Moving interface problems

for elliptic systems

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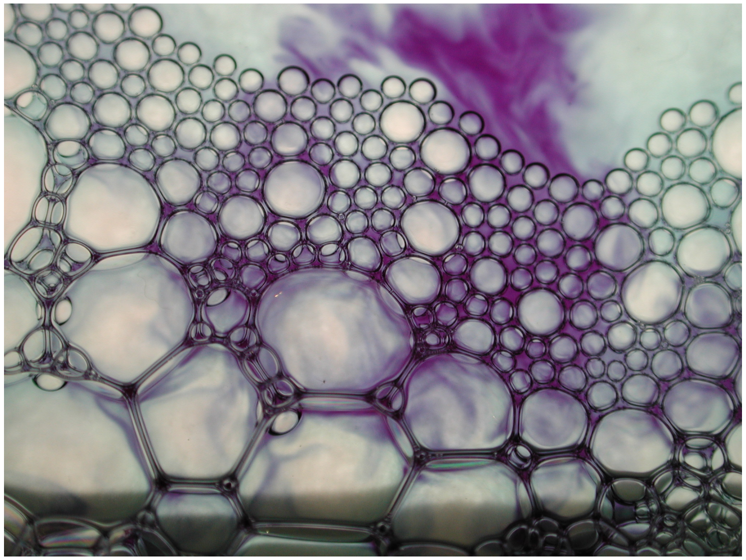
ALGORITHMS

Implicit semi-Lagrangian contouring moves interfaces
– with arbitrary topology
– subject to stiff interface velocity
using
* implicit interface representation
* implicit stiffly-stable time discretization

Locally-corrected spectral methods find velocity from
– overdetermined first-order elliptic systems in bulk phases
– geometric boundary conditions on moving interfaces
using
* boundary integral equations
* generalized Ewald summation
* local correction formulas
* geometric nonuniform fast Fourier transforms

MOVING INTERFACES



Multiphase Stokes flow

$$\begin{aligned} -\nu\Delta u + \nabla p &= f_\Gamma \delta_\Gamma \\ \nabla \cdot u &= 0 \\ V &= u \qquad \textbf{on } \Gamma \\ V &= S^{-1}(f_\Gamma \delta_\Gamma) \end{aligned}$$

Ostwald ripening

$$\begin{aligned} \Delta u &= 0 \\ u &= C \qquad \textbf{on } \Gamma \\ V &= [u_n]\, n \qquad \textbf{on } \Gamma \\ V &= \Lambda_\Gamma C \end{aligned}$$

STIFF INTERFACES

Normal velocity V on $\Gamma(t)$ depends on
– material properties, experimental parameters, . . .
– interface geometry, topology, dynamics, . . .

Sensitive dependence produces stiff interfaces

Curvature flow	Ostwald ripening	Surface diffusion
$V = C$	$V = \Lambda_\Gamma C$	$V = \Delta_\Gamma C$
$k = O(h^2)$	$k = O(h^3)$	$k = O(h^4)$

Computationally expensive dilemma
– explicit methods require tiny time steps
– implicit methods must solve nonlinear systems

