

# Slender and close: accurate Stokes flows for rigid particles in challenging geometries

Alex Barnett<sup>1</sup>
work with Anna Broms<sup>2</sup>, Anna-Karin Tornberg<sup>2</sup> and Dhairya Malhotra<sup>1</sup>

MIT Distinguished Seminar in CS&E, 4/17/25

<sup>1</sup>Center for Computational Mathematics, Flatiron Institute, Simons Foundation

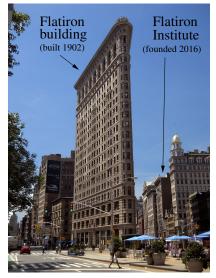
<sup>2</sup>Department of Mathematics, KTH, Sweden







# Flatiron Institute and the Center for Computational Math



A division of the Simons Foundation

CCM is one of five centers

others: biology astrophysics/astronomy quantum physics neuroscience

Each  $\approx 50$  researchers

#### CCM:

scientific computing numerical analysis biophysics / imaging computational statistics machine learning

Supports both basic research & software development / support

# My current/recent areas

- Numerical PDE linear, but complicated geometries wave scattering, acoustics, heat equation viscous fluid flow ← today
- Nonuniform FFTs and other signal processing lead developer of well-used software package: FINUFFT CPU+GPU. Inverse Fourier imaging (MRI, black hole), GP regression



 Various scientific computing / numerical analysis electronic structure (quantum) oscillatory differential equations bio-math (bio-mechanics, perfusion) protein imaging (cryo-EM), sampling (HMC)

Flatiron is a problem-rich environment. . .

... CCM is a hub for numerical advice / tools / collaboration

# Stokes flows with rigid bodies: motivations

Rheology: how do suspended particles change the effective viscosity?

Reynolds # Re=0: fluid inertia negligible

### Transport in shearing suspension:



(Souzy et al, '17)

mixing, super-diffusion, turbulence, at Re  $\approx 0\,$ 

# Stokes flows with rigid bodies: motivations

Rheology: how do suspended particles change the effective viscosity?

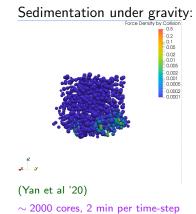
Reynolds # Re=0: fluid inertia negligible

### Transport in shearing suspension:



(Souzy et al, '17)

mixing, super-diffusion, turbulence, at Re pprox 0



# Stokes flows with rigid bodies: motivations

Rheology: how do suspended particles change the effective viscosity?

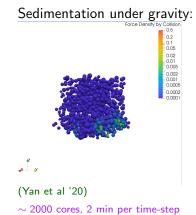
Reynolds # Re=0: fluid inertia negligible

### Transport in shearing suspension:



(Souzy et al, '17)

mixing, super-diffusion, turbulence, at Re pprox 0





cell biomechanics simulations (actin, nuclei)
active fluids: cilia. swimmers
nonzero slip velocity velice

(Nazockdast et al '15)

### Outline of today

1. Incompressible Stokes problems

resistance and mobility; challenges with existing methods

2. Method of fundamental solutions (MFS)

solve resistance and mobility for large collections of simple objects

3. Close-to-touching spheres

augmenting MFS using pair-wise lines of images

4. Slender bodies

replace common asymptotic approx. by convergent boundary integral equations (BIE)



# Outline of today

1. Incompressible Stokes problems

resistance and mobility; challenges with existing methods

2. Method of fundamental solutions (MFS)

solve resistance and mobility for large collections of simple objects

3. Close-to-touching spheres

augmenting MFS using pair-wise lines of images

4. Slender bodies

replace common asymptotic approx. by convergent boundary integral equations (BIE)

Goals throughout: tool-building. Design solvers that are. . .

- convergent solves the actual model with arbitrarily small error
- high order accurate
   effort grows weakly as error vanishes
- close to linear scaling in problem size number of particles or surface unknowns



assume: 1) Reynolds # Re  $\approx$  0 e.g.  $\mu$ m particles in H<sub>2</sub>O 2) no Brownian (thermal) forcing i.e. deterministic

Stokes Dirichlet BVP: solve for (u, p) vel, pressure in  $\Omega :=$  exterior of bodies  $\Omega_1, \dots, \Omega_B$ 

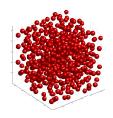
$$-\mu\Deltaoldsymbol{u}+
ablaoldsymbol{p}=oldsymbol{0}$$
 in  $\Omega$  local fluid force balance

$$abla \cdot {\it u} = 0 \quad \text{in } \Omega \quad \text{incompressible}$$

$$\| \boldsymbol{u}(\boldsymbol{x}) \| \to 0, \quad \| \boldsymbol{x} \| \to \infty$$
 decay condition

$$oldsymbol{u} = oldsymbol{u}_{\mathsf{BC}} := oldsymbol{v}_b + oldsymbol{\omega}_b imes (oldsymbol{x} - oldsymbol{c}_b)$$
 on  $\partial \Omega_b$ 

