# Solving Interface Problems on Cartesian Grids in the Boundary Integral Formulation

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**Modeling and Simulation of Interface Dynamics in Fluids/Solids and Their Applications**

National University of Singapore, May 14-18, 2018

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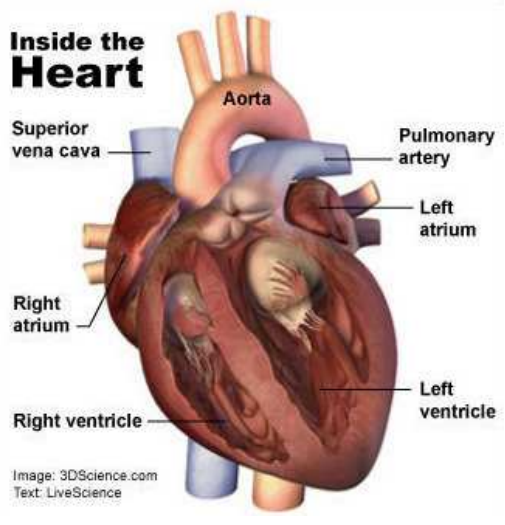
# Outline

- Motivation and Introduction
- Curve & Surface Representation/Discretization
- An Interface Problem around Closely Packed Cells
- The Poisson-Boltzmann Interface Problem
- The Hele-Shaw Free Boundary Problem
- A Stokes Moving Interface Problem

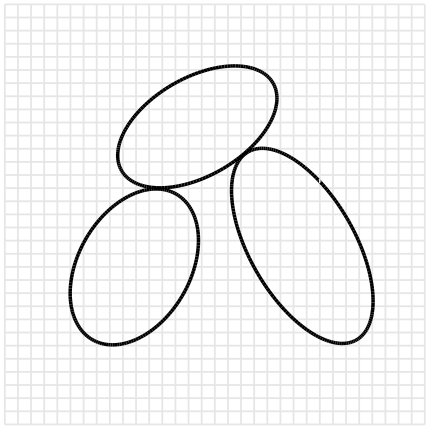
# Motivation and Introduction

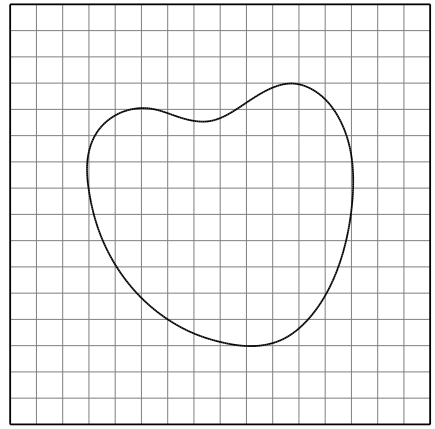
In physics and engineering applications, we often have to solve free boundary and moving interface problems such as

- motion of vesicles (blood cells)
- drops of one viscous fluid in another fluid
- the blood or electrical current flow in the beating heart



# We like Cartesian grid methods

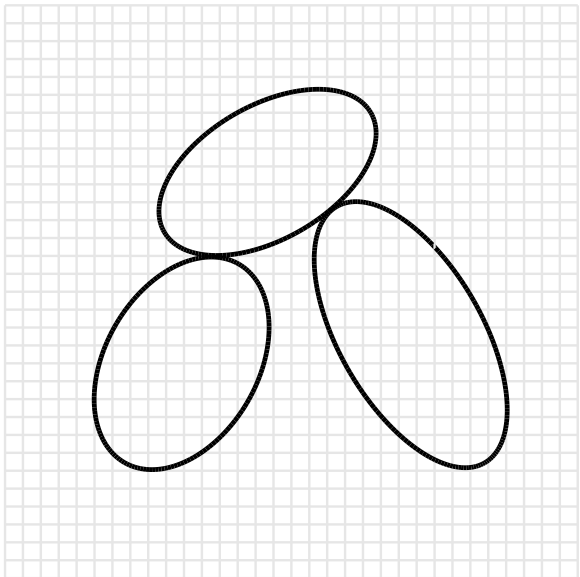


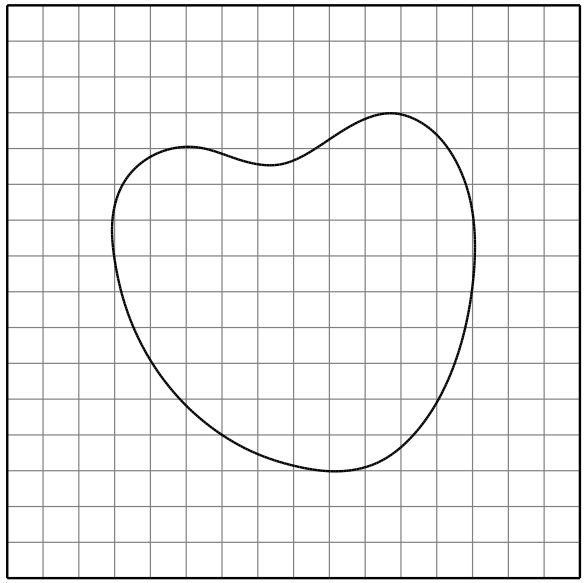


Some well-known Cartesian grid methods:

- Phase field method (Cahn & Hilliard 1958)
- Immersed boundary method (Peskin 1977)
- Grid-based boundary integral method (Mayo 1984)
- Front tracking method (Glimm, 1985)
- Level set method (Osher-Sethian, 1988)
- Immersed interface method (LeVeque & Li 1994)
- Augmented Immersed interface method (Li 1997)

# Reasons to love a special Cartesian grid method





A potential theory based Cartesian grid method takes full advantages of

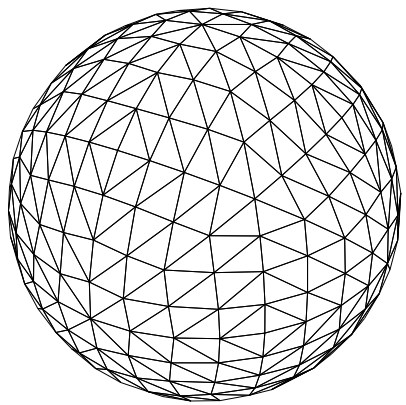
- well-conditioning property of boundary integral equations;
- fast elliptic solvers for the elliptic PDE on Cartesian grids;
- all those good points that a Cartesian grid method has.

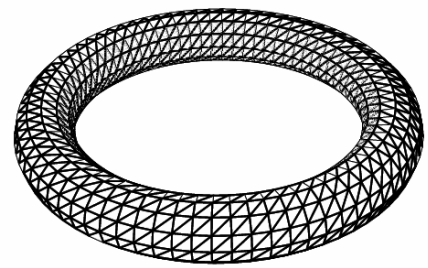
# Curve & Surface

# Representation/Discretization

# How to discretize the boundary, curve and surface?

With the traditional boundary integral method for free boundary and moving interface problems, we avoided the generation of (unstructured) volume grids but still have to discretize the boundary.

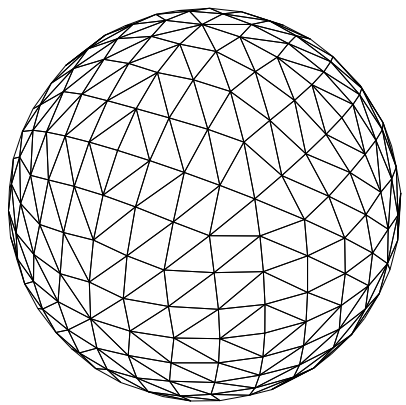


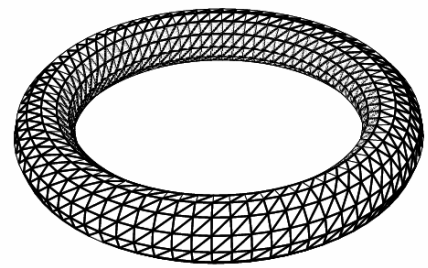


- Do we really need to make unstructured triangulation for the domain boundary/interface?

# How to discretize the boundary, curve and surface?

With the traditional boundary integral method for free boundary and moving interface problems, we avoided the generation of (unstructured) volume grids but still have to discretize the boundary.



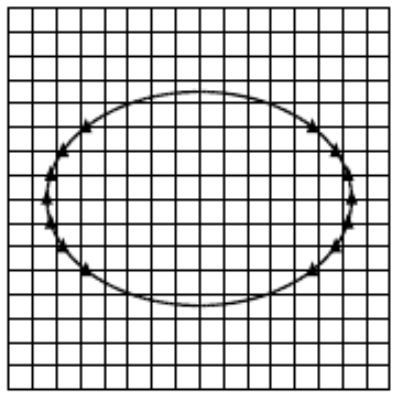


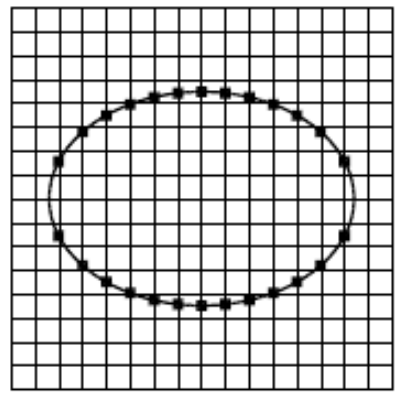
- Do we really need to make unstructured triangulation for the domain boundary/interface?

NO! NO! NO!

# Intersection Points with a Cartesian Grid

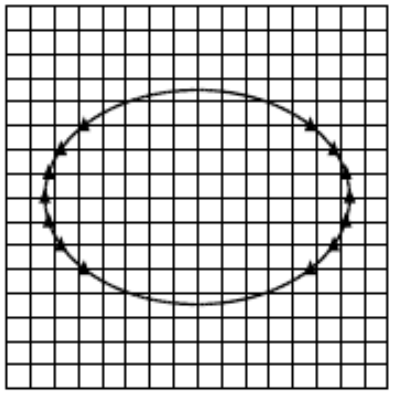
We discretize and represent the curve/surface by its intersection points with an underlying Cartesian grid.