IMPLICIT CONTOURING APPROACH

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

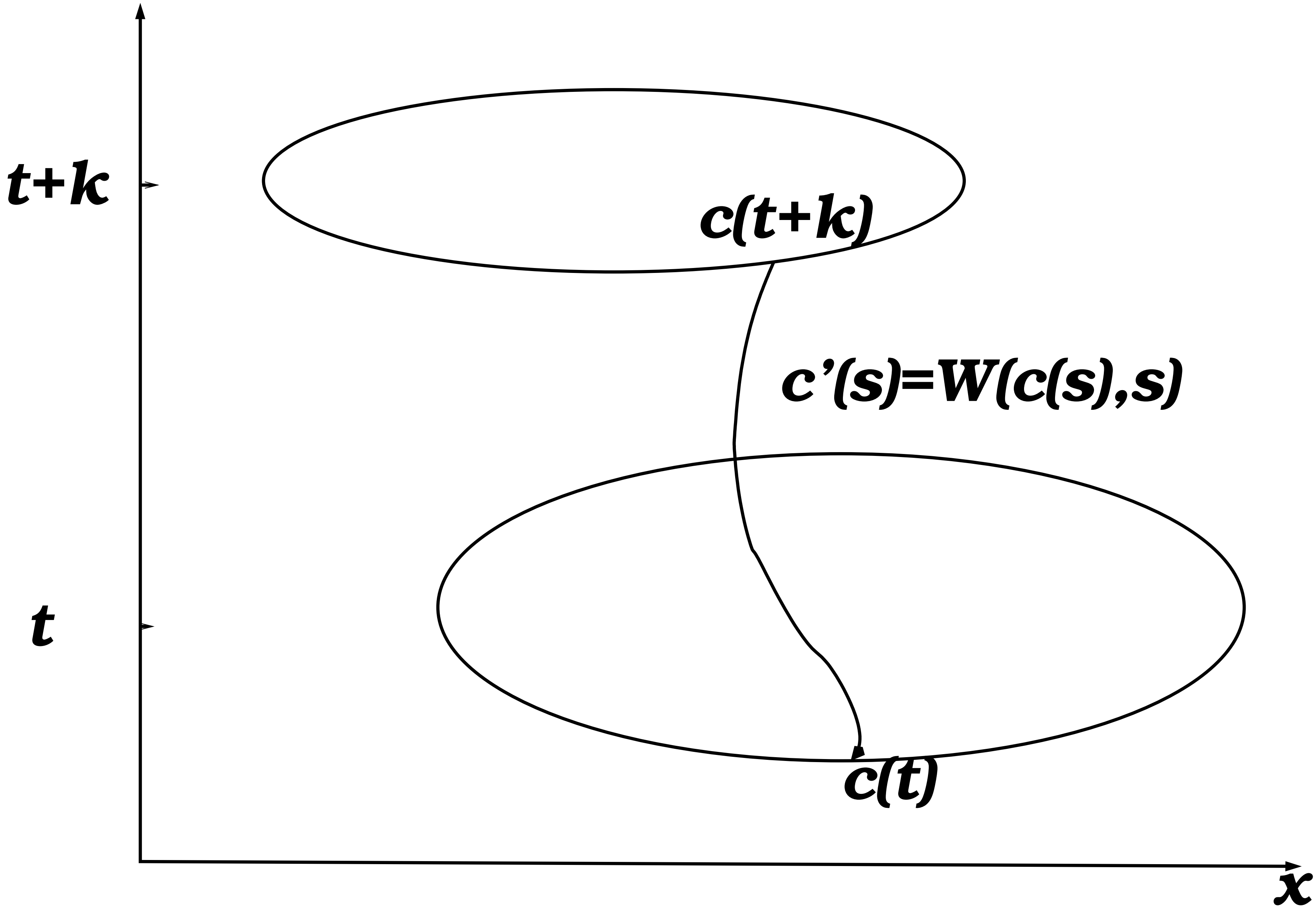
$$d(x) = \pm \min_{\gamma \in \Gamma(t)} \|x - \gamma\|$$

Extend $V(\gamma, t)$ to fictitious global velocity field $W(x, t)$ and transport values of d globally with velocity W

Contour: New interface $\Gamma(t + k)$ is zero set $\{x | \varphi(x) = 0\}$ of

$$\varphi(x) = d(\tilde{x})$$

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



t+k
c(t+k)
c'(s)=W(c(s),s)
t
c(t)
x

SEMI-LAGRANGIAN FORMULAS

Exact transported implicit representation is

$$\varphi(x) = d(c(t))$$

where $c(t)$ is foot at time t of backward characteristic $\dot{c}(s) = W(c(s), s)$ entering $x = c(t+k)$ at time $s = t + k$

