Introduction to the Immersed Boundary/Interface Method: I

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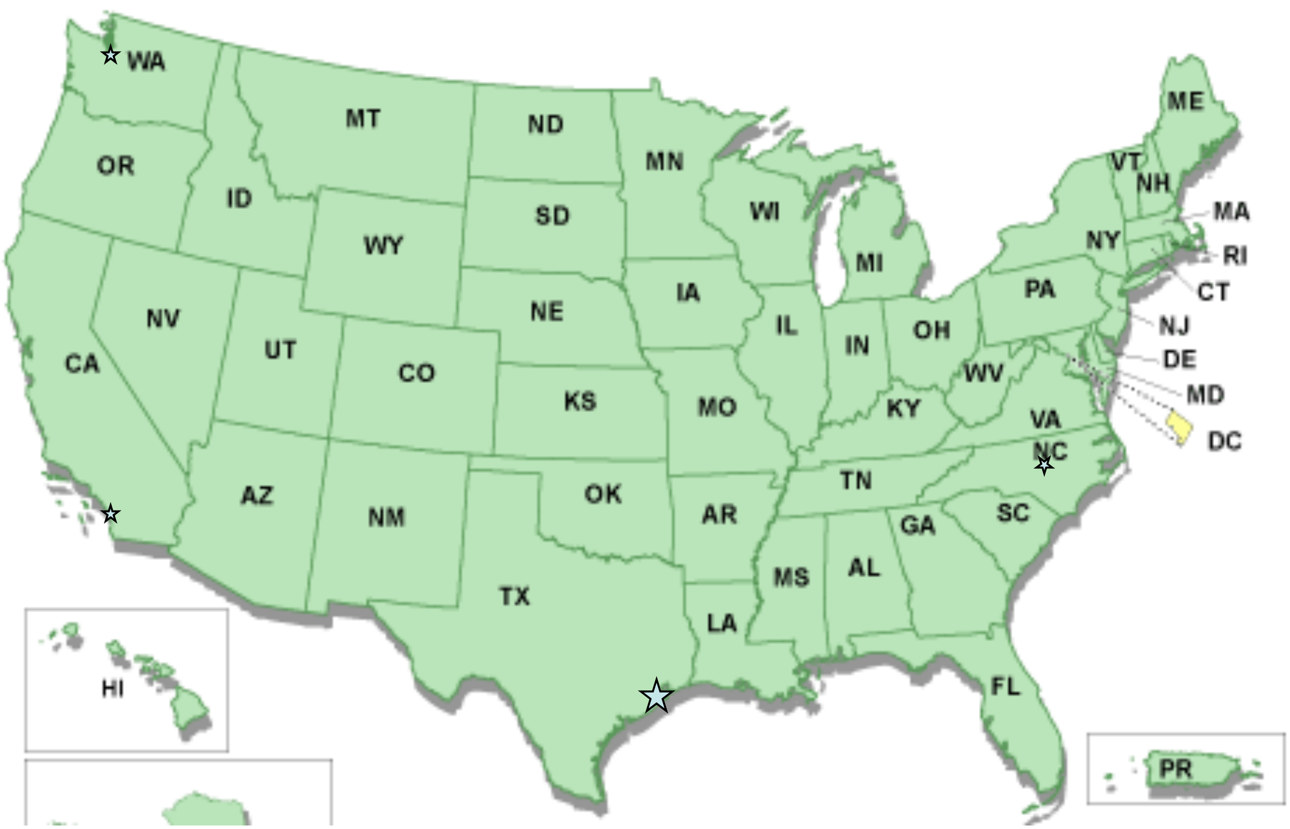
Where is NCSU?

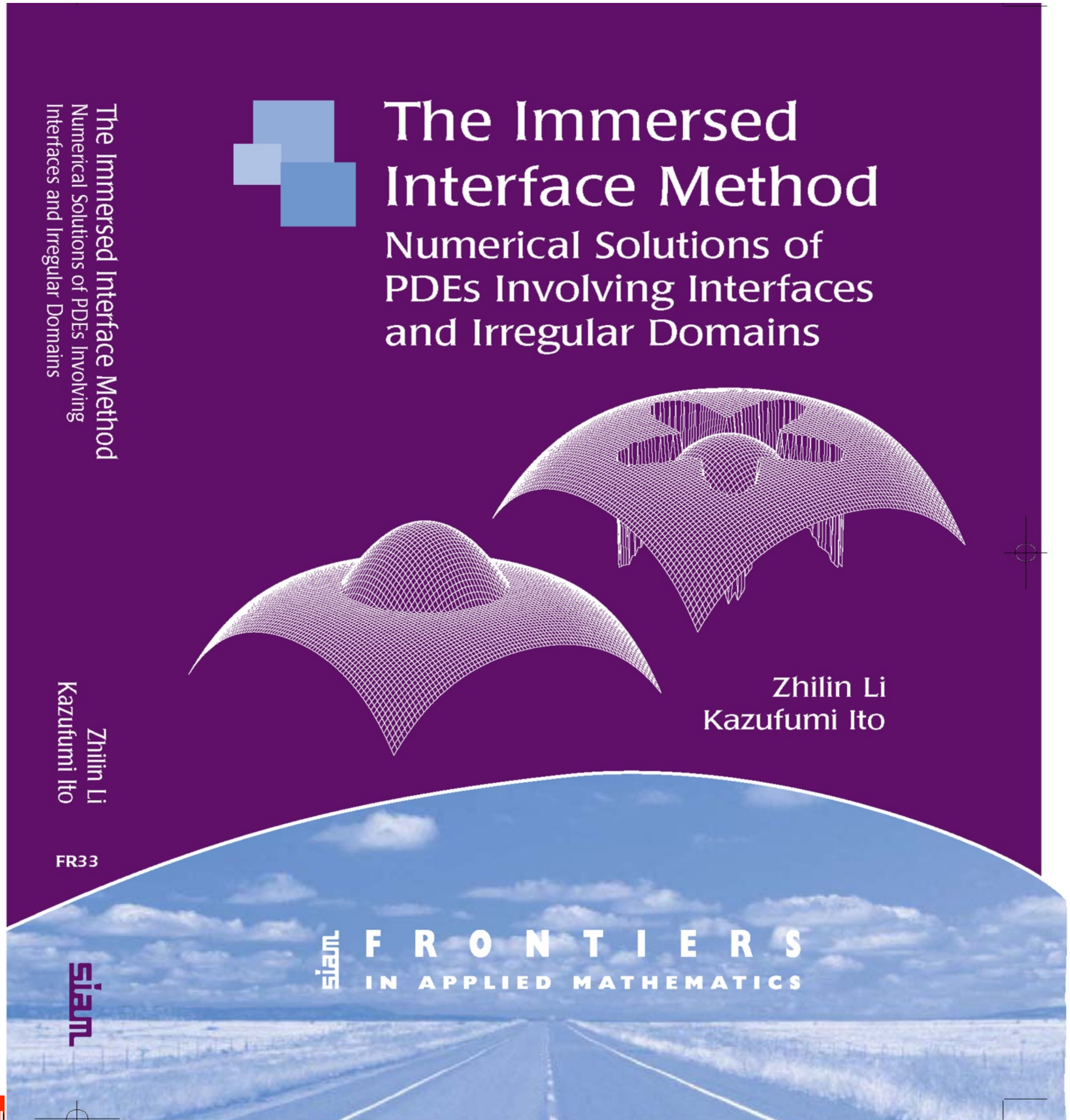


Where is NCSU? II

- Triangle: ***Duke (***private***)***, Durham; ***UNC*** (law/ medical), Chapel-Hill, ***NCSU*** (engineering), Raleigh
- Research Triangle (centroid): Head-quarter of ***IBM & Lenovo***
- Head-quarter of ***Red-Hat (Linux)***
- Home of ***SAS*** (largest statistics software, originated from NCSU)
- NSF Center: ***Samsi*** (Statistic and applied mathematics Institute)
- NISS, ARO, pharmaceutical, communications, ……

Outline

- ***Problems → PDES & Analysis/simulations***
  - *Can we model snowflakes?*
  - *Drop spreading*
  - *CFD and applications (flow past obstacles)*
- ***Numerical methods (IB, IIM, IFEM, Augmented IIM (idea, procedure, why & how)***
  - Why Cartesian/structured mesh?
  - IB → IIM, regular problem → Source terms (Peskin's IB model) → IIM → AIIM
- ***How to evolve free boundary/moving interface?***
  - Front tracking method
  - Level set method
- ***Conclusions***


The Immersed Interface Method
Numerical Solutions of PDEs Involving Interfaces and Irregular Domains
Zhilin Li
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FR33
siam
FRONTIERS
IN APPLIED MATHEMATICS

References

- R. LeVque & Z. Li: The immersed interface method for elliptic equations with discontinuous coefficients and singular sources, SIAM J. Numer. Anal. 31:1019--1044, 1994, cited ***1170***.
- The Immersed Interface Method: Numerical Solutions of PDEs Involving Interfaces and Irregular Domains, SIAM Frontiers in Applied Mathematics 33, 2006, Zhilin Li and Kazufumi Ito.
- New Cartesian grid methods for interface problems using the finite element formulationZ Li, T Lin, X Wu - Numerische Mathematik, 2003
- A Fast Iterative Algorithm for Elliptic Interface Problems, SIAM J. Numer. Anal., 35(1), 230–254.
- Accurate Solution and Gradient Computation for Elliptic Interface Problems with Variable Coefficients, SIAM J. Numer. Anal., 2017, 55(2), 570–597. (28 pages)

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Heat Propagation in Heterogeneous material

- Heat propagation through heterogeneous materials (*an interface problem*)

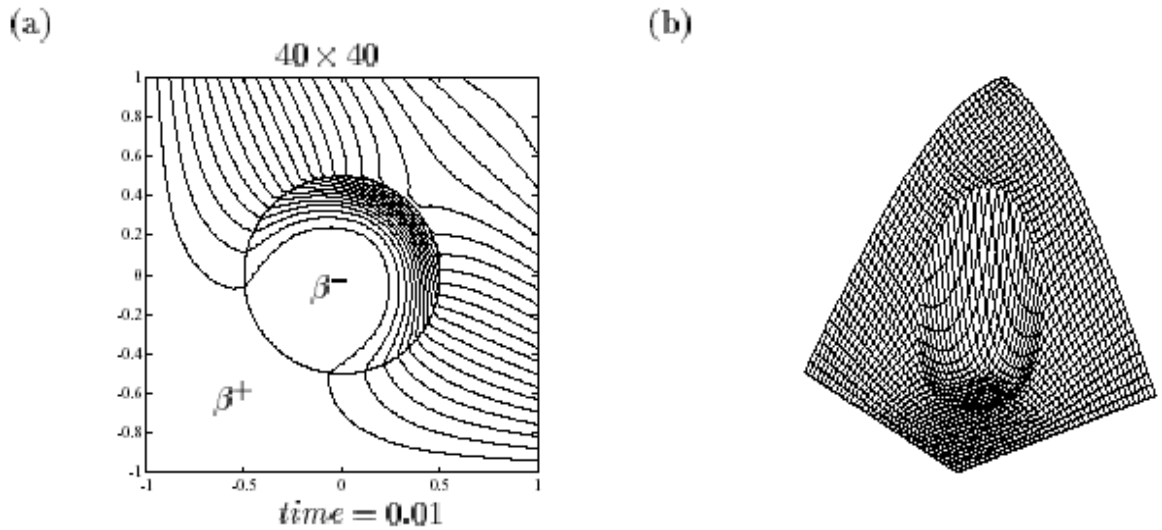

Figure 1.1: Heat propagation in different materials. (*a*) Contour plot of the temperature. (*b*) Mesh plot of the solution.

