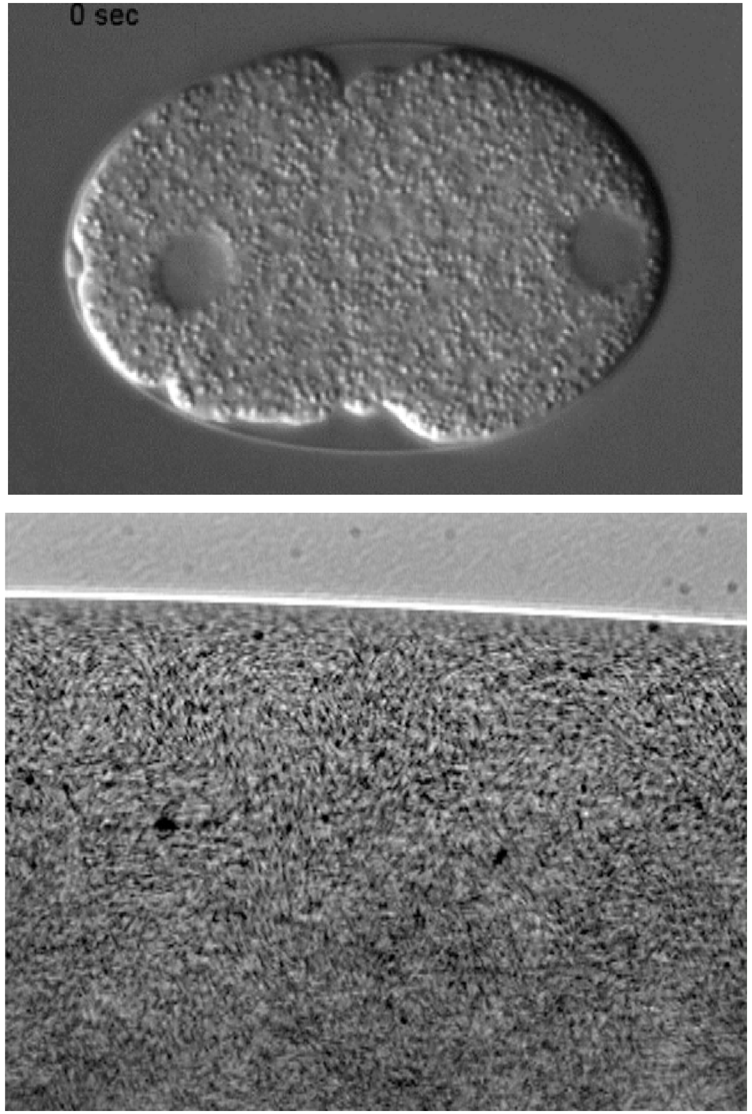
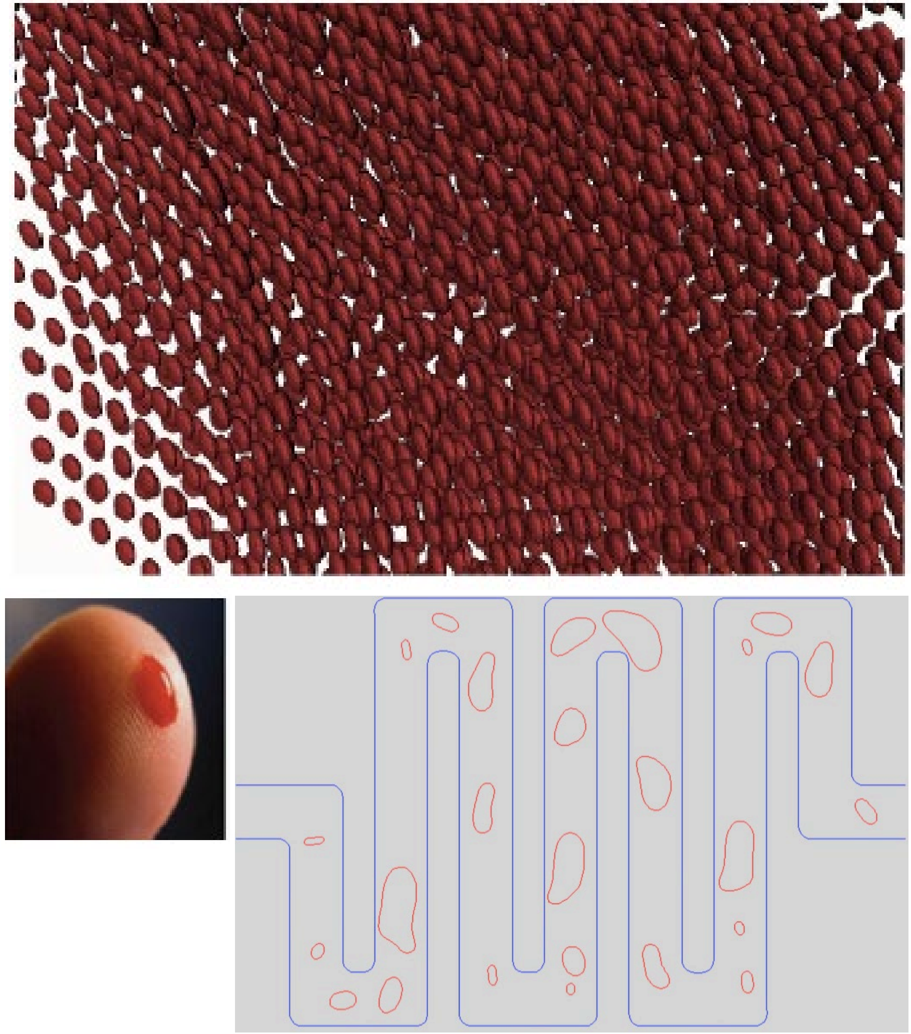
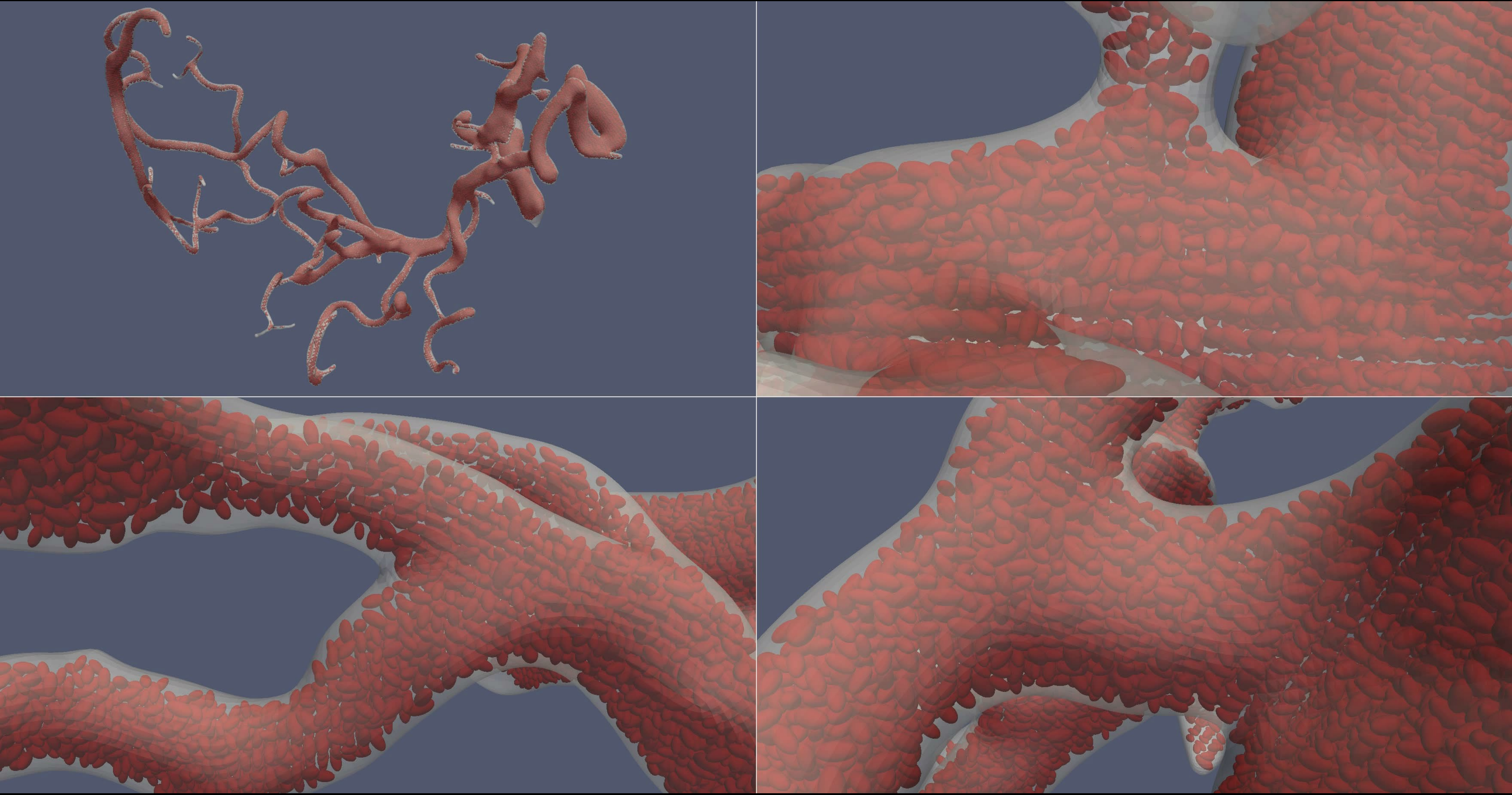
Potential theory for Stokes flow in three dimensions



