Numerical Methods for Geometric Motion

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McMaster Applied Math Seminar

Institute of Applied Mathematics

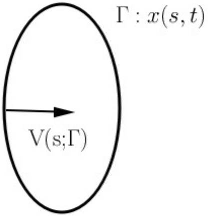
University of British Columbia

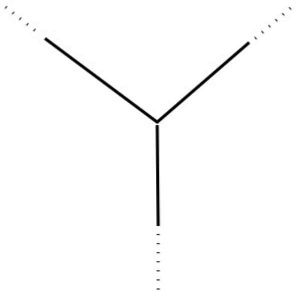
- Faculty participation from many departments.
- Interdisciplinary graduate programme.

Overview of the Talk

- Geometric Motion (2D Curvature Motion Example)
- Numerical Methods (Formulations)
- Sample of Generalized Problems
- Gradient Flow Dynamics

Geometric Motion - I





Examples:

- $V = \kappa$ (curvature)
- $V = -\kappa_{ss}$ (surface diffusion)
- Mullins-Sekerka (nonlocal)

Numerical Challenges:

- Topological changes
- Viscosity solutions
- Networks with junctions
- Stiff systems

Applications:

- Image processing
- Materials Science
- (Intrinsic Interest)

Geometric Motion-II

- "Geometric" means that the dynamics only depends on the curve shape.
- Only the normal velocity is needed to specify the dynamics.
- We will consider first 2D curvature motion of a simple, closed curve, $V = \kappa$.
- Gage, Hamilton, and Grayson: "every simple closed curve shrinks to a round point," (under curvature flow).
- Sethian movie
- Curvature flow arises as a sharp interface limit of the Allen-Cahn phase field model from materials science.

Derivation Allen-Cahn → Curvature Motion I

$$u_t = \epsilon^2 \Delta u - W'(u), \qquad W'(u) = u^3 - u$$

Allen and Cahn 1979

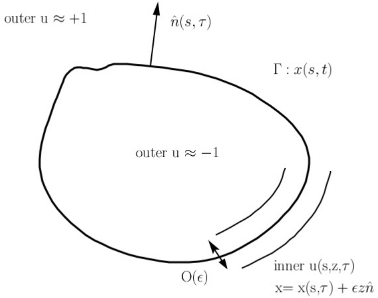
- For discussion, consider $\epsilon = 0$
- A-C is then an autonomous ODE with fixed points $u = \pm 1$ (stable) and $u = 0$ (unstable) at each space location
- Solutions tend to $u = \pm 1$ in $O(1)$ time
- With $\epsilon > 0$ there is an interface of width O(ϵ) that is formed between the two phases
- As $\epsilon \to 0$ the interface tends to a curve that moves with curvature motion in $O(1/\epsilon^2)$ time scale.
- Studying the limiting problem directly gives insight.

Allen-Cahn → Curvature Motion II

$$u_t = \epsilon^2 \Delta u - W'(u), \qquad W'(u) = u^3 + u$$

Outer solution $u = u^{(0)} + \epsilon u^{(1)} + \dots$

- $u(x(s,t),t) = 0$ describes the interface.
- $O(1)$: $u_t^{(0)} = -W'(u^{(0)})$ so $u^{(0)} \to \pm 1$.
- $O(\epsilon)$: $u_t^{(1)} = -W''(u^{(0)})u^{(1)} = -2u^{(1)}$ so $u^{(1)} \equiv 0$.



Allen-Cahn → Curvature Motion III

$$u_t = \epsilon^2 \Delta u - W'(u), \qquad W'(u) = u^3 + u$$

- $\tau = \epsilon^2 t$.
- $u_t = \epsilon V \partial u / \partial z + \ldots \; (V = \partial x / \partial \tau \cdot \hat{n})$
- $\epsilon^2 \Delta u = \partial^2 u / \partial z^2 - \epsilon \kappa \partial u / \partial z + \ldots$

Inner solution $u = u^{(0)} + \epsilon u^{(1)} + \ldots$

- $O(1) : \partial^2 u^{(0)} / \partial z^2 - W'(u^{(0)}) = 0.$ To match outer solution

$$u^{(0)}(z) = \tanh(z/2).$$

- $O(\epsilon) : \; V \partial u^{(0)} / \partial z = \partial^2 u^{(1)} / \partial z^2 - W''(u^{(0)}) u^{(1)} - \kappa \partial u^{(0)} / \partial z$
- Solvability condition $V = -\kappa$.