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Heat propagation through heterogeneous materials II

$$u_t = \nabla \cdot \beta \nabla u, \qquad -1 < x, y < 1$$

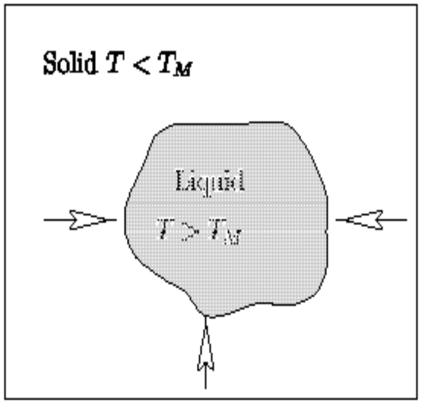
$$\beta = \begin{cases} 1 & \text{if } \; x^2 + y^2 \le \dfrac{1}{4} \\ 100 & \text{otherwise} \end{cases}$$

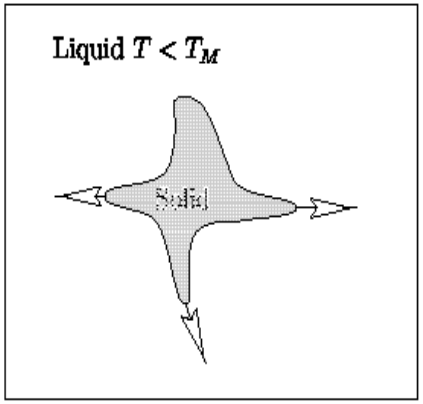
$$\begin{aligned} \text{BC:} \quad & u(x,1,t) = \sin((x+1)\pi/4), \\ & u(1,y,t) = \sin((y+1)\pi/4), \\ & u = 0 \qquad \text{elsewhere.} \end{aligned}$$

$$\text{IC} \quad u = 0, \quad [u] = 0, \quad [\beta u_n] = 0, \quad [u_n] \neq 0.$$

Formulations of Snowflakes (Crystal Growth)

- Heat equation with ***non-linear BC***



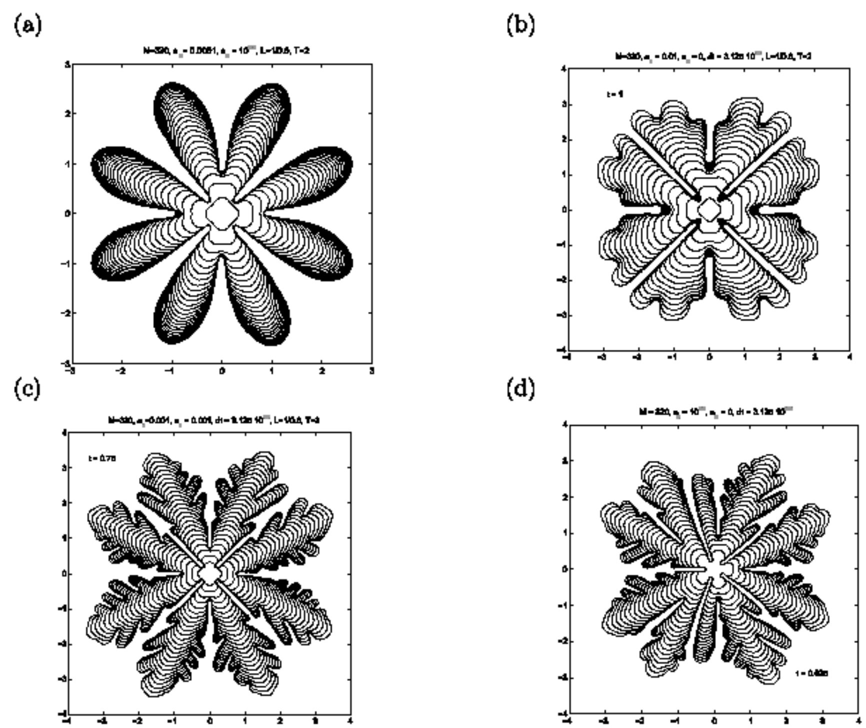


$$\rho c \frac{\partial T}{\partial t} = \nabla \bullet (\beta \nabla T), \quad \rho L V = -\left[\beta \frac{\partial T}{\partial n} \right]$$

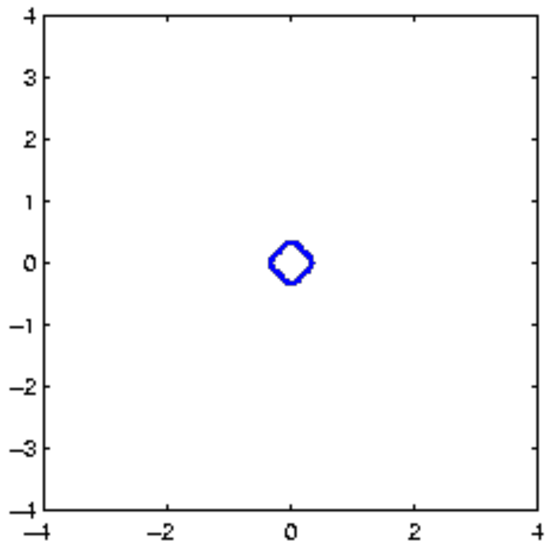
$$T(x,t) = -\varepsilon_c \kappa - \varepsilon_V V, \quad \frac{dX}{dt} \bullet n = V$$

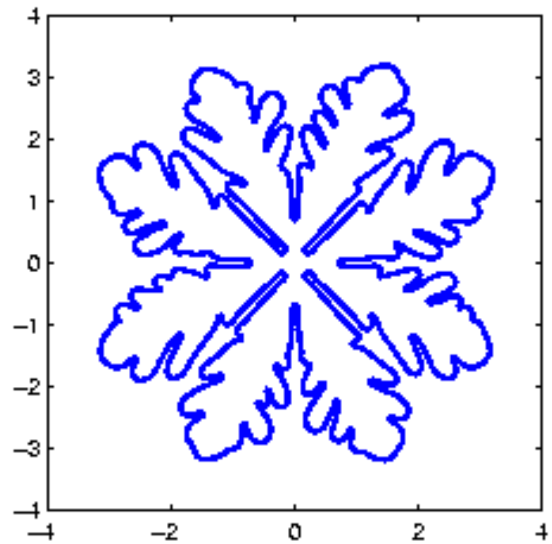
Stefan Problem and Crystal Growth

- ***Stability analysis:*** dynamically unstable for some medium modes (*exp(-k l t)*)



Simulation: Crystal Growth





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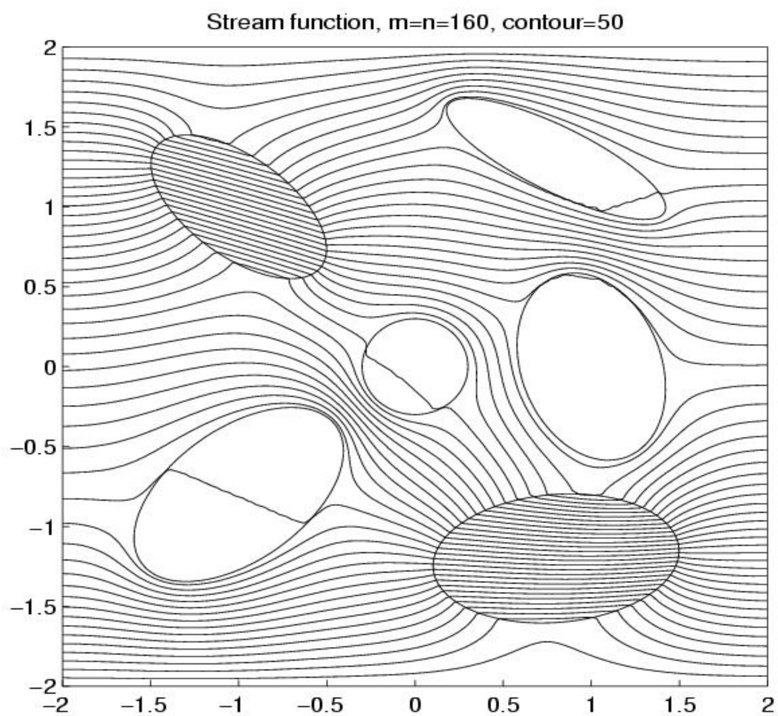
Underground Water Flow

- Ideal flow (steady state, potential flow)

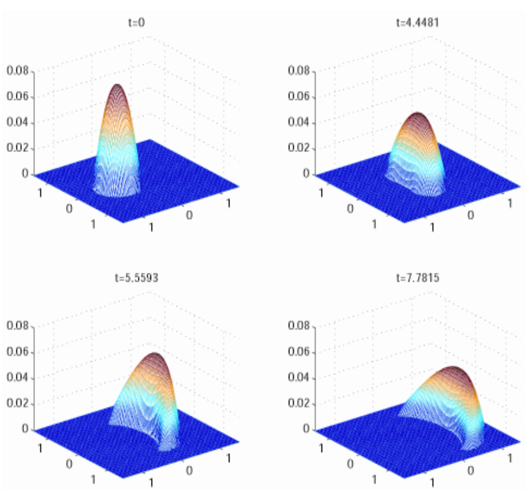
$$-\nabla \bullet (\beta \nabla u) = 0, \quad 1/\beta \text{ is the permeability}$$

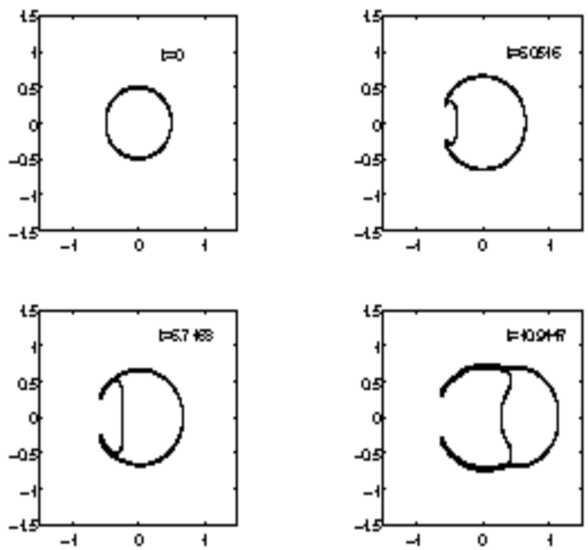
$$\left.\frac{\partial u}{\partial n}\right|_{x=a} = 1, \qquad \frac{\partial u}{\partial n} = 0 \;\; \text{along other sides}$$

