Immersed Interface Method

Anita Layton
Department of Mathematics, Duke University

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Numerical Challenges

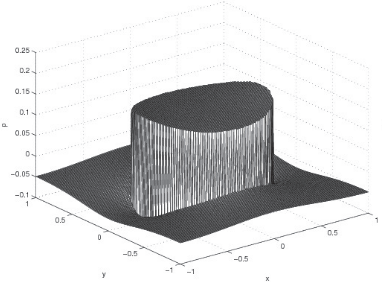
Singular boundary force introduces discontinuities in fluid solution.

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \mu \nabla^2 \mathbf{u} + \mathbf{F},$$

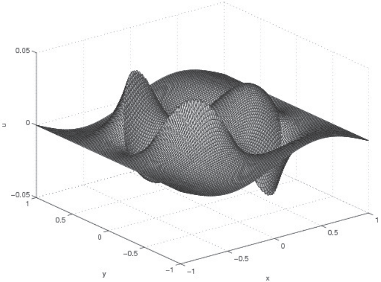
$$\nabla \cdot \mathbf{u} = 0$$

$$\mathbf{F}(\mathbf{x}, t) = \int_\Gamma \mathbf{f}(s, t)\delta(\mathbf{x} - \mathbf{X}(s, t))ds$$

Pressure

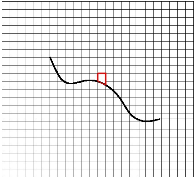


Velocity

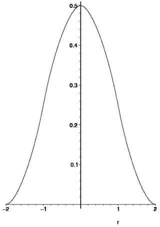


Solution Approaches

- Unstructured grid: requires mesh regeneration every time-step.



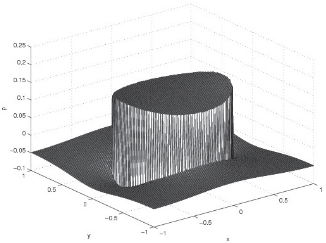
- Immersed bounadry method (Peskin, *Acta Numerica*, 2002): replaces singular δ by a smoother discrete δ_h.



- Immersed interface method (Li and Lai, *JCP*, 2001)

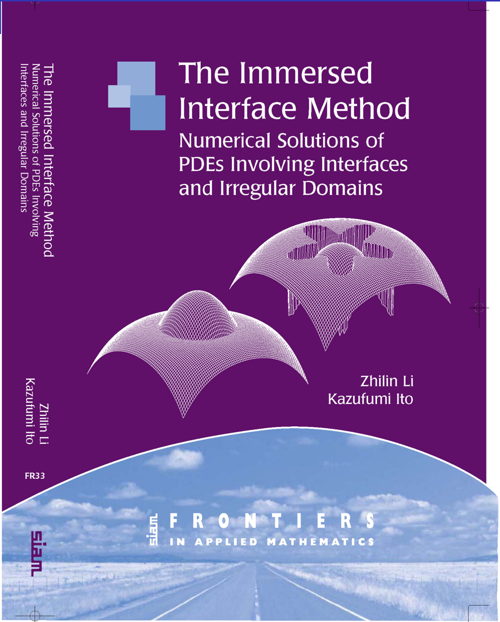
Features of Immersed Interface method

- Preserves sharp jumps in solutions and derivatives.



- Computes $\mathcal{O}(h^2)$ accurate solutions.
- Can be applied to problems other than immersed boundary problems.

Credits...


The Immersed Interface Method
Numerical Solutions of PDEs Involving Interfaces and Irregular Domains
Zhilin Li
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Zhilin Li
Kazufumi Ito
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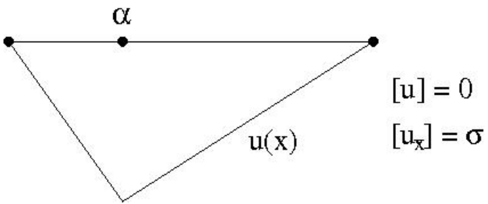
Example 1: Singular Sources

Delta function singularity

- Elastic material with two ends fixed and a point source
- Solution is continuous, but the derivatives are not!
- Standard numerical methods may have big errors.