Unique solution exists for any boundary data uBC



given rigid-body motion (Ladyzhenskaya '69)

assume: 1) Reynolds # Re  $\approx 0$  e.g.  $\mu$ m particles in H<sub>2</sub>O

2) no Brownian (thermal) forcing i.e. deterministic

**Stokes Dirichlet BVP**: solve for (u, p) vel, pressure

in 
$$\Omega:=$$
 exterior of bodies  $\Omega_1,\dots,\Omega_{\mathcal{B}}$ 

$$-\mu\Delta {m u} + 
abla p ~=~ {m 0} ~~{
m in}~ \Omega ~~{
m local}~ {
m fluid}~ {
m force}~ {
m balance}$$

$$abla \cdot {\it u} = 0 \quad \text{in } \Omega \quad \text{incompressible}$$

$$\|\boldsymbol{u}(\boldsymbol{x})\| \to 0, \quad \|\boldsymbol{x}\| \to \infty$$
 decay condition

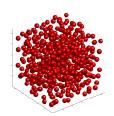
$$m{u} = m{u}_{BC} := m{v}_b + m{\omega}_b imes (m{x} - m{c}_b)$$
 on  $\partial \Omega_b$  given rigid-body motion

Unique solution exists for any boundary data  $\mathbf{u}_{\mathrm{BC}}$ 

(Ladyzhenskaya '69) We'll need surface traction (force) vector  $\mathbf{T} = \mathbf{T}[\mathbf{u}, p] := -p\mathbf{n} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \cdot \mathbf{n}$ 

Then from solution can extract net forces and torques on bth body:

$$m{F}_b = \int_{\partial\Omega_b} m{T} dS_{m{y}}$$
  $m{ au}_b = \int_{\partial\Omega_b} (m{y} - m{c}_b) imes m{T} dS_{m{y}}$ 



assume: 1) Reynolds # Re  $\approx 0$  e.g.  $\mu m$  particles in H<sub>2</sub>O

2) no Brownian (thermal) forcing i.e. deterministic

**Stokes Dirichlet BVP**: solve for (u, p) vel, pressure

in 
$$\Omega:=$$
 exterior of bodies  $\Omega_1,\dots,\Omega_{\mathcal{B}}$ 

$$-\mu\Delta {m u} + 
abla p ~=~ {m 0} ~~{
m in}~ \Omega ~~{
m local}~ {
m fluid}~ {
m force}~ {
m balance}$$

$$abla \cdot {\it u} = 0 \quad \text{in } \Omega \quad \text{incompressible}$$

$$\|\boldsymbol{u}(\boldsymbol{x})\| \to 0, \|\boldsymbol{x}\| \to \infty$$
 decay condition

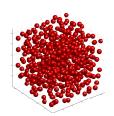
$$m{u} = m{u}_{ exttt{BC}} := m{v}_b + m{\omega}_b imes (m{x} - m{c}_b)$$
 on  $\partial \Omega_b$  given rigid-body motion

Unique solution exists for any boundary data uBC

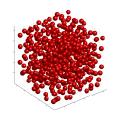
We'll need surface traction (force) vector  $\mathbf{T} = \mathbf{T}[\mathbf{u}, p] := -p\mathbf{n} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \cdot \mathbf{n}$ 

Then from solution can extract net forces and torques on 
$$b$$
th body:  $\mathbf{F}_b = \int_{\partial \Omega_b} \mathbf{T} dS_{\mathbf{y}} \qquad \mathbf{\tau}_b = \int_{\partial \Omega_b} (\mathbf{y} - \mathbf{c}_b) \times \mathbf{T} dS_{\mathbf{y}}$ 

"Resistance" problem: get  $\{ \mathbf{F}_b, \mathbf{\tau}_b \}_{b=1}^B$  from motions  $\{ \mathbf{v}_b, \boldsymbol{\omega}_b \}_{b=1}^B$   $\mathbf{F} = \mathcal{R} \mathbf{U}$  variant:  $\mathbf{u}_{\text{RC}}(\mathbf{x}) = \mathbf{v}_b + \boldsymbol{\omega}_b \times (\mathbf{x} - \mathbf{c}_b) - \mathbf{u}_0 + \mathbf{v}_{\text{slip}}$   $\leftarrow$  background flow  $\mathbf{u}_0$  and/or swimmers



assume: 1) Reynolds # Re  $\approx$  0 e.g.  $\mu$ m particles in H<sub>2</sub>O 2) no Brownian (thermal) forcing i.e. deterministic



Stokes Dirichlet BVP: solve for 
$$(\boldsymbol{u}, p)$$
 vel, pressure in  $\Omega :=$  exterior of bodies  $\Omega_1, \dots, \Omega_B$ 

$$-\mu\Delta m{u} + 
abla p = m{0}$$
 in  $\Omega$  local fluid force balance  $abla \cdot m{u} = 0$  in  $\Omega$  incompressible

$$\|oldsymbol{u}(oldsymbol{x})\| 
ightarrow 0, \quad \|oldsymbol{x}\| 
ightarrow \infty \quad ext{decay condition}$$

$$m{u} = m{u}_{ ext{BC}} := m{v}_b + m{\omega}_b imes (m{x} - m{c}_b)$$
 on  $\partial \Omega_b$  given rigid-body motion