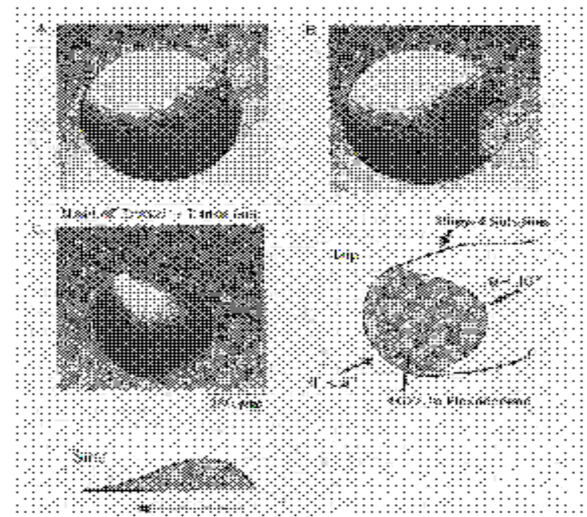


Drop Spreading

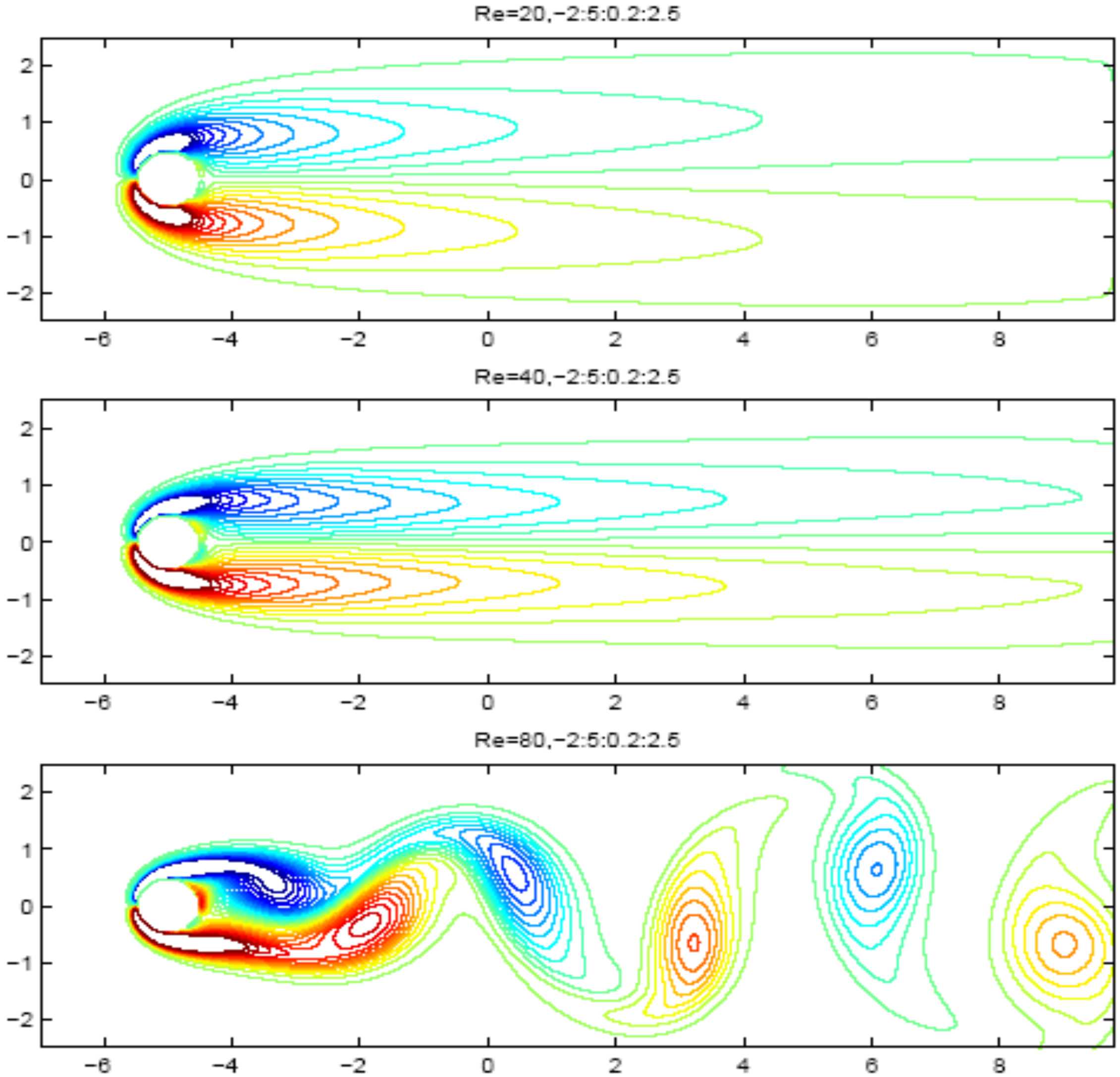
- A simplified model (Hunter, Li, Zhao): The velocity of the moving front $V=\theta_d - \theta_s$, *(difference* in dynamic and static contact angles). θ_d is computed from the Laplacian equation.



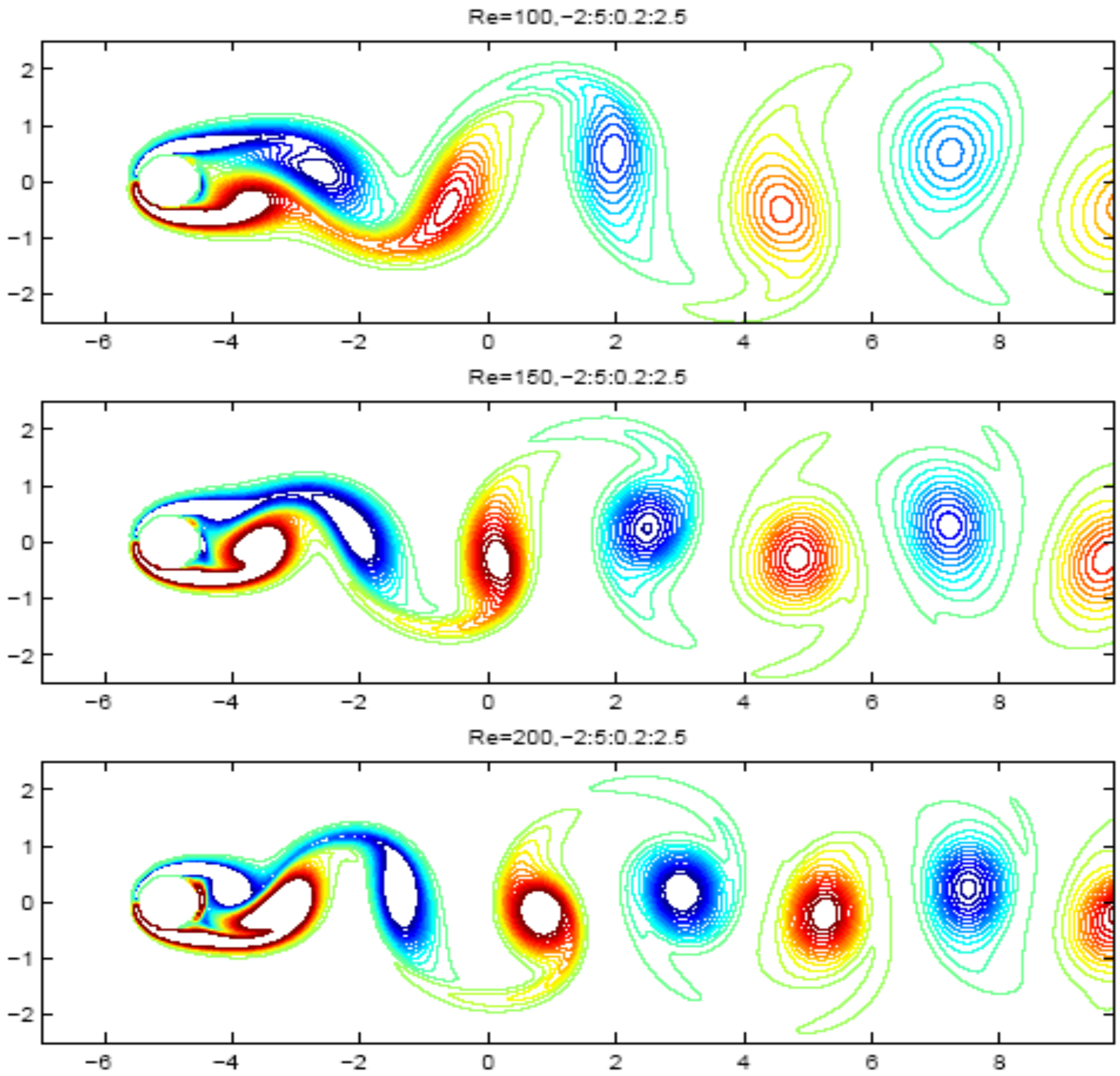




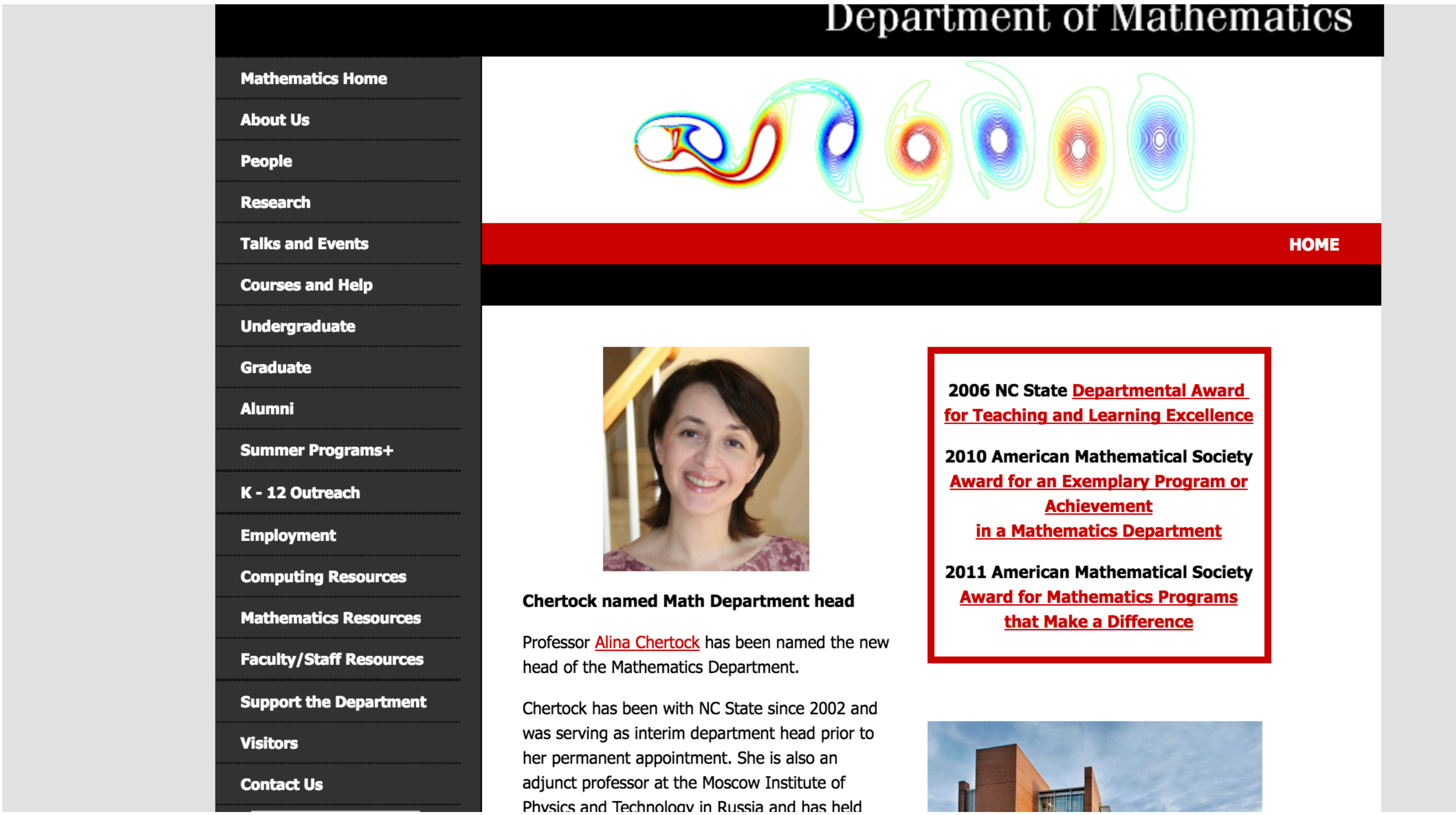
Flow pass a cylinder



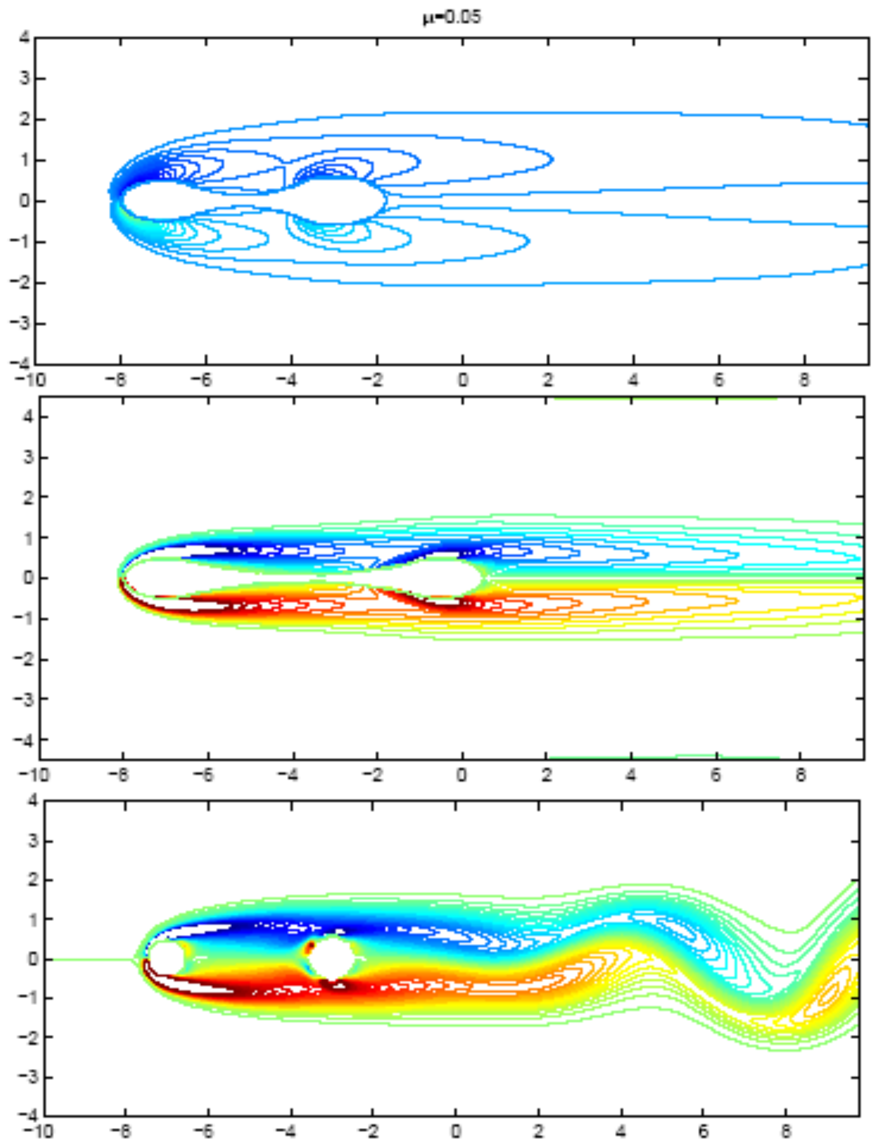
Flow pass a cylinder: II



Icon on Math Dept Web-page



Flow pass a dumbbell, two cylinders



Navier-Stokes Eqns with Interface

- The PDE model is the basis of Immersed Boundary (IB) method.

