Computing with Singular and Nearly Singular Integrals

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single or double layer potential on a curve in 2D or surface in 3D
the integral is nearly singular at points off the surface but nearby
use rectangular grids in coordinate systems
outline of the procedure:
(1) regularize, e.g., $1/r \mapsto 1/\delta$ for $r \to 0$
(2) standard quadrature over grid points
(3) corrections for regularization and discretization
corrections are found by local analysis near singularity
for closed surface in 3D use overlapping grids
and partition of unity (cf. O. Bruno)
curve or surface must be smooth
discrete integral equation for boundary value problem converges

Why Singular Integrals?

Solutions of $\Delta u = 0$ or $\Delta u = f$ in R^d
can be written as integrals with
$G(x)$, the fundamental solution,

$$\Delta G(x) = \delta(x)$$

$$G(x) = -\frac{1}{4\pi|x|} \qquad \text{in } R^3$$

$$G(x) = \frac{1}{2\pi}\log|x| \qquad \text{in } R^2$$

For $\Delta u = f$ in R^d, with decay at ∞,

$$u(x) \ = \ \int_{R^d} G(x-y) f(y)\, dy$$

Boundary value problems can be solved with
layer potentials on the boundary

Layer Potentials

$\Omega \subseteq R^d$ a bounded domain
For σ on $\partial\Omega$, the **single layer potential** is

$$u(x) = \int_{\partial\Omega} G(x-y)\sigma(y)\, dS(y)$$

$\Delta u = 0$ on $R^d - \Omega$, u continuous across $\partial\Omega$
$\partial u/\partial n$ has a jump at $\partial\Omega$
For μ on $\partial\Omega$, the **double layer potential** is

$$v(x) = \int_{\partial\Omega} \frac{\partial G(x-y)}{\partial n(y)} \mu(y)\, dS(y)$$

$\Delta v = 0$ on $R^3 - \Omega$, jumps at $\partial\Omega$

$$v(x\pm) = \mp\tfrac{1}{2}\mu(y) + \int_{\partial\Omega} \frac{\partial G}{\partial n(y)} \mu(y)\, dS(y)$$

Boundary Value Problems via Integral Equations

For μ on $\partial\Omega$, the **double layer potential** is

$$v(x) = \int_{\partial\Omega} \frac{\partial G(x-y)}{\partial n(y)} \mu(y)\, dS(y)$$

$\Delta v = 0$ on $R^3 - \Omega$, jumps at $\partial\Omega$

$$v(x\pm) = \mp\tfrac{1}{2}\mu(y) + \int_{\partial\Omega} \frac{\partial G}{\partial n(y)} \mu(y)\, dS(y)$$

To solve the Dirichlet problem

$$\Delta v = 0 \text{ in } \Omega,\ v = f \text{ on } \partial\Omega,$$

we solve an equation for μ on $\partial\Omega$,

$$\tfrac{1}{2}\mu(x) + \int_{\partial\Omega} \frac{\partial G(x-y)}{\partial n(y)} \mu(y)\, dS(y) = f(x)$$

a Fredholm integral equation of the second kind

Numerical Integration

Suppose $f : R^d \to R$ smooth and decaying at ∞.
Use regular grid points jh, $j \in Z^d$, $j = (j_1, \ldots, j_d)$,

$$I \;=\; \int_{R^d} f(x)\, dx\,, \quad S \;=\; \sum_{j \in Z^d} f(jh)\, h^d$$

For $\ell \geq d+1$, $\quad |S - I| \;\leq\; C_\ell\, h^\ell \|D^\ell f\|_{L^1}$
This follows from the Poisson Summation Formula:

$$(2\pi)^{-d/2} \sum_{j \in Z^d} f(jh)\, h^d = \sum_{k \in Z^d} \hat{f}(2\pi k/h)$$

where $\hat{f}$ is the Fourier transform

$$\hat{f}(k) = (2\pi)^{-d/2} \int_{R^d} f(x) e^{-ikx}\, dx$$

A single layer potential in $R^3 \;\approx\;$ an integral in R^2 with $1/|x|$
We want to use values only at grid points $x = jh$

A Simple Example

For $f : R^2 \to R$ smooth, decaying at ∞, $j = (j_1, j_2) \in Z^2$

$$\iint_{R^2} \frac{f(x)}{|x|}\, dx = \sum_{j \neq 0} \frac{f(jh)}{|jh|}\, h^2 \;+\; O(h)$$