Intracellular & bacterial flows

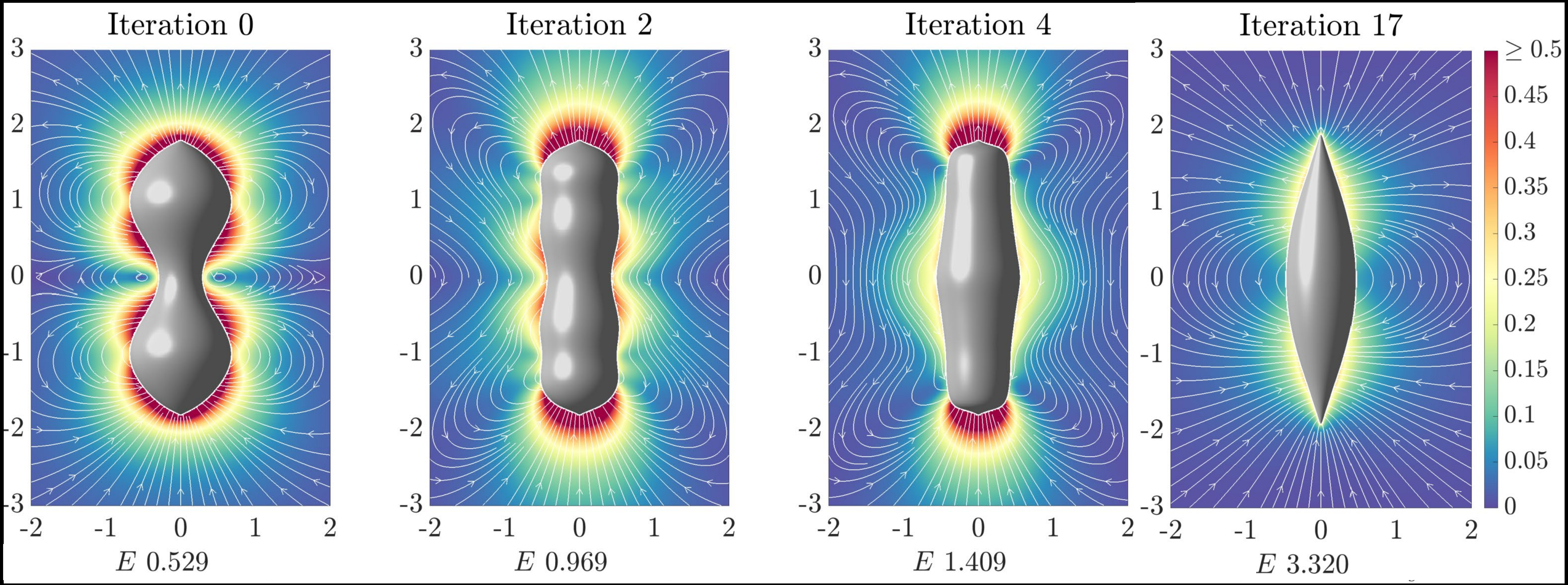


Blood flow



Lu, Morse, Rahimian, Stadler & Zorin, **SC’19**

Liu, Zhu, Guo, Bonnet & V-, **arXiv (2024)**



*Volume meshing avoided for (shape params * shape iterations) problems*

Outline

- **Formulation for different BVPs**
- **Boundary integral operator analysis**
- **Some numerics**

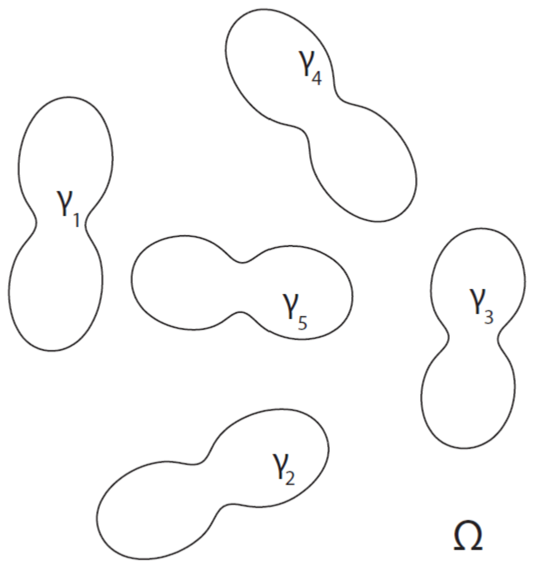
Stokes equations

$$-\mu\Delta\boldsymbol{u} + \nabla p = 0$$
$$\nabla\cdot\boldsymbol{u} = 0$$

Fundamental solution to Stokes equation in free space in $\mathbb{R}^3$:

$$G_{ij}(\boldsymbol{x},\boldsymbol{y}) = \frac{1}{8\pi\mu}\left(\frac{\delta_{ij}}{r} + \frac{r_i r_j}{r^3}\right), \quad i,j = 1,2,3$$

$$\boldsymbol{f} = -p\boldsymbol{n} + \mu(\nabla\boldsymbol{u} + \nabla^T\boldsymbol{u})\cdot\boldsymbol{n}$$



SLP Ansatz

$$\boldsymbol{u}(\boldsymbol{x}) = \mathcal{S}_\Gamma[\boldsymbol{\sigma}](\boldsymbol{x}) := \int_\Gamma G(\boldsymbol{x},\boldsymbol{y})\boldsymbol{\sigma}(\boldsymbol{y})dS(\boldsymbol{y})$$

$$p(\boldsymbol{x}) = \mathcal{Q}_\Gamma[\boldsymbol{\sigma}](\boldsymbol{x}) = \int_\Gamma Q(\boldsymbol{x},\boldsymbol{y})\boldsymbol{\sigma}(\boldsymbol{y})dS(\boldsymbol{y}), \quad Q_j(\boldsymbol{x},\boldsymbol{y}) = \frac{1}{4\pi\mu}\frac{r_j}{r^3}, \; j = 1,2,3$$

$$\boldsymbol{f}(\boldsymbol{x}) = \mathcal{K}_\Gamma[\boldsymbol{\sigma}](\boldsymbol{x}) = \int_\Gamma K(\boldsymbol{x},\boldsymbol{y})\boldsymbol{\sigma}(\boldsymbol{y})dS(\boldsymbol{y}), \quad K_{ij}(\boldsymbol{x},\boldsymbol{y}) = -\frac{3}{4\pi\mu}\frac{r_i r_j}{r^3}\frac{\boldsymbol{r}\cdot\boldsymbol{n}(\boldsymbol{x})}{r^2}, \quad \boldsymbol{x}\in\Gamma'$$

DLP Ansatz

$$\boldsymbol{u}(\boldsymbol{x}) = \mathcal{D}_\Gamma[\boldsymbol{\sigma}](\boldsymbol{x}) := \int_\Gamma D(\boldsymbol{x},\boldsymbol{y})\boldsymbol{\sigma}(\boldsymbol{y})dS(\boldsymbol{y})$$

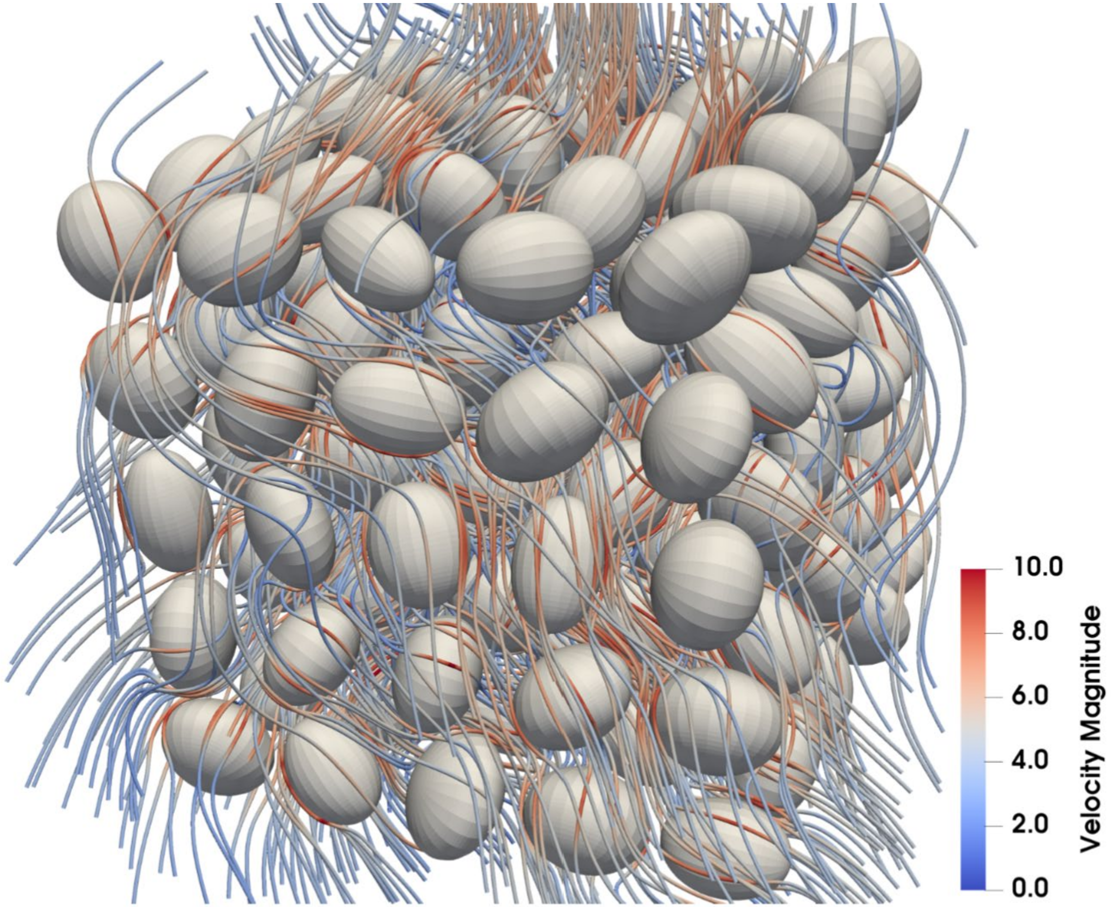
$$p(\boldsymbol{x}) = \mathcal{P}_\Gamma[\boldsymbol{\sigma}](\boldsymbol{x}) = \int_\Gamma P(\boldsymbol{x},\boldsymbol{y})\boldsymbol{\sigma}(\boldsymbol{y})dS(\boldsymbol{y}), \quad P(\boldsymbol{x},\boldsymbol{y}) = \frac{1}{2\pi\mu}\left(\frac{n_j(\boldsymbol{y})}{r^3} - 3\boldsymbol{r}\cdot\boldsymbol{n}(\boldsymbol{y})\frac{r_j}{r^5}\right)$$

$$\boldsymbol{f}(\boldsymbol{x}) = \mathcal{T}_\Gamma[\boldsymbol{\sigma}](\boldsymbol{x}) = \int_\Gamma T(\boldsymbol{x},\boldsymbol{y})\boldsymbol{\sigma}(\boldsymbol{y})dS(\boldsymbol{y})$$

$$T_{ij}(\boldsymbol{x},\boldsymbol{y}) = -\frac{3}{4\pi\mu}\left[\left(\frac{\boldsymbol{n}(\boldsymbol{y})\cdot\boldsymbol{n}(\boldsymbol{x})}{r^2} - 10d_{\boldsymbol{x}}d_{\boldsymbol{y}}\right)\frac{r_ir_j}{r^3} + d_{\boldsymbol{x}}d_{\boldsymbol{y}}\frac{\delta_{ij}}{r} + \frac{2}{3}\frac{n_i(\boldsymbol{x})n_j(\boldsymbol{y})}{r^3} + d_{\boldsymbol{x}}\frac{r_in_j(\boldsymbol{x})}{r^3} + d_{\boldsymbol{y}}\frac{r_jn_i(\boldsymbol{y})}{r^3}\right]$$

where $d_{\boldsymbol{x}} = \frac{\boldsymbol{r}\cdot\boldsymbol{n}(\boldsymbol{y})}{r^2}$, $d_{\boldsymbol{y}} = \frac{\boldsymbol{r}\cdot\boldsymbol{n}(\boldsymbol{x})}{r^2}$.