$$\frac{\partial u}{\partial t} + u \bullet \nabla u + \nabla p = \mu \Delta u + g$$

$$\nabla \bullet u = 0$$

$$u_{\partial \Omega} = \text{given velocity}$$

- Projection method:

$$\frac{u^* - u^k}{\Delta t} + (u \bullet \nabla u)^{k+1/2} + (\nabla p)^{k-1/2} = \frac{\mu}{2}(\Delta u^k + \Delta u^*) + F^{k+1/2} + C^k$$

$$\Delta \phi = \frac{\nabla \bullet u^*}{\Delta t} + C_2^k, \quad \frac{\partial \phi}{\partial \mathrm{n}} = 0$$

$$u^{k+1} = u^* - \Delta t \nabla \phi + C_3^k$$

$$\nabla p^{k+1/2} = \nabla p^{k-1/2} + \nabla \phi + C_4^k$$

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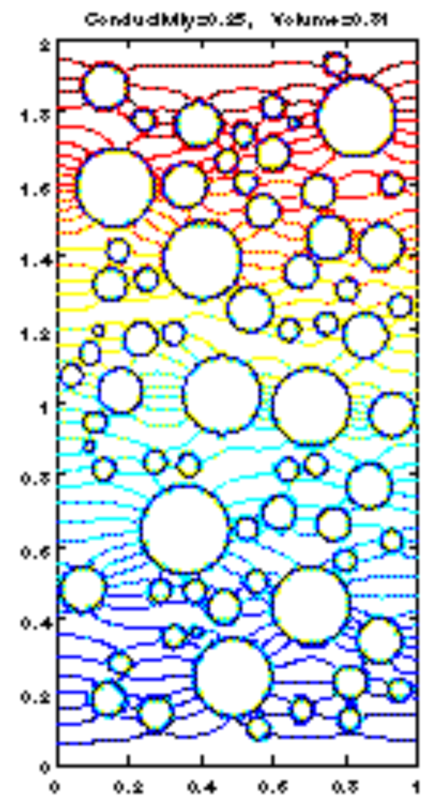
Permeability of concrete

- Estimate the permeability of concrete
  - Probability of random work
  - Laplacian equation exterior with Neumann BC.

$$\Delta u = 0, \quad \text{exterior}$$

$$\left.\frac{\partial u}{\partial n}\right|_{x=a} = 1, \qquad \frac{\partial u}{\partial n} = 0 \ \text{ along other sides}$$

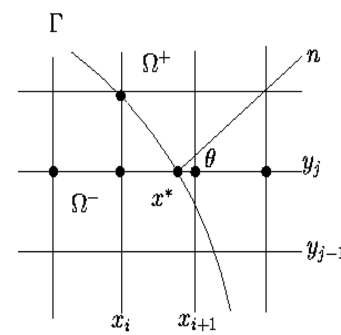


Numerical Simulations

- Analytic solutions are rarely available
- Approximate solutions
  - Analytic approach: series solution, asymptotic, perturbations, *etc*.
  - Use computers
- Numerical solutions using computers
  - **A mesh** (or a grid) Body fitted mesh, ***Cartesian***, ***structured*** or non-structured, mesh-free
  - **Discretization:** Finite difference/element, volume, …

Why Cartesian grid method?

Cartesian or ***adaptive*** Cartesian grids.
why?



- ***Simple (no grid generation)***
- ***Need less adaptively due to high resolution***
- ***Coupled with other Cartesian grid methods (FFT, level set method, Clawpack, structured multi-grid method)***
- ***Less cost for free boundary/moving interface problems, topological changes***

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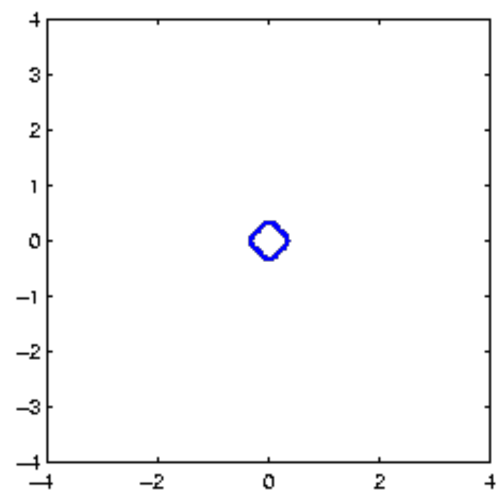
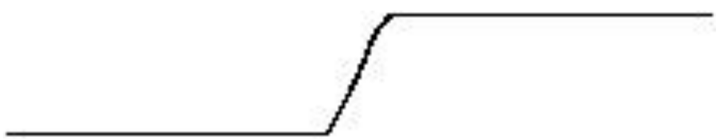
Simulation of free boundary moving interface Problems

- Solve the governing PDEs
  - Discontinuities in the coefficient, solution, flux, irregular domain …
- Evolve the free boundary or moving interface Problems
  - Front tracking (Lagrangian)
  - Level set method (Eulerian)
  - Volume of fractions (VOF)



A brief review of PDE solvers

- Peskin's *Immersed Boundary* (***IB***) method
- *Smoothing* method

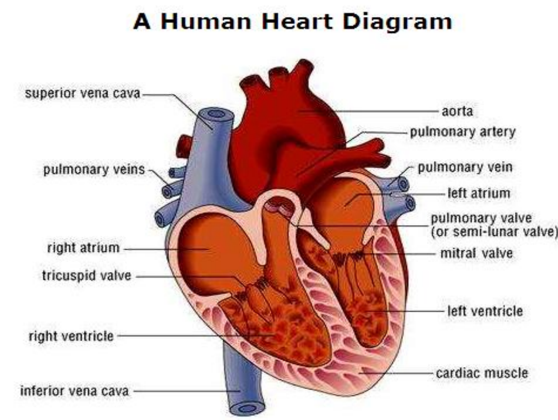


$$\beta_{i+\frac{1}{2}} = \left[\frac{1}{h} \int_{x_i}^{x_{i+1}} \beta^{-1}(x)\, dx \right]^{-1}$$

- Harmonic Averaging
- Integral equation, FMM (Greengard, Mayo et al.)
- FEM with body-fitted grid (Chen/Zou, Babuska…)
- IFEM (Z. Li, S. Hou & X-D Liu, J. Dolbow.. …)
- GFM (Fedkew), Hybrid method, Virture nodal
- IIM (LeVeque, Li, Lee, Calhoun, Zhao,…)
- Advantages and limitations …

Immersed boundary (IB)

- C. Peskin's IB method:
  - ***Modeling*** and simulation of heart beating/blood flow: treat the complicated boundary condition as a source distribution: *Irregular domain (with BC)→ rectangular box (no-BC)*



$$\rho\left(\frac{\partial u}{\partial t}+u\cdot\nabla u\right)+\nabla p=\nabla\bullet\mu(\nabla u+\nabla u^{T})+\cancel{\int_{\Gamma} f(s)\delta(x-X(s))\,ds}+g$$

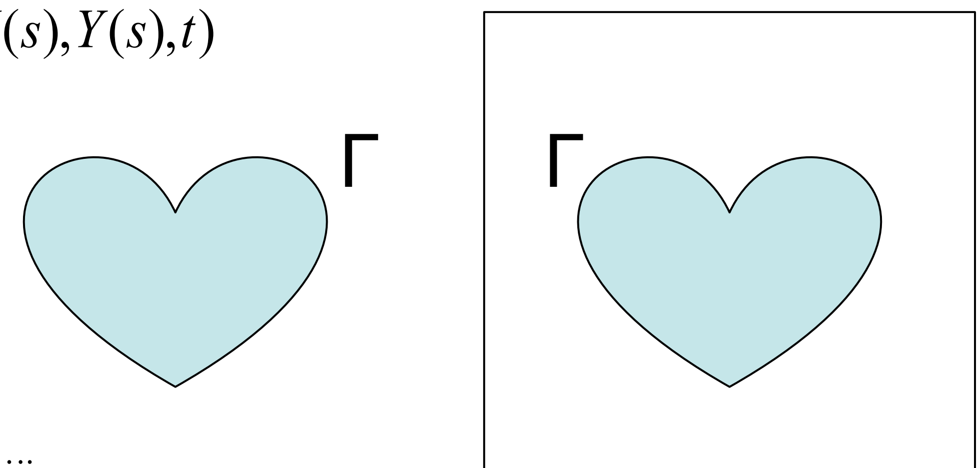
  - ***Numerics***: Use a discrete delta function to distribute the source to nearby grid points
  - Simple, robust, popular, application in bio-physics, biology, and many other areas
  - First order accurate, area conservation, non-sharp interface method

Immersed Boundary Method

- Immerse the heart into a rectangular box
- The NSE are defined on the entire box!
- The boundary condition is treated as a source distribution (Dirac delta function)

$$\rho\left(\frac{\partial u}{\partial t}+u\bullet\nabla u\right)+\nabla p=\nabla\bullet\mu(\nabla u+\nabla u^{T})+\int_{\Gamma} f(s)\delta(x-X(s))\,ds+g$$

$$\nabla\bullet u=0,\qquad \frac{d\Gamma}{dt}=u(X(s),Y(s),t)$$



A REU Project, 2010, NCSU

- IB (smoothing + discrete Delta function) may not converge for the following

$$(\beta u')' = C\delta(x-\alpha) + \bar{C}\delta'(x-\alpha)$$
$$u(0) = 0, \; u(1) = 0$$

- **QUESTION III:** ***What is the solution or the jump conditions for***

$$(\beta u')' = C\delta(x) + \bar{C}\delta'(x)$$
$$\text{linear BC at } x=0, \quad u(1) = 0\,?$$

- *Derived* the jump conditions; *Defined* (consistent) ***weak solution***; *Derived* relation of the weak solution with the *boundary conditions*; *Confirmed* theoretical results with numerical implementation.