Gradient Flow - I

Allen-Cahn dynamics are a gradient flow on the energy functional

$$\mathcal{E}(u) = \int \left(\frac{\epsilon^2}{2} |\nabla u|^2 + W(u) \right).$$

This can be seen by calculating (integrate by parts)

$$\frac{d\mathcal{E}}{dt} = \int u_t \left(-\epsilon^2 \Delta u + W'(u) \right).$$

Taking the dynamics to be

$$u_t = \epsilon^2 \Delta u - W'(u)$$

makes

$$\frac{d\mathcal{E}}{dt} \leq 0.$$

Gradient Flow - II

- Curvature motion inherits a gradient flow nature from Allen-Cahn.
- Energy $\mathcal{E} = L$ (curve length).
- Gradient flow

$$\frac{d\mathcal{E}}{dt} = -\int_{\Gamma} \kappa^2.$$

I: Level Set Methods

- Osher and Sethian 1988
- Γ described as the level set $\psi(x,t) = 0$
- Extend $V(\Gamma)$ smoothly to $V(x)$
- $\psi_t = -V|\nabla\psi|$ evolves all level sets with normal velocity V (Hamilton Jacobi equation).
- Curvature fits easily into this framework

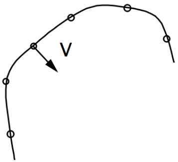
$$\kappa = \nabla \cdot \left(\frac{\nabla\psi}{|\nabla\psi|} \right)$$

- Extensive literature on efficient implementations.
- V can come from other models (not limited to geometric motion)

II: Convolution-Thresholding Methods.

- Ruuth 1998
- Let $\chi(t)$ be the characteristic set inside $\Gamma(t)$
- Solve $u_t = \Delta u$ with $u(x,0) = \chi(t)$
- $\{x : u(x,k) > 1/2\}$ approximates $\chi(t+k)$
- Spectral approximation with adaptive quadrature and nonuniform FFT to approximate the PDE problem to high accuracy
- Richard extrapolation in time stepping

III: Curve tracking x formulation



- $x(\sigma, t)$, with $x_t \cdot \hat{n} = V$
- Tangential velocity maintains scaled arc-length, impose this directly:

$$\frac{1}{2}\frac{\partial}{\partial\sigma}|x_\sigma|^2 = x_\sigma \cdot x_{\sigma\sigma} = 0 \quad \text{or} \quad |x_\sigma| = L$$

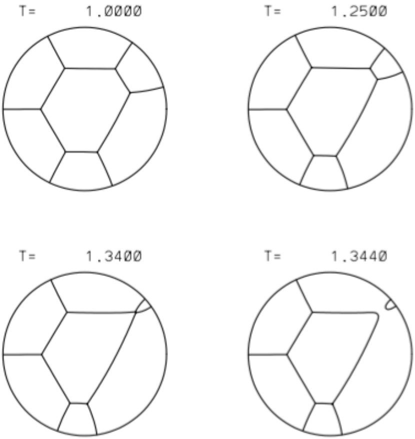
- Fix arbitrary constant in tangential velocity:

$$\int_0^1 x_t \cdot \hat{\tau} d\sigma = 0$$

- Curvature $\kappa = x_{\sigma\sigma} \cdot (x_\sigma)^\perp / L^3$
- FD discretization, implicit time stepping (index-1 DAE structure).