1. Porous media flow



Step 1:

ansatz: $$u(x) = u_\infty(x) + \Sigma_{k=1}^{n_b}(\mathcal{S}_k + \mathcal{D}_k)[\mu](x)$$

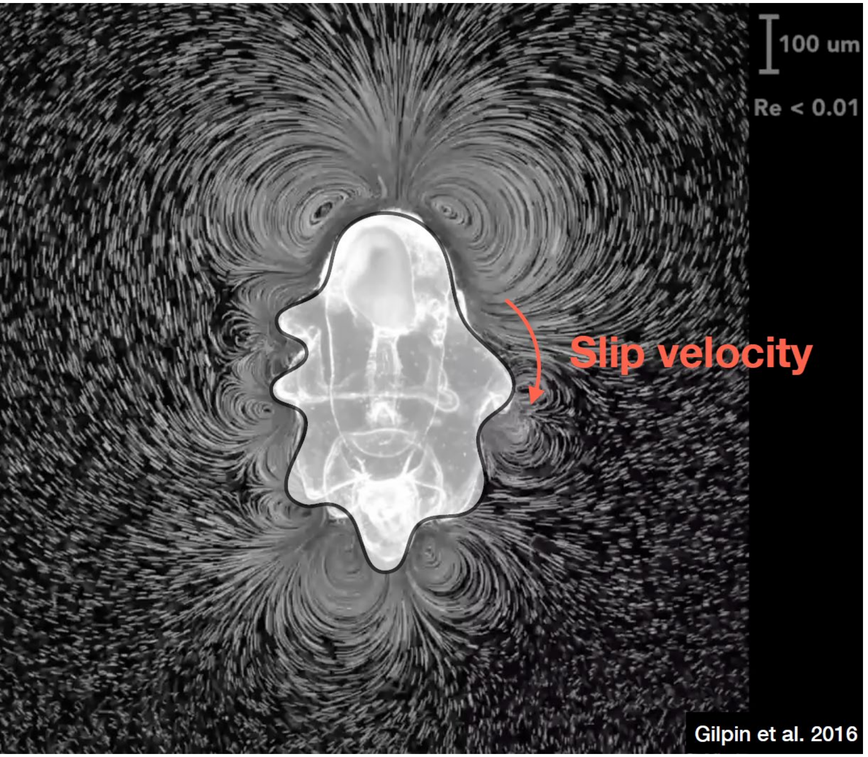
Step 2:

BIE: $$\left(\frac{1}{2}I + \Sigma_{k=1}^{n_b}(\mathcal{S}_k + \mathcal{D}_k)\right)[\mu](x) = -u_\infty(x)$$

Step 3:

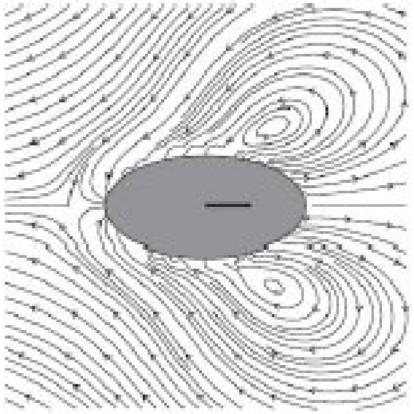
Evaluate the solution at targets

2. Microswimmers



$$u(x) = u_s(x) + v_k + \omega_k \times (x - x_k^c) \quad \forall \quad x \in \Gamma_k,$$

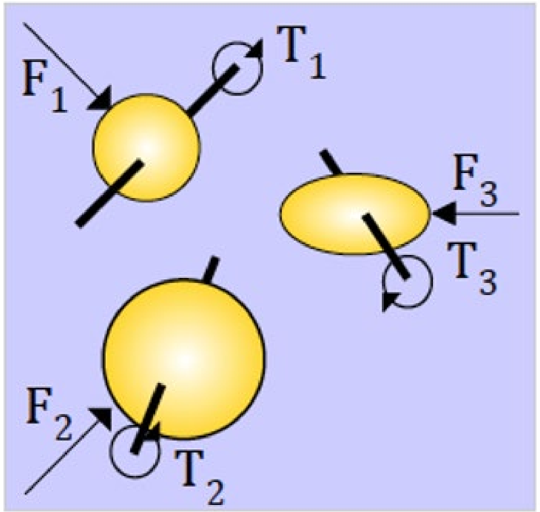
$$\int_{\Gamma_k} f \, d\Gamma = 0 \quad \text{and} \quad \int_{\Gamma_k} (x - x_k^c) \times f \, d\Gamma = 0.$$



Ansatz: $u(x) = \Sigma_{k=1}^{n_b} \left(\mathcal{S}_k + \mathcal{D}_k\right)[\mu](x).$

BIE: $\left(\frac{1}{2}I + \Sigma_{k=1}^{n_b} \left(\mathcal{S}_k + \mathcal{D}_k\right)\right)[\mu](x) = u_s(x) + v_i + \omega_i \times (x - x_i^c) \quad \text{for} \quad x \in \Gamma_i.$

3. Mobility problem



Surface Forces and Tractions

$$\int_{\Gamma_i} \boldsymbol{f}\, dS_y = \int_{\Gamma_i} \sigma \cdot \boldsymbol{n}\, dS_y = -\boldsymbol{F}_i,$$

$$\int_{\Gamma_i} (\boldsymbol{x} - \boldsymbol{x}_i^c) \times \boldsymbol{f}\, dS_y = -\boldsymbol{T}_i,$$

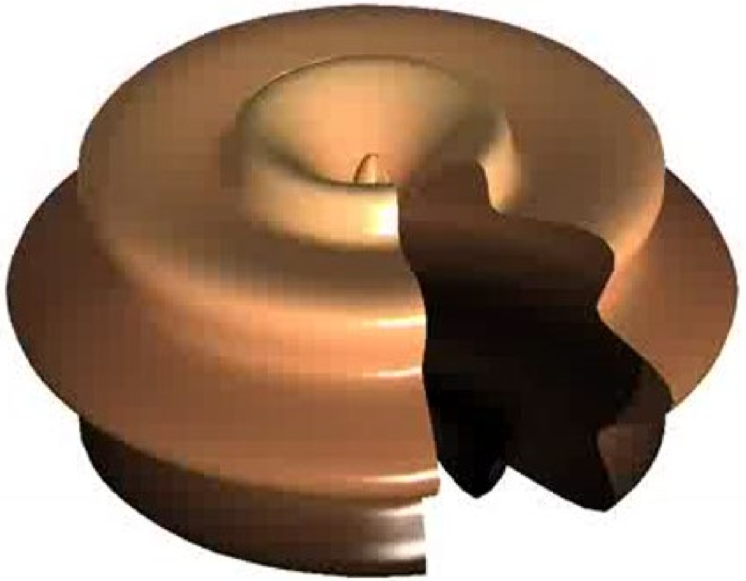
Ansatz: $\boldsymbol{u}(\boldsymbol{x}) = \Sigma_{k=1}^{n_b} \mathcal{S}_k[\boldsymbol{\mu} + \boldsymbol{\rho}](\boldsymbol{x}).$

Set: $\boldsymbol{\rho}_i = \dfrac{\boldsymbol{F}_i}{|\Gamma_i|} + \boldsymbol{\tau}_i^{-1} \boldsymbol{T}_i \times (\boldsymbol{x} - \boldsymbol{x}_i^c)$

BIE: $\left(\frac{1}{2}\boldsymbol{I} + \Sigma_{k=1}^{n_b} (\mathcal{K}_k + \mathcal{L}_k)\right) [\boldsymbol{\mu}](\boldsymbol{x}) = -\left(\frac{1}{2}\boldsymbol{I} + \Sigma_{k=1}^{n} \mathcal{K}_k\right) [\boldsymbol{\rho}](\boldsymbol{x})$

`Rachh & Greengard,` **`SINUM`**`, 2016`
`Corona, Greengard, Rachh & V-,` **`JCP`**`, 2017`