IIM in1D, simple case

- Equations:

$$u'' = f(x) + C\delta(x-\alpha)$$

$$u(0) = u_a \qquad u(1) = u_b$$

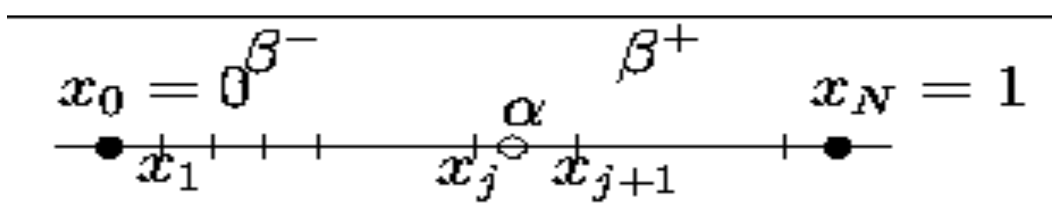
- Or

$$u'' = f(x), \quad x \in (0,\alpha) \cup (\alpha,1)$$

$$u(\alpha+) = u(\alpha-), \quad u'(\alpha+) = u'(\alpha-) + C$$

$$u(0) = u_a \qquad u(1) = u_b$$

- A uniform grid:



IIM in1D, simple case

- **Finite difference scheme:** *One finite difference equation at* ***every interior*** *grid point*
  - Regular grid: Standard central scheme

$$\frac{U_{i-1} - 2U_i + U_{i+1}}{h^2} = f(x_i), \quad x_j \le \alpha < x_{j+1}$$

$$i = 1, 2, \ldots, j-1, j+1, \ldots, n-1.$$

$$\frac{U_{j-1} - 2U_j + U_{j+1}}{h^2} = f(x_j) + C_j$$

$$\frac{U_j - 2U_{j+1} + U_{j+2}}{h^2} = f(x_{j+1}) + C_{j+1}$$

IIM for 1D problem & Analysis

- Equations:

$$(\beta u')' = f(x) + C\delta(x-\alpha)$$

$$u(0) = u_a \qquad\qquad u(1) = u_b$$

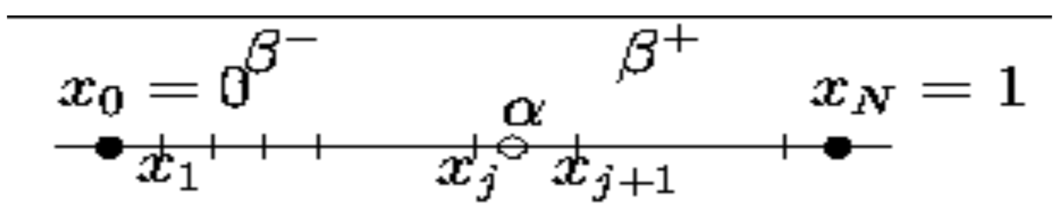
- Or

$$(\beta u')' = f(x), \quad x \in (0,\alpha) \cup (\alpha,1)$$

$$u(\alpha+) = u(\alpha-), \quad \beta^{+}u'(\alpha+) = \beta^{-}u'(\alpha-) + C$$

$$u(0) = u_a \qquad\qquad u(1) = u_b$$

- A uniform grid:



IIM for 1D problem, II

- Finite difference scheme: *One finite difference equation at* ***every interior*** *grid point*
  - Regular grid: Standard central scheme

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

$$i=1,2,\ldots,j-1,j+1,\ldots,n-1.$$

  - Irregular grid points, $x_j \quad and \quad x_{j+1}$

Derive FD at the two irregular grid points

- FD scheme:

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

- Determine the coefficients and the correction term
- Interface relations: $\gamma_{j-1}, \gamma_j, \gamma_{j+1}, C_j$

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

Derive FD at the irregular grid point, II

- Undetermined coefficient method to minimize the *local truncation error* at *α*

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

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

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

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

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

FD at the irregular grid point, III

- Taylor Expansion + interface relations + undetermined coefficient method

$$
\begin{aligned}
T_j &= \gamma_{j-1} u(x_{j-1}) + \gamma_j u(x_j) + \gamma_{j+1} u(x_{j+1}) - f_j - C_j \\
&= \gamma_{j-1}\left(u^- + u_x^-(x_{j-1}-\alpha) + \frac{(x_{j-1}-\alpha)^2}{2} u_{xx}^- + O(h^3)\right) \\
&\quad + \gamma_j\left(u^- + u_x^-(x_j-\alpha) + \frac{(x_j-\alpha)^2}{2} u_{xx}^-\right) \; + \; \gamma_{j+1}\frac{\beta^-}{\beta^+} C(x_{j+1}-\alpha) \\
&\quad + \gamma_{j+1}\left(u^- + \frac{\beta^-}{\beta^+} u_x^-(x_{j+1}-\alpha) + \frac{\beta^-}{\beta^+}\frac{(x_{j+1}-\alpha)^2}{2} u_{xx}^-\right) - f_j - C_j \\
&= u^-(\gamma_{j-1} + \gamma_{j-1} + \gamma_{j+1}) + u_x^-\left(\gamma_{j-1}(x_{j-1}-\alpha) + \gamma_j(x_j-\alpha)\right. \\
&\quad \left. + \gamma_{j+1}\frac{\beta^-}{\beta^+}(x_{j+1}-\alpha)\right) + u_{xx}^-\left(\gamma_{j-1}\frac{(x_{j-1}-\alpha)^2}{2} + \gamma_j\frac{(x_j-\alpha)^2}{2} + \right. \\
&\quad \left. \gamma_{j+1}\frac{\beta^-}{\beta^+}\frac{(x_{j+1}-\alpha)^2}{2}\right) - f_j - C_j
\end{aligned}
$$

Set-up equation

- The linear system for the coefficients:

$$\gamma_{j-1} + \gamma_{j-1} + \gamma_{j+1} = 0$$

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

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

- The correction term is

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

FD Scheme at irregular grid points

- It has been proved that if $\beta^-\beta^+ > 0$ then the solution exists and unique.

$$\begin{cases} \gamma_{j,1} = (\beta^- - [\beta](x_j - \alpha)/h)/D_j, \\ \gamma_{j,2} = (-2\beta^- + [\beta](x_{j-1} - \alpha)/h)/D_j, \\ \gamma_{j,3} = \beta^+/D_j, \end{cases}$$

$$\begin{cases} \gamma_{j+1,1} = \beta^-/D_{j+1}, \\ \gamma_{j+1,2} = (-2\beta^+ + [\beta](x_{j+2} - \alpha)/h)/D_{j+1}, \\ \gamma_{j+1,3} = (\beta^+ - [\beta](x_{j+1} - \alpha)/h)/D_{j+1}, \end{cases}$$

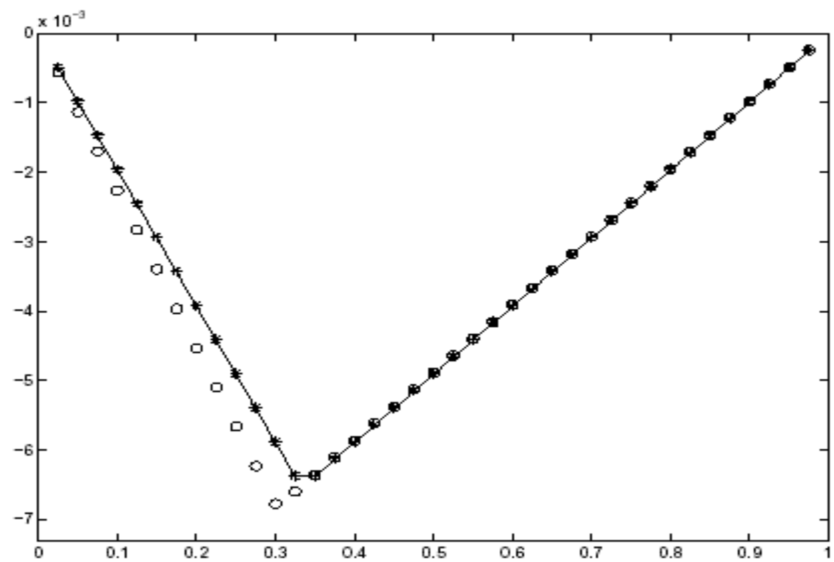
$$D_j = h^2 + [\beta](x_{j-1} - \alpha)(x_j - \alpha)/2\beta^-, \; D_{j+1} = h^2 - [\beta](x_{j+2} - \alpha)(x_{j+1} - \alpha)/2\beta^+$$

Theoretical Results

- The scheme is ***consistent*** and ***stable***.
- The scheme is ***2-nd accurate*** in the infinity norm (point-wise)
- No interface: back to the normal center FD scheme
- No delta function (C=0), then correction term is zero.
- If $\beta^+ = \beta^-$ then we have standard FD coefficients, only correction term!

An example and Comparison

- Eqn: $(\beta u')' = \delta(x-\alpha),\ u(0)=0,\ u(1)=0$
- Exact soln: $u(x) = \begin{cases} Bx(1-\alpha) \\ B\alpha(1-x) \end{cases}$ $\quad B = \dfrac{1}{\beta^{+}\alpha + \beta^{-}(1-\alpha)}$
- IIM exact
- Smoothing + discrete Delta



Error Estimates

- The determinant of the FD coefficient matrix satisfies

$$\det(A) = \begin{cases} CD_j & \text{If } \beta \text{ is piecewise cosntant} \\ C(D_j + O(h^3)) & \text{otherwise} \end{cases}$$

$$D_j = h^2 + [\beta](x_{j-1} - \alpha)(x_{j-1} - \alpha) / (2\beta^-) \geq h^2$$

$$\frac{\bar{C}}{h^2} \leq \gamma_k \leq \frac{C}{h^2} \quad \mathrm{C} = \frac{2\beta_{\max}^2}{\beta_{\min}}, \quad \bar{C} = \frac{2\beta_{\min}^2}{\beta_{\max}}$$

$$T_i = O(h^2), \quad T_j = O(h), \quad T_{j+1} = O(h), \quad \|E\|_\infty = O(h^2).$$

1D example II

- Many examples:

  http://www4.ncsu.edu/~zhilin/IIM/index.html

- Natural jump condition:

$$(\beta u')' = 12x^2, \; u(0)=0, \; u(1) = \frac{1}{\beta^+} + \left(\frac{1}{\beta^-} - \frac{1}{\beta^+} \right)\alpha^4$$

$$u(x) = \begin{cases} \dfrac{x^4}{\beta^-} & 0 < x < \alpha \\ \dfrac{x^4}{\beta^+} + \left(\dfrac{1}{\beta^-} - \dfrac{1}{\beta^+} \right)\alpha^4 & \alpha < x < 1 \end{cases}$$

1D example II

- Discontinuous coefficients only:

Table 2.1. *A grid refinement analysis of IIM and harmonic averaging (HV) for Example 2.2 with $\alpha = 1/2$, $\beta^- = 1$, $\beta^+ = 2$. Second order convergence in the infinity is verified.*

M	$\|\|E_M\|\|_\infty(IIM)$	ratio1/order1	ratio2	$\|\|E_M\|\|_\infty$(HV)	ratio3
20	2.6285^{-4}			5.0683^{-4}	
40	5.3523^{-5}	4.9110 (2.2960)		1.2787^{-4}	3.9634
80	1.5980^{-5}	3.3493 (1.7439)	16.4485	3.1842^{-5}	4.0161
160	3.3802^{-6}	4.7276 (2.2411)	15.8342	7.9779^{-6}	3.9912
320	9.9130^{-7}	3.4099 (1.7697)	16.1206	1.9923^{-6}	4.0043
640	2.1176^{-7}	4.6811 (2.2268)	15.9622	4.9835^{-7}	3.9978

Regular FD → IB → IIM

- Regular domain (rectangular, circles,..), no interface/ singularity

$$\Delta u = f(x)$$

BC (e.g. Dirichlet, Neuman, Mixed)

- The FD scheme at (x_i, y_j)

$$\frac{u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{i,j}}{h^2} = L_h u_{i,j} = f_{ij}$$

- ***AU=F; A***: Discrete Laplacian. Can be solved by a fast Poisson solver (e.g. ***FFT***, *$O(N^2)log(N)$), e.g.,* Fish-pack, or structured multigrid

Poisson Eqn. with singular sources

- **Interface problems**, simplified ***Peskin's IB*** model

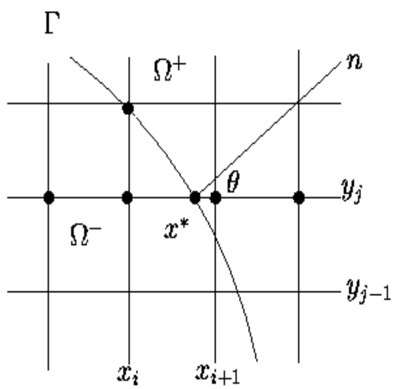
$$\Delta u = f(x) + \int_\Gamma c(s)\delta(x - X(s))ds + g$$

BC (e.g., Dirichlet, Neuman, Mixed)

- *Equivalent Problem*

$$\Delta u = f(x), \quad x \in \Omega \setminus \Gamma, \quad [u]_\Gamma = 0, \quad [\nabla u \bullet n]_\Gamma = \left[\frac{\partial u}{\partial n}\right]_\Gamma = C(s)$$

BC (e.g., Dirichlet, Neuman, Mixed)