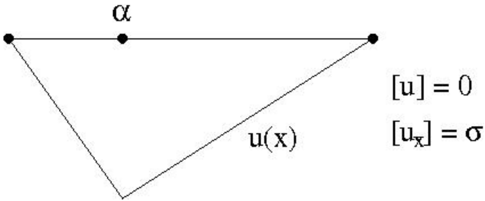
Example 1: Singular Sources

The equation

$$u''(x) = \sigma\delta(x-\alpha), \quad 0 < x < 1$$
$$u(0) = 0, \quad u(1) = 0$$

Equivalent problem

$$u'' = 0, \quad x \in (0,\alpha) \cup (\alpha, 1)$$
$$[u] = 0, \quad [u'] = \sigma$$



Example 2: Discontinuous Coefficients

Heat propagation through heterogeneous materials

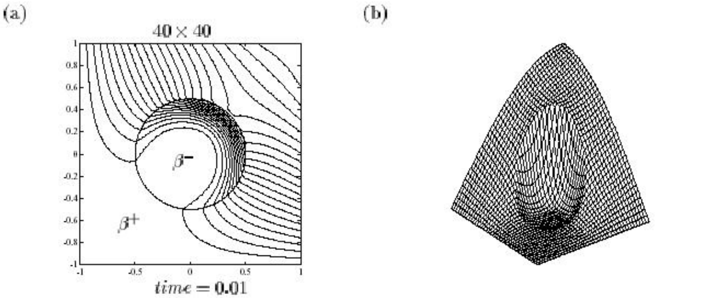


Figure 1.1: Heat propagation in different materials. (a) Contour plot of the temperature. (b) Mesh plot of the solution.

Example 2: Discontinuous Coefficients

Model equation, IC, and BC:

$$u_t = \nabla \cdot (\beta \nabla u), (x, y) \in [-1, 1] \times [-1, 1]$$

$$\beta = \begin{cases} 1, & x^2 + y^2 \leq \frac{1}{4} \\ 100, & \text{otherwise} \end{cases}$$

$$u(x, y, 0) = 0$$

$$u(-1, y, t) = u(x, -1, t) = 0$$

$$u(x, 1, t) = \sin((x + 1)\pi/4)$$

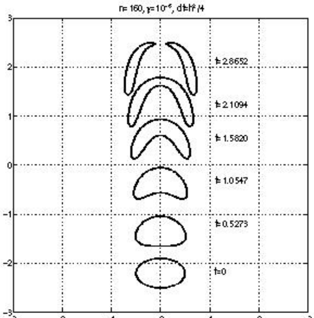
$$u(1, y, t) = \sin((y + 1)\pi/4)$$

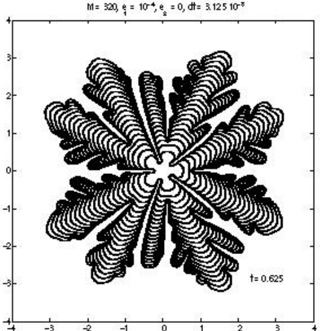
Other Examples

- 2D singular sources

$$-\nabla \cdot (\beta \nabla u) = f(x) + \int_{\Gamma} \nu(s)\delta(x - X(s))ds$$

- Multi-phase / singular sources
- Moving interface / free boundary
- Irregular domains



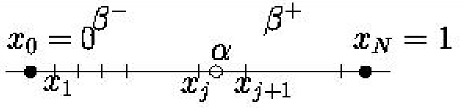


An 1D Example

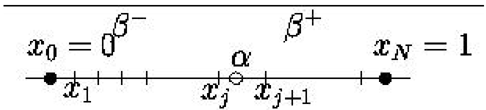
$$(\beta u')' = f(x) + \sigma\delta(x-\alpha)$$
$$u(0) = u_a, \quad u(1) = u_b$$

Equivalent problem:

$$(\beta u')' = f(x), \quad x \in (0,\alpha) \cup (\alpha,1)$$
$$u(\alpha^+) = u(\alpha^-), \quad \beta^+ u'(\alpha^+) = \beta^- u'(\alpha^-) + \sigma$$
$$u(0) = u_a, \quad u(1) = u_b$$



Finite-Difference Discretization



- Approximate solution at grid points $x_i = ih$, $i = 0, \ldots, N$.
- Regular grid points: standard centered difference scheme

$$\frac{\beta_{i-1}U_{i-1} - 2\beta_i U_i + \beta_{i+1}U_{i+1}}{h^2} = f(x_i)$$

  Local trunction error $\mathcal{O}(h^2)$ if u'''' exists.
- Irregular grid points, x_j and x_{j+1}, what to do?