Unique solution exists for any boundary data  $u_{BC}$  (Ladyzhenskaya '69)

We'll need surface traction (force) vector  $\mathbf{T} = \mathbf{T}[\mathbf{u}, p] := -p\mathbf{n} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \cdot \mathbf{n}$ Then from solution can extract net forces and torques on bth body:

$$m{F}_b = \int_{\partial\Omega_b} m{T} dS_{m{y}} \qquad \qquad m{ au}_b = \int_{\partial\Omega_b} (m{y} - m{c}_b) imes m{T} dS_{m{y}}$$
 "Resistance" problem: get  $\{m{F}_b, m{ au}_b\}_{b=1}^B$  from motions  $\{m{v}_b, m{\omega}_b\}_{b=1}^B$   $m{F} = \mathcal{R}m{U}$ 

variant:  $\mathbf{u}_{BC}(\mathbf{x}) = \mathbf{v}_b + \boldsymbol{\omega}_b \times (\mathbf{x} - \mathbf{c}_b) - \mathbf{u}_0 + \mathbf{v}_{slip}$   $\leftarrow$  background flow  $\mathbf{u}_0$  and/or swimmers

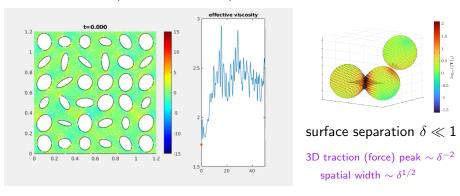
"Mobility" problem: its inverse formally  $\mathbf{U} = \mathcal{R}^{-1}\mathbf{F}$ , but don't compute that way!

### Challenges

 Elliptic BVP solve (long-range, all-to-all) needed each time-step moving geometry

### Challenges

- Elliptic BVP solve (long-range, all-to-all) needed each time-step moving geometry
- Close-touching (dense suspensions): strong lubrication forces



2D rheology of 25 neutrally-buoyant rigid ellipses, Wang-Nazockdast-B JCP '21

pressure near-singularities, diagonal force chains forming and breaking up

• Standard PDE solvers such as FEM impractical, rarely used

remeshing 3D exterior every time-step; unbounded domain;  $\nabla \cdot \textbf{\textit{u}} = 0$  constraint

- Standard PDE solvers such as FEM impractical, rarely used remeshing 3D exterior every time-step; unbounded domain;  $\nabla \cdot \mathbf{u} = 0$  constraint
- Discretize PDE on a grid must overlay the body boundaries, wrong if  $\delta$  <grid-spacing immersed boundary low-order (Peskin '72, Kallemov '26)
  - (Hansbo '14)
  - cut cell finite difference or FEM.

- Standard PDE solvers such as FEM impractical, rarely used remeshing 3D exterior every time-step; unbounded domain;  $\nabla \cdot \mathbf{u} = 0$  constraint
- Discretize PDE on a grid must overlay the body boundaries, wrong if δ <grid-spacing</li>
   immersed boundary low-order (Peskin '72, Kallemov '26)
  - cut cell finite difference or FEM

(Hansbo '14)

#### Green's function based: now don't need to discretize PDE...

- "Stokesian Dynamics" (chem. eng. community)
  - approximate long-range hydro. via "RPY tensor" (Brady-Bossis '88 etc)
  - add pair-wise lubrication approximation (Durlofsky et al '87)
     not convergent, except (Lefebvre-Lepot et al '15: lubrication, only 4 spheres)
- not convergent, except (Lerebyre-Lepot et al. 15. lubrication, only 4 spheres)
- Regularized Stokeslets / "rigid multiblobs" ad-hoc smoothing scale (Cortez '05)

- Standard PDE solvers such as FEM impractical, rarely used remeshing 3D exterior every time-step; unbounded domain;  $\nabla \cdot \mathbf{u} = 0$  constraint
- Discretize PDE on a grid must overlay the body boundaries, wrong if  $\delta$  <grid-spacing immersed boundary low-order (Peskin '72, Kallemov '26)
  - cut cell finite difference or FEM (Hansbo '14)

#### Green's function based: now don't need to discretize PDE...

- "Stokesian Dynamics" (chem. eng. community)
  - approximate long-range hydro. via "RPY tensor" (Brady-Bossis '88 etc)
  - add pair-wise lubrication approximation (Durlofsky et al '87)
     not convergent, except (Lefebvre-Lepot et al '15: lubrication, only 4 spheres)
- Regularized Stokeslets / "rigid multiblobs" ad-hoc smoothing scale (Cortez '05)
- Boundary integral equations (BIE)
   (Power–Miranda '87; state of art: af Klinteberg–Tornberg '16, Yan et al '20)

   potential theory using on-surface source density convergent, can be high-order

- Standard PDE solvers such as FEM impractical, rarely used remeshing 3D exterior every time-step; unbounded domain;  $\nabla \cdot \mathbf{u} = 0$  constraint
- $\bullet$  Discretize PDE on a grid must overlay the body boundaries, wrong if  $\delta$  <grid-spacing
  - immersed boundary low-order (Peskin '72, Kallemov '26)
  - cut cell finite difference or FEM

Green's function based: now don't need to discretize PDE...