- FD scheme *(x_i,y_j)*, regular/irregular

$$\frac{u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{i,j}}{h^2} = L_h u_{i,j} = f_{ij}$$

$$\frac{u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{i,j}}{h^2} = L_h u_{i,j} = f_{ij} + C_{ij}$$

Analysis of IB Method

- It is inconsistent! The local truncation error is O(1/h)!

$$\Delta u = f(x) + \int_{\Gamma} c(s)\delta(x - X(s))\,ds + g$$

BC (e.g., Dirichlet, Neuman, Mixed)

$$\frac{u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{i,j}}{h^2} = L_h u_{i,j} = f_{ij} + C_{ij}$$

$$C_{ij} = \sum_k C_k \delta_h(x_i - X_k)\delta_h(y_j - Y_k)\Delta s_k$$

- But it is first order convergent in the infinity norm!
- Rigorous proof by Z. Li, MathCom, 2014, in press
  - Obtain estimates of discrete Green with zero BC (function and their derivatives)!
  - Using the imaging technique to construct the Green function with the Green function in the entire space
  - Construct interpolation functions *C^1Q^5 and C^2Q^5*
  - Modified first and second discrete Green's theorem

IIM for a 2D Model Problem

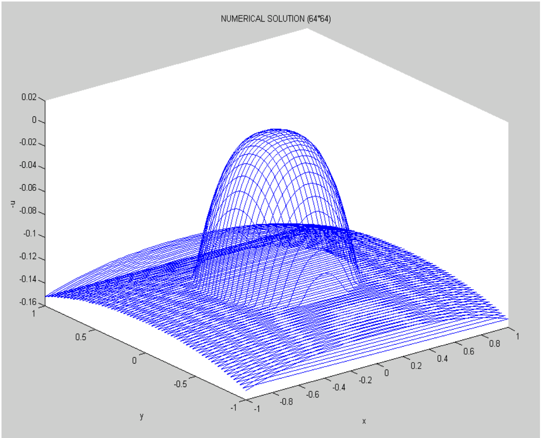
- Two equivalent forms

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

$$\iint_\Omega \beta\nabla u\cdot\nabla v\,dxdy = \iint_\Omega fv\,dx\,dy + \int_\Gamma c(s)v(X(s))\,ds$$

  - Equation on each domain coupled with the jump conditions

$$[u]=0,\ \text{or}\ [u]=w(s)\quad [\beta\nabla u\bullet n]=v(s)$$



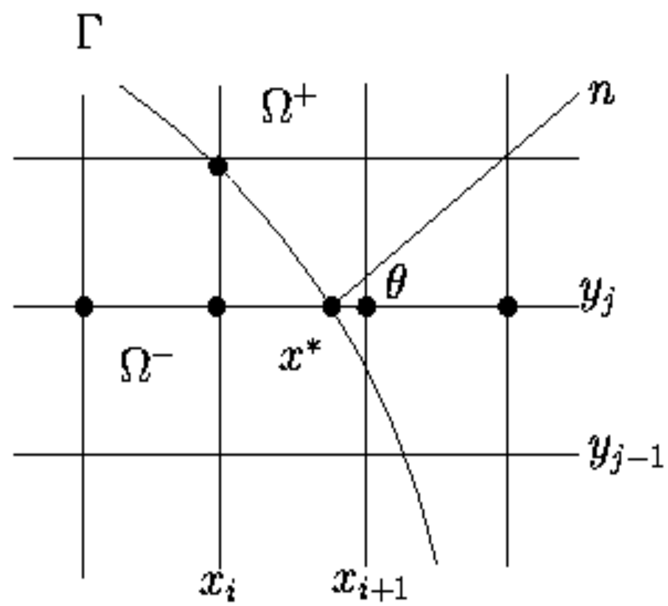
- Solution is not smooth or even discontinuous!

IIM for Singular Source

- [β]=0, i.e. continuous coefficient

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

$$[u] = w(s), \quad [\nabla u \bullet n] = v(s)$$



- Finite difference scheme (correction term only), one FFT

$$L_h u_{i,j} = f_{ij} + C_{ij}$$

Outline of IIM (Finite Difference)

- Simple Cartesian/adaptive Cartesian grids
- FD (algebraic) eqn at every grid point
  - Standard FD scheme away from the interface

$$
\begin{aligned}
(\beta u_x)_x \;+\; (\beta u_y)_y \approx\; & \\
& \frac{1}{h^2}\left\{\beta_{i+1/2,j}\left(U_{i+1,j}-U_{ij}\right)-\beta_{i-1/2,j}\left(U_{ij}-U_{i-1,j}\right)\right. \\
& \left.+\beta_{i,j+1/2}\left(U_{i,j+1}-U_{ij}\right)-\beta_{i,j-1/2}\left(U_{i,j}-U_{i,j-1}\right)\right\}.
\end{aligned}
$$

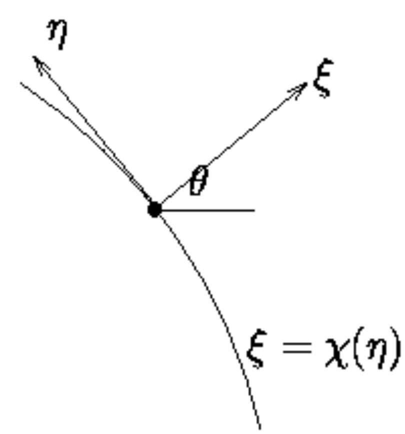
  - ***Modified FD scheme at grid points <u>near or on</u> the interface***

Key steps of IIM

- ***Un-determined coefficient method*** at grid point near/on the interface

$$(\beta u_x)_x + (\beta u_y)_y \approx \sum_{k}^{n_s} \gamma_k \, u\left(x_{i+i_k}, y_{j+j_k}\right) + C_{ij}$$

- Expand at on the interface from ***each side***!
- ***Use jump conditions*** to eliminate th quantities of one side in terms of the other
- Easier to do in the ***local coordinate***

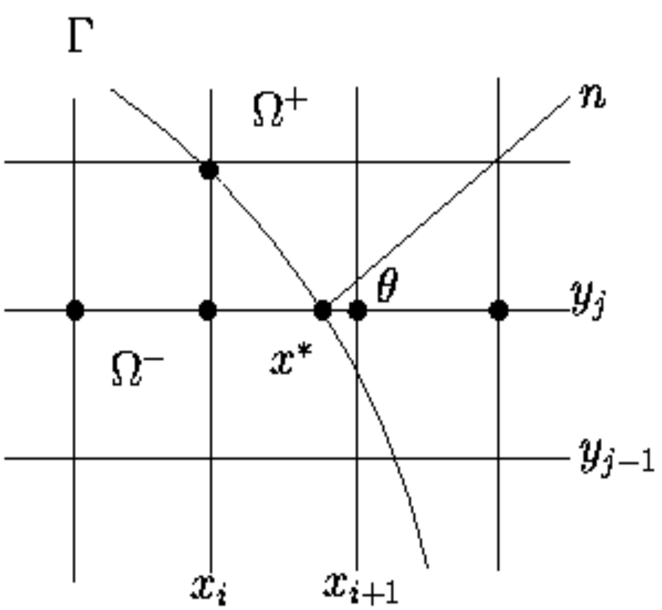


Set-up a system for FD coefficients

$$
\begin{aligned}
\{\, (\beta u_x)_x \;+\; (\beta u_y)_y \,\}^- &= \{\, (\beta u_\xi)_\xi + (\beta u_\eta)_\eta \,\}^- \\
&= \sum_k^{n_s} \gamma_k \, u\left(x_{i+i_k}, y_{j+j_k}\right) + C_{ij} \\
&= \sum_k^{n_s} \gamma_k \left\{ u^\pm + \xi_k \, u_\xi^\pm + \eta_k u_\eta^\pm + \cdots \right\} + C_{ij}
\end{aligned}
$$

$$(\;\;)^+ = (\;\;)^- \qquad \text{\& collect terms}$$

$$
\begin{aligned}
&= l_1(\gamma_1, \cdots, \gamma_{n_s}) u^- + l_2(\gamma_1, \cdots, \gamma_{n_s}) u_\xi^- \\
&\quad + l_3(\gamma_1, \cdots, \gamma_{n_s}) u_\eta^- + l_4(\gamma_1, \cdots, \gamma_{n_s}) u_{\xi\xi}^- \\
&\quad + l_5(\gamma_1, \cdots, \gamma_{n_s}) u_{\eta\eta}^- + l_6(\gamma_1, \cdots, \gamma_{n_s}) u_{\xi\eta}^- \\
&\quad + l_7(\gamma_1, \cdots, \gamma_{n_s}, [u], [\beta u_n]) + C_{ij}
\end{aligned}
$$



Interface Relations

- For homogeneous jump conditions, we get:

$$u^+ = u^- \qquad \text{known}$$

$$u_\eta^+ = u_\eta^-$$

$$u_\xi^+ = \rho\, u_\xi^-, \qquad \rho = \beta^-/\beta^+, \qquad \text{known}$$

$$u_{\xi\eta}^+ = \rho u_{\xi\eta}^- + (1-\rho)\; u_\eta^- \chi''$$

$$u_{\eta\eta}^+ = u_{\eta\eta}^- + (1-\rho)\; u_\xi^- \chi''$$

$$u_{\xi\xi}^+ = \rho u_{\xi\xi}^- + (\rho-1)\, u_{\eta\eta}^- + (\rho-1)\, u_\xi^- \chi''.$$

- It depends on the ***curvature***!

Set-up a system for FD coefficients

$$l_1(\gamma_1, \cdots, \gamma_{n_s}) = 0; \qquad l_2(\gamma_1, \cdots, \gamma_{n_s}) = \beta_\xi^-;$$

$$l_3(\gamma_1, \cdots, \gamma_{n_s}) = \beta_\eta^-; \qquad l_4(\gamma_1, \cdots, \gamma_{n_s}) = \beta^-;$$

$$l_5(\gamma_1, \cdots, \gamma_{n_s}) = \beta^-; \qquad l_6(\gamma_1, \cdots, \gamma_{n_s}) = 0.$$

- How many points in the stencil?
  - ns=6, original IIM
  - ns=5, 1-st order maximum principle preserving
  - ns=9, 2-nd order maximum principle preserving

Stability: Maximum principle preserving IIM

- Add ***maximum principle constraint***

$$\gamma_k \geq 0, \quad \text{if} \quad (i_k, j_k) \neq (0,0),$$

$$\gamma_k < 0, \quad \text{if} \quad (i_k, j_k) = (0,0), \text{the center}$$

- Set-up an optimization problem:

$$\min_{\gamma} \frac{1}{2} \sum_k (\gamma_k - g_k)^2 = \min_{\gamma} \frac{1}{2} \gamma^T H \gamma - \gamma^T g$$

$$s.t. \quad \begin{bmatrix} A_1 \\ A_2 \end{bmatrix} \gamma = b, \quad \gamma_k \geq 0, \quad \text{if} \quad (i_k, j_k) \neq (0,0),$$

$$\gamma_k < 0, \quad \text{if} \quad (i_k, j_k) = (0,0), \text{the center}$$

Maximum principal preserving IIM

- ns=9, nine-point stencil
- Correction term:
- Strictly ***theoretical proof*** of 2-nd order accuracy in infinity norm
- Zero jumps, zero correction (C = 0).
- No discontinuity in the coefficient **([β]=0)**., standard FD scheme of 5-point stencil (-->**FFT**)

$$\frac{U_{i-1,j}+U_{i+1,j}+U_{i,j-1}+U_{i,j+1}-4U_{i,j}}{h^2}=f_{ij}+C_{ij}$$

Convergence Analysis

Lemma 3.2. *Given a finite difference scheme L_h defined on a discrete set of interior points J_Ω for an elliptic PDE with a Dirichlet boundary condition. Assume the following conditions hold:*

1. *J_Ω can be partitioned into a number of disjoint regions*

$$J_\Omega = J_1 \cup J_2 \cup J_3 \cdots \cup J_{N_\Omega}, \qquad J_i \cap J_k = \emptyset, \qquad \text{if } i \neq k. \tag{3.36}$$

2. *The truncation error of the finite difference scheme at a grid point p satisfies*

$$|T_p| \le T_i, \quad \forall p \in J_i, \qquad i = 1,\, 2,\, \cdots,\, N_\Omega. \tag{3.37}$$

3. *There exists a non-negative mesh function ϕ defined on $\cup_{i=1}^{s} J_i$ satisfying*

$$L_h \phi_p \ge C_i > 0, \quad \forall p \in J_i, \qquad i = 1,\, 2,\, \cdots,\, N_\Omega. \tag{3.38}$$

Then the global error of the approximate solution $\{U_{ij}\}$ from the finite difference scheme at mesh points is bounded by

$$||E_h||_\infty \le \left(\max_{A \in J_{\partial\Omega}} \phi_A \right) \max_{1 \le i \le N_\Omega} \left\{ \frac{T_i}{C_i} \right\}, \tag{3.39}$$

where E_h is the difference of the exact solution of the differential equation and the approximate solution of the finite difference equations at the mesh points, and $J_{\partial\Omega}$ is the set that contains the boundary points.