4. Interfacial flows



Membrane energy

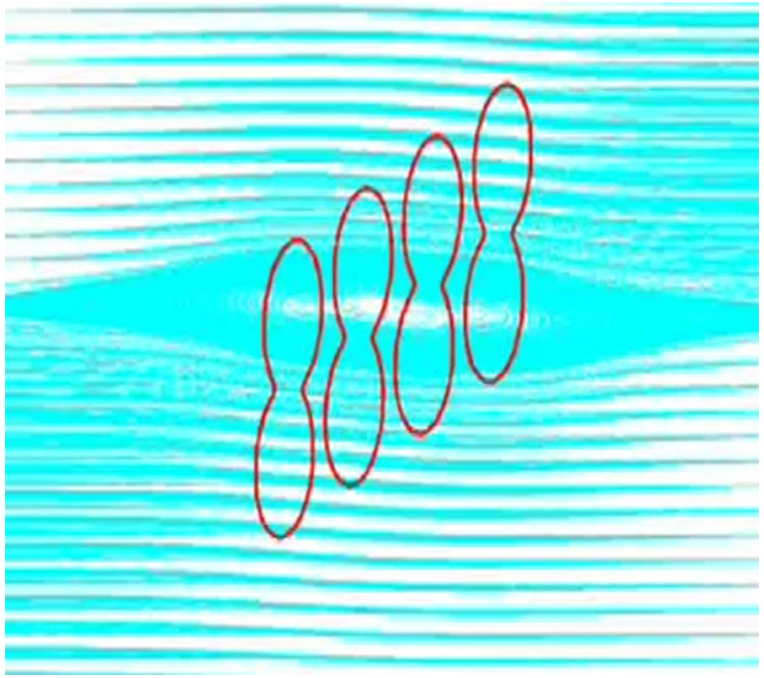
$$\varepsilon = \frac{1}{2}\kappa_B \int_\gamma H^2 d\gamma + \int_\gamma \sigma d\gamma$$

H - mean curvature; κ_B - bending modulus;

σ - membrane tension

Interfacial forces

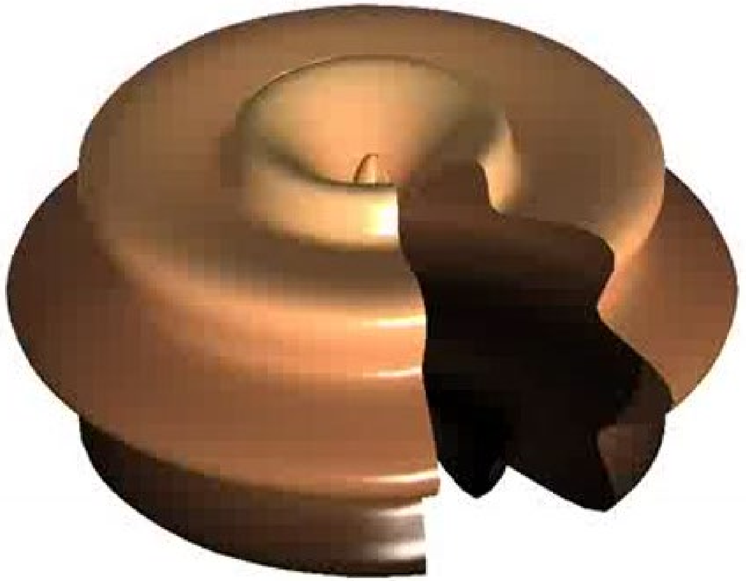
$$\begin{aligned} \mathbf{f}_b &= -\kappa_B(\triangle_\gamma H + 2H(H^2 - K))\mathbf{n} \\ \mathbf{f}_\sigma &= \sigma \triangle_\gamma \mathbf{x} + \nabla_\gamma \sigma \end{aligned}$$



Inextensibility Constraint

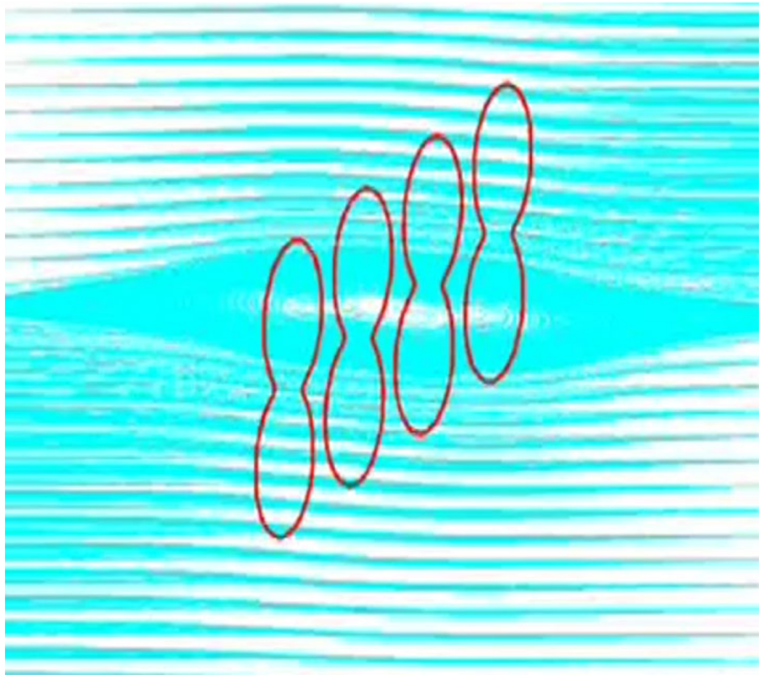
$$\mathrm{div}_\gamma \dot{\mathbf{x}} = 0$$

4. Interfacial flows



Boundary conditions

$$[\![\boldsymbol{u}(\boldsymbol{x})]\!] = \boldsymbol{0}, \quad [\![\boldsymbol{f}(\boldsymbol{x})]\!] = \boldsymbol{f}_b + \boldsymbol{f}_\sigma, \quad \boldsymbol{x} \in \gamma$$



Integro-differential equation for membrane evolution

$$\dot{\mathbf{x}} = \mathbf{v}_\infty + \mathcal{S}[\mathbf{f}_\sigma + \mathbf{f}_b]$$

$$\mathrm{div}_\gamma \mathcal{S}[\mathbf{f}_\sigma] = -\mathrm{div}_\gamma \left(\mathbf{v}_\infty + \mathcal{S}[\mathbf{f}_b]\right)$$

`Note:` **`Yuan-nan Young`**`'s talk (`**`Thu`**`)`

5. Multiphysics

- Surfactant-covered drops
- Multicomponent membranes

Surface chemistry + Stokes

Note: **Dan Fortunato**'s talk (**Fri**)

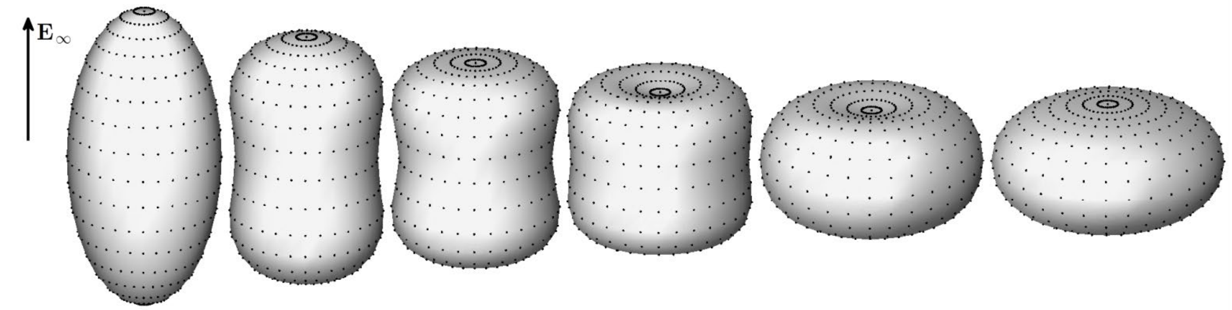
- Electrohydrodynamics

Laplace + Stokes

- Diffusiophoresis

Heat + Stokes

5. Multiphysics



$$
\begin{aligned}
-\Delta\phi &= 0 \quad \text{in} \quad \mathbb{R}^3 \setminus \gamma && \text{(potential equation)},\\
[\![\mathbf{n}\cdot(\sigma\nabla\phi)]\!]_\gamma &= 0 && \text{(current continuity)},\\
[\![\phi]\!]_\gamma &= V_m && \text{(transmembrane potential)},\\
-\nabla\phi(\mathbf{x}) \to \mathbf{E}_\infty(\mathbf{x}) \quad \text{as} \quad \|\mathbf{x}\| &\to \infty && \text{(far-field boundary condition)},\\
C_m\dot{V}_m + G_m V_m = -\mathbf{n}\cdot(\sigma_i\nabla\phi_i) \quad \text{on } &\gamma && \text{(conservation of electric current)}
\end{aligned}
$$

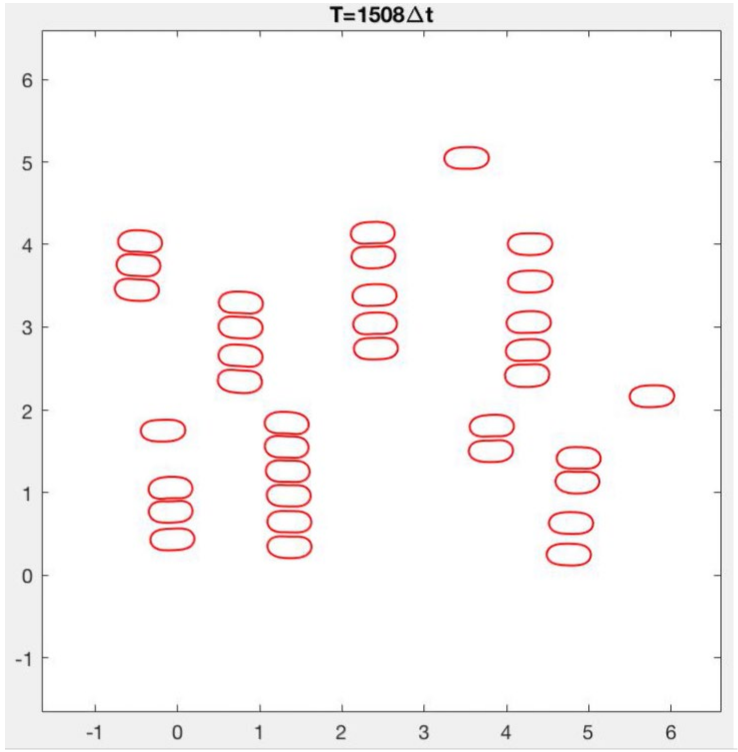
$$
\left[\!\left[\mathbf{n}\cdot(\Sigma^{el}+\Sigma^{hd})\right]\!\right]_\gamma = \mathbf{f}_m \quad \text{(membrane force balance)}
$$

$$
\phi(\mathbf{x}) = -\mathbf{E}_\infty\cdot\mathbf{x} + \mathcal{S}[q](\mathbf{x}) - \mathcal{D}[V_m](\mathbf{x})
$$

