FAST SEMI-LAGRANGIAN COMPUTATIONS WITH COMPLEX INTERFACES

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SINGULAR FLUID INTERFACES

- Classical fluid mechanics:
  - Kelvin-Helmholtz spirals roll-up
  - Oil-air interfaces cusp
  - Classical asymptotics assume simple topology
DENDRITIC SOLIDIFICATION

- Dendrite formation in plastic/steel/alloy solidification
  - Complex 3D branching instabilities
  - Simple physical models hard to solve
  - Ruins material by impurity segregation
OVERVIEW

• Goal: User-friendly solution of interface problems with:
  – complex dynamic interfacial geometry and topology
  – arbitrary physical phenomena in bulk phases

• Approach: Adaptive semi-Lagrangian contouring of signed distance to interface provides
  – Automatic topology evolution
  – Relaxed time step constraints
  – Adaptive $O(N \log N)$ spatial resolution
  – Modular velocity evaluation

• Results include:
  – Second-order adaptive 2D schemes for moving interfaces
  – Fast algorithms for dynamic computational geometry
  – Robust high-order accurate 2D contouring package
• Moving interface $\Gamma(t)$ is union of piecewise-smooth closed curves (2D) or surfaces (3D), parametrized by $X(t,s)$.

• Vector normal velocity $V = (X_t \cdot N)N$ is a functional of
  – transport processes (material PDEs and input data)
  – interface geometry, topology and dynamics
  – history of the system

• Typical functionals $V = F(\Gamma)$ include Ostwald ripening:

\[
\begin{align*}
\Delta u &= 0 \quad \text{off } \Gamma \\
\alpha u + \beta u_N &= g \quad \text{on } \partial B \\
 u &= C = \text{Curvature on } \Gamma \\
 V &= [u_N]N = DtN(C)N \quad \text{on } \Gamma
\end{align*}
\]
MODELS AND CHALLENGES

Passive transport

\[ V = F(x, t)N \]

⇒ need efficient resolution of complex structures

First-order geometry

\[ V = G(x, t, N) \]

⇒ need robust dynamic merging and faceting

Motion by curvature

\[ V = H(x, t, N, C) \]

⇒ need stable methods for disparate time scales
MATHEMATICAL THEORY

• **Local geometric motion** well-understood:
  - Explicit parametrization gives local existence and regularity theory for smooth solutions
  - Implicit parametrizations and viscosity solutions of Hamilton-Jacobi equations handle topology changes

• **Nonlocal problems** more challenging (and more realistic):
  - Local well-posedness with simple topology
  - Global existence for crystal growth
  - Counterexamples to smoothness
  - Many open problems
LINEARLY IMPLICIT APPROACH

- Represent interface $\Gamma(t)$ implicitly as zero set of signed distance

$$\varphi(x, t) = \pm \min_{\gamma \in \Gamma(t)} ||x - \gamma||$$

- Extract geometry from implicit representation by

$$N = \nabla \varphi / ||\nabla \varphi|| \quad \quad C = \nabla \cdot N$$

- Extend $V = \varphi_t \nabla \varphi / ||\nabla \varphi||^2$ to global velocity field $W$ and evolve $\varphi$ with velocity $W$ via linear advection equation

$$\varphi_t - W \cdot \nabla \varphi = 0$$

- Extract $\Gamma(t)$ by contouring $\varphi$. 
A CONTOURING PROBLEM

• Don’t move the interface! Characteristics will cross forward in time.

• Instead, ask every point $x$ at time level $t + k$ whether it could have come from an interface point $\tilde{x}$ at time $t$ with consistent velocity $V(\tilde{x}, t)$: Look back along characteristics.

• Finding the new interface $\Gamma(t+k)$ is a contouring problem: Find zero set $\{x | \psi(x) = 0\}$ of exact solution

$$\psi(x) = \varphi(x, t + k) = \varphi(\tilde{x}, t)$$

where $\tilde{x} = x(t)$ is foot at time $t$ of characteristic $\dot{x}(t) = W(x(t), t)$ entering $x = x(t + k)$ at time $t + k$. 
SEMI-LAGRANGIAN ADVECTION

- **Exact** solution to advection equation is

\[ \psi(x) = \varphi(x, t + k) = \varphi(\tilde{x}, t) \]

where \( \tilde{x} = x(t) \) is foot at time \( t \) of characteristic \( \dot{x}(t) = W(x(t), t) \) entering \( x = x(t + k) \) at time \( t + k \).

- **Explicit stable first-order** CIR predictor uses straight lines

\[ \tilde{x} \approx x + kW(x, t). \]

- **Second-order** trapezoidal corrector averages \( W \)

\[ \bar{\psi}(x) = \varphi(x + \frac{k}{2}W(\tilde{x}, t) + \frac{k}{2}\tilde{W}(x), t) \]

with extended velocity \( \tilde{W} \) built from velocity \( \tilde{V} = V(\tilde{\Gamma}) \) of zero set \( \tilde{\Gamma} \) of predicted \( \tilde{\psi} \).
SEMI-LAGRANGIAN SCHEMES

- CIR scheme is unusual: explicit yet unconditionally stable!

- Bad for hyperbolic conservation law $u_t + f(u)_x = 0$ because not in conservation form: moves shocks at wrong speed.

- Moving interface advection equation is not conservative, and signed distance function has no shocks.

- Semi-Lagrangian schemes are popular (but controversial) in meteorology where shocks are weak or nonexistent.