More precisely,

$$\iint \;=\; \sum + c_0 f(0) h \;+\; O(h^3)$$

where $c_0 \approx 3.900265$, $\quad c_0 \;=\; 4ab/(\sqrt{2} - 1)$,

$$a \;=\; 1 \;-\; 2^{-1/2} \;+\; 3^{-1/2} \;-\; 4^{-1/2} + \ldots$$
$$b \;=\; 1 \;-\; 3^{-1/2} \;+\; 5^{-1/2} \;-\; 7^{-1/2} + \ldots$$

The constant depends on the singularity.

For a surface with local coordinates $\alpha = (\alpha_1, \alpha_2)$,

$1/r = 1/\sqrt{g_{ij}\alpha_i\alpha_j}$, and c_0 depends on g_{ij}.

The constants are difficult to compute.

Quadrature of Singular Integrals

Integrate a homogeneous fcn times a smooth fcn
using regularly space points

General principle: Assume that
K is homogeneous in $x \in R^d$ of degree m,
$K(ax) = a^m K(x)$, $a > 0$, $x \neq 0$
$K(x)$ smooth for $x \neq 0$, $m \geq 1 - d$
$f(x)$ smooth, $f \to 0$ rapidly as $x \to \infty$

$$I = \int_{R^d} K(x) f(x)\, dx, \quad S = \sum_{j \neq 0} K(jh) f(jh)\, h^d$$

where $j \in Z^d$. Then

$$S - I \;=\; h^{d+m}(c_0 f(0) + C_1 h + C_2 h^2 + \dots)$$

(In our example, $m = -1,\ d = 2,\ d + m = 1$.)
Lyness '76; Goodman, Hou & Lowengrub '90
Again, c_0 is difficult to find.

Regularization?

First thing to try:

$$\frac{1}{|x|} \to \frac{1}{\sqrt{|x|^2 + \delta^2}}$$

Notice the regularized form

$$K_\delta(x) = K(x) s(|x|/\delta)\,, \qquad s(\rho) = \sqrt{\frac{\rho^2}{\rho^2 + 1}}$$

The error is $O(\delta)$, but we can make higher order kernels,
impose moment conditions
vortex methods, smooth particle hydrodynamics
We prefer more localized smoothing
Gaussian-based smoothing is much like Ewald summation

Quadrature with Regularization

Replace kernel K (degree m, $-d \le m \le 0$) with
$K_\delta(x) = K(x)s(x/\delta)$ or $K_\delta(x) = \delta^m K_1(x/\delta)$
Assume s is chosen so that
K_δ is smooth; $s \to 1$ at ∞
E.g., $K(x) = 1/|x|$, $K_\delta(x) = \mathrm{erf}(|x|/\delta)/|x|$
Now compare integral with sum:

$$I = \int_{R^d} K_\delta(x) f(x)\, dx, \quad S = \sum_j K_\delta(jh) f(jh)\, h^d$$

Again, if $\rho = \delta/h \ge \rho_0$,

$$S - I \;=\; h^{d+m}(c_0 f(0) + C_1 h + C_2 h^2 + \dots)$$

From the Poisson Summation Formula

$$c_0 = (2\pi)^{d/2} \sum_{n \ne 0} \hat{K}_\rho(2\pi n)$$

If K_ρ is smooth, the terms decrease rapidly. $\int K_\delta f \approx \int K f$?

Simple Example, Regularized Version

Use sum with regularized kernel:

$$\iint_{R^2} \frac{f(x)}{|x|}\, d^2x \;\approx\; \sum_{j\neq 0} \frac{f(jh)}{|jh|}\mathrm{erf}(|jh|/\delta)\, h^2$$

Smoothing error:

$$\iint_{R^2} \frac{f(x)}{|x|}(\mathrm{erf}(r/\delta)-1)\, d^2x \;=\; 2\pi\delta f(0)\int_0^\infty (\mathrm{erf}(\rho)-1)\, d\rho + O(\delta^3)$$

$$\iint_{R^2} \frac{f(x)}{|x|}\, d^2x \;=\; \iint_{R^2} \frac{f(x)}{|x|}\mathrm{erf}(r/\delta)\, d^2x \;+\; 2\sqrt{\pi}\delta f(0) \;+\; O(\delta^3)$$