FD Scheme at Irregular Gridpoints

- Un-determined coefficient method

$$\gamma_{j-1} U_{j-1} + \gamma_j U_j + \gamma_{j+1} U_{j+1} = f_j + C_j$$

- Determine coefficients and correction term

$$\gamma_{j-1}, \gamma_j, \gamma_{j+1}, C_j$$

- Make use of interface relations

$$u^+ = u^-, \quad u_x^+ = \frac{\beta^-}{\beta^+} u_x^- + \frac{\sigma}{\beta^+}, \quad u_{xx}^+ = \frac{\beta^-}{\beta^+} u_{xx}^-$$

FD Scheme at Irregular Gridpoints

Use un-determined coefficient method to minimize *local trunction error* at α (the solution is *piecewise smooth*):

$$T_j = \gamma_{j-1} u(x_{j-1}) + \gamma_j u(x_j) + \gamma_{j+1} u(x_{j+1}) - f_j - C_j$$

$$u(x_{j-1}) = u^- + u_x^-(x_{j-1} - \alpha) + \frac{(x_{j-1} - \alpha)}{2} u_{xx}^- + \mathcal{O}(h^3)$$

$$u(x_j) = u^- + u_x^-(x_j - \alpha) + \frac{(x_j - \alpha)}{2} u_{xx}^- + \mathcal{O}(h^3)$$

$$u(x_{j+1}) = u^+ + u_x^+(x_{j+1} - \alpha) + \frac{(x_{j+1} - \alpha)}{2} u_{xx}^+ + \mathcal{O}(h^3)$$

$$= u^- + \left(\frac{\beta^-}{\beta^+} u_x^- + \frac{\sigma}{\beta^+} \right)(x_{j+1} - \alpha) + \frac{\beta^-}{\beta^+} \frac{(x_{j+1} - \alpha)^2}{2} u_{xx}^- +$$

FD Scheme at Irregular Gridpoints

$$T_j = \gamma_{j-1} u(x_{j-1}) + \gamma_j u(x_j) + \gamma_{j+1} u(x_{j+1}) - f_j - C_j$$

Apply Taylor expansion, interface relations, un-determined coefficient method

$$\begin{aligned}
\Rightarrow T_j = {} & u^-(\gamma_{j-1} + \gamma_j + \gamma_{j+1}) \\
& + u_x^- \left(\gamma_{j-1}(x_{j-1} - \alpha) + \gamma_j (x_j - \alpha) + \gamma_{j+1} \frac{\beta^-}{\beta^+}(x_{j+1} - \alpha) \right) \\
& + u_{xx}^- \left(\gamma_{j-1} \frac{(x_{j-1} - \alpha)^2}{2} + \gamma_j \frac{(x_j - \alpha)^2}{2} \right. \\
& \qquad \left. + \gamma_{j+1} \frac{\beta^-}{\beta^+} \frac{(x_{j+1} - \alpha)^2}{2} \right) \\
& + \gamma_{j+1} \frac{\beta^-}{\beta^+} \sigma (x_{j+1} - \alpha) - f_j - C_j
\end{aligned}$$

Coefficients and Correction

The linear system for the coefficients

$$u^-(\gamma_{j-1} + \gamma_j + \gamma_{j+1}) = 0$$

$$\gamma_{j-1}(x_{j-1} - \alpha) + \gamma_j(x_j - \alpha) + \gamma_{j+1}\frac{\beta^-}{\beta^+}(x_{j+1} - \alpha) = 0$$

$$\gamma_{j-1}\frac{(x_{j-1} - \alpha)^2}{2} + \gamma_j\frac{(x_j - \alpha)^2}{2} + \gamma_{j+1}\frac{\beta^-}{\beta^+}\frac{(x_{j+1} - \alpha)^2}{2} = \beta^-$$

The correction term

$$C_j = \sigma\gamma_{j+1}\frac{\beta^-}{\beta^+}(x_{j+1} - \alpha)$$

Key Steps of IIM

1. Un-determined coefficient method at grid points near/on the interface

$$\gamma_{j-1} U_{j-1} + \gamma_j U_j + \gamma_{j+1} U_{j+1} = f_j + C_j$$

2. Expand $u(x_i + jh)$ at $u(\alpha)$ on the interface from each side.
3. Use jump conditions to express the quantities of one side in terms of the other
4. Choose coefficients and correction term to minimize local trunction errors.