Explicit CIR scheme uses straight lines with old W

$$\varphi(x) = d(x - kW(x, t))$$

Implicit CIR solves functional equation

$$\varphi(x) = d(x - kW(x, t + k))$$

for φ and unknown extended normal velocity

$$W(x, t + k) = E_{\varphi} V_{\varphi}(x)$$

Mesh-free functional approach $\Rightarrow$ Only resolve interface

IMPLICIT SLC

Solve implicit SLC equation

$$F(\varphi) := \varphi(x) - d(x - kW(x, t+k)) = 0$$

with unknown extended interface velocity

$$W(x, t+k) = E_{\varphi} V_{\varphi}(x)$$

Update φ **with damped Newton** $DF(\varphi)\delta\varphi = -F(\varphi)$

$$(I - D\left[d(x - kE_{\varphi}V_{\varphi}(x)]\right)\delta\varphi(x) = d(x - kE_{\varphi}V_{\varphi}(x)) - \varphi(x)$$

$$\varphi \leftarrow \varphi + \theta\delta\varphi$$

where $\theta \in [0, 1]$ **reduces** $\|F(\varphi)\|$

(With Ian Sammis, Mathematics, UC Davis)

FRECHET DERIVATIVES

Chain rule for Newton operator $DF(g)$ composes

– **Signed distance gradient $\nabla d(x - kE_\varphi V_\varphi)$**

– **Extension variation from nearest point $\gamma \in \Gamma$ to x**

$$DE_\varphi V \delta\varphi(x) = D_\gamma V \cdot \left(\|\nabla\varphi\| I + \|\gamma - x\| D^2\varphi\right)^{-1} \|\gamma - x\| \nabla\delta\varphi(x)$$

– **Interface velocity variation DV_φ composed of**

* **problem-independent geometric variations**

$$Dn \cdot \delta\varphi = \left(I - \frac{\nabla\varphi\nabla\varphi^T}{\|\nabla\varphi\|^2}\right)\frac{\nabla(\delta\varphi)}{\|\nabla\varphi\|}$$

* **problem-dependent elliptic system**

EXAMPLES OF ELLIPTIC SYSTEMS

Poisson/Helmholtz/Yukawa/ ...

$$\Delta u + \omega u = f$$

Stokes

$$-\Delta u + \nabla p = f, \qquad \nabla \cdot u = 0$$

Low-frequency Maxwell

$$\nabla \times E = -\frac{i\omega}{c} H \qquad \nabla \cdot E = 4\pi\rho$$

$$\nabla \times H = \frac{i\omega}{c} E + \frac{4\pi}{c} j \qquad \nabla \cdot H = 0$$

FIRST-ORDER SYSTEMS

Second-order system of partial differential equations

$$\sum_{ijl} a_{ijkl}\partial_i\partial_j v_l + \sum_{jl} b_{jkl}\partial_j v_l + \sum_l c_{kl} v_l = f_k \qquad \textbf{in } \Omega$$

$$\sum_l \alpha_{kl} v_l + \sum_{jl} \beta_{kjl}\partial_j v_l = g_k \qquad \textbf{on } \Gamma = \partial\Omega$$

equivalent to first-order system

$$Au = \sum_j A_j \partial_j u + A_0 u = f \qquad \textbf{in } \Omega$$

$$Bu = g \qquad \textbf{on } \Gamma$$

for vector u of v and first derivatives $\partial_j v$

SQUARE BUT NOT ELLIPTIC

2D Poisson equation

$$\Delta v = f \qquad \textbf{in } \Omega$$

$$\alpha v + \beta \partial_n v = g \qquad \textbf{on } \Gamma$$

equivalent to 3×3 **system for** v **and derivatives:**

$$Au = \begin{bmatrix} \partial_1 & -1 & 0 \\ \partial_2 & 0 & -1 \\ 0 & \partial_1 & \partial_2 \end{bmatrix} \begin{bmatrix} v \\ \partial_1 v \\ \partial_2 v \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ f \end{bmatrix}$$

$$Bu = \begin{bmatrix} \alpha & \beta n_1 & \beta n_2 \end{bmatrix} \begin{bmatrix} v \\ \partial_1 v \\ \partial_2 v \end{bmatrix} = g$$