After this correction, the total error is

smoothing error + discretization error $= O(\delta^3) + O(he^{-c_0\delta^2/h^2})$

E.g., $f(x) = e^{-x^2}$, $\delta = 2h$, error $\approx .3\delta^3 = 2.4h^3$ if h not too small

Discretization error can be corrected to $O(h^2e^{-c_0\delta^2/h^2})$

Single Layer Potential on a Surface

For single layer potential on a surface, y on or near surface,

$$u(y) = \iint_S G(y-x)f(x)\,dS = \iint G(y-x(\alpha))\,f(x(\alpha))\,J(\alpha)\,d^2\alpha$$

with coordinates $\alpha = (\alpha_1, \alpha_2)$, $G(x) = -1/4\pi|x|$
Regularize and discretize: $G_\delta(x) = G(x)\text{erf}(|x|/\delta)$, $\alpha = (j_1 h, j_2 h)$

$$u(y) \approx \sum_{j \in Z^2} G_\delta(y - x(jh))f(x(jh))\,J(jh)\,h^2$$

Error in two parts: $\int - \sum_\delta = (\int - \int_\delta) + (\int_\delta - \sum_\delta)$
Smoothing correction $= (\delta/2)(1 + \delta\eta H)(|\eta|\text{erfc}|\eta| - e^{-\eta^2}/\sqrt{\pi})$
where y is at (normal) distance b from x_0 on the surface;
$\eta = b/\delta$; and $H =$ mean curvature at x_0.
Smoothing error $O(\delta^3)$ after correction.
Discretization error $O(he^{-c_0\delta^2/h^2})$, correctable to $O(h^2 e^{-c_0\delta^2/h^2})$

Smoothing Correction, Nearly Singular Case

$$\text{error} = \iint (G_\delta - G)\,(y - x(\alpha))f(\alpha)\,d^2\alpha$$

For y near Γ, let $y = x(0) + bn(0)$, over $\alpha = 0$

Use special coordinates $\alpha = (\alpha_1, \alpha_2)$ such that for $\alpha = 0$,

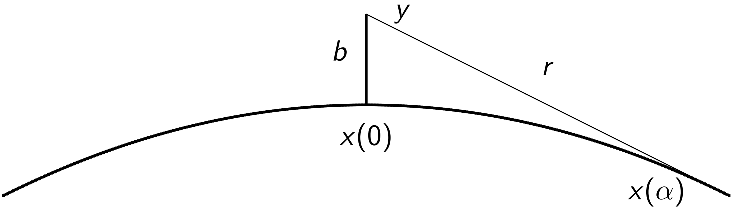
- g_{ij} is identity; Christoffel symbols are zero
- tangent vectors are principal directions of curvature

$(G_\delta - G)$ is a function of r/δ, rapidly varying for small δ

$$r^2 = |x(\alpha) - y|^2 = |\alpha^2| + b^2 + O(|\alpha|^3 + b^3)$$

Change variables, $\alpha \to \xi$, define $\xi = \xi(\alpha, b)$ so $r^2 = \xi^2 + b^2$

Rescale (ξ, b) by δ, expand integrand in δ



The Dirichlet Problem in 3D

Ω a bounded domain, $\mathcal{S}$ the boundary

$$\Delta u = 0 \quad \text{in } \Omega\,, \qquad u = g \quad \text{on } \mathcal{S}$$

For some f on $\mathcal{S}$

$$u(y) = \int_{\mathcal{S}} \frac{\partial}{\partial n(x)} G(x-y) f(x)\, dS(x)$$

$$\frac{\partial}{\partial n(x)} G(x-y) \;=\; \frac{n(x)\cdot(x-y)}{4\pi|x-y|^3}\,.$$

Solve the integral equation for f:

$$\frac{1}{2} f(x) \,+\, \int_{\mathcal{S}} K(x,x') f(x')\, dS(x') \;=\; g(x)\,, \qquad x \in \mathcal{S}$$

