Numerical Methods for Geometric Motion

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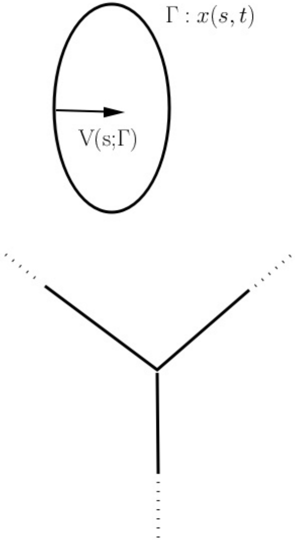
Overview of the Talk

- Geometric Motion basics
- Comparison of numerical methods for local velocities (*i.e.* curvature motion). High level: historical.
- Extension to nonlocal velocities (generalized Mullins-Sekerka) New work: technical

Geometric Motion Definition



Examples:

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

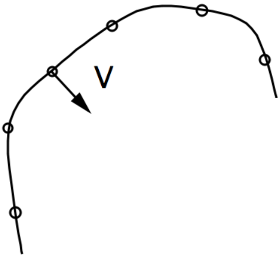
Numerical Challenges:

- Topological changes
- Viscosity solutions
- Networks with junctions

Applications:

- Materials Science
- Image processing
- Intrinsic Interest

Basic Discretization: Tracking



- Normal speed V "given".
- Track points as a discrete approximation, updating the point locations using a small time step.
- Tangential speed is arbitrary.
- There are other approaches with strengths and weaknesses, discussed in the next section.

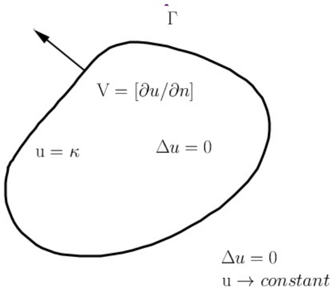
Allen-Cahn $\rightarrow$ Curvature Motion

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

Allen and Cahn 1979

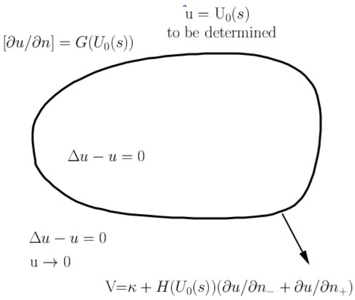
- For discussion, consider $\epsilon = 0$
- A-C is then an autonomous ODE with fixed points $u = \pm 1$ (stable) and $u = 0$ (unstable) at each space location
- Solutions tend to $u = \pm 1$ in O(1) time
- With $\epsilon > 0$ there is an interface of width O(ϵ) that is formed between the two phases
- 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 and is easier computationally.

Mullins-Sekerka Flow



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

New Problem



- Limit of an activator-inhibitor reaction diffusion problem (Gierer-Meinhardt system with saturation)
- u is the inhibitor (global), v the activator (local to the curve)
- $\mathcal{G}$ and $\mathcal{H}$ involve the inner solution for the activator
- Moyles and Ward, Studies in Applied Math 2016

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.
- Sethian movie

Level Set Methods: Pros and Cons

Pros:

- Handles topological changes
- Computes viscosity solutions
- Easy extension to 3D
- Existing software
- Extended to curves on surfaces MacDonald, Ruuth

Cons:

- Difficult to get high accuracy
- Difficult to implement implicitly
- Cannot handle junctions

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

Convolution-Thresholding Methods: Pros and Cons

Pros:

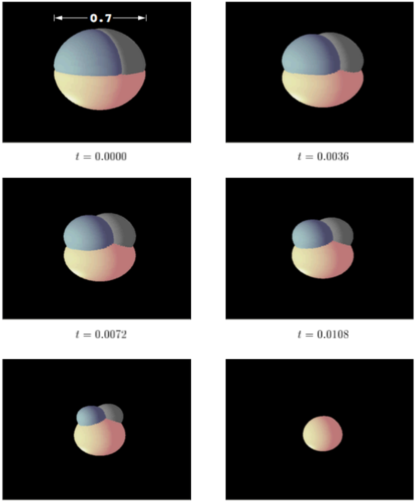
- Handles topological changes
- Easy extension to 3D
- Junctions
- High accuracy

Cons:

- Limited application
- Cannot handle mixed junctions

Convolution-Thresholding Methods: Old Picture

Ruuth



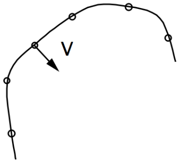
$t = 0.0000$ $t = 0.0036$

$t = 0.0072$ $t = 0.0108$

$t = 0.0144$ $t = 0.0180$

Esedoglu: new movie

IV: Curve tracking x formulation



- $x_t \cdot \hat{n} = V$
- 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:

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

- Curvature $\kappa = x_{\sigma\sigma} \cdot (x_\sigma)^\perp / L^3$

Curve tracking x formulation: Pros and Cons

Pros:

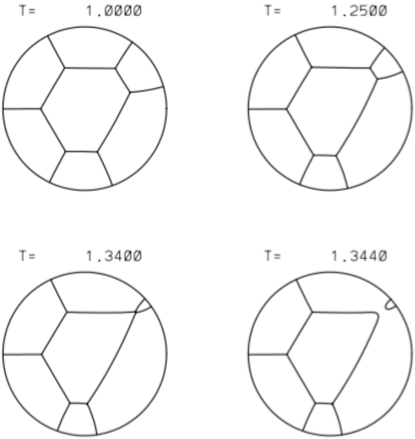
- High spatial accuracy
- Arbitrary time stepping (fully implicit)
- Handles mixed junctions

Cons:

- Does not handle topological changes
- No (easy) extension to 3D: Nurnberg

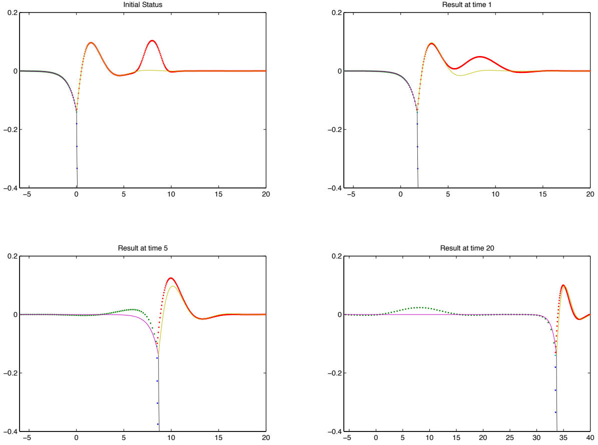
Surface tracking for other problems: Glimm, Krasny

Curve tracking x example: crystal grain evolution



Bronsard and Wetton 1995

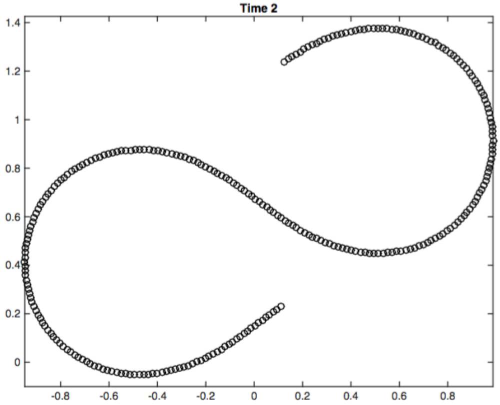
Curve tracking x example: quarter loop



Pan and Wetton 2008

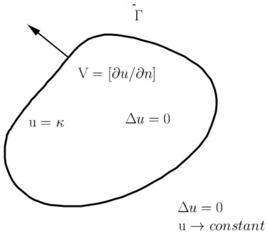
Curve tracking x example: general local motion

$V(\kappa, \kappa_{ss}, L)$



Wetton 2011 unpublished

Mullins Sekerka

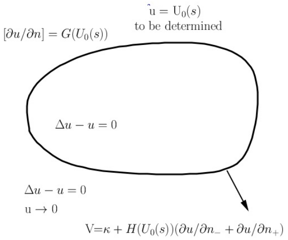


- Zhu, Chen and Hou 1995
- Angle tracking formulation, spectral in σ
- Single layer potential formulation

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

- Singular boundary integral problem to match $u = \kappa$.
- Potential $f(s)$ is exactly $V = [\partial u / \partial n]$.
- Stiffest evolution term is spectrally diagonal, IMEX method

Generalized Mullins Sekerka problem



- Moyles and Wetton, JCP 2015
- x tracking formulation, second order finite differences in σ, fully implicit in time
- 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.

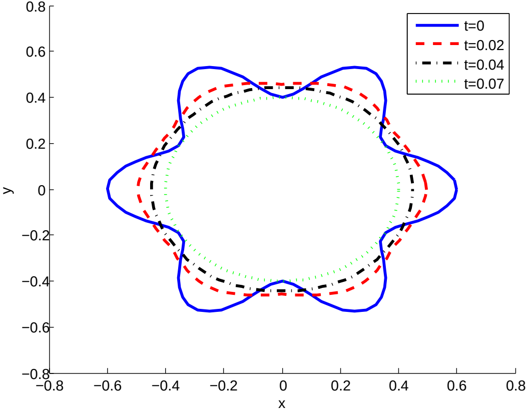
Generalized Mullins Sekerka problem cont.