System not elliptic: $\sum_j k_j A_j$ **singular!**

OVERDETERMINED BUT ELLIPTIC

2D Poisson equation

$$\Delta v = f \qquad \textbf{in } \Omega$$

$$\alpha v + \beta \partial_n v = g \qquad \textbf{on } \Gamma$$

also equivalent to overdetermined 4×3 elliptic system

$$Au = \begin{bmatrix} \partial_1 & -1 & 0 \\ \partial_2 & 0 & -1 \\ 0 & -\partial_2 & \partial_1 \\ 0 & \partial_1 & \partial_2 \end{bmatrix} \begin{bmatrix} v \\ \partial_1 v \\ \partial_2 v \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ f \end{bmatrix}$$

$$Bu = \begin{bmatrix} \alpha & \beta n_1 & \beta n_2 \end{bmatrix} \begin{bmatrix} v \\ \partial_1 v \\ \partial_2 v \end{bmatrix} = g$$

Compatibility conditions make system overdetermined but elliptic: $\sum_j k_j A_j$ injective for $k \neq 0$.

SOLVABILITY

Ellipticity of first-order system

$$Au = \sum_j A_j \partial_j u + A_0 u = f \qquad \text{in } \Omega$$

implies solvability for any directional derivative

$$\partial_n u = \sum_i n_i \partial_i u$$

using left inverse

$$A_n^\dagger = \left(\sum_j n_j A_j \right)^\dagger = (A_n^* A_n)^{-1} A_n^*$$

Integrate

$$\partial_n u = A_n^\dagger (f - A_T \partial_T u - A_0 u)$$

inward to solve boundary value problem

ALTERNATING DIRECTION IMPLICIT

Separable second-order equations in rectangles

$$-\Delta u = Au + Bu = -\partial_1^2 u - \partial_2^2 u = f, \qquad A, B > 0$$

efficiently solved by essentially optimal ADI iteration

$$(s^2 + A)(s^2 + B)u^{m+1} = (s^2 - A)(s^2 - B)u^m + 2f$$

Error mode $e^{ik^T x}$ **damped by symbol**

$$\sigma(k_1)\sigma(k_2) = \left(\frac{s^2 - k_1^2}{s^2 + k_1^2}\right)\left(\frac{s^2 - k_2^2}{s^2 + k_2^2}\right)$$

Fast damping over geometric range

$$\frac{1}{\sqrt{2}} \le \frac{|k_1|}{s} \le \sqrt{2} \quad \rightarrow \quad |\sigma_1(k_1)| \le \frac{1}{3}$$

– $O(\epsilon)$ **damping in** $O(\log N \log \epsilon)$ **sweeps**

– **with** $s = 1, 2, 4, 8, 16, \ldots, N$

ADI FOR SYSTEMS

Choose sweep direction n

$$\sum_j A_j \partial_j u = \sum_{ij} A_i (n_i n_j + \delta ij - n_i n_j) \partial_j u = A_n \partial_n u + A_T \partial_T u$$

Left-invert A_n **and shift by 1/length scale** s**:**

$$su + \partial_n u + B_0 u = su + f - B_T \partial_T u$$

Error mode $\mathrm{e}^{\mathrm{i}k^T x} I$ **damped by matrix symbol**

$$\rho(k) = \prod_n (s + \mathrm{i}k_n + B_0)^{-1} (s - \mathrm{i}B_T k_T)$$

Damping factors 0.5, 0.1, 0.005 with 4, 8, 16 sweep directions

POTENTIAL THEORY

Given fundamental solution $G = G_x$ **of adjoint system**

$$-\partial_1 G A_1 - \partial_2 G A_2 + G A_0 = \delta_x I \qquad \text{in box } Q \supset \Omega$$