Iteration with $0 < \beta < 1$

$$f^{n+1} = (1-\beta) f^n - 2\beta T f^n + 2\beta g$$

Use overlapping coordinate grids, partition of unity

E.g., for sphere, two stereographic projections

Integrals on the Boundary Surface $\mathcal{S}$

Use grids in coordinate patches $X^\sigma : U^\sigma \to \mathcal{S}$, $U^\sigma \subseteq R^2$
partition of unity $\psi^\sigma(x)$, with $\Sigma_\sigma \psi^\sigma(x) \equiv 1$
e.g. $\psi^\sigma = \phi^\sigma / \sum_\tau \phi^\tau$, $\phi^\sigma(X^\sigma(\alpha)) = \exp(-r^2/(r^2 - |\alpha|^2)$, $|\alpha| \leq r$
grid points $x_i^\sigma = X^\sigma(ih)$ in support of ψ^σ

$$\int_{\mathcal{S}} F(x')\, dS(x') = \sum_\sigma \int_{U_\sigma} F(X^\sigma(\alpha))\psi^\sigma(X^\sigma(\alpha))A^\sigma(\alpha)d\alpha$$

Integral equation with subtraction and discrete version:

$$f(x) + \int_{\mathcal{S}} K(x,x')[f(x') - f(x)]\, dS(x') = g$$

$$f_i^\sigma + \sum_{j,\tau} K_{ij}^{\sigma\tau} \psi_j^\tau [f_j^\tau - f_i^\sigma] A_j^\tau\, h^2 + g_i^\sigma$$

with $K_{ij}^{\sigma\tau} = K_\delta(x_i^\sigma, x_j^\tau)$, $K_\delta(x,x') = n(x') \cdot \nabla G_\delta(x' - x)$
$\nabla G_\delta(x' - x) = \nabla G(x' - x) s(|x - x'|/\delta)$,
$s(r) = \operatorname{erf}(r) - (2/\sqrt{\pi})(r - 2r^3/3)e^{-r^2}$, $O(\delta^5)$ smoothing error

The Integral Equation on $\mathcal{S}$

Theorem. For h, δ small, $\delta/h \geq \rho_0$,
the discrete integral eq'n has a unique solution;
the iteration converges to the discrete solution;
and as $h, \delta \to 0$,

$$|f_i^\sigma - f(x_i^\sigma)| \leq C_1\delta^5 + C_2 h^2 e^{-c_0\delta^2/h^2}$$

e.g, if $\delta = ch^q$, $q < 1$, error $= O(h^{5q})$
c_0 depends on coordinate systems
proof uses Hölder norms to maintain
agreement in overlaps

Nearly Singular Integrals on $\mathcal{S}$

For y in Ω, near $\mathcal{S}$,

$$u(y) \,=\, \int_{\mathcal{S}} \frac{\partial}{\partial n(x)} G(x-y)[f(x)-f(x_0)]\, dS(x) \,+\, f(x_0)$$

Start with the sum

$$S \,=\, \sum_{\sigma,j} n(x_j^\sigma)\cdot\nabla G_\delta(x_j^\sigma - y)[f(x_j^\sigma)-f(x_0)]\psi_j^\sigma A_j^\sigma h^2$$

with errors $O(\delta^2)$ and $O(he^{-c_0\delta^2/h^2})$. Corrected sum is

$$\tilde{u}(y) \,=\, S \,+\, f(x_0) \,+\, T_1 \,+\, \Sigma_\sigma T_2^\sigma\,,$$

$$|\tilde{u}(y)-u(y)| \le C_1\delta^3 + C_2 h^2 e^{-c_0\delta^2/h^2}$$

Error is almost $O(h^3)$

Corrections for Nearly Singular Integrals

Suppose $y = x_0 + bn_0$, x_0 on $\mathcal{S}$. Smoothing correction:

$$T_1 \ = \ \delta^2(\Delta_{\mathcal{S}} f(x_0))(\eta/4)(|\eta|\mathrm{erfc}|\eta| - e^{-\eta^2}/\sqrt{\pi})$$

where $\Delta_{\mathcal{S}}$ = surface Laplacian, $\eta = b/\delta$, $\rho = \delta/h$
Discretization correction:

$$T_2^\sigma = -h \sum_{r=1}^{2} c_r \psi^\sigma(\alpha_0) \frac{\partial(f \circ X^\sigma)}{\partial \alpha_r}(\alpha_0)$$