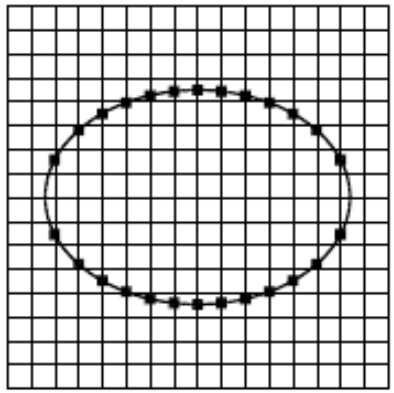


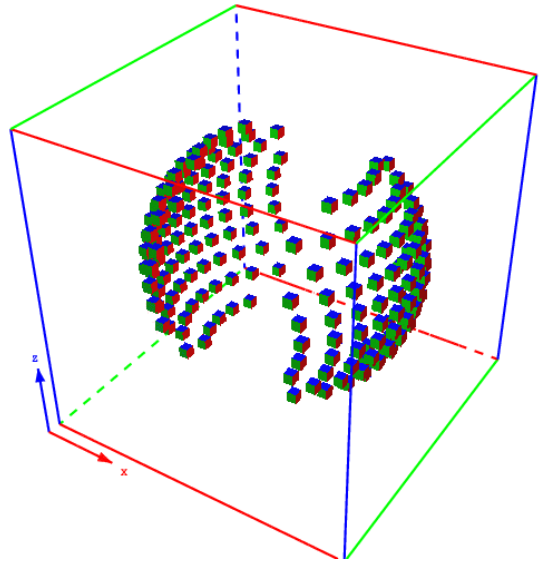


- **Advantage 1**. No triangulation of the surface/boundary is needed for the curve/surface representation and discretization.

# Second advantage of this method

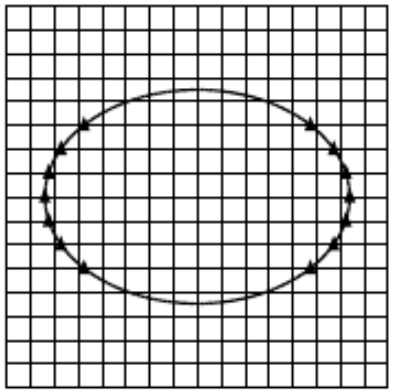


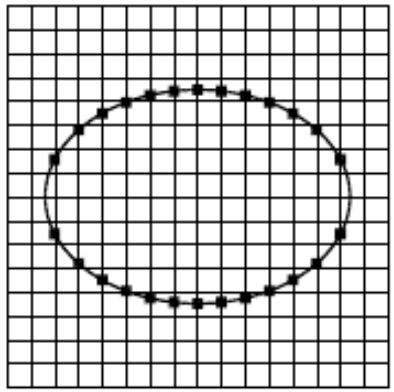


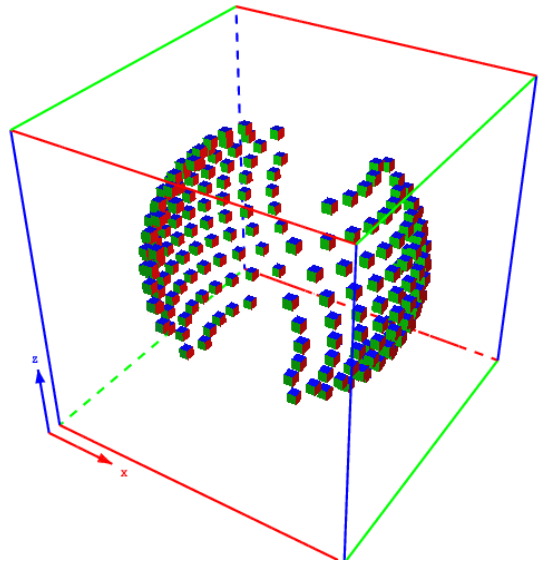


- **Advantage 2**. A locally uniform stencil for interpolation or differentiation can be easily found at any point on the curve/surface.

# Third advantage of this method





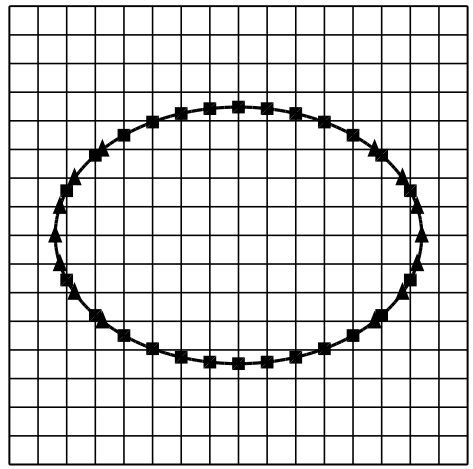


- **Advantage 3**. The intersection points can be used as quadrature points for boundary integrals with super-algebraic convergence (Wilson 2010, Beale-Ying-Wilson 2016).

  Provided $g(\mathbf{x}) \in C^{2m}(\Gamma)$, it can be shown (Wilson, 2010)

$$\left| \int_\Gamma g(\mathbf{x})\, ds_{\mathbf{x}} - h^{d-1} \sum_{\ell=1}^{d} \sum_{\mathbf{x}_j \in R_{h,\ell}} \frac{\rho_\ell(\mathbf{n}(\mathbf{x}_j))\, g(\mathbf{x}_j)}{|\mathbf{n}(\mathbf{x}_j) \cdot \mathbf{e}_\ell|} \right| \leq C h^{2m}$$

# Comments on the Interface Representation Strategy



- W.-J. Ying and W.-C. Wang, A kernel-free boundary integral method for implicitly defined surfaces, Journal of Computational Physics, Vol. 252, pp. 606-624, 2013.

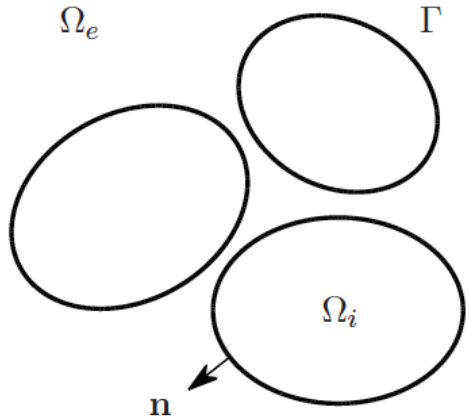
- J. Thomas Beale and W.-J. Ying, Solution of the Dirichlet problem by a finite difference analog of the boundary integral equation, submitted to Numerische Mathematik, 2018.

# I. An Interface Problem on Closely Packed/Clustered Cells

# A Steady-state Interface Problem

Let

$$\Phi(\mathbf{p}) = \begin{cases} \Phi_i(\mathbf{p}) & \mathbf{p} \in \Omega_i \\ \Phi_e(\mathbf{p}) & \mathbf{p} \in \Omega_e \end{cases}.$$




The Laplace equation:

$$\triangle\Phi(\mathbf{p}) = 0 \qquad \mathbf{p} \in \Omega_i \cup \Omega_e.$$

Interface conditions:

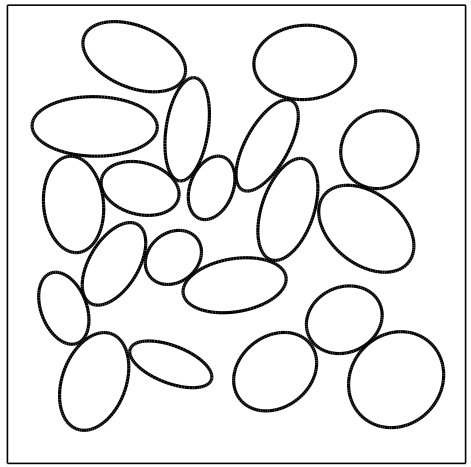
$$\Phi_i(\mathbf{p}) - \Phi_e(\mathbf{p}) = V_m(\mathbf{p}) \qquad \text{on } \Gamma,$$

$$\sigma_i \frac{\partial \Phi_i(\mathbf{p})}{\partial \mathbf{n_p}} - \sigma_e \frac{\partial \Phi_e(\mathbf{p})}{\partial \mathbf{n_p}} = 0 \qquad \text{on } \Gamma.$$

Far field condition:

$$\Phi_e(\mathbf{p}) \to 0 \qquad \text{as } |\mathbf{p}| \to \infty.$$

# Similar Interface Problems



- Drops of one viscous fluid in another fluid, two-phase flows (e.g., Zenchenko 2000, Pozrikidis 2001)
- Motion of vesicles (blood cells) (e.g., Veerapaneni et al. 2011)
- Many other multi-component flows, multiphase materials and evolution of microstructures (e.g., Akaiwa et al. 2001, Thornton et al. 2004, Lowengrub et al. 2007)

# Boundary Integral Equation

Let

$$\psi(\mathbf{p}) = \frac{\partial \Phi_i(\mathbf{p})}{\partial \mathbf{n_p}} - \frac{\partial \Phi_e(\mathbf{p})}{\partial \mathbf{n_p}} \qquad \text{on } \Gamma.$$

The potential $\Phi(\mathbf{p})$ to the interface problem can be represented as

$$\Phi(\mathbf{p}) = \int_\Gamma \frac{\partial G(\mathbf{q}-\mathbf{p})}{\partial \mathbf{n_q}} V_m(\mathbf{q})\, ds_\mathbf{q} - \int_\Gamma G(\mathbf{p}-\mathbf{q})\, \psi(\mathbf{q})\, ds_\mathbf{q}.$$

The boundary integral equation on the interface reads

$$\frac{1}{2}\psi(\mathbf{p}) + \mu \int_\Gamma \frac{\partial G}{\partial \mathbf{n_p}} \psi(\mathbf{q})\, ds_\mathbf{q} = \mu \int_\Gamma \frac{\partial^2 G}{\partial \mathbf{n_p} \partial \mathbf{n_q}} V_m(\mathbf{q})\, ds_\mathbf{q}$$

with $\mu = \dfrac{\sigma_e - \sigma_i}{\sigma_e + \sigma_i} \in (-1, 1)$.