Numerical Results

Example

$$(\beta u')' = \delta(x - \alpha)$$
$$u(0) = 0, \quad u(1) = 0$$

with $\beta^- = 1$, $\beta^+ = 100$, and $\alpha = 1/3$.

The exact solution is

$$u(x) = \begin{cases} Bx(1-\alpha), & 0 \le x \le \alpha \\ B\alpha(1-x), & \alpha < x \le 1 \end{cases}$$

where $B = -1/(\beta^+\alpha + \beta^-(1-\alpha))$.

Numerical Results

Compare accuracy of

1. IIM
2. Smoothing + discrete delta:
   Smooth $\beta(x)$ using

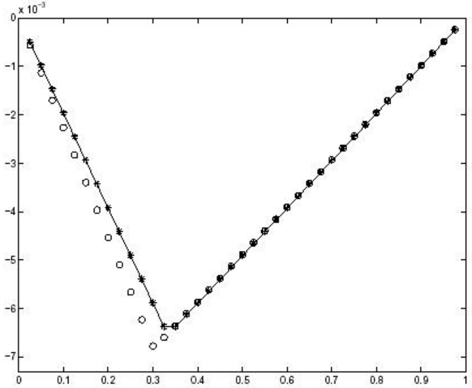
$$\beta_\epsilon(x) = \beta^- + (\beta^+(x) - \beta^-(x))H_\epsilon(x-\alpha)$$

$$H_\epsilon(x) = \begin{cases} 0, & x < -\epsilon \\ \frac{1}{2}\left(1 + \frac{x}{\epsilon} + \frac{1}{\pi}\sin\frac{\pi x}{\epsilon}\right), & |x| \leq \epsilon \\ 1, & x > \epsilon \end{cases}$$

   Use discrete cosine delta function

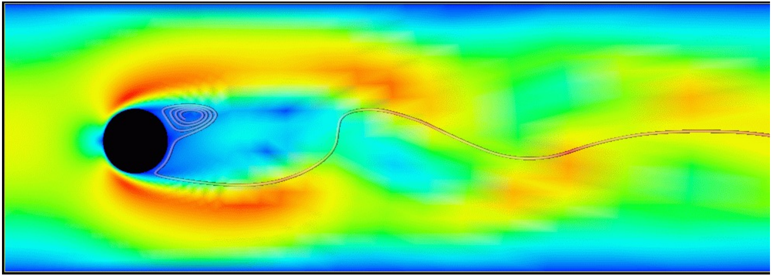
$$\delta_\epsilon(x) = \begin{cases} \frac{1}{4\epsilon}\left(1 + \cos\frac{\pi x}{2\epsilon}\right), & |x| < 2\epsilon \\ 0, & |x| \geq 2\epsilon \end{cases}$$

Results and Comparison



Solid line: exact solution
* IIM; ∘ smoothing + discrete delta ($\epsilon = 2h$).
$h = 1/40$.

IIM for Immersed Boundary Problems



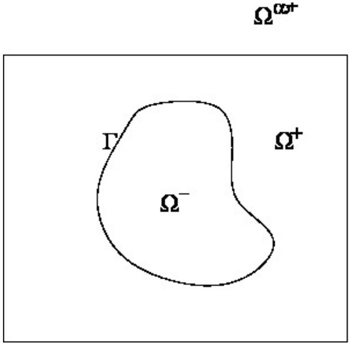
IIM for Stokes Equations

Stokes problem with a singular source on a closed curve Γ

$$\nabla p = \mu \Delta u + F$$

$$\nabla \cdot u = 0$$

$$F = \int_\Gamma f(s)\delta(x - X(s))\; ds$$



Jump Conditions

Anita Layton
Department of Mathematics, Duke University

(LeVeque and Li, *SINUM*, 1994)
Assume no-slip along the immersed boundary,

$$\frac{\partial}{\partial t} X(s,t) = u\left(X(s,t)\right)$$

Balancing forces in the normal and tangential directions, we can express the jump conditions in terms of the boundary forces ($\hat{f}_1 = \mathbf{f} \cdot \mathbf{n}, \hat{f}_2 = \mathbf{f} \cdot \tau$):

$$[p] = \hat{f}_1, \quad [p_n] = \frac{\partial}{\partial \tau} \hat{f}_2,$$
$$[u] = [v] = 0, \quad [\mu u_n] = \hat{f}_2 \sin\theta, \quad [\mu v_n] = \hat{f}_2 \cos\theta$$