(Hansbo '14)

- "Stokesian Dynamics" (chem. eng. community)
  - approximate long-range hydro. via "RPY tensor" (Brady-Bossis '88 etc.)
    - add pair-wise lubrication approximation (Durlofsky et al '87)
- not convergent, except (Lefebvre-Lepot et al '15: lubrication, only 4 spheres)
- Regularized Stokeslets / "rigid multiblobs" ad-hoc smoothing scale (Cortez '05)
- Boundary integral equations (BIE)
   (Power–Miranda '87; state of art: af Klinteberg–Tornberg '16, Yan et al '20)

   potential theory using on-surface source density convergent, can be high-order
- Collisons? prevented explicitly, with an artificially inflated radius e.g. 1.1R :(

"potential theory with off-surface sources" convergent, can be high-order used for acoustics, electromagnetics; rarely for Stokes

"potential theory with off-surface sources" convergent, can be high-order used for acoustics, electromagnetics; rarely for Stokes

Fundamental soln. 
$$\mathbb{S}(\pmb{x}, \pmb{y}) := \frac{1}{8\pi\mu} \left( \frac{\mathbb{I}}{\|\pmb{x} - \pmb{y}\|} + \frac{(\pmb{x} - \pmb{y})(\pmb{x} - \pmb{y})^T}{\|\pmb{x} - \pmb{y}\|^3} \right)$$

Stokeslet tensor.  $u(x) = \mathbb{S}(x, y)f$  flow field due to point force f at  $y \in \mathbb{R}^3$  a) solves PDE  $\forall x \neq y$ , b) incompressible, c) has decay  $||u|| \to 0$ 

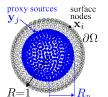


"potential theory with off-surface sources" convergent, can be high-order used for acoustics, electromagnetics; rarely for Stokes

Fundamental soln. 
$$\mathbb{S}(\boldsymbol{x}, \boldsymbol{y}) := \frac{1}{8\pi\mu} \left( \frac{\mathbb{I}}{\|\boldsymbol{x} - \boldsymbol{y}\|} + \frac{(\boldsymbol{x} - \boldsymbol{y})(\boldsymbol{x} - \boldsymbol{y})^T}{\|\boldsymbol{x} - \boldsymbol{y}\|^3} \right)$$
  
Stokeslet tensor.  $\boldsymbol{u}(\boldsymbol{x}) = \mathbb{S}(\boldsymbol{x}, \boldsymbol{y})\boldsymbol{f}$  flow field due to point force  $\boldsymbol{f}$  at  $\boldsymbol{y} \in \mathbb{R}^3$ 

a) solves PDE  $\forall \pmb{x} 
eq \pmb{y}$ , b) incompressible, c) has decay  $\|\pmb{u}\| o 0$ 





Choose "proxy" sources discretizing an interior surface Representation:  $u(x) = \sum_{i=1}^{N} \mathbb{S}(x, y_i) \lambda_i$  omit p(x) formula

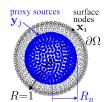
"potential theory with off-surface sources" convergent, can be high-order used for acoustics, electromagnetics; rarely for Stokes

Fundamental soln. 
$$\mathbb{S}(\pmb{x},\pmb{y}) \coloneqq \frac{1}{8\pi\mu} \left( \frac{\mathbb{I}}{\|\pmb{x}-\pmb{y}\|} + \frac{(\pmb{x}-\pmb{y})(\pmb{x}-\pmb{y})^T}{\|\pmb{x}-\pmb{y}\|^3} \right)$$

Stokeslet tensor.  $u(x) = \mathbb{S}(x,y)f$  flow field due to point force f at  $y \in \mathbb{R}^3$ 

a) solves PDE  $\forall \pmb{x} 
eq \pmb{y}$ , b) incompressible, c) has decay  $\|\pmb{u}\| o 0$ 





Choose "proxy" sources discretizing an interior surface

Representation: 
$$u(x) = \sum_{j=1}^{N} \mathbb{S}(x, y_j) \lambda_j$$
 omit  $p(x)$  formula

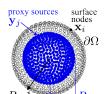
Enforce BC by collocation on nodes  $\mathbf{x}_i \in \partial \Omega$ :

$$\sum_{j=1}^{N} \mathbb{S}(\mathbf{x}_i, \mathbf{y}_j) \lambda_j = \mathbf{u}_{\mathsf{BC}}(\mathbf{x}_i), \qquad i = 1, \dots, M$$

abbrev:  $G\lambda = u_{BC}$  G target-from-source matrix,  $3M \times 3N$ 

"potential theory with off-surface sources" convergent, can be high-order used for acoustics, electromagnetics; rarely for Stokes

Fundamental soln. 
$$\mathbb{S}(\boldsymbol{x}, \boldsymbol{y}) := \frac{1}{8\pi\mu} \left( \frac{\mathbb{I}}{\|\boldsymbol{x} - \boldsymbol{y}\|} + \frac{(\boldsymbol{x} - \boldsymbol{y})(\boldsymbol{x} - \boldsymbol{y})^T}{\|\boldsymbol{x} - \boldsymbol{y}\|^3} \right)$$
  