# Boundary Integral Equation (continued)

The boundary integral equation can be re-written concisely as

$$\frac{1}{2}\psi + \mu\,\mathcal{M}^*\psi = \mu\,\mathcal{N}V_m + \jmath_m \qquad \text{on } \Gamma$$

where $\mathcal{M}^*$ and $\mathcal{N}$ are the integral operators defined on the interface

$$\begin{aligned}(\mathcal{M}^*\psi)(\mathbf{p}) &= \frac{\partial}{\partial \mathbf{n_p}} \int_\Gamma G(\mathbf{p}-\mathbf{q})\psi(\mathbf{q})\, ds_\mathbf{q} \\ (\mathcal{N}V_m)(\mathbf{p}) &= \frac{\partial}{\partial \mathbf{n_p}} \int_\Gamma \frac{\partial G(\mathbf{p}-\mathbf{q})}{\partial \mathbf{n_q}} V_m(\mathbf{q})\, ds_\mathbf{q}.\end{aligned}$$

# Iterative methods for the BIE

Since the spectrum of the operator $\mathcal{M}^*$ is contained in the interval $-\frac{1}{2} < \lambda \leq \frac{1}{2}$ (e.g., refer to Kress 1999), the boundary integral equation

$$\frac{1}{2}\psi + \mu\mathcal{M}^*\psi = \mu\mathcal{N}V_m + \jmath_m$$

can be efficiently solved by the Richardson iteration:

$$\psi^{(\nu+1)} = (1-\beta)\,\psi^{(\nu)} + 2\beta\left[(\mu\,\mathcal{N}V_m + \jmath_m) - \mu\,\mathcal{M}^*\psi^{(\nu)}\right]$$

for $\nu = 0, 1, 2, \cdots$, which converges to the exact solution for $0 < \beta < 2/(1+\mu)$.

# Potential solution to the interface problem

After the unknown density $\psi$ is solved from the BIE

$$\frac{1}{2}\psi + \mu\mathcal{M}^*\psi = \mu\mathcal{N}V_m + \jmath_m \qquad \text{on} \quad \Gamma,$$

the potential solution $\Phi(\mathbf{p})$ can be computed by

$$\Phi(\mathbf{p}) = \mathcal{M}V_m - \mathcal{L}\psi \qquad \text{for} \quad \mathbf{p} \in \mathbb{R}^2 \setminus \Gamma.$$

Here, $\mathcal{M}V_m$ and $\mathcal{L}\psi$ are respectively the double layer and single layer boundary integrals given by

$$\begin{aligned} (\mathcal{L}\psi)(\mathbf{p}) &= \int_\Gamma G(\mathbf{p}-\mathbf{q})\psi(\mathbf{q})\, ds_\mathbf{q}, \\ (\mathcal{M}V_m)(\mathbf{p}) &= \int_\Gamma \frac{\partial G(\mathbf{q}-\mathbf{p})}{\partial \mathbf{n}_\mathbf{q}} V_m(\mathbf{q})\, ds_\mathbf{q}. \end{aligned}$$

# An issue on closely packed cells

On closely packed cells, the single layer, double layer, adjoint double layer and hyper-singular boundary integrals,

$$
\begin{aligned}
(\mathcal{L}\psi)(\mathbf{p}) &= \int_\Gamma G(\mathbf{p}-\mathbf{q})\psi(\mathbf{q})\, ds_{\mathbf{q}}, \\
(\mathcal{M}V_m)(\mathbf{p}) &= \int_\Gamma \frac{\partial G(\mathbf{q}-\mathbf{p})}{\partial \mathbf{n}_{\mathbf{q}}} V_m(\mathbf{q})\, ds_{\mathbf{q}}, \\
(\mathcal{M}^*\psi)(\mathbf{p}) &= \frac{\partial}{\partial \mathbf{n}_{\mathbf{p}}} \int_\Gamma G(\mathbf{p}-\mathbf{q})\psi(\mathbf{q})\, ds_{\mathbf{q}}, \\
(\mathcal{N}V_m)(\mathbf{p}) &= \frac{\partial}{\partial \mathbf{n}_{\mathbf{p}}} \int_\Gamma \frac{\partial G(\mathbf{p}-\mathbf{q})}{\partial \mathbf{n}_{\mathbf{q}}} V_m(\mathbf{q})\, ds_{\mathbf{q}},
\end{aligned}
$$

become nearly singular. It is hard to accurately evaluate the nearly singular boundary integrals with the standard quadrature method (e.g., Atkinson 1997).

# Source of the nearly singularity

For example, when the evaluation point $\mathbf{p}$ on one component of the interface is very close to another component of the interface $\Gamma$, the double layer potential

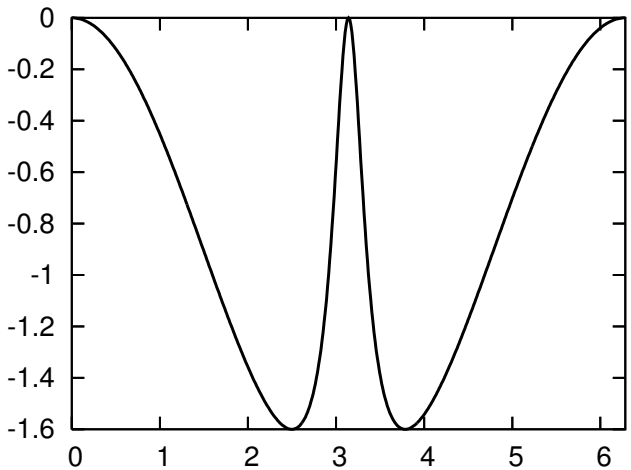
$$\mathcal{M}\varphi(\mathbf{p}) = \int_{\Gamma} \mathbf{n_q} \cdot \nabla G(\mathbf{q}-\mathbf{p})\, \varphi(\mathbf{q})\, d\mathbf{s_q}$$

with

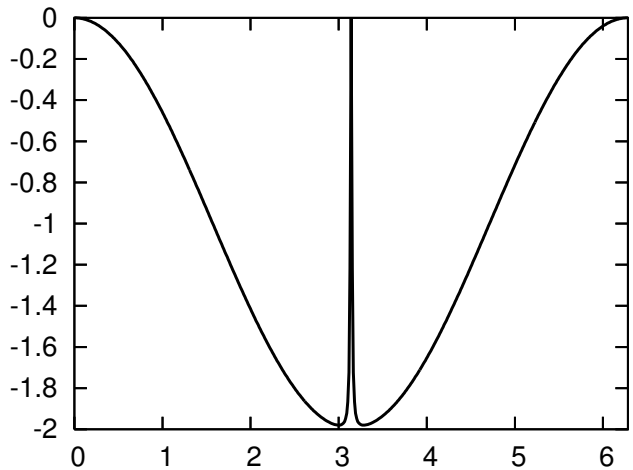
$$G(\mathbf{q}-\mathbf{p}) = \frac{1}{2\pi} \ln|\mathbf{q}-\mathbf{p}| \quad \text{and} \quad \nabla G(\mathbf{q}-\mathbf{p}) = \frac{1}{2\pi} \frac{\mathbf{q}-\mathbf{p}}{|\mathbf{q}-\mathbf{p}|^2}$$

is a nearly singular integral because in this case the kernel behaves like $|\mathbf{q}-\mathbf{p}|^{-1}$ and has very large variation.

# Two Plots of Nearly Singular Integrand Function




(a) $\rho = 0.8$




(b) $\rho = 0.9$

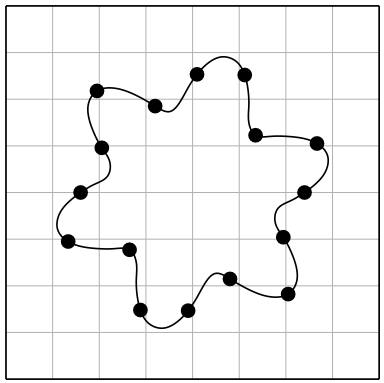
Figure: Integrand function at a point close to a circular curve

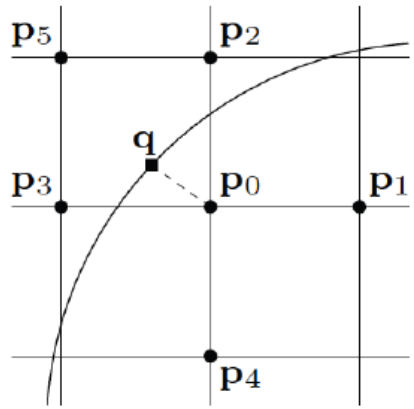
# People are working hard on nearly singular integrals

- Use a large number of points in the Nyström method
- Locally interpolate the density of a boundary integral and then evaluate at a set of finer points (Atkinson 1997, Gedney 2003)
- Structured grid-based correction method (Mayo 1985, McKenney 1996, Strain 2007)
- Regularization and asymptotic analysis-based method (Goodman 1990, Schwab-Wendland 1992, Lowengrub 1993, Beale and Lai 2001/2004, Ying-Beale 2013)
- Recent quadrature-by-expansion (QBX) Nyström method (Klöckner, Barnett and L. Greengard et al. 2012)
- Many other works, including Bremer et. al. 2010, Helsing and Ojala 2008, Helsing, 2009, 2013 and Barnett 2013.