Ansatz

$$
\left(\frac{1}{2} + \eta\,\mathcal{S}'\right) q = \eta\,\mathbf{E}_\infty\cdot\mathbf{n} + \eta\,\mathcal{D}'[V_m]
$$

BIE



V-. JCP 2016; Wu & V-. JFM 2019

BIO Analysis

Scalar Spherical Harmonics

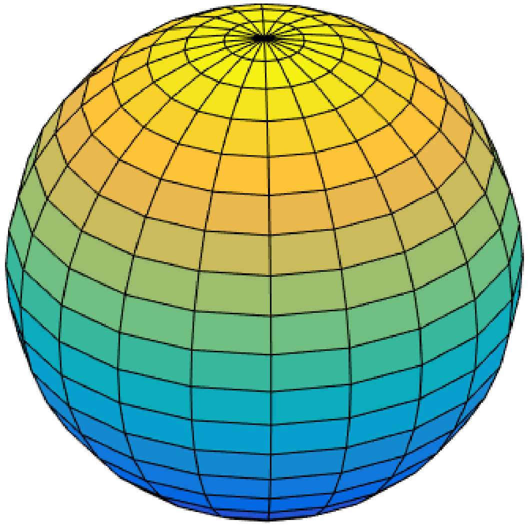
$$Y_n^m(\theta,\phi) = \sqrt{\frac{2n+1}{4\pi}}\sqrt{\frac{(n-|m|)!}{(n+|m|)!}}\,P_n^{|m|}(\cos\theta)\,e^{im\phi}$$

$$\left\{\phi_k = \frac{2\pi k}{2p+2},\ k=0,\dots,2p+1\right\}$$

$$\{\theta_j = \cos^{-1}(t_j), j=0,\dots p\}\,,$$

$$f(\theta,\phi) = \sum_{n=0}^{p}\sum_{m=-n}^{n} f_n^m\, Y_n^m(\theta,\phi) = \sum_{n=0}^{p}\sum_{m=-n}^{n} f_n^m\, P_n^m(\cos\theta)\cdot e^{im\phi}.$$

$$f_n^m = \int_0^{\pi}\int_0^{2\pi} f(\theta,\phi)\overline{Y_n^m(\theta,\phi)}\sin\theta\, d\theta\, d\phi$$



Vector Spherical Harmonics

$$\begin{aligned}
\boldsymbol{V}_n^m &= \nabla_\gamma Y_n^m(\theta,\phi) - (n+1)Y_n^m(\theta,\phi)\boldsymbol{e}_r(\theta,\phi),\\
\boldsymbol{W}_n^m &= \nabla_\gamma Y_n^m(\theta,\phi) + nY_n^m(\theta,\phi)\boldsymbol{e}_r(\theta,\phi),\\
\boldsymbol{X}_n^m &= \boldsymbol{e}_r(\theta,\phi)\times\nabla_\gamma Y_n^m(\theta,\phi),
\end{aligned}$$

Signatures of integral operators

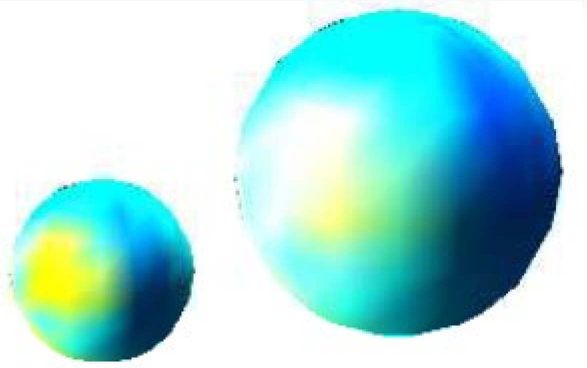
	$\boldsymbol{V}_n^m$	$\boldsymbol{W}_n^m$	$\boldsymbol{X}_n^m$
$\mathcal{S}$	$\dfrac{n}{(2n+1)(2n+3)}$	$\dfrac{n+1}{(2n+1)(2n-1)}$	$\dfrac{1}{2n+1}$
$\mathcal{D}_+$	$\dfrac{2n^2+4n+3}{(2n+1)(2n+3)}$	$\dfrac{2(n-1)(n+1)}{(2n+1)(2n-1)}$	$\dfrac{n-1}{2n+1}$
$\mathcal{D}_-$	$\dfrac{-2n(n+2)}{(2n+1)(2n+3)}$	$\dfrac{-(2n^2+1)}{(2n+1)(2n-1)}$	$\dfrac{-(n+2)}{2n+1}$
$\mathcal{K}_+$	$\dfrac{-2n(n+2)}{(2n+1)(2n+3)}$	$\dfrac{-(2n^2+1)}{(2n+1)(2n-1)}$	$\dfrac{-(n+2)}{2n+1}$
$\mathcal{K}_-$	$\dfrac{2n^2+4n+3}{(2n+1)(2n+3)}$	$\dfrac{2(n-1)(n+1)}{(2n+1)(2n-1)}$	$\dfrac{n-1}{2n+1}$

Single layer evaluation

$$\mathcal{S}[\boldsymbol{V}_n^m](r,\theta,\phi) = \begin{cases} \dfrac{n}{(2n+1)(2n+3)}\boldsymbol{V}_n^m r^{-n-2} & r \geq 1 \\ \dfrac{n}{(2n+1)(2n+3)}\boldsymbol{V}_n^m r^{n+1} + \dfrac{n+1}{4n+2}\boldsymbol{W}_n^m (r^{n-1} - r^{n+1}) & r \leq 1 \end{cases}$$

$$\mathcal{S}[\boldsymbol{W}_n^m](r,\theta,\phi) = \begin{cases} \dfrac{n+1}{(2n+1)(2n-1)}\boldsymbol{W}_n^m r^{-n} + \dfrac{n}{4n+2}\boldsymbol{V}_n^m (r^{-n-2} - r^{-n}) & r \geq 1 \\ \dfrac{n+1}{(2n+1)(2n-1)}\boldsymbol{W}_n^m r^{n-1} & r \leq 1 \end{cases}$$

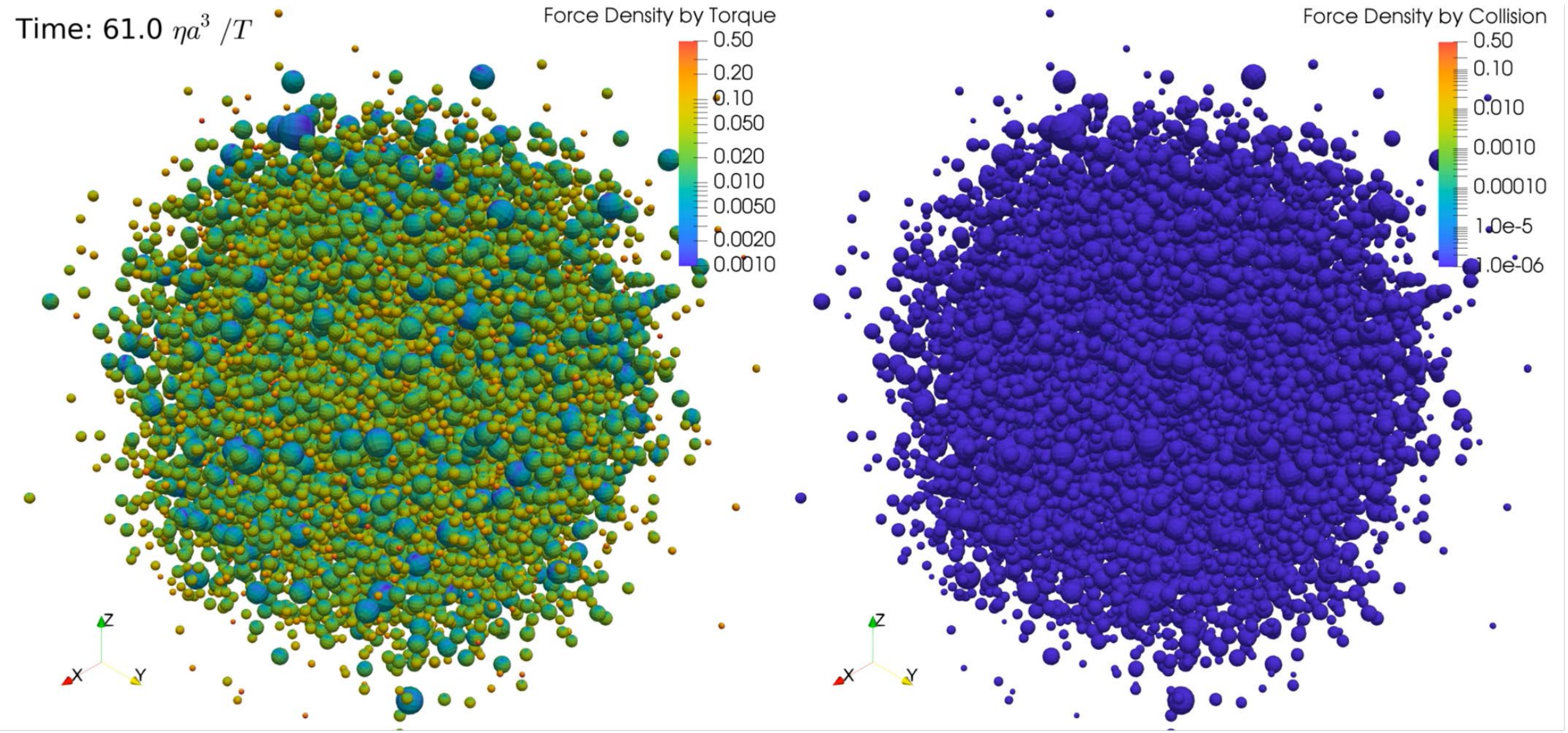
$$\mathcal{S}[\boldsymbol{X}_n^m](r,\theta,\phi) = \begin{cases} \dfrac{1}{2n+1}\boldsymbol{X}_n^m r^{-n-1} & r \geq 1 \\ \dfrac{1}{2n+1}\boldsymbol{X}_n^m r^{n} & r \leq 1. \end{cases}$$