Convergence Analysis

Theorem 3.3. *Let $u(x, y)$ be the exact solution to (3.1) and (3.2a)-(3.2b) with $\sigma \geq 0$, and a Dirichlet boundary condition. Assume that: (1). The optimization problem (3.25)-(3.26) with the constraints (3.20) using the standard compact 9-point stencil has a solution $\{\gamma_k\}$ at every irregular grid points; (2). The solution $u(x, y)$ has up to third order piecewise continuous partial derivatives; (3). The mesh spacing h is sufficiently small; (4). The following inequalities are true:*

$$|\gamma_k| \leq \frac{C_1}{h^2} \quad \text{and} \quad \sum_{\xi_k \geq 0} \gamma_k \xi_k \geq \frac{C_2}{h}. \tag{3.40}$$

Then we have the following error estimate for $\{U_{ij}\}$, the solution of the finite difference scheme obtained from the maximum principle immersed interface method

$$\|u(x_i, y_j) - U_{ij}\|_\infty \leq Ch^2, \tag{3.41}$$

where the constant C depend on the underlying grid and interface, as well as u, f, and β.

Zhilin LI

Convergence Analysis

Proof: Consider the solution to the following interface problem

$$\begin{aligned} \nabla \cdot \beta \nabla \phi &= 1, \\ [\phi] = 0, \qquad [\beta \phi_{\boldsymbol{n}}] = 1, &\quad \phi_{\partial\Omega} = 1. \end{aligned} \tag{3.42}$$

From the results in [11, 44], we know that the solution ϕ exists, and it is unique and piecewise continuous. Therefore the solution is also bounded. Let

$$\bar{\phi}(x,y) = \phi(x,y) + \left| \min_{(x,y)\in\Omega} \phi(x,y) \right|. \tag{3.43}$$

Note that the second term in the right hand side is a constant. If (3.40) is true, then we know that

$$L_h \bar{\phi}(x_i, y_j) \ge \begin{cases} 1 + O(h^2), & \text{if } (x_i, y_j) \text{ is a regular grid point,} \\ \displaystyle\sum_{\xi_k \ge 0} \gamma_k \xi_k \ge \frac{C_2}{h} + O(1), & \text{if } (x_i, y_j) \text{ is an irregular grid point.} \end{cases}$$

the first inequality above still holds. At regular grid points we have

$$\frac{|T_{ij}|}{L_h \bar{\phi}(x_i, y_j)} \le \frac{C_3 h^2}{1}.$$

At irregular grid points where (3.40) is satisfied, we have

$$\frac{|T_{ij}|}{L_h \bar{\phi}(x_i, y_j)} \le \frac{C_4 h}{C_2/h} = \frac{C_4}{C_2} h^2$$

A benchmark example

- Variable & discontinuous coefficients, singular source

$$\nabla \bullet (\beta \nabla u) = f(x) + \int_\Gamma C\delta(x - X(s))ds$$

$$f(x,y) = 8\left(x^2 + y^2\right) + 4$$

$$\beta(x,y) = \begin{cases} x^2 + y^2 + 1, & \text{if } x^2 + y^2 \le 1/4 \\ b & \end{cases}$$

$$u(x,y) = \begin{cases} x^2 + y^2, & \text{if } x^2 + y^2 \le 1/4 \\ \left(1 - \frac{1}{8b} - \frac{1}{b}\right)/4 + \left(\frac{r^4}{2} + r^2\right)/\mathrm{b} + C\log(2r)/b & \end{cases}$$

An Example

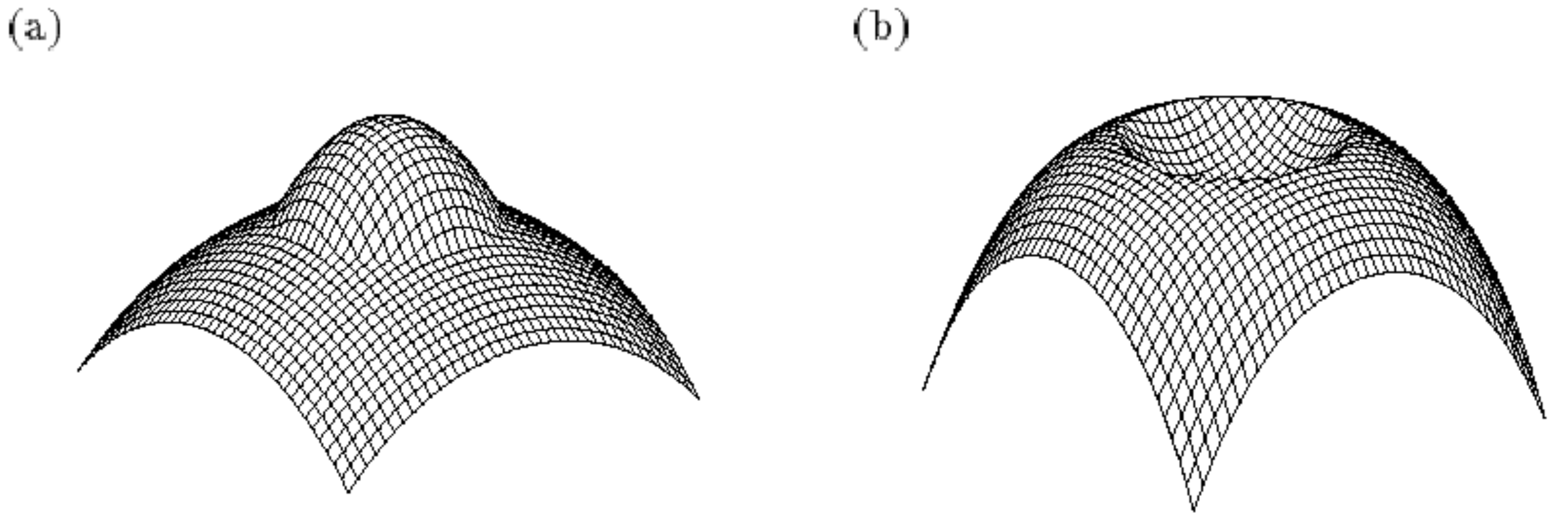


Figure 2.5: The solutions for Example 2.2. (a) The function u for the case $b = 10$, $C = 0.1$. (b) The function $-u$ in the case $b = -3$, $C = 0.1$.

An Example: grid refinement analysis

Table 3.1. *A grid refinement analysis of the maximum principle preserving scheme for Example 3.1 with* $b = 10$, $C = 0.1$, *and* $N_{coarse} = 6$. *Average second order convergence is confirmed.*

N_{finest}	N_b	n_l	$\|\| E_N \|\|_\infty$	order
42	40	4	$4.8638e\ 10^{-4}$	
82	80	5	$1.4476e\ 10^{-4}$	1.7484
162	160	6	$3.0120\ 10^{-5}$	2.2649
322	320	7	$8.2255\ 10^{-6}$	1.8726
642	640	8	$2.0599\ 10^{-6}$	1.9975

An Example: grid refinement analysis

Table 3.2. *A grid refinement analysis of the maximum principle preserving scheme for Example 3.1 with* $N_{coarse} = 9$. *Second order convergence is confirmed.*

N_{finest}	N_b	n_l	$b = 1000,\ C = 0.1$ $\|\| E_N \|\|_\infty$	order	$b = 0.001,\ C = 0.1$ $\|\| E_N \|\|_\infty$	order
34	40	3	$5.1361\ 10^{-4}$		9.3464	
66	80	4	$8.2345\ 10^{-5}$	2.7598	2.0055	2.3204
130	160	5	$1.8687\ 10^{-5}$	2.1878	$5.8084\ 10^{-1}$	1.8280
258	320	6	$4.0264\ 10^{-6}$	2.2394	$1.3741\ 10^{-1}$	2.1031
514	640	7	$9.430\ 10^{-7}$	2.1059	$3.5800\ 10^{-2}$	1.9514

Discontinuous Solution

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

$$u(x,y) = \begin{cases} x^2 - y^2, & \text{if } x^2 + 4y^2 \le 1 \\ \sin(x)\cos(y) & \end{cases}$$

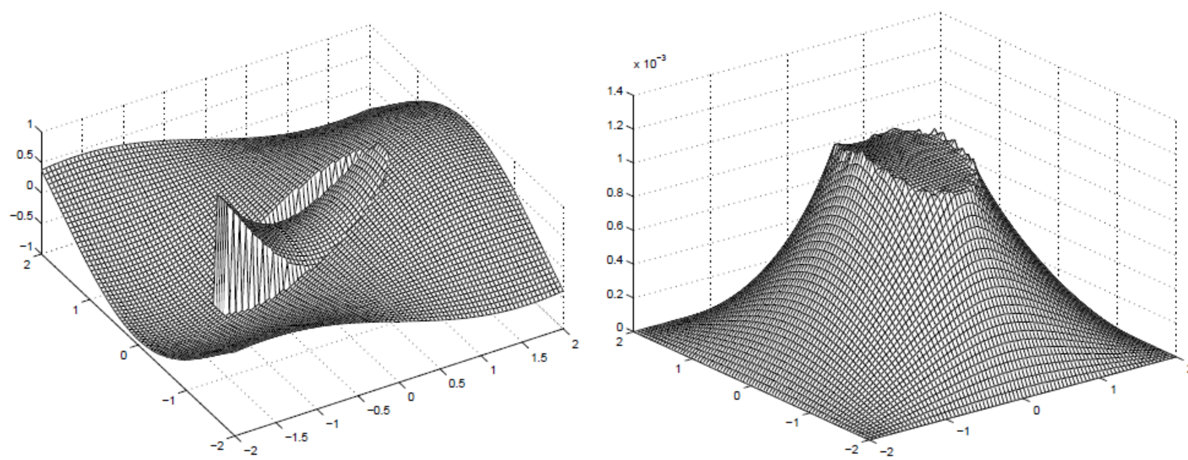


Figure 3.3. *(a). The solution of Example 3.2 with jumps in the solution as well as in the normal derivative. The parameters are* $\beta^+ = 1$, $\beta^- = 100$, *and* $N_{finest} = 82$. *(b). The error plot with the same parameters. The error distribution is better than that obtained from the six-point immersed interface method.*

A grid refinement analysis

Table 3.3. *A grid refinement analysis of maximum principle preserving scheme for Example 3.2 with $N_{coarse} = 9$, average second order convergence is confirmed.*

N_{finest}	N_b	n_l	$\beta^+ = 1000, \beta^- = 1$		$\beta^+ = 1, \beta^- = 1000$	
			$\| E_N \|_\infty$	order	$\| E_N \|_\infty$	order
34	40	3	$1.8322\ 10^{-1}$		$8.0733\ 10^{-3}$	
66	80	4	$3.5224\ 10^{-3}$	5.9574	$3.0371\ 10^{-3}$	1.4739
130	160	5	$4.5814\ 10^{-5}$	3.0090	$7.1981\ 10^{-4}$	2.1238
258	320	6	$1.4240\ 10^{-5}$	1.7049	$1.6876\ 10^{-4}$	2.1162
514	640	7	$3.1501\ 10^{-6}$	2.1887	$2.7407\ 10^{-5}$	2.6371