# A Cartesian grid-based evaluation method

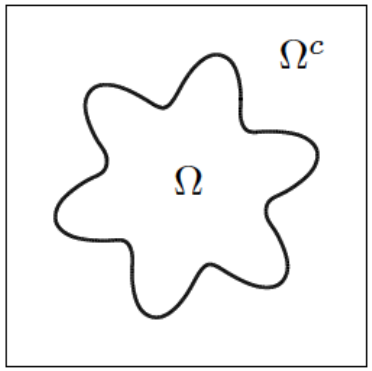
**Main idea**: use a Cartesian grid-based solution to approximate a boundary or volume integral (generalization of A. Mayo 1984 and Z. Li 1997).

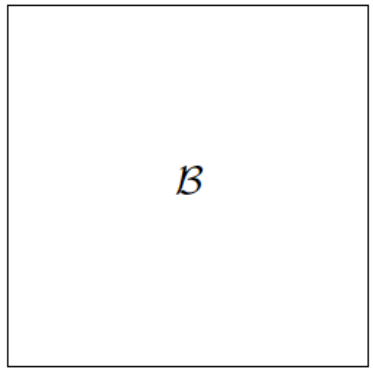





- **Step 1**. on a Cartesian grid, solve an equivalent, simple interface problem, whose solution is the boundary or volume integral to be evaluated.
- **Step 2**. interpolate the grid solution to get values of the boundary integral at discretization points of the interface.

# Reinterpretation of the double layer boundary integral

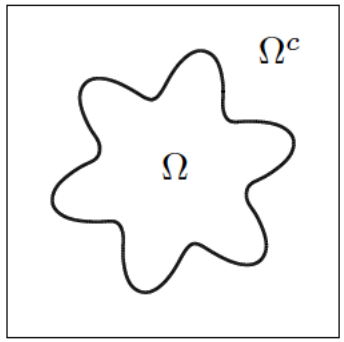


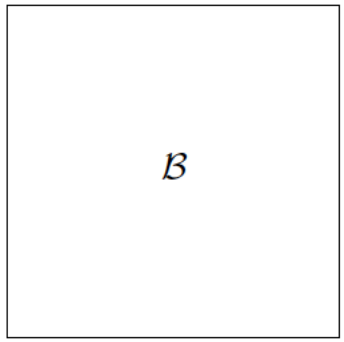




The double layer boundary integral $w = \mathcal{M}\varphi = \int_\Gamma \frac{\partial G}{\partial \mathbf{n}} \varphi \, ds$ is the solution to the simple interface problem,

$$
\begin{aligned}
\triangle w &= 0 \quad \text{in } \mathcal{B} \setminus \Gamma, \\
w^+ &= w^- + \varphi \quad \text{on } \Gamma, \\
\mathbf{n} \cdot \nabla w^+ &= \mathbf{n} \cdot \nabla w^- \quad \text{on } \Gamma, \\
w &= \mathcal{M}\varphi \quad \text{on } \partial\mathcal{B}.
\end{aligned}
$$

# Reinterpretation of the single layer boundary integral



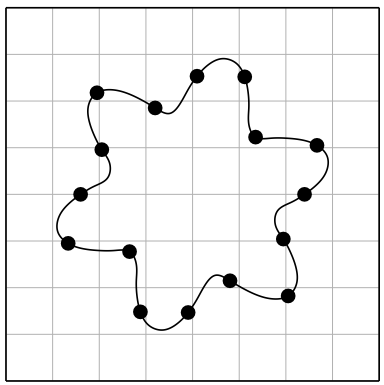



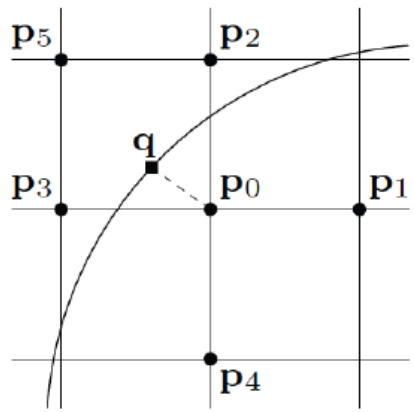

The single layer potential $v(\mathbf{p}) = -\mathcal{L}\psi = -\int_\Gamma G(\mathbf{q},\mathbf{p})\psi\, ds_\mathbf{q}$ is the solution to the simple interface problem,

$$\begin{aligned}
\triangle v &= 0 \quad \text{in } \mathcal{B}\setminus\Gamma,\\
v^+ &= v^- \quad \text{on } \Gamma,\\
\mathbf{n}\cdot\nabla v^+ &= \mathbf{n}\cdot\nabla v^- + \psi \quad \text{on } \Gamma,\\
v &= -\mathcal{L}\psi \quad \text{on } \partial\mathcal{B}.
\end{aligned}$$

# Same for the adjoint and hyper-singular integrals

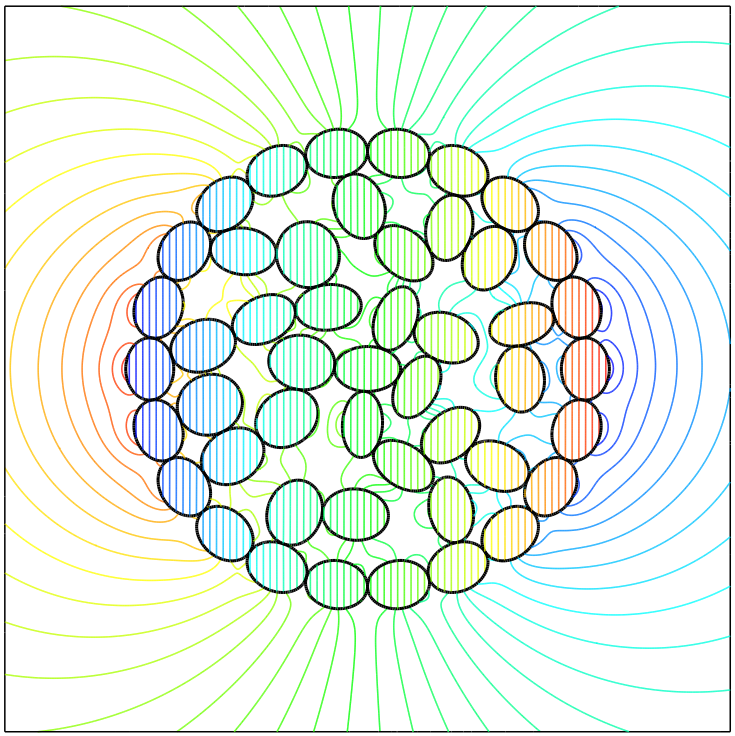
For the adjoint double layer and hyper-singular boundary integrals, $\mathcal{M}^*\psi$ and $\mathcal{N}\varphi$, we also solve the same simple interface problems that are equivalent to $\mathcal{L}\psi$ and $\mathcal{M}\varphi$. The only difference is at the interpolation part of the two-step procedure below.

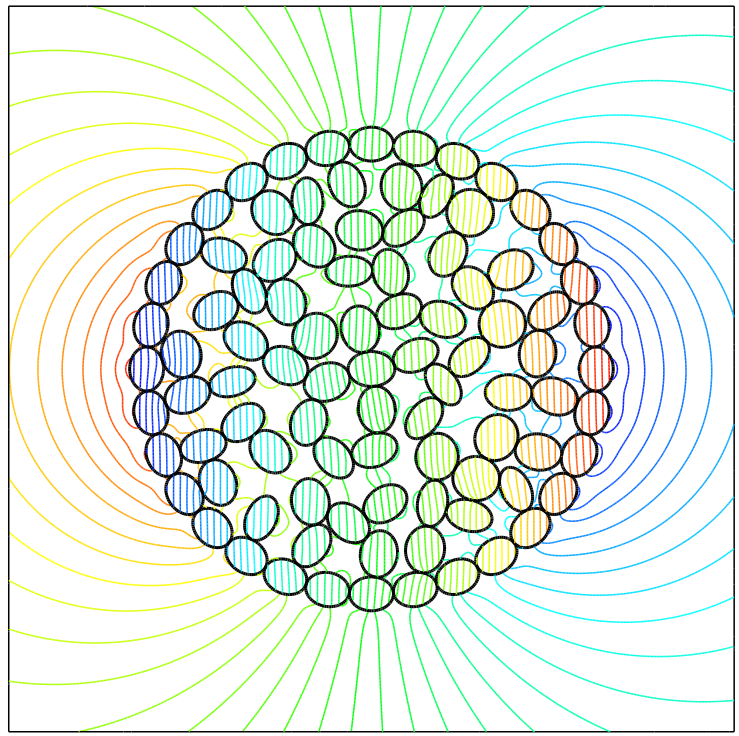





- **Step 1**. on a Cartesian grid, solve a simple interface problem, whose solution is $\mathcal{L}\psi$ or $\mathcal{M}\varphi$.
- **Step 2**. interpolate the grid solution to get normal derivatives of $\mathcal{L}\psi$ or $\mathcal{M}\varphi$ at discretization points of the interface.

# Numerical solutions by the Cartesian Grid Method





# Numerical results of the example with 48 random cells

Table: results by a second-order version of the Cartesian grid method

| grid size | $512^2$ | $1024^2$ | $2048^2$ | $4096^2$ |
|---|---|---|---|---|
| M | 32 | 64 | 128 | 256 |
| #Richardson | 36 | 35 | 35 | 36 |
| $\|\mathbf{e}_h^{int}\|_\infty$ | 2.31E-1 | 2.47E-2 | 3.60E-3 | 2.51E-4 |
| $\|\mathbf{e}_h^{ext}\|_\infty$ | 1.97E-1 | 2.13E-2 | 3.46E-3 | 2.69E-4 |
| CPU (secs) | 1.01E+1 | 3.91E+1 | 1.58E+2 | 6.54E+2 |

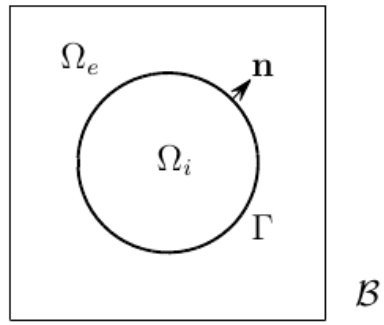
Table: results by a fourth-order version of the Cartesian grid method

| grid size | $512^2$ | $1024^2$ | $2048^2$ | $4096^2$ |
|---|---|---|---|---|
| M | 32 | 64 | 128 | 256 |
| #Richardson | 38 | 35 | 36 | 36 |
| $\|\mathbf{e}_h^{int}\|_\infty$ | 8.73E-2 | 3.54E-3 | 2.81E-4 | 9.72E-6 |
| $\|\mathbf{e}_h^{ext}\|_\infty$ | 5.52E-2 | 2.80E-3 | 2.70E-4 | 9.42E-6 |
| CPU (secs) | 1.40E+1 | 4.82E+1 | 1.93E+2 | 7.89E+2 |

# II. The Poisson-Boltzmann interface problem in biophysics

# The Poisson-Boltzmann interface problem

Assume $\Omega_i \cap \Omega_e = \emptyset$, $\partial\Omega_i \cap \partial\Omega_e = \Gamma$ and $\Omega_i \cup \Gamma \cup \Omega_e = \mathcal{B}$.