$$c_r = \frac{\rho\eta}{2} \sum_{s=1}^{2} \sum_{n \in Q} a(n,s) \sin\left(2\pi n \cdot \nu\right) \frac{g^{rs} n_s}{\|n\|} E(\eta, \pi\rho\|n\|)$$

$$E(p,q) = e^{2pq}\mathrm{erfc}(p+q) + e^{-2pq}\mathrm{erfc}(-p+q)$$

$$Q = \{n = (n_1, n_2) \in Z^2 : n_2 \geq 0, n \neq 0\}$$

$\|n\| = \sqrt{g^{ij} n_i n_j}$; $a = 1$ mostly; $|n\text{th term}| \ \leq \ C\rho\exp(-c_0\rho n^2)$, indep't of y

The Dirichlet Problem on the Sphere

$$(1/2)f + Kf = g$$

$$f(x) = 1.75((Mx)_1 - 2(Mx)_2)(7.5(Mx)_3^2 - 1.5)$$

$$g(x) = (4/7)f(x)\,, \qquad u(x) = g(x/|x|)|x|^3$$

$$M = \begin{pmatrix} 1/\sqrt{3} & 0 & -2/\sqrt{6} \\ 1/\sqrt{3} & 1/\sqrt{2} & 1/\sqrt{6} \\ 1/\sqrt{3} & -1/\sqrt{2} & 1/\sqrt{6} \end{pmatrix}$$

Errors in the Integral Equation on the Sphere

		$\delta = .5h^{2/3}$			$\delta = .75h^{2/3}$		
$1/h$	Grid Points	δ/h	Rel Err	Order	δ/h	Rel Err	Order
8	610	1.00	5.1E-4		1.50	3.6E-4	
16	2490	1.26	6.1E-5	3.1	1.89	1.4E-5	4.7
32	10026	1.59	4.0E-6	3.9	2.38	1.7E-6	3.1
64	40138	2.00	6.3E-8	6.0	3.00	1.7E-7	3.3

The Dirichlet Problem on the Sphere, (cont'd)

$$(1/2)f + Kf = g$$

$$f(x) = 1.75((Mx)_1 - 2(Mx)_2)(7.5(Mx)_3^2 - 1.5)$$

$$g(x) = (4/7)f(x)\,, \qquad u(x) = g(x/|x|)|x|^3$$

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Errors at Nearby Points

	Irreg	$\delta = .5h^{2/3}$		$\delta = .75h^{2/3}$		$\delta = 2h$	
$1/h$	Points	Rel Err	Order	Rel Err	Order	Rel Err	Order
8	606	3.1E-3		6.9E-3		1.5E-2	
16	2546	5.3E-4	2.6	1.7E-3	2.0	2.0E-3	2.9
32	10470	1.3E-4	2.0	4.3E-4	2.0	2.6E-4	3.0
64	42282	3.2E-5	2.0	1.1E-4	2.0	3.2E-5	3.0

The Dirichlet Problem on an Ellipsoid

$$\mathcal{S} : x_1^2 + x_2^2 + x_3^2/2 = 1$$

$$u(x) = \exp\left((Mx)_1 + 2(Mx)_2\right) \cos \sqrt{5}(Mx)_3)$$

$$(1/2)f + Kf = g$$

Set $g = u$ on $\mathcal{S}$; f is unknown.
Solve integral equation for f, compute $u(y)$ near $\mathcal{S}$

Errors at Nearby Points

	Irreg	$\delta = .5h^{2/3}$		$\delta = .75h^{2/3}$		$\delta = 2h$	
$1/h$	Points	Rel Err	Order	Rel Err	Order	Rel Err	Order
8	798	4.1E-3		7.8E-3		1.3E-2	
16	3330	3.1E-4	3.8	1.0E-3	3.0	1.2E-3	3.4
32	13614	7.6E-5	2.0	2.5E-4	2.0	1.5E-4	3.0
64	54914	1.9E-5	2.0	6.2E-5	2.0	1.9E-5	3.0

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Math. Comp. 70 (2001), 977-1029.