Gauss theorem

$$\int_\Omega \partial_j \left(G A_j u\right) \, \mathrm{d}x = \int_\Gamma n_j G A_j u \, \mathrm{d}\gamma$$

implies boundary integral equation

$$\frac{1}{2} u(\gamma) + \int_\Gamma G_\gamma(\sigma) A_n(\sigma) u(\sigma) \, \mathrm{d}\sigma = \int_\Omega G_\gamma(y) f(y) \, \mathrm{d}y \quad \text{on } \Gamma$$

where $A_n(\gamma) = \sum n_j(\gamma) A_j$

PROJECTED INTEGRAL EQUATION

Project out boundary condition $Bu = g$ **with** $P(\gamma) = I - B^*B$

Solve well-conditioned square system

$$\frac{1}{2}\mu(\gamma) + \int_\Gamma P(\gamma)G_\gamma(\sigma)A_n(\sigma)\mu(\sigma)\mathrm{d}\sigma = \rho(\gamma)$$

for projected unknown $\mu = Pu$ **with data**

$$\rho(\gamma) = P(\gamma)\int_\Omega G_\gamma(y)f(y)\,\mathrm{d}y + P(\gamma)\int_\Gamma G_\gamma(\sigma)A_n(\sigma)B^*g(\sigma)\,\mathrm{d}\sigma$$

Recover $u = \mu + B^*g$ **on** Γ **and**

$$u(x) = \int_\Omega G_x(y)f(y)\,\mathrm{d}y + \int_\Gamma G_x(\sigma)A_n(\sigma)u(\sigma)\,\mathrm{d}\sigma \qquad \textbf{in}\,\Omega$$

Need fast algorithm for $G_\gamma(\sigma)$

FUNDAMENTAL SOLUTION IN A BOX

Fourier series in box enclosing Γ gives fundamental solution

$$G_x(y) = \sum_{k \in Z^d} \mathrm{e}^{-\mathrm{i}k^T x} s(k)^{-1} a^*(k) \mathrm{e}^{\mathrm{i}k^T y}$$

where $s = a^* a$ is positive definite Hermitian matrix and

$$a(k) = \mathrm{i} \sum_{j=1}^{d} k_j A_j + A_0$$

Filter with $\mathrm{e}^{-\tau s}$ for exponentially fast convergence:

$$G_x(y) = \sum_{\|k\| \le N} \mathrm{e}^{-\mathrm{i}k^T x} \mathrm{e}^{-\tau s(k)} s(k)^{-1} a^*(k) \mathrm{e}^{\mathrm{i}k^T y}$$

up to $O(\mathrm{e}^{-\tau N^2})$ truncation error and $O(\tau)$ local error

GENERALIZED EWALD SUMMATION

Fundamental solution is smooth rapidly-converging series

$$G_\tau(x) = \sum \mathrm{e}^{-\tau s(k)} s(k)^{-1} a^*(k) \mathrm{e}^{-\mathrm{i}k^T x}$$

plus local asymptotic error expansion

$$E_\tau = (I - \mathrm{e}^{-\tau S}) S^{-1} A^* = \left(\tau - \frac{\tau^2}{2!} S + \frac{\tau^3}{3!} S^2 - \cdots \right) A^*$$

with local differential operators A^* and $S = A^* A$

Implies many local correction methods for Laplace, Helmholtz, Stokes, . . .