The Poisson-Boltzmann interface problem reads

$$\begin{aligned} \nabla \cdot (\epsilon_i \nabla u_i) &= \rho_i && \text{in } \Omega_i, \\ \nabla \cdot (\epsilon_e \nabla u_e) - \kappa^2 \sinh(u_e) &= \rho_e && \text{in } \Omega_e, \end{aligned}$$

subject to the interface conditions

$$u_i - u_e = g \quad \text{and} \quad \epsilon_i \, \partial_{\mathbf{n}} u_i - \epsilon_e \, \partial_{\mathbf{n}} u_e = J \qquad \text{on } \Gamma$$

and the boundary condition $u_e = 0$ on $\partial\mathcal{B}$.

# Computational difficulties

- Heterogeneity and nonlinearity of the PDE

$$\begin{aligned} \nabla \cdot (\epsilon_i \nabla u_i) &= \rho_i \qquad \text{in } \Omega_i, \\ \nabla \cdot (\epsilon_e \nabla u_e) - \kappa^2 \sinh(u_e) &= \rho_e \qquad \text{in } \Omega_e. \end{aligned}$$

- Geometric complexity of the interface $\Gamma$ (such as the surface of macro-molecules)
- Discontinuities of the potential or its normal derivative across the interface

$$u_i - u_e = g \quad \text{and} \quad \epsilon_i \, \partial_{\mathbf{n}} u_i - \epsilon_e \, \partial_{\mathbf{n}} u_e = J \qquad \text{on } \Gamma$$

Refer to the review paper by Lu-Zhou-Holst-McCammon (2008).

# The linearized PBE is a variable coefficient PBE

We solve the nonlinear PBE with the Newton method.

The linearized PBE in the $m^{th}$ Newton iteration is a variable coefficient PB equation

$$\nabla \cdot \left(\epsilon_e \nabla\right) u_e^{m+1} - \kappa^2 \cosh\left(u_e^m\right) u_e^{m+1} = \epsilon_e f_e^m$$

with

$$f_e^m = \epsilon_e^{-1}\left[\rho_e + \kappa^2 \sinh\left(u_e^m\right) - \kappa^2 \cosh\left(u_e^m\right) u_e^m\right].$$

# The linearized PBE by the Cartesian grid method

The linearized Poisson-Boltzmann interface problem,

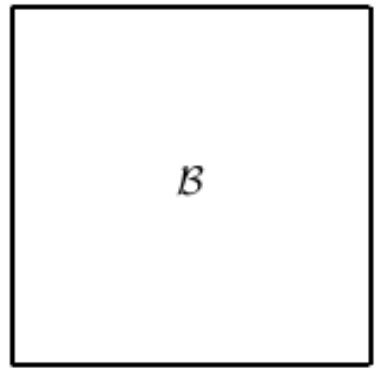
$$\begin{aligned} \nabla \cdot (\epsilon_i \nabla u_i^{m+1}) &= \epsilon_i f_i \qquad \text{in } \Omega_i, \\ \nabla \cdot (\epsilon_e \nabla u_e^{m+1}) - \kappa^2 \cosh(u_e^m)\, u_e^{m+1} &= \epsilon_e f_e^m \qquad \text{in } \Omega_e, \end{aligned}$$

subject to the interface conditions

$$u_i^{m+1} - u_e^{m+1} = g \quad \text{and} \quad \epsilon_i\, \partial_{\mathbf{n}} u_i^{m+1} - \epsilon_e\, \partial_{\mathbf{n}} u_e^{m+1} = J \qquad \text{on } \Gamma$$

and the boundary condition $u_e^{m+1} = 0$ on $\partial\mathcal{B}$, is solved with the Cartesian grid based boundary integral method.

# Two Green's functions




We introduce two Green's functions $G = G(\mathbf{q};\mathbf{p})$ and $K = K(\mathbf{q};\mathbf{p})$ that satisfy, for $\mathbf{p} \in \mathcal{B}$,

$$\begin{aligned} \triangle G(\mathbf{q};\mathbf{p}) &= \delta(\mathbf{q}-\mathbf{p}) \qquad \mathbf{q} \in \mathcal{B} \\ G(\mathbf{q};\mathbf{p}) &= 0 \qquad \mathbf{q} \in \partial\mathcal{B} \end{aligned}$$

and

$$\begin{aligned} \triangle K(\mathbf{q};\mathbf{p}) - \epsilon_e^{-1}\kappa^2 \cosh(u_e^m)\, K(\mathbf{q};\mathbf{p}) &= \delta(\mathbf{q}-\mathbf{p}) \qquad \mathbf{q} \in \mathcal{B} \\ K(\mathbf{q};\mathbf{p}) &= 0 \qquad \mathbf{q} \in \partial\mathcal{B}. \end{aligned}$$

# Boundary and Volume Integrals

For functions $\psi(\mathbf{q})$ and $\varphi(\mathbf{q})$ defined on the interface $\Gamma$, let

$$L_e\psi \equiv \int_\Gamma K(\mathbf{q};\mathbf{p})\psi(\mathbf{q})\,ds_\mathbf{q}, \quad M_i\varphi \equiv \int_\Gamma \frac{\partial G(\mathbf{q};\mathbf{p})}{\partial \mathbf{n}_\mathbf{q}}\varphi(\mathbf{q})\,ds_\mathbf{q}$$

be the single layer and double layer boundary integrals,

$$M_e^*\psi \equiv \int_\Gamma \frac{\partial K(\mathbf{q};\mathbf{p})}{\partial \mathbf{n}_\mathbf{p}}\psi(\mathbf{q})\,ds_\mathbf{q}, \quad N_i\varphi \equiv \frac{\partial}{\partial \mathbf{n}_\mathbf{p}}\int_\Gamma \frac{\partial G(\mathbf{q};\mathbf{p})}{\partial \mathbf{n}_\mathbf{q}}\varphi(\mathbf{q})\,ds_\mathbf{q}$$

be the adjoint double layer and hyper-singular boundary integrals, and

$$\mathcal{G}\rho_i \equiv \int_{\Omega_i} G(\mathbf{q};\mathbf{p})f_i(\mathbf{q})\,d\mathbf{q}, \quad \mathcal{K}\rho_e^m \equiv \int_{\Omega_e} K(\mathbf{q};\mathbf{p})f_e^m(\mathbf{q})\,d\mathbf{q}.$$

be the interior and exterior volume integrals, respectively.

# Boundary Integral Equations

In terms of the boundary and volume integral operators, we get the boundary integral system below

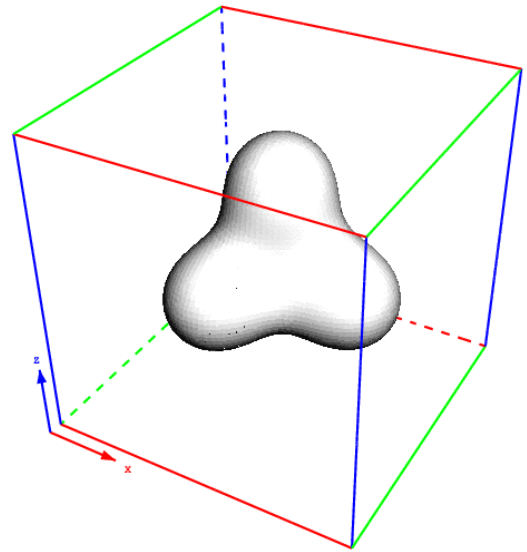
$$\begin{bmatrix} 1/2 + M_i & L_e \\ \mu N_i & 1/2 + M_e^* \end{bmatrix} \begin{bmatrix} \varphi^{m+1} \\ \psi^{m+1} \end{bmatrix} = \begin{bmatrix} g + \mathcal{K}\rho_e^m - \mathcal{G}\rho_i \\ J/\epsilon_e + \partial_{\mathbf{n_p}}(\mathcal{K}\rho_e^m - \mu\,\mathcal{G}\rho_i) \end{bmatrix}.$$

The solution to the linearized Poisson-Boltzmann interface problem is computed by

$$\begin{aligned} u_i^{m+1}(\mathbf{p}) &= \mathcal{G}f_i + M_i\,\varphi^{m+1} \qquad \text{in } \Omega_i, \\ u_e^{m+1}(\mathbf{p}) &= \mathcal{K}f_e^m - L_e\psi^{m+1} \qquad \text{in } \Omega_e. \end{aligned}$$

**Remark:** All boundary and volume integrals encountered are evaluated by the Cartesian grid-based boundary integral method.