- Efficiency: concentrate resolution at the interface. In semi-Lagrangian schemes, each solution evaluation $\psi(x)$ is completely independent, so adaptive gridding requires no global effort.
GEOMETRIC ALGORITHMS

- Need efficient algorithms for
  - Contouring:
    \[ \psi \longrightarrow \Gamma = \{ x | \psi(x) = 0 \} \]
  - Distancing:
    \[ \Gamma \longrightarrow \psi = \pm \text{distance to } \Gamma \]
  - Extension:
    \[ V \longrightarrow W \text{ extending } V \text{ off } \Gamma \]

- All provided by refinements of quadtree mesh structure:
Adaptive quadtree meshes zoom in on $\Gamma$ with cell size proportional to distance $|\varphi|$.

Signed distance $\varphi$ is evaluated exactly to eliminate time step restrictions.
FAST GEOMETRIC ALGORITHMS

• Quadtree-based fast signed distance computation
  – Cells track nearby points
  – Compute distance near $N$-element interface in $O(N \log N)$
  – Guaranteed search strategy

• Fast stable velocity extension
  – Nearest-point extension discontinuous at medial axis
  – Quadtree interpolant continuous and stable

• Produce smooth accurate contours of $\psi$
  – Evaluate at arbitrary points for subgrid accuracy
  – Conflict between topological consistency and accuracy
EFFICIENT DISTANCING

- Voronoi diagram of $\Gamma$ optimal in principle, but inefficient in practice—compact Voronoi diagram under development

- Quadtree with cell size proportional to distance computes distance efficiently for points near $\Gamma$

- Guarantees exact signed distance: the nearest element in $T^*$ may not be optimal, but rules out exterior of $T^{**}$ to limit search area
QUADTREE TRACKS NEARBY $\Gamma$ POINTS

- Quadtree cells $C$ built with pointers to all points of $\Gamma$ inside concentric triples $T$
- Standard condition for Whitney decomposition, fast multipole method
- Costs $O(N \log N)$ with $N$ elements in $\Gamma$
VELOCITY EXTENSION

• Nearest-point extension \( W(x) = V(\text{nearest } \gamma \in \Gamma \text{ to } x) \) discontinuous on medial axis where nearest point jumps

• Whitney extension (1934) evaluates in quadtree cells and builds continuous function by partition of unity

• Numerical version interpolates on triangulated quadtree: cheap, stable, independent of the physical problem
QUADTREE CONTOURING

- Build distance tree for $\Gamma$ from semi-Lagrangian $\psi$

- Build Delaunay triangulation of vertices

- Find exact polygonal zero set of piecewise-linear interpolant to vertex values $\Rightarrow$ consistent topology

- Cost $O(N \log N)$ if $\Gamma$ has $N$ elements

- Increase accuracy, preserve topological consistency via subgrid refinement because $\psi(x)$ available off grid
CONSISTENCY VS ACCURACY

\[ V = N \]

\[ V = DtN(C)N \]
- Safeguard topology:
  — segments don’t cross
  — points don’t leave triangles
HIGH-ORDER ADAPTIVE CONTOURING

- **Binary triangle tree** refines triangulation of quadtree

- **Piecewise quadratic** $C^1$ Bezier micropatches: Clough-Tocher, Powell-Sabin, triangle-split-square, ...

- **Accurate cubic contouring:**
  - panel patches for robust topology detection
  - enclose zero sets with gradient-projected-polyhedron algorithm
  - guaranteed quadratic convergence
  - produces $G^2$ cubic spline segments in 2D

- **New natural neighbor interpolant for scattered data.**

- **Josh Levenberg, PhD thesis 2003;**
  open source package in preparation.
NEARLY SINGULAR CONTOURS

\[ \epsilon + L(x)L(y) \]

\[ \epsilon + L(x, y)E(x, y) \]

\[ \epsilon + L(x, y)E(x, y) \]
GEOMETRIC EXAMPLES
OSTWALD RIPENING BY POTENTIAL THEORY

• Velocity $V = DtN(F(N, C))N = u_NN$ where
  $\Delta u = 0 \text{ off } \Gamma(t) = \Gamma_1 \cup \cdots \cup \Gamma_m$ and
  $u = F(N, C)$ on $\Gamma(t)$.

• Mikhlin double layer potential representation

  $$2\pi u(x) = \int_{\Gamma} (1 + \partial_N \log |x - s|) \mu(s) ds + \sum_k a_k \log |x - s_k|$$

  gives second-kind integral equation on $\Gamma$

  $$\pi \mu(x) + \int_{\Gamma} (1 + \partial_N \log |x - s|) \mu(s) ds + \sum_k a_k \log |x - s_k| = 2\pi F(N, C)$$

  plus constraints

  $$\sum_k a_k = 0, \quad \int_{\Gamma_k} \mu(s) ds = 0 \quad k < m$$
VELOCITY DISCRETIZATION

- Integral equation spectrally accurate with trapezoidal rule
- Fast solution by GMRES because eigenvalues cluster
- Even faster with fast multipoles
- Cost $O(N \log N)$ per time step with $N$ elements on curve
- Accurate normal derivative from Cauchy-Riemann equations and spectral derivative
FACETED RIPENING

- Velocity \( V = (1 + \epsilon \cos(\theta(N)))(DtN(C) + \delta)N \)
GOLD SINTERING EXPERIMENTS
CONCLUSIONS

- General problem
  move interface with velocity functional \( V = F(\Gamma) \)
determined by technological situation.

- Solved with efficient \( O(N \log N) / \text{step} \) modular approach.

- Velocity modules require
  fast PDE solvers/geometry engines.

- Fast robust accurate contouring schemes
  surprisingly important in material problems.