Stokeslet tensor.  $\boldsymbol{u}(\boldsymbol{x}) = \mathbb{S}(\boldsymbol{x}, \boldsymbol{y})\boldsymbol{f}$  flow field due to point force  $\boldsymbol{f}$  at  $\boldsymbol{y} \in \mathbb{R}^3$  a) solves PDE  $\forall \boldsymbol{x} \neq \boldsymbol{y}$ , b) incompressible, c) has decay  $\|\boldsymbol{u}\| \to 0$ 



Choose "proxy" sources discretizing an interior surface Representation:  $u(x) = \sum_{j=1}^N \mathbb{S}(x, y_j) \lambda_j$  omit p(x) formula

Enforce BC by collocation on nodes  $x_i \in \partial \Omega$ :

$$\sum_{j=1}^{N} \mathbb{S}(\mathbf{x}_i, \mathbf{y}_j) \lambda_j = \mathbf{u}_{BC}(\mathbf{x}_i), \qquad i = 1, \dots, M$$

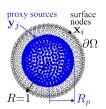
abbrev:  $G\lambda = u_{BC}$  G target-from-source matrix,  $3M \times 3N$ 

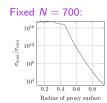
If proxy surface *well-separated* from  $\partial\Omega$ :

- 1) functions  $\mathbb{S}(\cdot, \mathbf{y}_j)$  on  $\partial\Omega$  are **smooth**: simple quadrature e.g.  $M\approx 1.3N$
- 2) representation accurate for flow eval. arbitrarily close to and on  $\partial\Omega$

contrast BIE: technical singular quadratures needed on  $\partial\Omega$ , near-singular ones close to  $\partial\Omega$ 

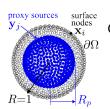
### ... but MFS does have a catch!



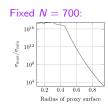


Intuitively:  $\sigma_{\min}$  controlled by the degree- $\sqrt{N}$  sph. harmonic which decayed like  $(R_p/R)^{\sqrt{N}}$ 

### but MFS does have a catch!



Condition #  $\kappa(G) := \frac{\sigma_{\text{max}}}{\sigma_{\text{min}}} \gtrsim 10^8$ grows (root) exponentially in N growth rate worse as proxy  $R_p$  shrinks but small  $R_p$  needed for small errors!

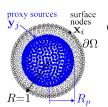


Intuitively:  $\sigma_{\min}$  controlled by the degree- $\sqrt{N}$  sph. harmonic which decayed like  $(R_p/R)^{\sqrt{N}}$ 

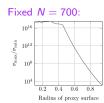
Consequence: iterative solution impossible need least-squares:  $\min_{\lambda \in \mathbb{R}^{3N}} \|G\lambda - \mathbf{u}_{BC}\|_{2}$  ... with  $\|\lambda\|^{2}$  not needlessly big

unlike well-conditioned BIF

### ... but MFS does have a catch!



 $\begin{array}{ll} \text{Condition} \ \# & \kappa(\textit{G}) := \frac{\sigma_{\max}}{\sigma_{\min}} \gtrsim 10^8 \\ \text{grows (root) exponentially in } \textit{N} \\ \text{growth rate worse as proxy } \textit{R}_{\textit{p}} \text{ shrinks} \\ \text{but small } \textit{R}_{\textit{p}} \text{ needed for small errors!} \end{array}$ 

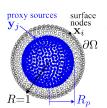


Intuitively:  $\sigma_{\min}$  controlled by the degree- $\sqrt{N}$  sph. harmonic which decayed like  $(R_p/R)^{\sqrt{N}}$ 

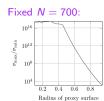
Consequence: iterative solution impossible unlike well-conditioned BIE need least-squares:  $\min_{\lambda \in \mathbb{R}^{3N}} \|G\lambda - u_{\text{BC}}\|_2$  ... with  $\|\lambda\|^2$  not needlessly big

Direct soln via SVD:  $G = U\Sigma V^T$ , where  $\Sigma = \text{diag}\{\sigma_k\}$  cost  $\mathcal{O}(N^3)$  pick cut-off  $\epsilon$  (e.g.  $10^{-12}$ ), set  $\Sigma^+ := \text{diag}\{\sigma_k^{-1} \text{ if } \sigma_k > \epsilon \sigma_1, \text{ else } 0\}$ 

### ... but MFS does have a catch!



 $\begin{array}{ll} \text{Condition} \ \# & \kappa(\textit{G}) := \frac{\sigma_{\max}}{\sigma_{\min}} \gtrsim 10^8 \\ \text{grows (root) exponentially in } \textit{N} \\ \text{growth rate worse as proxy } \textit{R}_{\textit{p}} \text{ shrinks} \\ \text{but small } \textit{R}_{\textit{p}} \text{ needed for small errors!} \end{array}$ 



Intuitively:  $\sigma_{\min}$  controlled by the degree- $\sqrt{N}$  sph. harmonic which decayed like  $(R_p/R)^{\sqrt{N}}$ 