Solving the Stokes Equations Using IIM

1. Given boundary configuration $\Gamma(t_n)$, compute boundary force $\mathbf{f}$.
2. With $\mathbf{f}$, compute jump conditions.
3. Solve three Poisson problems:

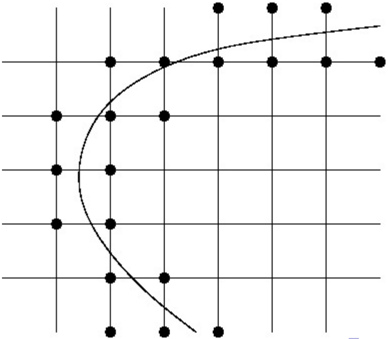
$$\Delta p = \nabla \cdot F, \quad \Delta u = \frac{1}{\mu} p_x, \quad \Delta v = \frac{1}{\mu} p_y$$

Solving the Stokes Equations using IIM

For pressure

$$\frac{1}{h^2}\left(P_{i+1,j} + P_{i-1,j} - 4P_{i,j} + P_{i,j+1} + P_{i,j-1}\right) = C_{i,j}$$

At regular grid points $C_{i,j} = 0$, at irregular grid points, $C_{i,j}$ is determined using the un-determined coefficient method as before.



Solving the Stokes Equations using IIM

For velocity

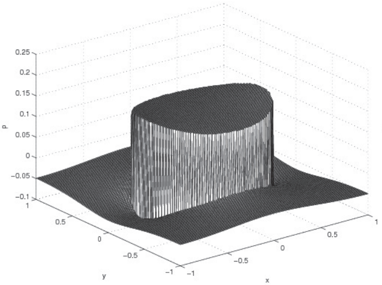
$$\frac{1}{h^2}\left(U_{i+1,j} + U_{i-1,j} - 4U_{i,j} + U_{i,j+1} + U_{i,j-1}\right) = \frac{1}{\mu}(P_x)_{i,j} + \hat{C}_{i,j}$$

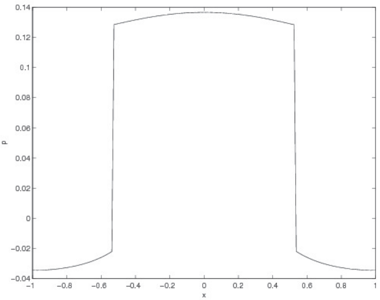
Update Γ:

$$X^{n+1} = X^n + \Delta t U(X^n)$$

Stokes Example

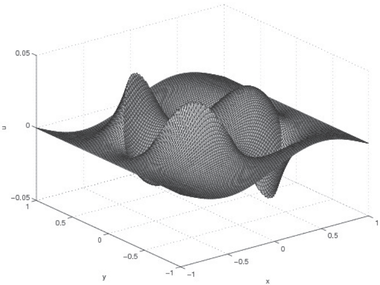
Pressure:

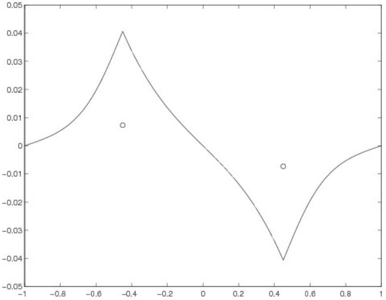




Stokes Example

Velocity (u):





Alternative: Boundary Integral Solution

Stokes solutions are given by the boundary integrals

$$p(\mathbf{x}) = \int_\Gamma \nabla G(\mathbf{x}-\mathbf{y})\mathbf{f}(\mathbf{y})ds(\mathbf{y})$$

$$\mathbf{u}(\mathbf{x}) = \int_\Gamma V(\mathbf{x}-\mathbf{y})\mathbf{f}(\mathbf{y})ds(\mathbf{y}).$$

∇G and V are determined by the spatial dimensions and boundary conditions. For 2D free space,

$$\nabla G(\mathbf{x}) = \frac{\mathbf{x}}{2\pi|\mathbf{x}|^2}$$

$$V(\mathbf{x}) = \frac{1}{4\pi}\begin{bmatrix} -\log|\mathbf{x}| + \frac{x_1^2}{|\mathbf{x}|^2} & \frac{x_1x_2}{|\mathbf{x}|^2} \\ \frac{x_1x_2}{|\mathbf{x}|^2} & -\log|\mathbf{x}| + \frac{x_2^2}{|\mathbf{x}|^2} \end{bmatrix}$$

Two Problems with Integral Solutions

Using boundary integrals eliminate the need for corrections, but...

