self-similar if } S_n = 0 \end{cases}
  \]

\[
S_n(C, \eta, J, \Psi, \lambda) = (n\Psi - 2)J + \frac{\eta^{3/2}}{2\lambda^3} n(n^2 - 1)(A_1(n^2 + 1) + A_2)
\]

\[
A_1(C, \eta) = Ce^{-\eta}(-4\eta^2 + 10\eta - 2) - 2(1 - C)
\]

\[
A_2(C, \eta) = Ce^{-\eta}(8\eta^2 - 22\eta + 5) + 5(1 - C)
\]

\[
\hat{\gamma} = \frac{\nu_0 M_1 M_2}{M_1 + M_2}, \quad \hat{J} = \frac{\lambda^3 J}{2\pi \gamma} \quad \text{and} \quad \eta = \left( \frac{\lambda}{R} \right)^2 \quad \Psi = \frac{M_1 - M_2}{M_1 + M_2}
\]

- Mode selection if the initial shape is a mode-mixture?
Linear stability analysis #2

• If the initial shape is a mode mixture, in 2D, the flux for the fastest growth mode:

\[
\text{mode } n_{\text{max}} \text{ such that } \frac{\partial S}{\partial n} = 0, \text{ mode } n_{\text{max}} \text{ dominates the shape.}
\]

The maximum growth rate:

\[
G_{\text{max}} = \frac{\eta}{\lambda^5} S_{n_{\text{max}}} (C, \eta, J, \Psi, \lambda).
\]

\[n_{\text{max}} \text{ and } G_{\text{max}} \text{ as a function of } \eta, J = 230, \Psi = 1, \eta = (\lambda / R)^2.\]

• Mode with zero growth rate if \( J = J_R \)

\[
J_R = -\frac{n(n^2-1)(A_1(n^2+1)+A_2)\lambda^3}{2a^3(n\Psi-2)} \sim 1/R^3
\]
Preliminary numerical results

- Implement the rescaling scheme in a boundary integral formulation to speed up the evolution.

\[ R(0) = 1 + 0.05\sin(4\theta), C = 0, \nu_0 = 0.1, \lambda = 1, J = 20. \]

- Check the linear theory and convergence.

analytical solution:

\[ \frac{\delta}{R} \left( t \right) = \frac{\delta}{R} \left( 0 \right) R^{n^2 - 2} \exp \left[ \frac{\lambda^3}{6J} n (n^2 - 1)(2n^2 - 3)(R^3 - 1) \right] \]

<table>
<thead>
<tr>
<th>dt</th>
<th>C=0 error</th>
<th>convergence rate</th>
<th>C=0.5 error</th>
<th>convergence rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.25E-5</td>
<td>1.0545E-6</td>
<td></td>
<td>5.2700E-6</td>
<td></td>
</tr>
<tr>
<td>6.25E-6</td>
<td>2.6363E-7</td>
<td>1.9996</td>
<td>2.1253E-6</td>
<td>1.3101</td>
</tr>
<tr>
<td>3.125E-6</td>
<td>6.5906E-8</td>
<td>2.0000</td>
<td>7.1026E-7</td>
<td>1.5812</td>
</tr>
<tr>
<td>1.56125E-6</td>
<td>1.6367E-8</td>
<td>2.0000</td>
<td>1.8584E-7</td>
<td>1.9343</td>
</tr>
</tbody>
</table>

Error = |A(t) - A(0)|
Long time simulations

- Unstable growth for $C=0$ and $C=0.5$, $R(0) = 1 + 0.01\sin(4\theta), \nu_0 = 0.1, \lambda = 1, J = 230$.

- Self-similar solutions using $R(0) = 1 + 0.05(\cos(2\theta) - \cos(3\theta)), \nu_0 = 0.1, \lambda = 1, J = J_R / 1 \sim 1 / R^3$.

Ref: M. Zhao, J. Lowengrub, A. Belmonte, X. Li, S. Li, manuscript.
A shrinking Hele-Shaw bubble problem

- The problem

\[ u = -\frac{h^2}{12\eta} \nabla P, \quad \nabla \cdot u = -\frac{1}{h \, dt} \frac{dh}{dt} \]

- Equations:

\[
\begin{align*}
\mathbf{u} &= -h^2(t) \nabla P, \text{ in } \Omega \\
\nabla \cdot \mathbf{u} &= \frac{\dot{h}(t)}{h(t)}, \text{ in } \Omega \\
\nabla^2 P &= \frac{\dot{h}(t)}{h^3(t)}, \text{ in } \Omega \\
[P] &= \tau \kappa, \text{ on } \partial \Omega \\
V &= -h^2(t) \frac{\nabla P}{\partial n}, \text{ on } \partial \Omega \\
\nabla^2 \tilde{P} &= 0, \text{ in } \Omega \\
[\tilde{P}] &= \tau \kappa - \frac{\dot{h}(t)}{4h^3(t)} |\mathbf{x}|^2, \text{ on } \partial \Omega \\
\tilde{V} &= -h^2(t) \frac{\nabla \tilde{P}}{\partial n}, \text{ on } \partial \Omega \\
\tilde{V} &= V + \frac{\dot{h}(t)}{2h(t)} \mathbf{x} \cdot \mathbf{n}
\end{align*}
\]