# Numerical Results for the Nonlinear PBE in 3D

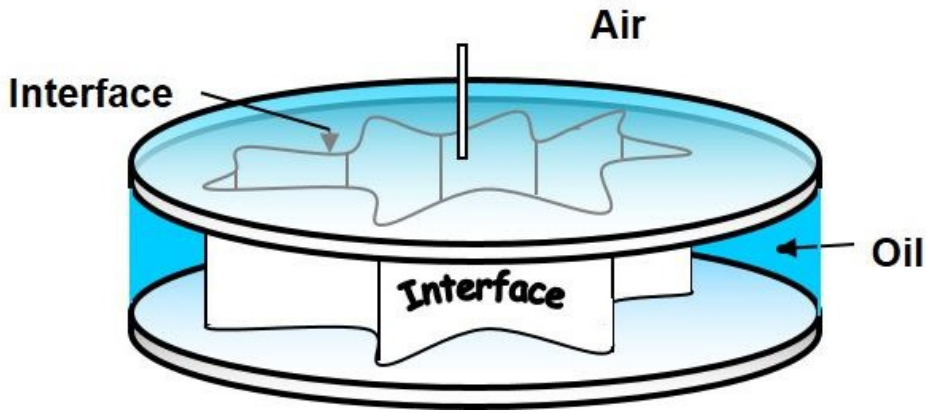


| grid size | #NEWTON | #GMRES | $\|e_h\|_\infty$ | CPU (sec) |
|---|---|---|---|---|
| $128^3$ | 4 | 16 | 1.89E-4 | 3.60E+2 |
| $256^3$ | 4 | 16 | 4.73E-5 | 2.86E+3 |
| $512^3$ | 4 | 16 | 1.45E-5 | 2.53E+4 |

$u_i = exp(x - 0.6y + 0.8z)$ and $u_e = \sin(\pi x)\sin(\pi y)\sin(\pi z)$.
$\mathcal{B} = (-1, 1)^3$, $\epsilon_i = 1$, $\epsilon_e = 4$ and $\kappa = 1$. $\text{tol}_{newton} = 10^{-8}$, $\text{tol}_{gmres} = 10^{-8}$, and $\text{tol}_{multigrid} = 10^{-10}$.

# III. The Hele-Shaw Free Boundary Problem

# The Hele-Shaw Flow Problem




Experiment: two parallel, closely spaced plates sandwich a viscous fluid; another less viscous fluid is injected into the system; the interface experiences Saffman-Taylor instability.

Saffman-Taylor instability $\rightarrow$ Viscous Fingering

- Application: oil recovery in petroleum engineering, crystal growth, tumor growth

# The Hele-Shaw Flow Problem (PDEs)

Let $\Omega(t) \subset \mathbb{R}^2$ be an unbounded domain with smooth boundary $\Gamma(t)$, which depends on time $t > 0$. The pressure unknown $p = p(\mathbf{x})$ satisfies the Poisson equation

$$\begin{aligned} \triangle p &= J\,\delta(\mathbf{x}-\mathbf{z}) \qquad \text{in } \Omega(t), \\ p &= \sigma\kappa \qquad \text{on } \Gamma(t). \end{aligned}$$

Let $\mathbf{n}$ be the unit outward normal on the boundary $\Gamma(t)$. The boundary $\Gamma(t)$ moves by the velocity $\partial_{\mathbf{n}} p$ in the direction of $\mathbf{n}$. For a point $\mathbf{x}(t) \in \Gamma(t)$, its motion is governed by the ODE

$$\mathbf{n} \cdot \frac{d\mathbf{x}(t)}{dt} = \frac{\partial p}{\partial \mathbf{n}}.$$

# Boundary Integral Equation Formulation

Let $v(\mathbf{x}) = \dfrac{J}{2\pi} \ln |\mathbf{x} - \mathbf{z}|$. We first solve the equivalent BIE

$$-\frac{1}{2}\varphi(\mathbf{x}) + \int_{\Gamma(t)} \frac{\partial G(\mathbf{y}, \mathbf{x})}{\partial \mathbf{n}_\mathbf{y}} \varphi(\mathbf{y})\, ds_\mathbf{y} = -v(\mathbf{x}) + \sigma\kappa \qquad \text{for } \mathbf{x} \in \Gamma(t),$$

then compute the normal derivative

$$\frac{\partial \mathbf{w}(\mathbf{x})}{\partial \mathbf{n}_\mathbf{x}} = \frac{\partial}{\partial \mathbf{n}_\mathbf{x}} \int_{\Gamma(t)} \frac{\partial G(\mathbf{y}, \mathbf{x})}{\partial \mathbf{n}_\mathbf{y}} \varphi(\mathbf{y})\, ds_\mathbf{y} \qquad \text{for } \mathbf{x} \in \Gamma(t),$$

finally move a point $\mathbf{x}$ on the curve $\Gamma(t)$ by the ODE

$$\mathbf{n} \cdot \frac{d\mathbf{x}(t)}{dt} = \frac{\partial w(\mathbf{x})}{\partial \mathbf{n}} + \frac{\partial v(\mathbf{x})}{\partial \mathbf{n}}.$$

# Rescaling

A rescaling technique (Li-Lowengrub-Leo, 2007) and (Zhao-Ying-Lowengrub-Li, 2017) is applied so that the domain area is unchanged during the simulation.

Rescale the spatial and temporal variables, $(x, t) \to (\bar{\mathbf{x}}, \bar{t})$:

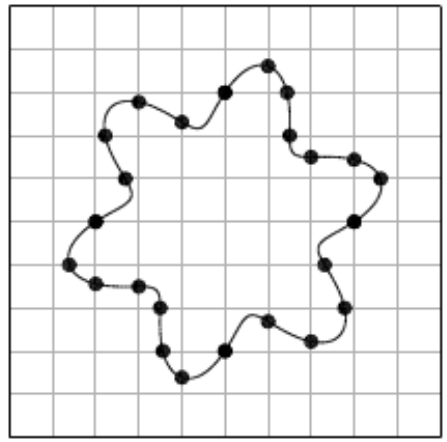
$$\mathbf{x}(\alpha, t) = \bar{R}(\bar{t})\bar{\mathbf{x}}(\alpha, \bar{t}), \quad \bar{t} = \int_0^t \frac{1}{\bar{\rho}(t')} dt'.$$

- the normal velocity in the rescaled frame $\bar{V}$,

$$\bar{V}(\bar{t}) = \frac{\bar{\rho}}{\bar{R}} V(t(\bar{t})) - \frac{\bar{\mathbf{x}} \cdot \mathbf{n}}{\bar{R}} \frac{d\bar{R}}{d\bar{t}}$$

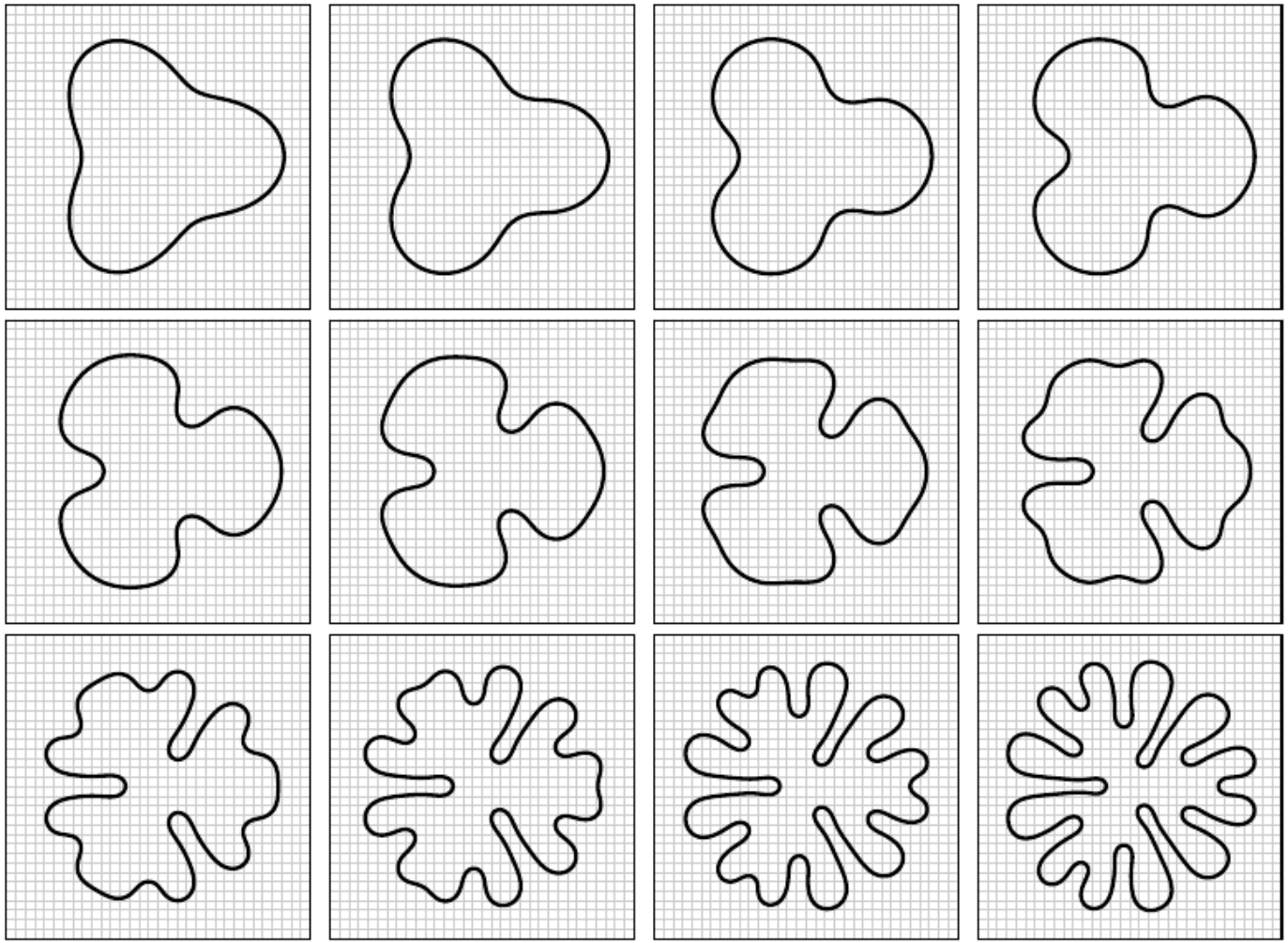
- $\frac{d\bar{A}}{d\bar{t}} = \frac{1}{2} \int_{\bar{\Gamma}(\bar{t})} \bar{\mathbf{n}} \cdot \frac{d\bar{\mathbf{x}}}{d\bar{t}} d\bar{s} = \frac{1}{2} \int_{\bar{\Gamma}(\bar{t})} \bar{V} d\bar{s} = 0 \to \frac{d\bar{R}}{d\bar{t}} = \frac{\pi \bar{\rho} \bar{J}}{\bar{A}(0)\bar{R}}$