Also effective for volume and layer potentials

HIGHER-ORDER GAUSS THEOREM

Gauss theorem differentiates indicator function $\omega(x)$ of set Ω:

$$\int_\Omega \partial_j u \, \mathrm{d}x = \int_\Gamma n_j u \, \mathrm{d}\gamma \quad \Leftrightarrow \quad \partial_j \omega = n_j \delta_\Gamma$$

Geometry in second-order derivatives

$$\partial_j \partial_k \omega(x) = (\partial_j n_k)\delta_\Gamma + n_j n_k \partial_n \delta_\Gamma$$

Volume potential of discontinuous function $f\omega$ splits:

$$\int_\Omega G_x(y) f(y) \, \mathrm{d}y = B(f\omega) = B_F(f\omega) + B_L(f\omega)$$

Local correction B_L satisfies product rule:

$$B_L(f\omega)(x) = \tau \left((A^* f(x))\omega(x) - \sum_j A_j^* f(x) n_j(x) \delta_\Gamma(x) \right) + O(\tau^2)$$

SPECTRAL INTEGRAL EQUATION

Fourier series for fundamental solution separates variables

$$G_r(x-y) = \sum \mathrm{e}^{-\mathrm{i}k^T x} \mathrm{e}^{-\tau s(k)} s(k)^{-1} a^*(k) \mathrm{e}^{\mathrm{i}k^T y}$$

Converts integral equation to semi-separated form

$$\left(\frac{1}{2} - MRT\right)\mu(\gamma) = \rho(\gamma)$$

Solve in Fourier space by identity

$$\left(\frac{1}{2} - MRT\right)^{-1} = 2 + 2MR\left(\frac{1}{2} - TMR\right)^{-1} T$$

– $T\rho$ **computes Fourier coefficients of** $(A_n\rho)\delta_\Gamma$
– R **applies filtered inverse of elliptic operator in Fourier space**
– M **evaluates and projects Fourier series on** Γ

Compresses system and boundary conditions to matrix

$$(TMR)_{kq} = \int_\Gamma A_n(\sigma) P(\sigma) \mathrm{e}^{-\mathrm{i}(k-q)^T\sigma}\, \mathrm{d}\sigma\, \mathrm{e}^{-\tau s(q)} s(q)^{-1} a^*(q)$$

NONUNIFORM FFT

Standard FFT works on uniform equidistant mesh

Nonuniform FFT works on arbitrary point sources:
- smooth point sources into Gaussians
- evaluate Gaussians on uniform mesh
- compute Fourier coefficients by FFT
- divide out smoothing of each coefficient

Integral operator and density ρ require Fourier coefficients of soup of piecewise polynomials P_q on simplices T_q (points, segments, triangles, tetrahedra, ...)

$$\widehat{f}(k) = \sum_q \int_{T_q} \mathrm{e}^{\mathrm{i}k^T x} P_q(x)\,\mathrm{d}x$$

Similar to semiconductor mask computations

GEOMETRIC NONUNIFORM FFT

Geometric NUFFT evaluates Fourier coefficients of soup in arbitrary dimension and codimension

Follow model of NUFFT for point sources, but
– integrating Gaussians over simplices intractable,
so smooth with piecewise-polynomial B-spline kernels
– then evaluate smoothed distributions on uniform mesh,
– apply standard FFT,
– unsmooth with guaranteed error bounds

Exact quadrature: split simplices between uniform grid cells where smoothing kernels are polynomial

(With Ian Sammis, Mathematics, UC Davis)

WORK IN PROGRESS

Stabilize stiff moving interfaces with
– fast approximate Jacobians from boundary integral equation
– exponentially fitted time stepping methods

Extract **explicit highest-derivative terms**
in Frechet derivative of

$$
\begin{aligned}
u &= B^*g + \left(\frac{1}{2} - MRT\right)^{-1} \rho \\
&= B^*g + \left(2 + 2MR\left(\frac{1}{2} - TMR\right)^{-1} T\right)(P\Omega f + MRTB^*g) \\
&\approx B^*g + (2 + MRT)(P\Omega f + MRTB^*g)
\end{aligned}
$$

where g depends on geometry of interface

Ostwald ripening of a perturbed linear interface
has $V \approx HD^3$ where H is Hilbert transform