Vico, Greengard & Gimbutas, **Num. Math. (2014)**; Corona & V-, **JCP (2018)**

Applications

- **Avoid quadrature** altogether for spherical suspensions



Yan, Corona, Malhotra, V- & Shelley, **JCP** 2020

Applications

- **Avoid quadrature** altogether for spherical suspensions

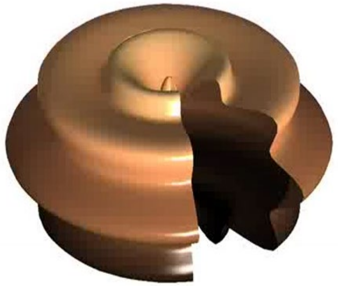
- **Preconditioning**

Theorem 5.2 (Inextensibility operator). *On the unit sphere, the spherical harmonic functions are eigenfunctions of the inextensibility operator $\mathcal{L}$ defined as*

$$\mathcal{L}\sigma = div_\gamma \mathcal{S}[\sigma \Delta_\gamma \mathbf{x} + \nabla_\gamma \sigma].$$

and

$$\mathcal{L}Y_n^m = -\frac{n(n+1)(2n^2+2n-1)}{(2n-1)(2n+1)(2n+3)} Y_n^m.$$



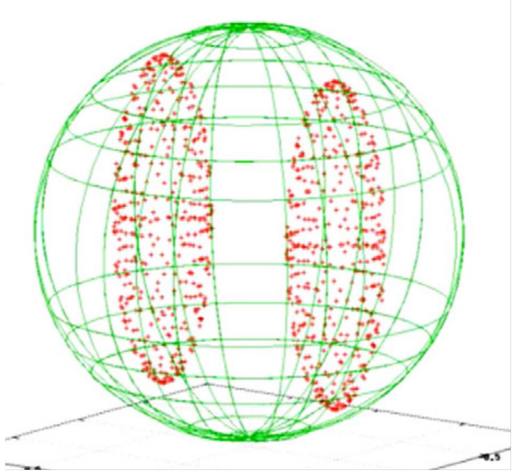
V-, Rahimian, Biros & Zorin **JCP (2011)**

- **Small deformation theory**

  Vlahovska, **ARFM (2019)**

- **Fast multiple-particle scattering**

  Gimbutas & Greengard, **JCP (2013)**



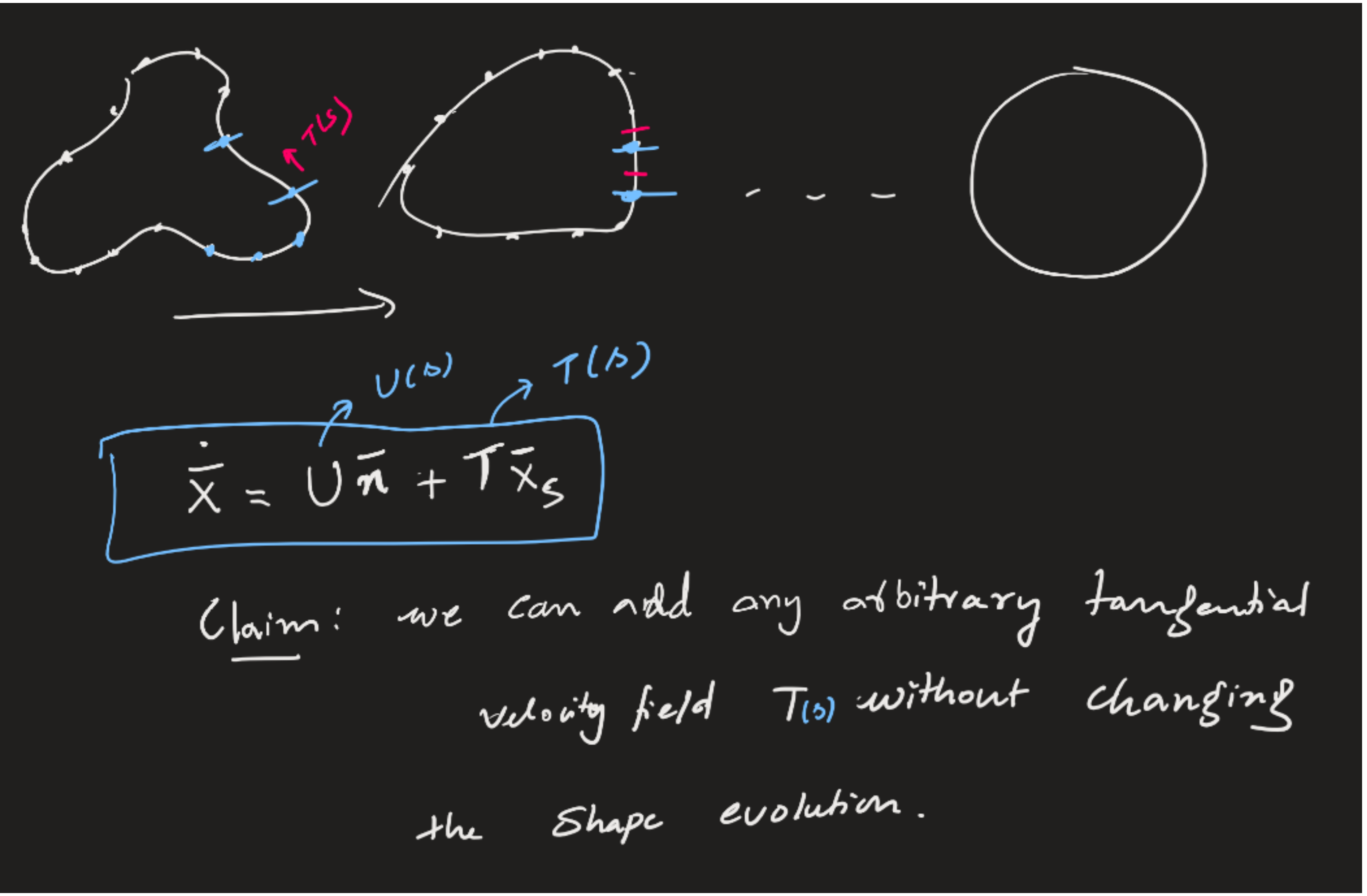
Generalizations: **Kausik Das & Tianyue (Choco) Li's posters**

Numerics

- Wall, periodic BCs
- Reparameterization
- Aliasing, expanded forms
- Singular quadrature
- Fast solvers
- Collision detection and resolution

Note: **Bryce Palmer**'s talk (**Thu**)

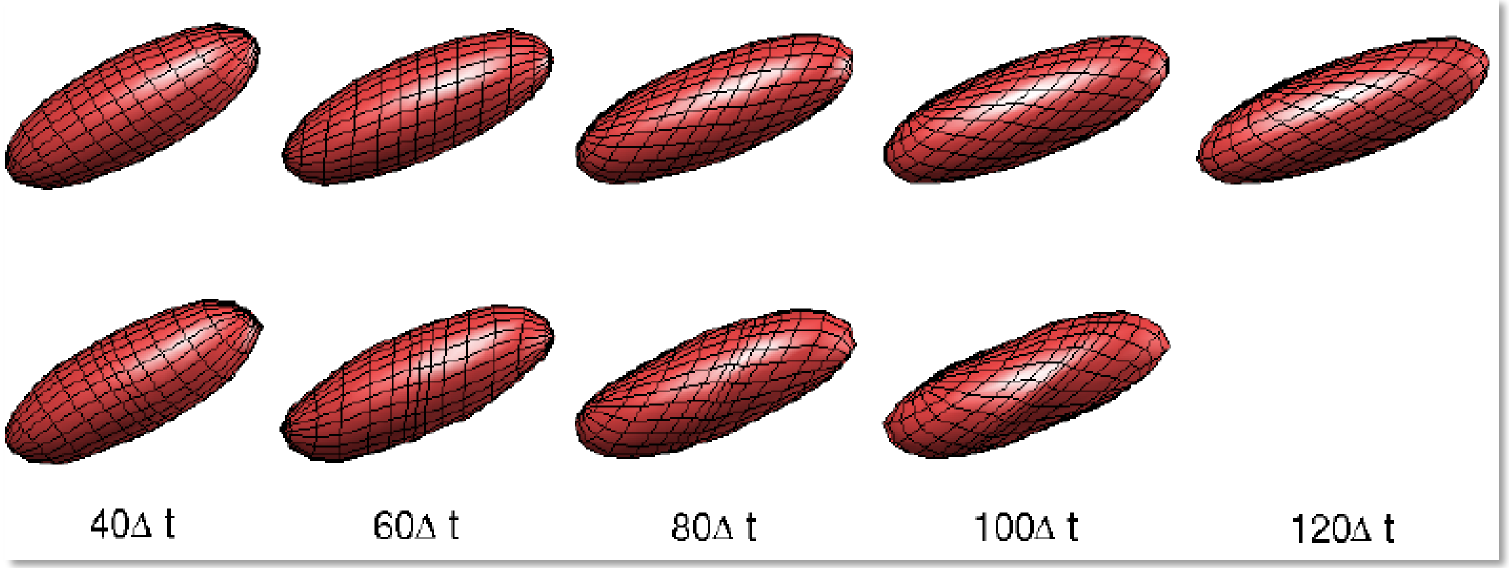
Reparameterization



- Equiarclength parameterization to help construct implicit methods
- Adaptive discretization to resolve physics better

Hou, Lowengrub & Shelley, **JCP** 1994

Reparameterization



- Define a mesh quality measure *E*

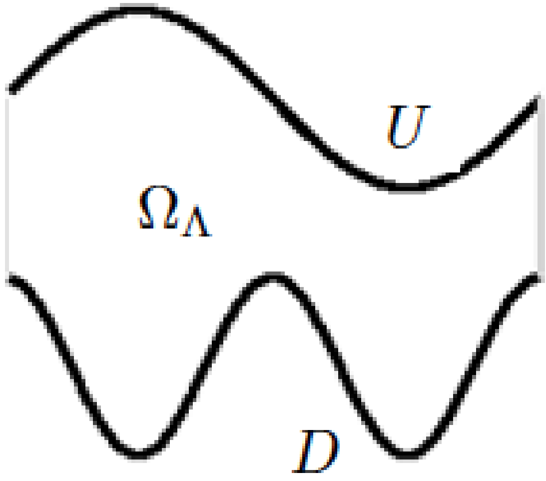
$$\dot{\mathbf{y}} + (I - \mathbf{n}(\mathbf{y}) \otimes \mathbf{n}(\mathbf{y}))\nabla E(\mathbf{y}) = 0$$