# Procedure for the Interface Moving

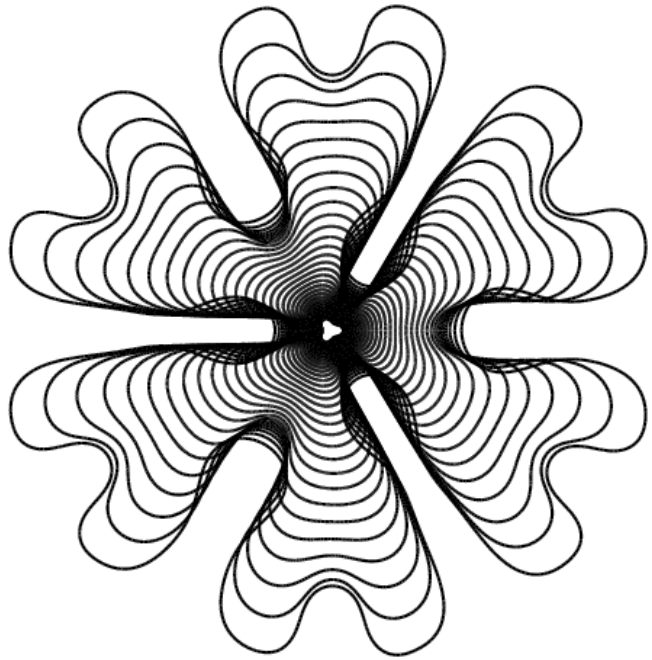


- **Step A**. find the intersection points of the initial interface with an underlying Cartesian grid.
- **Step B**. solve the BIE and move the intersection points explicitly with the computed velocities.
- **Step C**. construct local parabolic curves or surfaces to find their intersection points with the underlying Cartesian grid; go back to **Step A** and continue the interface advancing.

# Snapshots of the rescaled Hele-Shaw interfaces



# Free Boundaries by the Hele-Shaw Flow



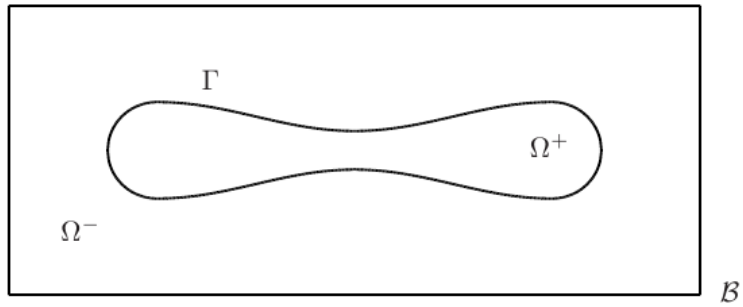
The initial curve is the three-fold curve

$$\begin{cases} x(\theta) &= [1-\delta+\delta\cos(3\theta)]\cos\theta \\ y(\theta) &= [1-\delta+\delta\cos(3\theta)]\sin\theta \end{cases} \qquad \text{for} \quad \theta \in [0,\, 2\pi),$$

with $\delta = 0.2$.

# IV. A Moving Interface Problem of the Stokes Equations

# An Interface Problem of the Stokes Equations



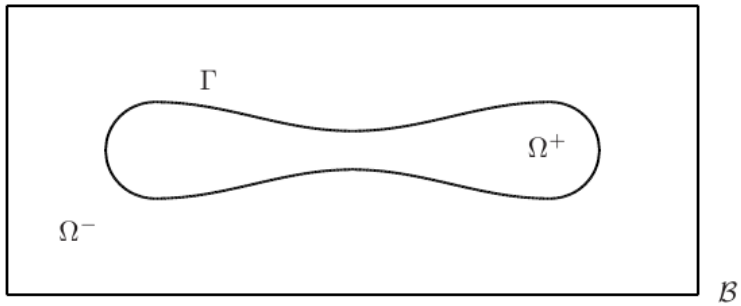

Let

$$\boldsymbol{\sigma}^{\pm} = \boldsymbol{\sigma}^{\pm}(\mathbf{u}^{\pm}, p^{\pm}) = -p^{\pm}\mathbf{I} + \mu^{\pm}\left(\nabla\mathbf{u}^{\pm} + (\nabla\mathbf{u}^{\pm})^{T}\right)$$

be the stress tensors. The Stokes equations read

$$\begin{aligned}
-\mu^{+}\triangle\mathbf{u}^{+} + \nabla p^{+} &= 0 \quad \text{in } \Omega^{+},\\
-\mu^{-}\triangle\mathbf{u}^{-} + \nabla p^{-} &= 0 \quad \text{in } \Omega^{-},\\
\nabla\cdot\mathbf{u}^{+} &= 0 \quad \text{in } \Omega^{+},\\
\nabla\cdot\mathbf{u}^{-} &= 0 \quad \text{in } \Omega^{-}.
\end{aligned}$$

# A Stokes Interface Problem (continued)




The two-phase Stokes flow is subject to the interface condition

$$\begin{aligned} \mathbf{u}^+ - \mathbf{u}^- &= 0 \qquad \text{on } \Gamma(t), \\ \boldsymbol{\sigma}^+ \mathbf{n} - \boldsymbol{\sigma}^- \mathbf{n} &= \gamma \kappa \, \mathbf{n} \qquad \text{on } \Gamma(t), \end{aligned}$$

and the "no-slip" boundary conditions

$$\mathbf{u} = 0 \qquad \text{on } \partial\mathcal{B}.$$

The normal velocity of a point on the interface $\Gamma(t)$ is given by

$$\mathbf{n} \cdot \frac{\partial \mathbf{x}}{\partial t} = \mathbf{n} \cdot \mathbf{u} \qquad \text{on } \Gamma(t).$$

In order to rewrite the interface problem of PDEs as boundary integral equations, we introduce two scaled pressure variables

$$q^+ = \frac{p^+}{\mu^+} \quad \text{and} \quad q^- = \frac{p^-}{\mu^-}.$$

Then we replace the momentum equations by

$$\begin{aligned} \triangle \mathbf{u}^+ - \nabla q^+ &= 0 \qquad \text{in } \Omega^+, \\ \triangle \mathbf{u}^- - \nabla q^- &= 0 \qquad \text{in } \Omega^-. \end{aligned}$$

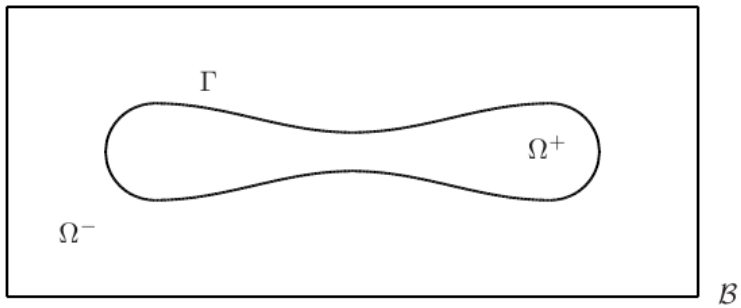
Let

$$\boldsymbol{\tau}^\pm = \boldsymbol{\tau}^\pm(\mathbf{u}^\pm, q^\pm) = -q^\pm \mathbf{I} + \left(\nabla \mathbf{u}^\pm + (\nabla \mathbf{u}^\pm)^T\right)$$

be the scaled stress tensors. We replace the second interface condition by

$$\mu^+ \boldsymbol{\tau}^+ \mathbf{n} - \mu^- \boldsymbol{\tau}^- \mathbf{n} = \gamma \kappa \, \mathbf{n} \qquad \text{on } \Gamma(t).$$

# Green's functions




Let $(\mathbf{G}_{\mathbf{v}}^{(k)}, G_q^{(k)})$ be the Green function pair of the Stokes equations

$$\begin{aligned} \Delta \mathbf{G}_{\mathbf{v}}^{(k)} + \nabla G_q^{(k)} &= \mathbf{e}^{(k)} \delta(\mathbf{x} - \mathbf{y}) \quad \text{in } \mathcal{B}, \\ \nabla \cdot \mathbf{G}_{\mathbf{v}}^{(k)} &= 0 \quad \text{in } \mathcal{B}, \\ \mathbf{G}_{\mathbf{v}}^{(k)} &= 0 \quad \text{on } \partial\mathcal{B}, \end{aligned}$$

for $k = 1, \cdots, d$. Here, $\mathbf{e}^k$ is the $k^{th}$ unit vector in $\mathbb{R}^d$.

# Derivation of Boundary Integral Equations

The velocity to the Stokes interface problem takes the form

$$u_k = -\int_\Gamma \mathbf{G}_{\mathbf{u}}^{(k)} \cdot \boldsymbol{\psi}\, ds$$

for $k = 1, \cdots, d$, with the density $\boldsymbol{\psi} = \boldsymbol{\tau}^+\mathbf{n} - \boldsymbol{\tau}^-\mathbf{n} \in \mathbb{R}^d$.
By the discontinuity properties of $\boldsymbol{\tau}^\pm\mathbf{n}$, we have

$$\begin{aligned} \boldsymbol{\tau}^+\mathbf{n} &= \frac{1}{2}\boldsymbol{\psi} + \mathcal{T}(\boldsymbol{\psi}) \qquad \text{on } \Gamma, \\ \boldsymbol{\tau}^-\mathbf{n} &= -\frac{1}{2}\boldsymbol{\psi} + \mathcal{T}(\boldsymbol{\psi}) \qquad \text{on } \Gamma. \end{aligned}$$

Here, $\mathcal{T}$ is the traction operator.