Consequence: iterative solution impossible unlike well-conditioned BIE need least-squares:  $\min_{\pmb{\lambda} \in \mathbb{R}^{3N}} \| G \pmb{\lambda} - \pmb{u}_{\text{BC}} \|_2$  ... with  $\| \pmb{\lambda} \|^2$  not needlessly big

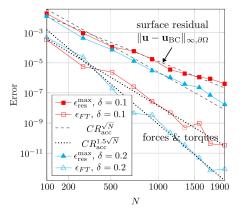
Direct soln via SVD:  $G = U\Sigma V^T$ , where  $\Sigma = \mathrm{diag}\{\sigma_k\}$  cost  $\mathcal{O}(N^3)$  pick cut-off  $\epsilon$  (e.g.  $10^{-12}$ ), set  $\Sigma^+ := \mathrm{diag}\{\sigma_k^{-1} \text{ if } \sigma_k > \epsilon \sigma_1, \text{ else } 0\}$  then  $\lambda \approx V\Sigma^+(U^T \mathbf{u}_{\mathrm{BC}}) =: G^+\mathbf{u}_{\mathrm{BC}}$  a (possibly regularized) pseudoinverse

Note:  $G^+$  should never be filled! Backward stable iff apply the two matvecs in above order

However, MFS effective for simple smooth bodies  $N, M \sim 10^3$ , SVD  $\sim$  few secs

# MFS small example

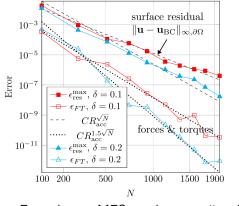
MFS discretization solving resistance for B=2 unit spheres:  $R_p=0.6$ 



Separations  $\delta = 0.1$ ,  $\delta = 0.2$ Error in forces and torques hits  $10^{-10}$  by  $N \approx 1700$  convergence root-exponential for some rate  $R_{\rm acc}(\delta)$  smaller  $\delta \Rightarrow$  slower conv.

# MFS small example

MFS discretization solving resistance for B = 2 unit spheres:  $R_p = 0.6$ 



Separations  $\delta = 0.1$ ,  $\delta = 0.2$ 

Error in forces and torques hits  $10^{-10}$  by  $N\approx 1700$  convergence root-exponential for some rate  $R_{\rm acc}(\delta)$ 

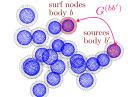
smaller  $\delta \Rightarrow$  slower conv.

- For spheres, MFS needs same # unknowns as BIE for same error
   BIE uses elaborate vector spherical harmonic close-eval. (Corona-Veerapaneni '18)
- MFS (as BIE) can handle more general smooth shapes (Liu-B '15)

$$\begin{bmatrix} G^{(11)} & G^{(12)} & \dots & G^{(1B)} \\ G^{(21)} & G^{(22)} & \dots & \dots \\ \vdots & \vdots & \ddots & \vdots \\ G^{(B1)} & \dots & \dots & G^{(BB)} \end{bmatrix} \begin{bmatrix} \boldsymbol{\lambda}^{(1)} \\ \vdots \\ \boldsymbol{\lambda}^{(B)} \end{bmatrix} = \begin{bmatrix} \boldsymbol{u}_{\mathsf{BC}}^{(1)} \\ \vdots \\ \boldsymbol{u}_{\mathsf{BC}}^{(B)} \end{bmatrix}$$

abbrev:  $G\lambda = u_{BC}$  huge  $3MB \times 3NB$ , ill-cond.  $\Rightarrow$  can't solve iteratively

$$\begin{bmatrix} G^{(11)} & G^{(12)} & \dots & G^{(1B)} \\ G^{(21)} & G^{(22)} & \dots & \dots \\ \vdots & \vdots & \ddots & \vdots \\ G^{(B1)} & \dots & \dots & G^{(BB)} \end{bmatrix} \begin{bmatrix} \boldsymbol{\lambda}^{(1)} \\ \vdots \\ \boldsymbol{\lambda}^{(B)} \end{bmatrix} = \begin{bmatrix} \boldsymbol{u}_{\mathsf{BC}}^{(1)} \\ \vdots \\ \boldsymbol{u}_{\mathsf{BC}}^{(B)} \end{bmatrix}$$



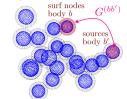
abbrev:  $G\lambda = \mathbf{u}_{BC}$  huge  $3MB \times 3NB$ , ill-cond.  $\Rightarrow$  can't solve iteratively