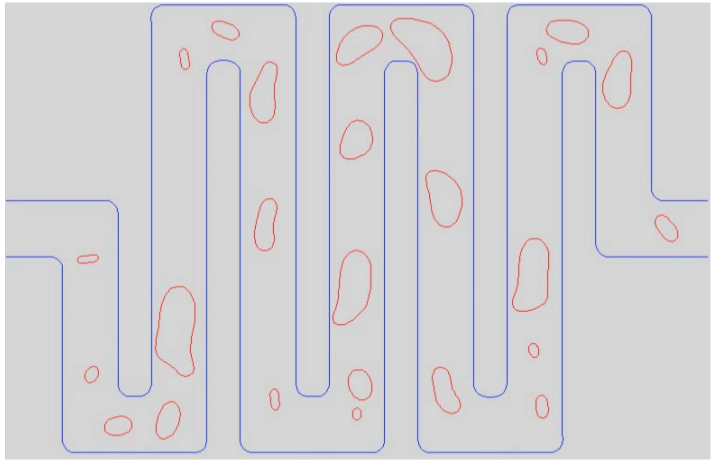
$$\nabla E = \sum_{n>_{cutoff},m} \langle Y_n^m, \mathbf{y}\rangle \, Y_n^m$$

V-, Rahimian, Biros & Zorin **JCP (2011)**; Sorgentone & Tornberg **JCP (2018)**

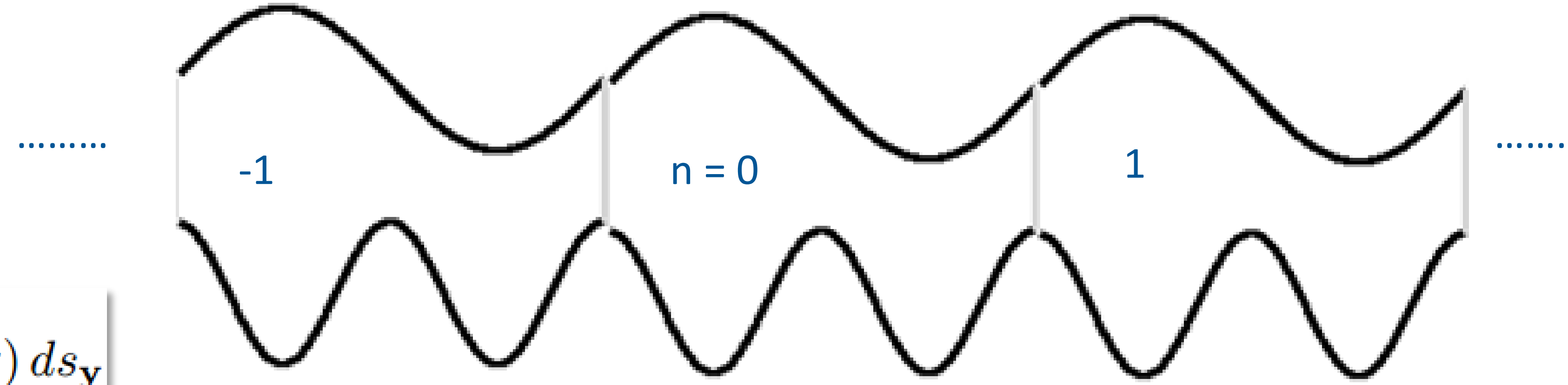
Periodic BCs

$$
\begin{aligned}
(\mathbf{u}, p) \quad & \text{Stokes in } \Omega_\Lambda \\
\mathbf{u} = \mathbf{v}_U \ & \text{on } U \\
\mathbf{u} = \mathbf{v}_D \ & \text{on } D \\
\mathbf{u}(\mathbf{x}+\mathbf{d}) - \mathbf{u}(\mathbf{x}) = 0, \quad & \mathbf{x} \in \Omega_\Lambda \\
p(\mathbf{x}+\mathbf{d}) - p(\mathbf{x}) = p_{\text{drive}}, \quad & \mathbf{x} \in \Omega_\Lambda .
\end{aligned}
$$



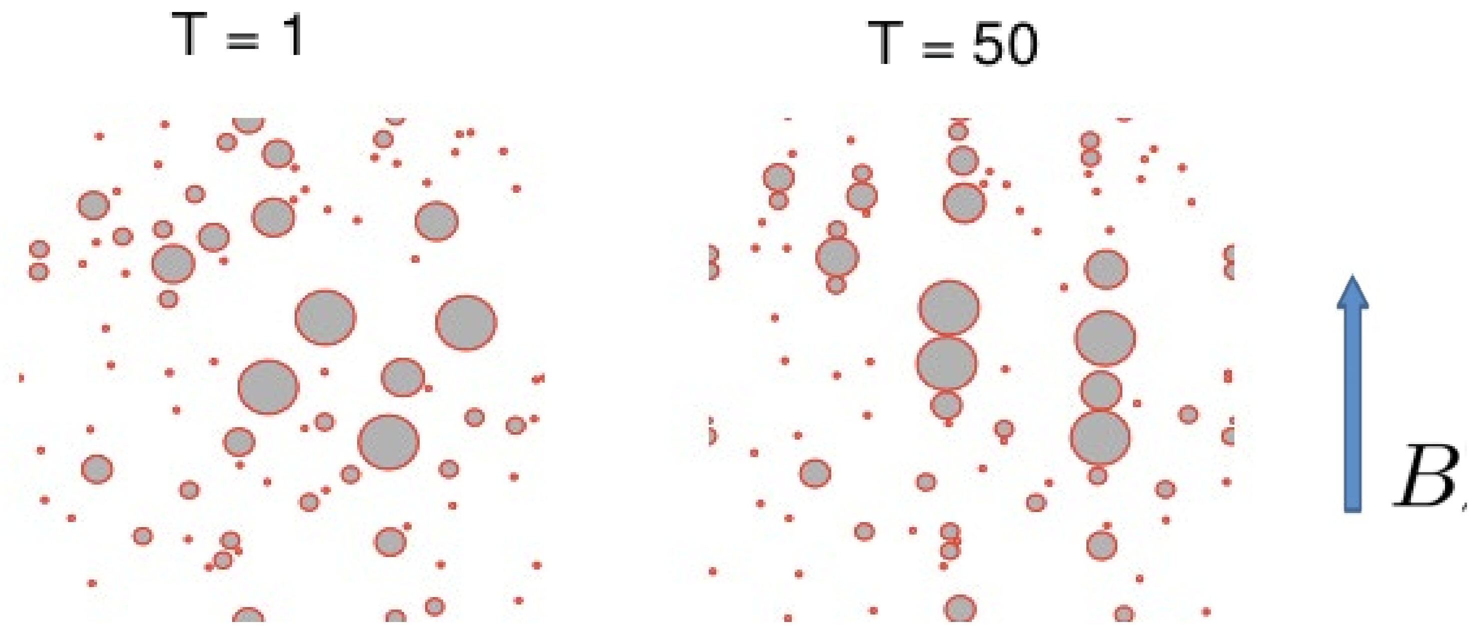


Periodic Green's functions



$$
\mathbf{u}(\mathbf{x}) = \sum_{n\in\mathbb{Z}} \int_\Gamma D(\mathbf{x}, \mathbf{y} + n\mathbf{d})\, \boldsymbol{\tau}(\mathbf{y})\, ds_{\mathbf{y}}
$$

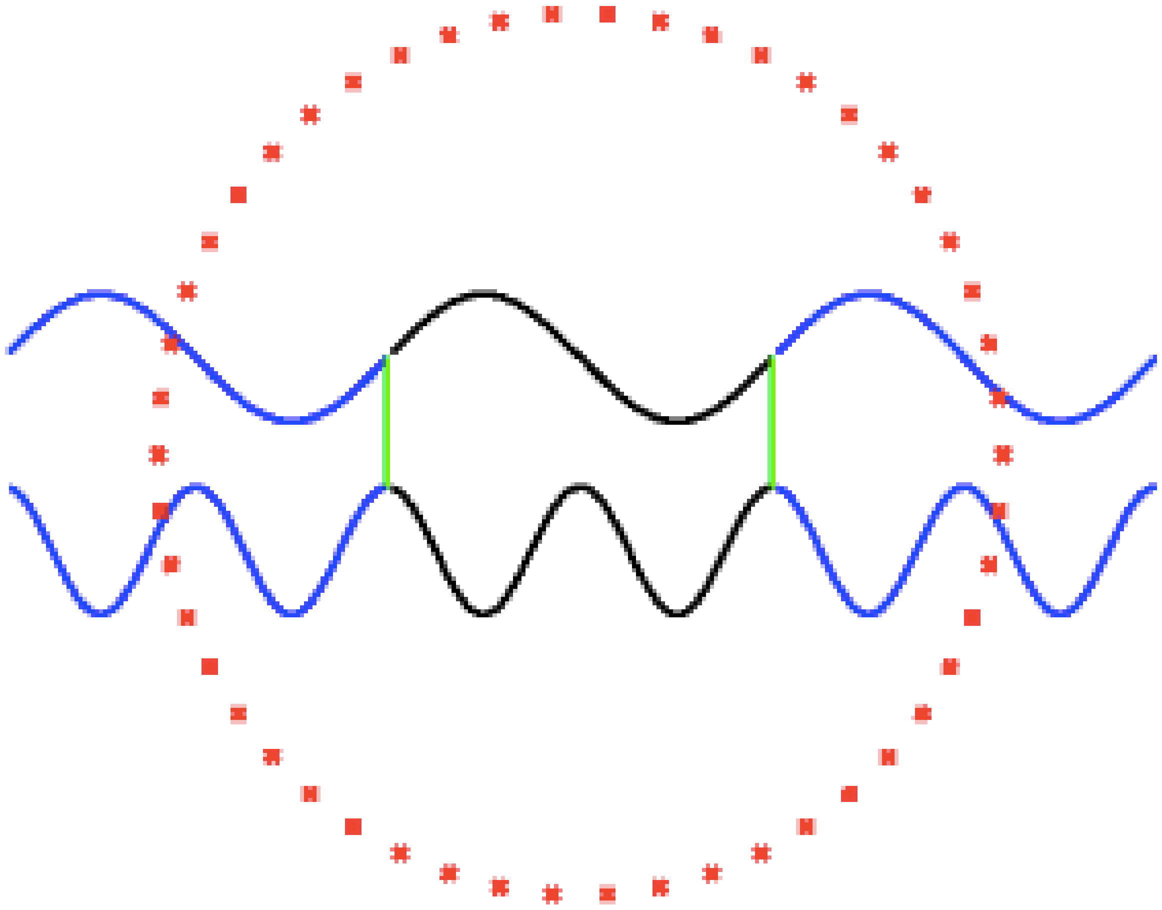
Periodic BCs



MHD of soft particles

What we want: ``FMMable scheme''