Ref. Picture from EO Dias, et al., PRE.
Linear stability analysis

- Shape evolution
  \[ r_\Sigma(\theta, t) = R(t) + \delta(t) \cdot \cos(k\theta) \]
  \[
  \left( \frac{\delta}{R} \right)^{-1} \frac{d}{dt} \left( \frac{\delta}{R} \right) = \frac{\dot{h}k}{2h} - \frac{\tau h^2 (k^3 - k)}{R^3} \]
  \[
  \frac{\delta}{R} = \left( \frac{\delta}{R} \right)_0 h^\frac{k}{2} (t) e^{\alpha(k)} \int_0^t h^{7/2}(s) ds
  \]
  \[
  \alpha(k) = \tau h_0^3/2 R_0^3 (k - k^3)
  \]


- Shrinking instability with unstable modes
  \[ k < \sqrt{1 + \frac{hR^3}{2\tau h^3}} \]
  \[ \text{for } h > 0 \]

- What about self-similar solution?
  \[ h(t) = (1 - \frac{7}{2}ct)^{-\frac{2}{7}}, \text{ where } c = 2(3k^2 - 1)\tau \]

- If \( h(t) \) is a linear or exponential function, the interface evolution will have two stage. In the first stage the perturbation grows rapidly while shrinking. There exist a critical time \( t^* \) when the perturbation gains its maximum. After that the perturbation will shrink, and the interface will reduce to a circle, eventually vanish.

For \( h(t) = e^t \), \( t^* = \frac{2}{7} \ln \beta^{-1}(k) \), \( (\frac{\delta}{R})_{max} = (\frac{\delta}{R})_0 \beta^{-k/7}(k) e^{-\frac{2}{7} \alpha(k) \beta^{-\frac{7}{2}}(k)} \)

\[ \beta(k) = 2\tau h_0^3/2 R_0^3 (k^2 - 1) \]
Preliminary numerical results #1

- Implement the rescaling scheme in a boundary integral formulation to slow down the evolution

\[ R(0) = 1 + 0.01\cos(4\theta), \tau = 1e - 4, N = 4096, \Delta t = 1e - 4 \]

original \( h(T)=e^T \Rightarrow h(t) = 1 + 0.5t \)

\[ \frac{\delta}{R}(t) = (1 + 0.5t)^2 \exp\left[\frac{120\tau}{7}(1 - (1 + 0.5t)^{7/2})\right] \]

<table>
<thead>
<tr>
<th>dt</th>
<th>error</th>
<th>convergent rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>4E-4</td>
<td>3.711E-8</td>
<td>2.001</td>
</tr>
<tr>
<td>2E-4</td>
<td>9.272E-9</td>
<td>2.009</td>
</tr>
<tr>
<td>1E-4</td>
<td>2.302E-9</td>
<td>2.079</td>
</tr>
<tr>
<td>5E-5</td>
<td>5.449E-10</td>
<td></td>
</tr>
</tbody>
</table>
Preliminary numerical results #2

$R(0) = 1 + 0.01(\cos(3\theta) + \sin(7\theta) + \cos(15\theta) + \sin(25\theta))$

$\tau = 1e^{-4}, N = 4096, \Delta t = 5e^{-5}$

original $h(T) = e^T$ slow down to $h(t) = 1 + 0.5t$


Ref: M. Zhao, J. Lowengrub, A. Belmonte, X. Li, S. Li, manuscript.
Preliminary numerical results #3: self-similarity?

\[ R(0) = 1 + 0.02(\cos(3\theta) + \sin(7\theta) + \cos(15\theta) + \sin(25\theta)), \tau = 1e - 4, N = 4096, \Delta t = 1e - 4 \]

original \( h(T) = (1 + 3.5cT)^{-2/7} \) for self-similar shrinking speed up to \( h(t) = e^t \) in the rescaled frame. \( c = 2\tau(3 \cdot 3^2 - 1) \)
Rescaling implemented in Cartesian Grid Method

W. Ying: Kernel-free Boundary Integral Evaluation Method, which does not need to know the fundamental solution or Green function associated with the elliptic operator.

\[
\frac{dx(t)}{dt} = -\gamma \kappa n(x)
\]

Ref: W. Ying, X. Li, S. Li, manuscript.
A summary on Hele-Shaw problem

- Generalized the classical theory to account for flux, which leads to a unifying perspective capable of describing:
  - generation and suppression of the Mullins-Sekerka instability, Saffman-Taylor instability
  - control of the evolving shape by adjusting boundary conditions
- Developed the general idea to balance the time scales of the macro-scale driving force and the micro-scale interfacial properties
- Constructed morphology diagrams by analogy with phase diagrams for systems in equilibrium
- Confirmed theoretical and numerical findings by the Hele-Shaw experiments

Extension
- Thermodynamic interpretation, proof (B. Hu…)?
  - universal shapes may be metastable extrema of an appropriate energy functional of this open system (or entropy maximizers)
- 3D: theory and nonlinear simulations (have some preliminary results)
- Anisotropy (Glicksman and Lowengrub)
- Other non-equilibrium systems: thin film growth, bio-membrane (S. Veerapaneni), tumor problem (E. Turian), etc.