Block-diag. ("1-body") right-precondition: insert  $\lambda^{(b)} = G^{(bb)} + \mu^{(b)}$ , b = 1, ..., B

$$\begin{bmatrix} G^{(11)}G^{(11)+} & G^{(12)}G^{(22)+} & \dots & G^{(1B)}G^{(BB)+} \\ G^{(21)}G^{(11)+} & G^{(22)}G^{(22)+} & \dots & \dots \\ \vdots & \vdots & \ddots & \vdots \\ G^{(B1)}G^{(11)+} & \dots & \dots & G^{(BB)}G^{(BB)+} \end{bmatrix} \begin{bmatrix} \boldsymbol{\mu}^{(1)} \\ \vdots \\ \boldsymbol{\mu}^{(B)} \end{bmatrix} = \begin{bmatrix} \boldsymbol{u}_{\mathsf{BC}}^{(1)} \\ \vdots \\ \boldsymbol{u}_{\mathsf{BC}}^{(B)} \end{bmatrix}$$

changes basis to **surface vel.** unknowns  $\mu^{(b)}$ , just as in "direct BIE" diag. blocks: projectors onto Col  $G^{(bb)}$ , rank-deficient since M>N  $\Rightarrow$  replace by I

$$\begin{bmatrix} G^{(11)} & G^{(12)} & \dots & G^{(1B)} \\ G^{(21)} & G^{(22)} & \dots & \dots \\ \vdots & \vdots & \ddots & \vdots \\ G^{(B1)} & \dots & \dots & G^{(BB)} \end{bmatrix} \begin{bmatrix} \boldsymbol{\lambda}^{(1)} \\ \vdots \\ \boldsymbol{\lambda}^{(B)} \end{bmatrix} = \begin{bmatrix} \boldsymbol{u}_{\mathsf{BC}}^{(1)} \\ \vdots \\ \boldsymbol{u}_{\mathsf{BC}}^{(B)} \end{bmatrix}$$



abbrev:  $G\lambda = \mathbf{u}_{BC}$  huge  $3MB \times 3NB$ , ill-cond.  $\Rightarrow$  can't solve iteratively

Block-diag. ("1-body") right-precondition: insert  $\lambda^{(b)} = G^{(bb)} + \mu^{(b)}$ , b = 1, ..., B

$$\begin{bmatrix} I & G^{(12)}G^{(22)+} & \dots & G^{(1B)}G^{(BB)+} \\ G^{(21)}G^{(11)+} & I & \dots & \dots \\ \vdots & \vdots & \ddots & \vdots \\ G^{(B1)}G^{(11)+} & \dots & \dots & I \end{bmatrix} \begin{bmatrix} \boldsymbol{\mu}^{(1)} \\ \vdots \\ \boldsymbol{\mu}^{(B)} \end{bmatrix} = \begin{bmatrix} \boldsymbol{u}_{\mathsf{BC}}^{(1)} \\ \vdots \\ \boldsymbol{u}_{\mathsf{BC}}^{(B)} \end{bmatrix}$$

changes basis to **surface vel.** unknowns  $\mu^{(b)}$ , just as in "direct BIE" diag. blocks: projectors onto Col  $G^{(bb)}$ , rank-deficient since M>N  $\Rightarrow$  replace by I

$$\begin{bmatrix} G^{(11)} & G^{(12)} & \dots & G^{(1B)} \\ G^{(21)} & G^{(22)} & \dots & \dots \\ \vdots & \vdots & \ddots & \vdots \\ G^{(B1)} & \dots & G^{(BB)} \end{bmatrix} \begin{bmatrix} \boldsymbol{\lambda}^{(1)} \\ \vdots \\ \boldsymbol{\lambda}^{(B)} \end{bmatrix} = \begin{bmatrix} \boldsymbol{u}_{\mathsf{BC}}^{(1)} \\ \vdots \\ \boldsymbol{u}_{\mathsf{BC}}^{(B)} \end{bmatrix}$$

abbrev:  $G\lambda = \mathbf{u}_{BC}$  huge  $3MB \times 3NB$ , ill-cond.  $\Rightarrow$  can't solve iteratively

Block-diag. ("1-body") right-precondition: insert 
$$\lambda^{(b)} = G^{(bb)}^+ \mu^{(b)}$$
,  $b = 1, \dots, B$ 

$$\begin{bmatrix} I & G^{(12)}G^{(22)+} & \dots & G^{(1B)}G^{(BB)+} \\ G^{(21)}G^{(11)+} & I & \dots & \dots \\ \vdots & \vdots & \ddots & \vdots \\ G^{(B1)}G^{(11)+} & \dots & \dots & I \end{bmatrix} \begin{bmatrix} \boldsymbol{\mu}^{(1)} \\ \vdots \\ \boldsymbol{\mu}^{(B)} \end{bmatrix} = \begin{bmatrix} \boldsymbol{u}_{\mathsf{BC}}^{(1)} \\ \vdots \\ \boldsymbol{u}_{\mathsf{BC}}^{(B)} \end{bmatrix}$$

changes basis to **surface vel.** unknowns  $oldsymbol{\mu}^{(b)}$ , just as in "direct BIE"

diag. blocks: projectors onto Col  $G^{(bb)}$ , rank-deficient since  $M > N \implies$  replace by I

abbrev:  $G\mu= extbf{\emph{u}}_{ extsf{BC}}$  huge, square, well-cond.  $\Rightarrow$  iter. solve (Liu–B '15, Stein–B, '22)

# Iterative solution of $\tilde{G}\mu=u_{\scriptscriptstyle \mathrm{BC}}$ for resistance prob.

We use GMRES as solver each iteration needs matvec  $\mathbf{u} \leftarrow \tilde{G} \mu$ 