Proxy surfaces

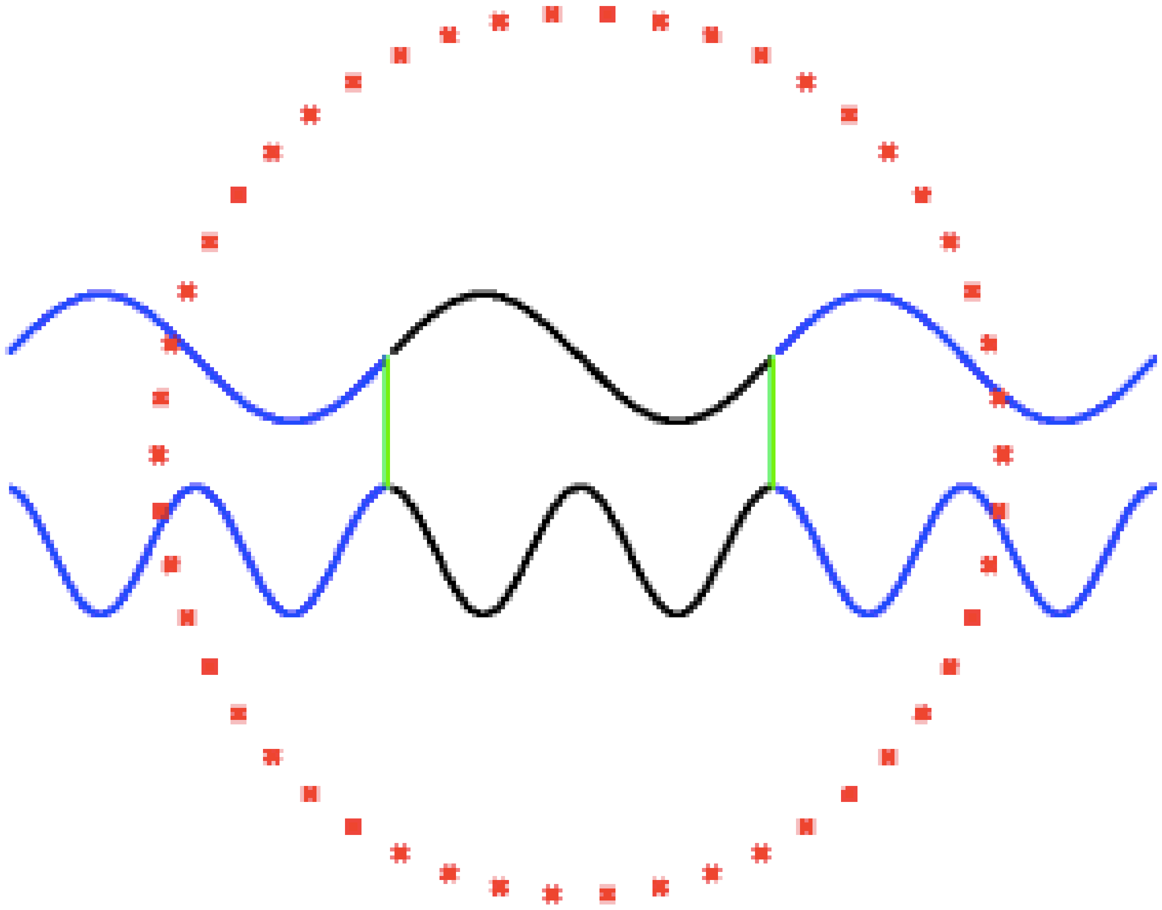


1. $\mathbf{u} = \mathcal{D}_{\Gamma}^{\text{near}} \boldsymbol{\tau} + \sum_{m=1}^{M} \mathbf{c}_m \phi_m$

2. $\phi_m(\mathbf{x}) = S(\mathbf{x}, \mathbf{y}_m)$

Anderson, **SISC**, 1992; Ying, Biros, Zorin, **JCP**, 2004; Barnett, Greengard, **BITNUM**, 2011
Marple, Barnett, Gillman & V-. **SISC**, 2016; Barnett, Marple, V- & Zhao. **CPAM**, 2018

Proxy surfaces



1. $\mathbf{u} = \mathcal{D}_\Gamma^{\text{near}} \boldsymbol{\tau} + \sum_{m=1}^{M} \mathbf{c}_m \phi_m$

2. $\phi_m(\mathbf{x}) = S(\mathbf{x}, \mathbf{y}_m)$

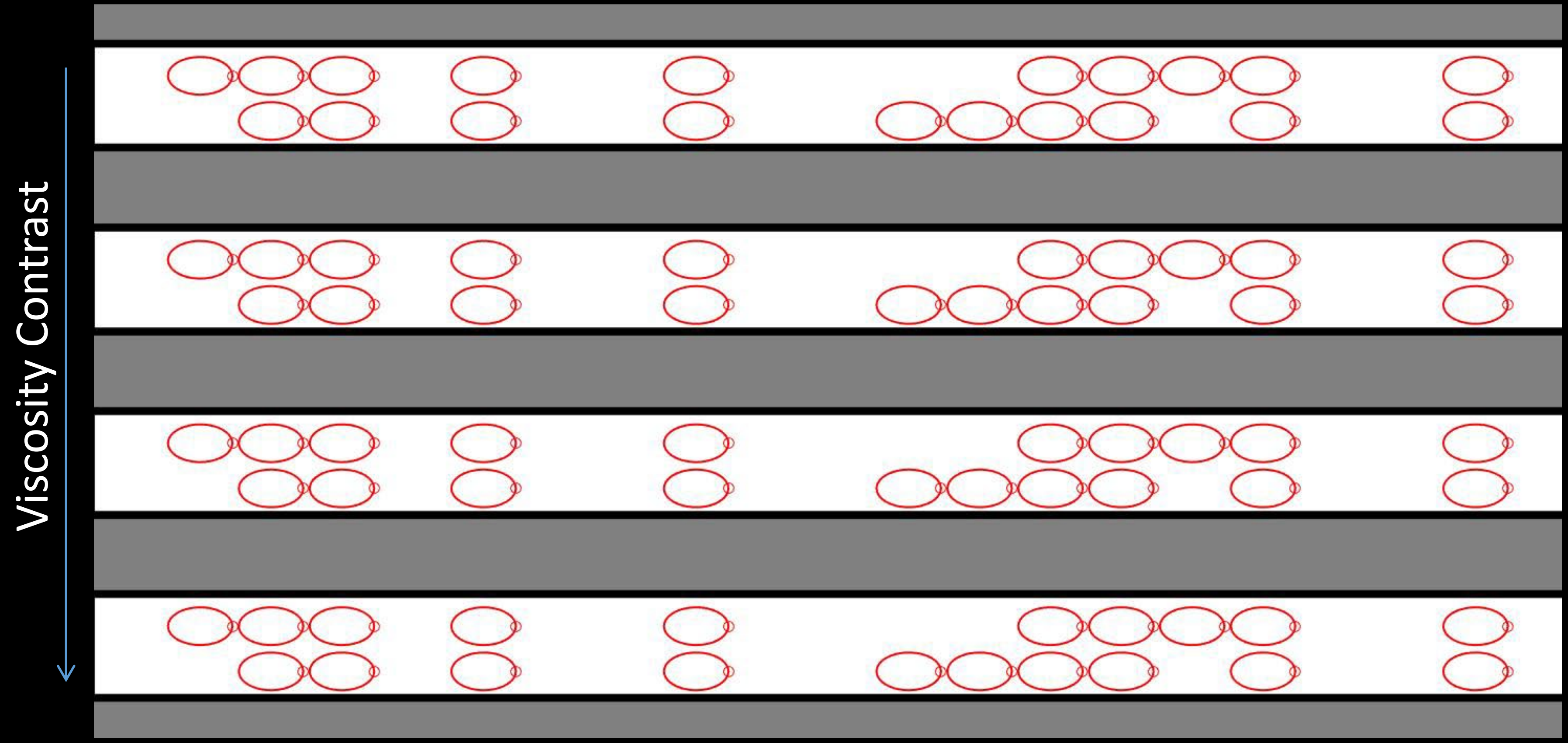
3. Apply Dirichlet BCs on walls

4. Apply periodic BCs

5. $\begin{bmatrix} A & B \\ C & Q \end{bmatrix} \begin{bmatrix} \boldsymbol{\tau} \\ \boldsymbol{c} \end{bmatrix} = \begin{bmatrix} \boldsymbol{v} \\ \boldsymbol{g} \end{bmatrix}$

Anderson, **SISC**, 1992; Ying, Biros, Zorin, **JCP**, 2004; Barnett, Greengard, **BITNUM**, 2011
Marple, Barnett, Gillman & V-. **SISC**, 2016; Barnett, Marple, V- & Zhao. **CPAM**, 2018

Periodic flows



Direct solvers for wall BCs

Note: **Gunnar Martinsson**'s breakout room (**Wed**)

Summary

- Stokes BVPs
  - First vs second kind formulations
  - Multiphysics applications
  - Optimization and inverse problems
- Boundary integral operator analysis
  - Generalizations
- Numerical BIE/IDE solvers
  - Fast solvers
  - Periodic BCs
  - Collision resolution
  - Close evaluation
  - Stable time-steppers

Thank You!