Incompressible Fluid Flow

Euler equations, no viscosity, density $= 1$:

$$v_t + (v \cdot \nabla)v + \nabla p = 0\,, \quad \nabla \cdot v = 0$$

Navier-Stokes equations, viscous fluid, density $= 1$:

$$v_t + (v \cdot \nabla)v + \nabla p = \nu \Delta v\,, \quad \nabla \cdot v = 0$$

Reynolds number $Re = \frac{LU}{\nu}$, $L =$ length scale, $U =$ velocity scale
integrals are useful in the two extremes!
low viscosity, high Re: Euler (no viscosity) in interior,
viscosity still important at boundary layers
high viscosity, low Re: drops of viscous fluids; small scales; biology

Inviscid Flow, Vorticity

$\omega = \nabla \times v$, the vorticity
For Euler flow (no viscosity)

$$\omega_t + (v \cdot \nabla)\omega = (\omega \cdot \nabla v)$$

stretching; right side = 0 in 2D; integral form due to Cauchy

$$v(x,t) = \int K(x-x')\omega(x',t)\, d^3x' , \quad K(x) = -\frac{1}{4\pi}\frac{x}{|x|^3}\times$$

"vortex method": $dx_j/dt = v(x_j,t)$,

$$\omega \approx \sum \omega_j(t)\delta_j(x - x_j(t)) , \quad v \approx \sum K_\delta(x - x_j(t))\omega_j(t)\, h^3$$

plus some means of stretching $\omega_j(t)$ in 3D
A. Leonard; A. Chorin; smooth particle hydrodynamics
convergence theory O. Hald, Beale & A. Majda, many more
G.-H. Cottet & P. D. Koumoutsakos, Vortex Methods

Vortex Sheets

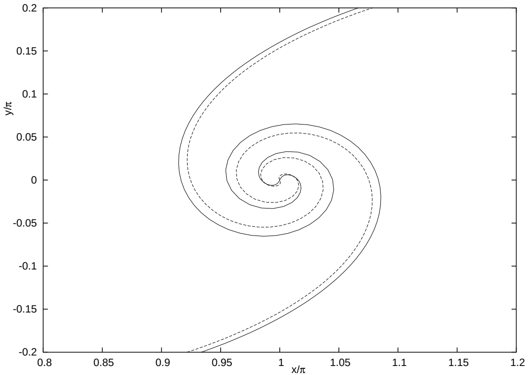
a sheet of vorticity behind an airplane wing rolls up
2D model, inviscid, potential flow above and below, $v = \nabla\phi$
evolution for interface alone, Kelvin-Helmholtz instability
regularized calculations by R. Krasny (1986)

$$\frac{\partial \overline{z}}{\partial t}(\xi, t) \;=\; \int K(\xi, \xi')\gamma(\xi', t)\, d\xi' \,,$$

$$K(\xi, \xi') = \frac{1}{2\pi i}\,\frac{1}{z(\xi, t) - z(\xi', t)}$$

or periodic version with $1/z \to \frac{1}{2}\cot\,(z/2)$
G. Baker and Beale ('04), more general
different densities above & below, choice of reg'z'n

Roll-Up of a Vortex Sheet (Krasny)



Gaussian (solid); Krasny (dashed)

Water Waves

usual model: inviscid, potential flow, vacuum above

$\Delta\phi = 0$ below surface, ϕ determined by value on surface

surface moves with fluid velocity

$$\phi_t + \frac{1}{2}|\nabla\phi|^2 + gy = 0$$

Surface $X = X(\alpha_1, \alpha_2, t)$, two evolution eq'ns on surface

$$X_t = \dots, \quad \phi_t = \dots$$

From ϕ on surface we have $\nabla_S\phi$. We need $\partial\phi/\partial n$.

$\phi \mapsto \partial\phi/\partial n$ with $\Delta\phi = 0$ below

This is the Dirichlet-to-Neumann map!

  Fredholm equation of second kind; cf. Colton & Kress

  uses normal derivative of a double layer potential

boundary integral methods have been used in 2D since 1970's

  why would people in England, Norway, Netherlands care?

several groups have 3D codes

Stokes Flow or Creeping Flow

large viscosity, slow flow, quasi-steady
neglect $v_t + (v \cdot \nabla)v$ in Navier-Stokes equations

$$-\nu \Delta v + \nabla p = F \,, \quad \nabla \cdot v = 0$$

interfacial conditions lead to layer potential representations
fluid moves, velocity needed only on interface
boundary integrals have long been used; Acrivos, Pozrikidis
drop of one fluid in another

Heat potentials: L. Greengard & J. Strain, others
Biros, L. Ying, & Zorin