# Boundary Integral Equations

By the discontinuity properties above, from the interface condition,

$$\mu^+ \boldsymbol{\tau}^+ \mathbf{n} - \mu^- \boldsymbol{\tau}^- \mathbf{n} = \gamma \kappa \, \mathbf{n} \qquad \text{on} \quad \Gamma(t),$$

we get the second kind Fredholm BIEs

$$\frac{1}{2}\boldsymbol{\psi} + \omega \mathcal{T}(\boldsymbol{\psi}) = \frac{\gamma \kappa}{\mu^+ + \mu^-} \mathbf{n} \qquad \text{on} \quad \Gamma.$$

Here, $\omega = \dfrac{\mu^+ - \mu^-}{\mu^+ + \mu^-}$ is the Atwood ratio.

We may also solve the corresponding discrete system by a Krylov subspace iterative method with the boundary integral $\mathcal{T}(\boldsymbol{\psi})$ evaluated indirectly.

# Simple Interface Problem for the Integral Evaluation

The single layer boundary integral

$$u_k = -\int_\Gamma \mathbf{G}_{\mathbf{u}}^{(k)} \cdot \boldsymbol{\psi}\, ds \qquad \text{for} \quad k = 1, \cdots, d,$$

is the velocity solution to the interface problem below

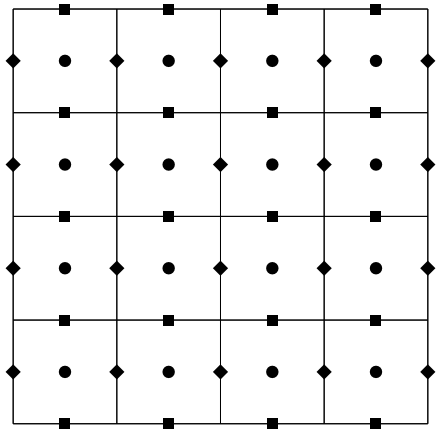
$$\begin{aligned} \triangle \mathbf{u} - \nabla q &= 0 \qquad \text{in} \quad \mathcal{B} \setminus \Gamma, \\ \nabla \cdot \mathbf{u} &= 0 \qquad \text{in} \quad \mathcal{B} \setminus \Gamma, \end{aligned}$$

subject to the interface conditions

$$\begin{aligned} \mathbf{u}^+ - \mathbf{u}^- &= 0 \qquad \text{on} \quad \Gamma, \\ \boldsymbol{\tau}^+ \mathbf{n} - \boldsymbol{\tau}^- \mathbf{n} &= \boldsymbol{\psi} \qquad \text{on} \quad \Gamma, \end{aligned}$$

and the "no-slip" boundary condition on $\partial\mathcal{B}$.

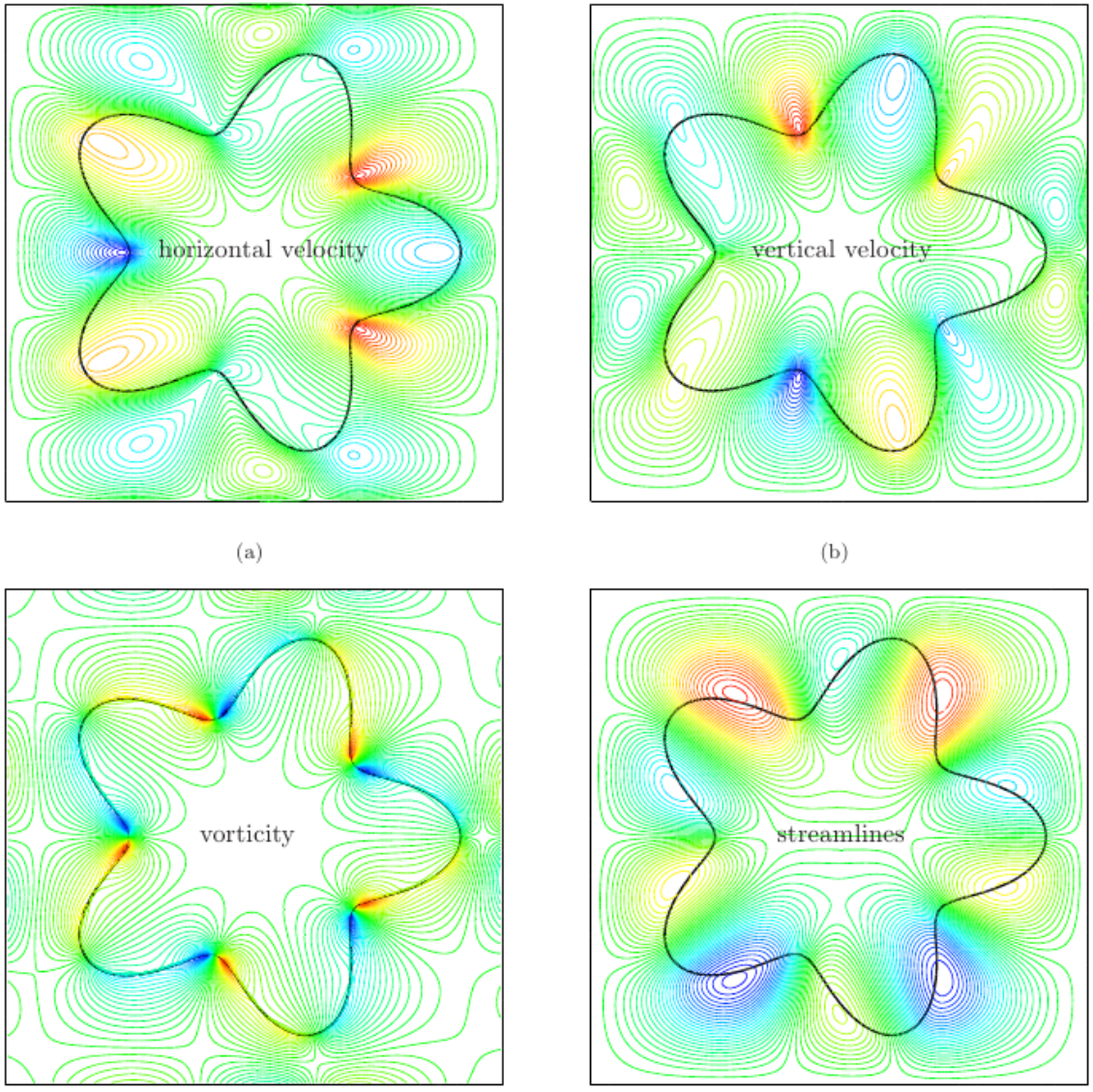
# Discretization of the Simple Interface Problem



By the Cartesian grid-based boundary integral method, to evaluate the boundary integrals, we solve the simple interface problem with the marker and cell (MAC) scheme on the staggered grid.

$$
\begin{aligned}
\triangle_h \mathbf{u}_h - \nabla_h q_h &= 0 \quad \text{in } \mathcal{B}, \\
\nabla_h \cdot \mathbf{u}_h &= 0 \quad \text{in } \mathcal{B}, \\
[\mathbf{u}_h] &= 0 \quad \text{on } \Gamma, \\
[\boldsymbol{\tau}_h \mathbf{n}] &= \psi_h \quad \text{on } \Gamma, \\
\mathbf{u}_h &= 0 \quad \text{on } \partial B.
\end{aligned}
$$

# Two-phase flow around a star-shaped interface




(a) (b) (c) (d)

# Efficiency and Accuracy Results in Three Space Dimensions

Example 1. The domain is an ellipsoid in 3D.

| grid size | #GMRES | $\|\mathbf{u}-\mathbf{u}_h\|_\infty$ | $\|p-p_h\|_\infty$ |
|---|---|---|---|
| $128\times128\times128$ | 14 | 1.18E-3 | 1.70E-2 |
| $256\times256\times256$ | 14 | 1.62E-4 | 4.61E-3 |
| $512\times512\times512$ | 14 | 3.33E-5 | 1.13E-3 |

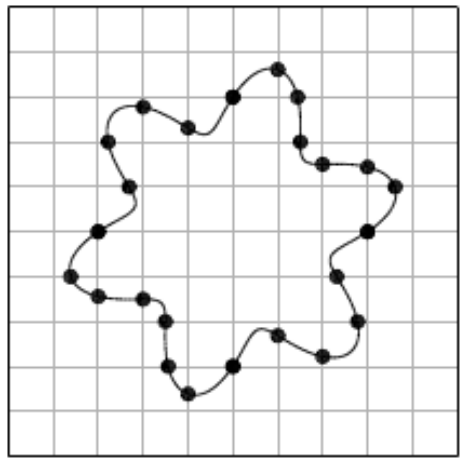
Example 2. The domain is a torus in 3D.

| grid size | #GMRES | $\|\mathbf{u}-\mathbf{u}_h\|_\infty$ | $\|p-p_h\|_\infty$ |
|---|---|---|---|
| $128\times128\times128$ | 23 | 3.65E-3 | 2.54E-2 |
| $256\times256\times256$ | 23 | 3.81E-4 | 8.13E-3 |
| $512\times512\times512$ | 23 | 9.17E-5 | 2.22E-3 |

**Remark:** These two examples are for the Dirichlet BVP of the Stokes system on fixed (time-independent) domains.

# Summary

1. Use intersection points of the curve or surface with an underlying Cartesian grid for representation and discretization.



2. The method solves interface problems in the boundary integral formulation and takes full advantages of

- well-conditioning property of boundary integral equations;
- fast elliptic solvers for the elliptic PDE on Cartesian grids;
- all those good points that a Cartesian grid method has.


# Thank you!