- Accuracy. The kernels V and ∇G are singular!

$$\nabla G(\mathbf{x}) = \frac{\mathbf{x}}{2\pi|\mathbf{x}|^2}, \quad V(\mathbf{x}) = \frac{1}{4\pi}\begin{bmatrix} -\log|\mathbf{x}| + \frac{x_1^2}{|\mathbf{x}|^2} & \frac{x_1 x_2}{|\mathbf{x}|^2} \\ \frac{x_1 x_2}{|\mathbf{x}|^2} & -\log|\mathbf{x}| + \frac{x_2^2}{|\mathbf{x}|^2} \end{bmatrix}$$

  Near the immersed interface, nearly singular integrals give rise to large quadrature errors.

- Efficiency. Using boundary integrals to compute solution values at N^2 grid-points takes $\mathcal{O}(N^3)$ time.

Accuracy: Modified Stokeslets

Replace point source by a "blob" (Cortez, *SISC*, 2001)

$$\phi_\epsilon(r) = \frac{3\epsilon^3}{2\pi(r^2+\epsilon^2)^{5/2}}$$

Then the Green's function of $\Delta G = \delta$ becomes regularized:

$$G(r) = \frac{1}{2\pi}\log(r) \Rightarrow G_\epsilon(r) = \frac{1}{2\pi}\left(\log(\sqrt{r^2+\epsilon^2}+\epsilon) - \frac{\epsilon}{\sqrt{r^2+\epsilon^2}}\right)$$

where $r = |\mathbf{x}|$. Stokes solutions are given by the boundary integrals, e.g.,

$$p(\mathbf{x}) = \int_\Gamma \nabla G_\epsilon(\mathbf{x}-\mathbf{y})\mathbf{f}(\mathbf{y})ds(\mathbf{y})$$

Accuracy: Modified Stokeslets

But Stokes solutions computed using the regularized Green's function are smooth near the boundary, i.e., the jump discontinuities in p and in the derivatives of $\mathbf{u}$ are not preserved.

This leads to $\mathcal{O}(h)$ errors in $\mathbf{u}$ and $\mathcal{O}(1)$ errors in p.

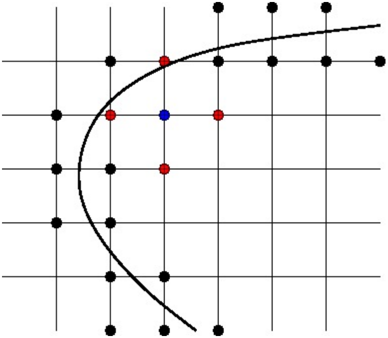
To achieve better accuracy, corrections can be added:

$$p(\mathbf{x}) = \sum_k \nabla G_\epsilon(\mathbf{x} - \mathbf{s}_k) f(\mathbf{s}_k) \Delta s + T_1(\mathbf{x}) + T_2(\mathbf{x}) + \mathcal{O}(\Delta s^2 + \epsilon^2)$$

where T_1 and T_2 correct for the quadrature and regularization errors (Beale and Lai, *SINUM*, 2001).

Efficiency: Hybrid Approach

- Combine boundary integrals with mesh-based solver.
- Compute integral solutions only near boundary (cost: $\mathcal{O}(N^2)$), enough values to form discrete five-point Laplacian at irregular grid points.



Hybrid Approach

Solve three Poisson problems:

$$\Delta_h p = \begin{cases} \frac{p_{i+1,j}+p_{i,j+1}-4p_{i,j}+p_{i-1,j}+p_{i,j-1}}{h^2}, & \text{irreg points} \\ 0, & \text{reg points} \end{cases}$$

p values in RHS Laplacian computed using modified Stokeslets.

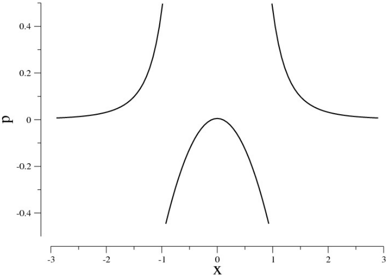
$$\Delta_h u = \begin{cases} \frac{\mathbf{u}_{i+1,j}+\mathbf{u}_{i,j+1}-4\mathbf{u}_{i,j}+\mathbf{u}_{i-1,j}+\mathbf{u}_{i,j-1}}{h^2}, & \text{irreg points} \\ \nabla p, & \text{reg points} \end{cases}$$

$\mathbf{u}$ values in RHS Laplacian computed using modified Stokeslets.
∇p computed using finite difference.