Algorithm, efficiency analysis

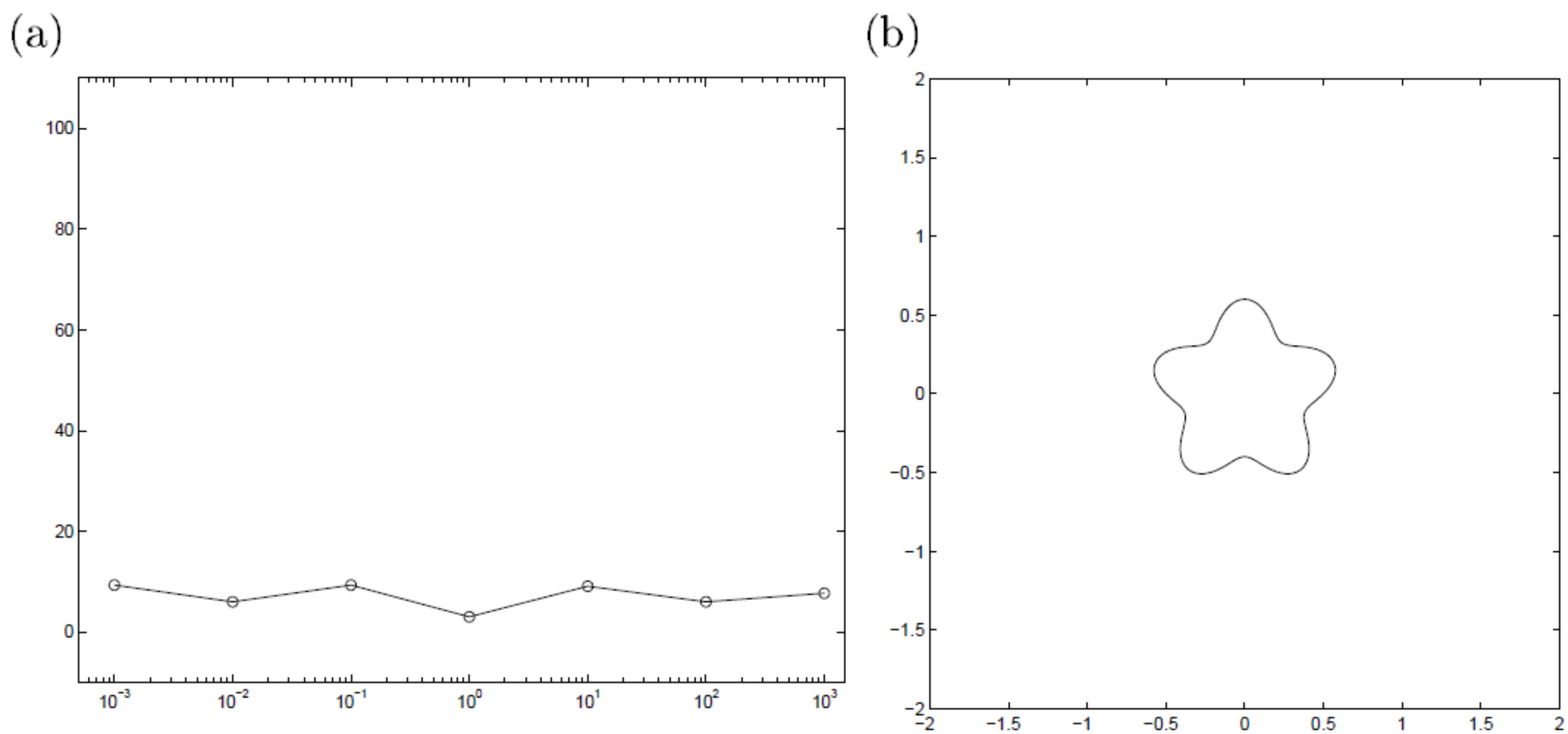


Figure 3.4. *(a). A plot of percentage of the CPU time used for dealing with interfaces versus* $\log(\beta^+/\beta^-)$. *The axes are about* $[10^{-3},\ 10^3] \times [0,\ 100]$.

Algorithm, efficiency analysis

Table 3.4. *The CPU time for Example 3.2 with different parameters using an IBM SP2 machine. The outputs vary with machines.*

N_{finest}	N_b	n_l	N_{coarse}	β^-	β^+	CPU time (s)
130×130	160	5	9	10	1	0.03
258×258	320	6	9	1	1	0.03
258×258	320	6	9	1	100	0.05
258×258	320	6	9	1	10000	0.06
258×258	320	6	9	100	1	0.06
258×258	320	6	9	10000	1	3.29
514×514	640	7	9	1	1000	0.15
514×514	640	7	9	1000	1	0.35

IIM in 3D

- IIM in 3D (Li, Deng,Ito) using a level set representation

$$\Delta u = f(x) + \int_{\Gamma(s_1,s_2)} v(s_1,s_2)\delta(x - X(s_1,s_2))\,ds$$

$$[u] = w(s_1,s_2), \quad [\nabla u \bullet n] = v(s_1,s_2)$$

- A regular grid point: standard central 7-point stencil

$$\sum_{m}^{n_s} \gamma_m U_{i+i_m,j+j_m,k+k_m} - \sigma_{ijk} U_{ijk} = f_{ijk} + C_{ijk},$$

$$\gamma_{i\pm1,j,k} = \frac{\beta_{i\pm1/2,j,k}}{h^2}, \qquad \gamma_{i,j\pm1,k} = \frac{\beta_{i,j\pm1/2,k}}{h^2},$$

$$\gamma_{i,j,k\pm1} = \frac{\beta_{i,j,k\pm1/2}}{h^2},$$

$$\gamma_{i,j,k} = -\left(\sum \gamma_{i\pm1,j,k} + \sum \gamma_{i,j\pm1,k} + \sum \gamma_{i,j,k\pm1} \right),$$

IIM in 3D, at an irregular grid

- A local coordinates

$$\left\{ \begin{array}{lcl} \xi &=& (x-X)\,\alpha_{x\xi} + (y-Y)\,\alpha_{y\xi} + (z-Z)\,\alpha_{z\xi} \\ \eta &=& (x-X)\,\alpha_{x\eta} + (y-Y)\,\alpha_{y\eta} + (z-Z)\,\alpha_{z\eta} \\ \tau &=& (x-X)\,\alpha_{x\tau} + (y-Y)\,\alpha_{y\tau} + (z-Z)\,\alpha_{z\tau}, \end{array} \right.$$

- cosines computed from level set function

$$\boldsymbol{\xi} = \frac{\nabla\varphi}{|\nabla\varphi|} = (\varphi_x,\ \varphi_y,\ \varphi_z)^T \Big/ \sqrt{\varphi_x^2+\varphi_y^2+\varphi_z^2},$$

$$\boldsymbol{\eta} = (\varphi_y,\ -\varphi_x,\ 0)^T \Big/ \sqrt{\varphi_x^2+\varphi_y^2},$$

$$\boldsymbol{\tau} = \frac{\mathbf{s}}{|\mathbf{s}|}, \qquad \text{where} \ \ \mathbf{s} = (\varphi_x\varphi_z,\ \varphi_y\varphi_z,\ -\varphi_x^2-\varphi_y^2)^T.$$

IIM in 3D, at an irregular grid

- Interface relations:
  - 2 given
  - 8 derived
- The rest process is the same
  - Need surface derivatives of jumps

$$
\begin{aligned}
u^+ &= u^- + w, \\
u^+_\xi &= \frac{\beta^-}{\beta^+}\, u^-_\xi + \frac{v}{\beta^+}, \\
u^+_\eta &= u^-_\eta + w_\eta, \\
u^+_\tau &= u^-_\tau + w_\tau, \\
u^+_{\eta\tau} &= u^-_{\eta\tau} + (u^-_\xi - u^+_\xi)\chi_{\eta\tau} + w_{\eta\tau}, \\
u^+_{\eta\eta} &= u^-_{\eta\eta} + (u^-_\xi - u^+_\xi)\chi_{\eta\eta} + w_{\eta\eta}, \\
u^+_{\tau\tau} &= u^-_{\tau\tau} + (u^-_\xi - u^+_\xi)\chi_{\tau\tau} + w_{\tau\tau}, \\
u^+_{\xi\eta} &= \frac{\beta^-}{\beta^+}\, u^-_{\xi\eta} + \left(u^+_\eta - \frac{\beta^-}{\beta^+}\, u^-_\eta\right)\chi_{\eta\eta} + \left(u^+_\tau - \frac{\beta^-}{\beta^+}\, u^-_\tau\right)\chi_{\eta\tau} \\
&\quad + \frac{\beta^-_\eta}{\beta^+}\, u^-_\xi - \frac{\beta^+_\eta}{\beta^+}\, u^+_\xi + \frac{v_\eta}{\beta^+}, \\
u^+_{\xi\tau} &= \frac{\beta^-}{\beta^+}\, u^-_{\xi\tau} + \left(u^+_\eta - \frac{\beta^-}{\beta^+}\, u^-_\eta\right)\chi_{\eta\tau} + \left(u^+_\tau - \frac{\beta^-}{\beta^+}\, u^-_\tau\right)\chi_{\tau\tau} \\
&\quad + \frac{\beta^-_\tau}{\beta^+} u^-_\xi - \frac{\beta^+_\tau}{\beta^+} u^+_\xi + \frac{v_\tau}{\beta^+}, \\
u^+_{\xi\xi} &= \frac{\beta^-}{\beta^+}\, u^-_{\xi\xi} + \left(\frac{\beta^-}{\beta^+} - 1\right) u^-_{\eta\eta} + \left(\frac{\beta^-}{\beta^+} - 1\right) u^-_{\tau\tau} + \\
&\quad u^+_\xi \left(\chi_{\eta\eta} + \chi_{\tau\tau} - \frac{\beta^+_\xi}{\beta^+}\right) - u^-_\xi \left(\chi_{\eta\eta} + \chi_{\tau\tau} - \frac{\beta^-_\xi}{\beta^+}\right) \\
&\quad + \frac{1}{\beta^+}\left(\beta^-_\eta u^-_\eta - \beta^+_\eta u^+_\eta\right) + \frac{1}{\beta^+}\left(\beta^-_\tau u^-_\tau - \beta^+_\tau u^+_\tau\right) \\
&\quad + \frac{1}{\beta^+}\left([\sigma]u^- - \sigma^+[u]\right) + \frac{[f]}{\beta^+} - w_{\eta\eta} - w_{\tau\tau}.
\end{aligned}
$$

IIM in 3D, an example

- Exact soln:

$$u(\mathbf{x}) = \begin{cases} r^2, & \text{if } r \le \frac{1}{2}, \\ (1 - \frac{1}{8\,b} - \frac{1}{b})/4 + (\frac{r^4}{2} + r^2)/b + C\,\log(2r)/b, & \text{if } r > \frac{1}{2}, \end{cases}$$

$$\beta = \begin{cases} x^2 + y^2 + z^2 + 1, & x^2 + y^2 + z^2 \le 1 \\ b, & x^2 + y^2 + z^2 > 1 \end{cases}$$

N	$b = 1$		$b = 10$		$b = 1000$	
	$\Vert E_N \Vert_\infty$	ratio	$\Vert E_N \Vert_\infty$	ratio	$\Vert E_N \Vert_\infty$	ratio
26	1.247×10^{-3}		1.525×10^{-3}		3.485×10^{-3}	
52	3.979×10^{-4}	3.134	5.240×10^{-4}	2.910	1.111×10^{-3}	3.137
104	9.592×10^{-5}	4.148	1.010×10^{-4}	5.188	1.605×10^{-4}	6.922

Zhilin LI

IIM in 3D, example of multi-connected domain

where

$$S_1(x,y,z) = (x-0.2)^2 + 2(y-0.2)^2 + z^2 - 0.01,$$

$$S_2(x,y,z) = 3(x+0.2)^2 + (y+0.2)^2 + z^2 - 0.01.$$

Table 4.2. *A grid refinement analysis for the multi-connected domain with* $M = N = L$.

N	$\beta^+ = 1,\ \beta^- = 1$		$\beta^+ = 1000,\ \beta^- = 1$	
	$\Vert E_N \Vert_\infty$	ratio	$\Vert E_N \Vert_\infty$	ratio
52	3.108×10^{-2}		2.032×10^{-2}	
104	6.758×10^{-3}	4.599	4.771×10^{-3}	4.259

Table 4.3. *Comparison of the CPU time (in seconds) of the SOR method and the AMG method with* $M = N = L$.

N	Example 3.1 in 3D ($b = 10^7$)		Multi-connected domain ($\beta^+ = 10^4,\ \beta^- = 1$)	
	SOR	AMG	SOR	AMG
20	0.21	1.57	0.06	0.83
40	27.51	25.56	29.62	13.89
80	1410.54	265.26	1464.57	265.84