- Discretize with N points in $\sigma \in [0,1]$.
- Use discrete unknowns X, F, U_0, V and L $(5N+1)$.
- Backward Euler time stepping
- $(X^{n+1} - X^n) \cdot (D_1 X^{n+1}/L)^\perp - kV^{n+1} = 0$ normal velocity (N)
- $|D_+ X^{n+1}|^2 - (L^{n+1})^2 = 0$ scaled arc length (N)
- $\sum (X^{n+1} - X^n) \cdot D_1 X^{n+1} = 0$ arbitrary tangential constant (1)
- $\mathbf{M_1} F^{n+1} - U_0^{n+1} = 0$ singular integral equation (N)
- $F^{n+1} - \mathcal{G}(U_0^{n+1}) = 0$ matching condition (N)
- $D_2 X^{n+1} \cdot (D_1 X^{n+1})^\perp / L^3 + \mathcal{H}(U_0^{n+1}) \mathbf{M_2} F^{n+1} - V^{n+1} = 0$ velocity (N)
- Nonlinear system solved with Newton's iterations
- $\mathbf{M_1}$ and $\mathbf{M_2}$ are dense, other Jacobian blocks are sparse.

Generalized Mullins Sekerka problem cont.

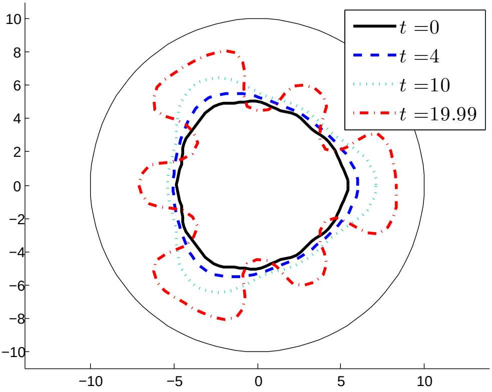
- Problem has an index-1 DAE structure, high order accurate time stepping is possible.
- Product trapezoid rule used for the singular integral. Errors $O(h^2 \log h)$, $h = \Delta\sigma$.
- Higher order quadrature is possible Alpert 1999, Quaife 2011.
- We use a direct solver. Iterative Krylov subspace solvers could be possible, $\mathbf{M_1}$ and $\mathbf{M_2}$ can be applied efficiently using fast multipole techniques.
- The $U_0(\Gamma)$ sub-problem can fail to have a solution and there are non-unique solutions.

Generalized Mullins Sekerka problem results I



Possible bifurcations in the $U_0(\Gamma)$ sub-problem

Generalized Mullins Sekerka problem results II



3-mode buckling (Movie)

Summary

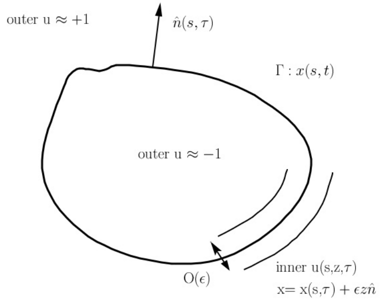
- Some history and comparison of methods for local geometric motion
- New framework to handle a general class of 2D nonlocal geometric motion problems. Easy to adapt to new problem structures.
- Fully implicit time stepping.
- Current implementation is low order, but efficient and high order methods are possible.

Allen-Cahn → Curvature Motion cont.

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

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

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



Allen-Cahn $\rightarrow$ Curvature Motion cont.

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

- $\tau = \epsilon^2 t$.
- z is the interface normal direction, scaled by ϵ.
- $u_t = \epsilon V \partial u / \partial z + \ldots$ $(V = \partial x / \partial \tau \cdot \hat{n})$
- $\epsilon^2 \Delta u = \partial^2 u / \partial z^2 - \epsilon \kappa \partial u / \partial z + \ldots$

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 $V = -\kappa$.

III: Curve tracking angle formulation

$$x_t = V\hat{n} + U\hat{\tau}$$

- Tangential velocity U to be determined
- Curve length $L(t)$ can change.
- Scaled arc length $\sigma = s/L \in [0,1]$, $\hat{\tau} = x_\sigma/L$, $\hat{n} = \hat{\tau}^\perp$
- Write $x_\sigma = L(\cos\theta, \sin\theta)$. Use θ and U as unknowns.
- Differentiate equation with σ, equate $\hat{n}$ and $\hat{\tau}$ components:

$$\begin{aligned} \hat{\tau} &: \quad \dot{L} = -V\theta_\sigma + U_\sigma \\ \hat{n} &: \quad L\theta_t = V_\sigma + U\theta_s \end{aligned}$$

- Curvature $\kappa = \theta_s = \theta_\sigma/L$.
- Stiffest term $\theta_t \sim \theta_{\sigma\sigma}$.

Curve tracking angle formulation: Pros and Cons

Pros:

- High spatial accuracy
- Efficient IMEX time stepping

Cons:

- Does not handle topological changes
- No extension to 3D
- Not a natural formulation for junctions