- Solve Poisson problems using FFT, $\mathcal{O}(N^2 \log N)$.

Resolving Boundary Layers

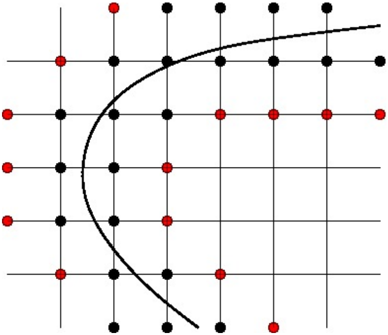
- Stiff boundary forces may generate a steep gradient in the solutions near the boundary.
- Even though the solutions are "smooth" away from the boundary, finite-difference approximation of the Laplacian may have large discretization errors.
- Remedy: Expanding the "band" where we use boundary integrals to compute the discrete Laplacian.



Resolving Boundary Layers

$$\Delta_h p = \begin{cases} \frac{p_{i+1,j}+p_{i,j+1}-4p_{i,j}+p_{i-1,j}+p_{i,j-1}}{h^2}, & \text{inside band} \\ 0, & \text{outside band} \end{cases}$$

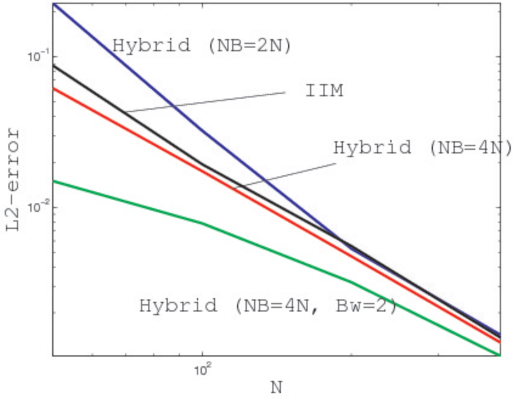
$$\Delta_h u = \begin{cases} \frac{\mathbf{u}_{i+1,j}+\mathbf{u}_{i,j+1}-4\mathbf{u}_{i,j}+\mathbf{u}_{i-1,j}+\mathbf{u}_{i,j-1}}{h^2}, & \text{inside band} \\ \nabla p, & \text{outside band} \end{cases}$$



Stokes Example

Interface is a unit circle.

$$\mathbf{f}(\theta) = 14\sin(7\theta)\mathbf{x}(\theta), \quad p(r,\theta) = \begin{cases} r^{-7}\sin(7\theta), & r \geq 1 \\ -r^{7}\sin(7\theta), & r < 1 \end{cases}$$



Immersed Boundary Problem with NS Flows

(Li and Lai, *JCP*, 2001)

Navier-Stokes Equations with Singular sources

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \mu \nabla^2 \mathbf{u} + \mathbf{F},$$

$$\nabla \cdot \mathbf{u} = 0$$

$$\mathbf{u}|_{\partial\Omega} = \mathbf{u}_b$$

$$\mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0$$

$$\mathbf{F}(\mathbf{x}, t) = \int_\Gamma \mathbf{f}(s, t)\delta(\mathbf{x} - \mathbf{X}(s, t))ds$$

IIM for Navier-Stokes

IIM from t_n to t_{n+1} can be written as

$$\frac{\mathbf{u}^* - \mathbf{u}^n}{\Delta t} + (\mathbf{u} \cdot \nabla_h \mathbf{u})^{n+\frac{1}{2}} = -\nabla_n p^{n-\frac{1}{2}} + \frac{\mu}{2}\left(\nabla_h^2 \mathbf{u}^* + \nabla_h^2 \mathbf{u}^n\right) + \mathbf{C}_1^n,$$

where

$$(\mathbf{u} \cdot \nabla_h \mathbf{u})^{n+\frac{1}{2}} = \frac{2}{3}(\mathbf{u} \cdot \nabla_h \mathbf{u})^n - \frac{1}{3}(\mathbf{u} \cdot \nabla_h \mathbf{u})^{n-1} + \mathbf{C}_2^n$$