Junctions - I

Crystal Grains

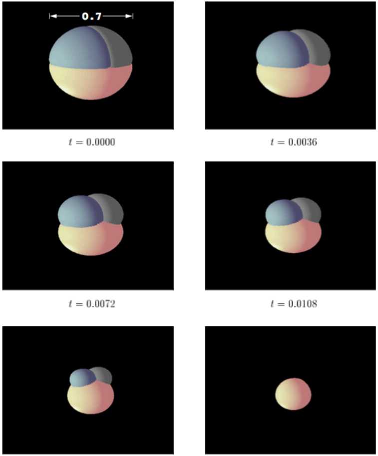


Bronsard and Wetton 1995

Junctions - II

3D Crystal Grains

Ruuth

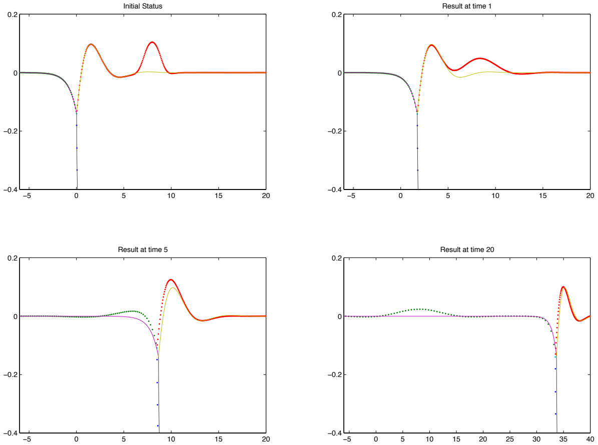


$t = 0.0000$ $t = 0.0036$ $t = 0.0072$ $t = 0.0108$ $t = 0.0144$ $t = 0.0180$

Esedoglu

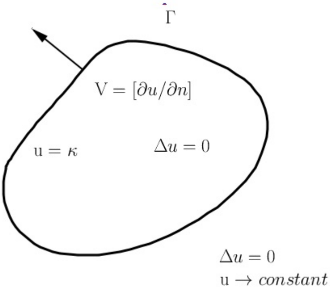
Junctions -III

Quarter Loop



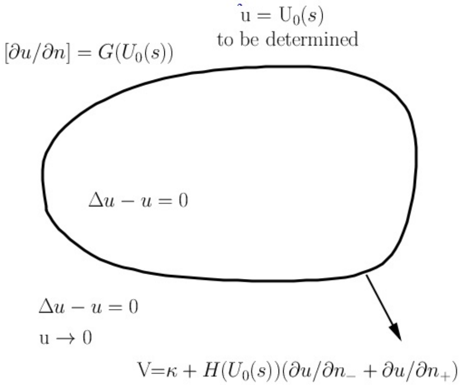
Pan and Wetton 2008

Mullins-Sekerka Flow



- Mullins and Sekerka 1963
- Sharp interface limit of Cahn Hilliard equations, Pego 1989 and Alikakos, Bates, and Chen 1994

Generalized Mullins Sekerka -I



- Limit of an activator-inhibitor reaction diffusion problem.
- u is the inhibitor (global), v the activator (local to the curve)
- G and H involve the inner solution for the activator
- Moyles and Ward

Generalized Mullins Sekerka -II

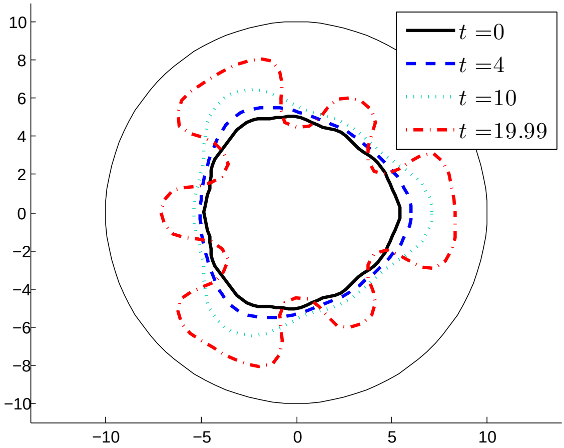
- Moyles and Wetton
- x tracking formulation
- Single layer potential formulation

$$u(y) = \frac{1}{2\pi} \int_{\Gamma} K_0(|x - y|) f(s) ds$$

- Singular boundary integral problem to match $u = U_0(s)$.
- $f(s) = [\partial u / \partial n]$, and $\partial u / \partial n_+ + \partial u / \partial n_-$ can be determined from f with a non-singular integral.
- FD discretization in space, implicit time stepping.
- Trapezoid rule used for the singular integral. Errors $O(h^2 \log h)$, $h = \Delta\sigma$.

Generalized Mullins Sekerka - III

Results



Gradient Flow for $\mathcal{E}(\Gamma)$

Example

- Adhesion Energy

$$\mathcal{E} = L \int_0^1 \frac{1}{2}\kappa^2 \, d\sigma + L^2 \int_0^1 \int_0^1 G(|d|^2) \, d\sigma \, d\sigma' + A(L - L_0)^2$$

- G has a minimum at a prescribed distance.
- Gradient flow velocity Promislow:

$$V = \left(\Delta_s + \frac{\kappa^2}{2} - \mathbb{B}(\sigma) \right) \kappa - \mathbb{A}(\sigma) \cdot n(s).$$

where

$$\mathbb{A}(s) := 4L \int_0^1 2G'(|d|^2); d\sigma'$$

and

$$\mathbb{B}(s) := 2L \int_0^1 G(|d|^2); d\sigma'$$

- x tracking results movie.

General x Code

- Ongoing (just started) project for an open source code that can handle a variety of (local) geometric motion velocities.
- Up to sixth order terms (fourth order in curvature).
- Adaptive implicit time stepping.
- Direct solves for Newton iterations.

Summary

- Some history of methods for curvature motion.
- Some more general geometric motion examples (Wetton focussed).
- Proposed open source framework to handle a general class of 2D local geometric motion problems.