The projection step is as follows

$$\nabla_h \phi^{n+1} = \frac{\nabla_h \cdot \mathbf{u}^*}{\Delta t} + \mathbf{C}_3^n$$

$$\frac{\partial \phi^{n+1}}{\partial \mathbf{n}} = 0$$

$$\mathbf{u}^{n+1} = \mathbf{u}^* - \Delta t \nabla_h \phi^{n+1} + \mathbf{C}_4^n$$

$$\nabla_h p^{n+\frac{1}{2}} = \nabla_h p^{n-\frac{1}{2}} + \nabla_h \phi^{n+1} + \mathbf{C}_5^n$$

Determining the Correction Terms

Let $u(x)$ be a piecewise twice differentiable function. Assume that $u(x)$ and its derivatives have jumps $[u]$, $[u_x]$, and $[u_{xx}]$ at $x^* = x + \alpha h$, then

$$\frac{u(x+h) - u(x-h)}{2h} = \begin{cases} u'(x) + \frac{C(x,\alpha)}{2h} + \mathcal{O}(h^2), & 0 \leq \alpha \leq 1 \\ u'(x) - \frac{C(x,\alpha)}{2h} + \mathcal{O}(h^2), & -1 \leq \alpha < 0 \end{cases}$$

$$\frac{u(x+h) - 2u(x) + u(x-h)}{h^2} = u''(x) + \frac{C(x,\alpha)}{h^2} + \mathcal{O}(h)$$

where

$$C(x,\alpha) = [u] + [u_x](1 - |\alpha|)h + [u_{xx}]\frac{(1 - |\alpha|)^2 h^2}{2}$$

Determining the Correction Terms for $\mathbf{C}_1^n$

1. From $(\mathbf{u} \cdot \nabla_h \mathbf{u})^n$

$$-\frac{3}{4h}\left([u_x^n](x_{i+1}-x^*)+[u_{xx}^n]\frac{(x_{i+1}-x^*)^2}{2}\right)u^n(x^*,y_j)$$

2. From $(\mathbf{u} \cdot \nabla_h \mathbf{u})^{n-1}$

$$\frac{1}{4h}\left([u_x^n](x_{i+1}-x^*)+[u_{xx}^n]\frac{(x_{i+1}-x^*)^2}{2}\right)u^n(x^*,y_j)$$

3. From $\nabla_h p^{n-\frac{1}{2}}$

$$-\frac{1}{2h}\left([p^{n-\frac{1}{2}}]+[p_x^{n-\frac{1}{2}}](x_{i+1}-x^*)\right)$$

4. From $\mu\Delta_h(u^n/2)$

$$-\frac{\mu}{2h^2}\left([u_x^n](x_{i+1}-x^*)+[u_{xx}^n]\frac{(x_{i+1}-x^*)^2}{2}\right)$$

The Velocity Decomposition Approach

(Beale and Layton, *JCP* 2009)

$$\mathbf{u} = \mathbf{u}_s + \mathbf{u}_r$$

The Stokes solution satisfies

$$\nabla p_s = \mu \nabla^2 \mathbf{u}_s + \mathbf{f}, \quad \nabla \cdot \mathbf{u}_s = 0$$

Substituting into the Navier-Stokes equations:

$$\begin{aligned} \frac{\partial(\mathbf{u}_s + \mathbf{u}_r)}{\partial t} + \mathbf{u} \cdot \nabla (\mathbf{u}_s + \mathbf{u}_r) &= -\nabla(p_s + p_r) \\ &+ \mu \nabla^2 (\mathbf{u}_s + \mathbf{u}_r) + \mathbf{f}, \\ \Rightarrow \frac{\partial \mathbf{u}_r}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u}_r &= -\nabla p_r + \mu \nabla^2 \mathbf{u}_r + \mathbf{f_b}, \\ \nabla \cdot \mathbf{u}_r &= 0, \\ \mathbf{f}_b &= -\frac{\partial \mathbf{u}_s}{\partial t} - \mathbf{u} \cdot \nabla \mathbf{u}_s \end{aligned}$$

Summary

Some recent applications of the IIM:

- Free boundary problem with moving contact lines;
- Immersed interface finite element methods;
- Navier-Stokes equations in irregular domains;
- Surfactant-laden drop-drop interactions;
- Stokes equations with discontinuous viscosity;
- Navier-Stokes equations with discontinuous viscosity;
- Tracking interface using the level-set method;
- Higher than second-order accuracy;
- More: today's talks!