 $\tilde{G}$  is way too big to fill or store!

minimizes residual in the Krylov subspace

# Iterative solution of $\tilde{G}\mu=u_{\scriptscriptstyle \mathrm{BC}}$ for resistance prob.

We use GMRES as solver

minimizes residual in the Krylov subspace

each iteration needs matvec  ${\it u} \leftarrow \tilde{\it G} \mu$ 

 $\tilde{G}$  is way too big to fill or store! But can do matvec fast in 3 steps:

1) 
$$\lambda^{(b)} = G^{(bb)^+} \mu^{(b)}, b = 1, ..., B$$

each block uses 2-step  $V\Sigma^+(U^Toldsymbol{\mu}^{(b)})$ 

We use GMRES as solver

minimizes residual in the Krylov subspace

each iteration needs matvec  $oldsymbol{u} \leftarrow ilde{G} oldsymbol{\mu}$ 

 $\tilde{G}$  is way too big to fill or store! But can do matvec fast in 3 steps:

1) 
$$\boldsymbol{\lambda}^{(b)} = G^{(bb)^+} \boldsymbol{\mu}^{(b)}$$
,  $b = 1, \dots, B$  each block uses 2-step  $V\Sigma^+(U^T \boldsymbol{\mu}^{(b)})$ 

2) 
$$\boldsymbol{u}_{i}^{(b)} = \sum_{b'=1}^{B} \sum_{j=1}^{N} \mathbb{S}(\boldsymbol{x}_{i}^{(b)}, \boldsymbol{y}_{j}^{(b')}) \boldsymbol{\lambda}_{j}^{(b')}$$
  $i = 1, ..., N, b = 1, ..., B$  all-to-all

We use GMRES as solver

minimizes residual in the Krylov subspace

each iteration needs matvec  $oldsymbol{u} \leftarrow ilde{G} oldsymbol{\mu}$ 

 $\tilde{G}$  is way too big to fill or store! But can do matvec fast in 3 steps:

1) 
$$\boldsymbol{\lambda}^{(b)} = G^{(bb)^+} \boldsymbol{\mu}^{(b)}$$
,  $b=1,\ldots,B$  each block uses 2-step  $V\Sigma^+(U^T \boldsymbol{\mu}^{(b)})$ 

2) 
$$\boldsymbol{u}_{i}^{(b)} = \sum_{b'=1}^{B} \sum_{j=1}^{N} \mathbb{S}(\boldsymbol{x}_{i}^{(b)}, \boldsymbol{y}_{j}^{(b')}) \boldsymbol{\lambda}_{j}^{(b')}$$
  $i = 1, ..., N, b = 1, ..., B$  all-to-all

Stokes fast multipole method, linear cost in # sources+targets (Tornberg-Greengard '08)

Black-box software: FMM3D (Rachh et al), PVFMM (Malhotra), STKFMM (Wen et al)

Parallel throughput  $10^4$  to  $10^5$  pts/sec/core, depending on requested tolerance

We use GMRES as solver

minimizes residual in the Krylov subspace

each iteration needs matvec  $oldsymbol{u} \leftarrow ilde{G} oldsymbol{\mu}$ 

 $\tilde{G}$  is way too big to fill or store! But can do matvec fast in 3 steps:

1) 
$$\boldsymbol{\lambda}^{(b)} = G^{(bb)^+} \boldsymbol{\mu}^{(b)}$$
,  $b = 1, \dots, B$  each block uses 2-step  $V\Sigma^+(U^T \boldsymbol{\mu}^{(b)})$ 

2) 
$$\mathbf{u}_{i}^{(b)} = \sum_{b'=1}^{B} \sum_{j=1}^{N} \mathbb{S}(\mathbf{x}_{i}^{(b)}, \mathbf{y}_{j}^{(b')}) \lambda_{j}^{(b')}$$
  $i = 1, ..., N, b = 1, ..., B$  all-to-all

Stokes fast multipole method, linear cost in # sources+targets (Tornberg-Greengard '08)

Black-box software: FMM3D (Rachh et al), PVFMM (Malhotra), STKFMM (Wen et al)

Parallel throughput 10<sup>4</sup> to 10<sup>5</sup> pts/sec/core, depending on requested tolerance

3) 
$$\boldsymbol{u}_i^{(b)} = \boldsymbol{u}_i^{(b)} - G^{(bb)} \boldsymbol{\lambda}^{(b)} + \boldsymbol{\mu}^{(b)}, \quad b=1,\ldots,B$$
 replaces diag. blocks by  $l$ .

We use GMRES as solver

minimizes residual in the Krylov subspace

each iteration needs matvec  $oldsymbol{u} \leftrightarrow ilde{G} \mu$ 

 $\tilde{G}$  is way too big to fill or store! But can do matvec fast in 3 steps:

1) 
$$\boldsymbol{\lambda}^{(b)} = G^{(bb)^+} \boldsymbol{\mu}^{(b)}$$
,  $b = 1, \dots, B$  each block uses 2-step  $V\Sigma^+(U^T \boldsymbol{\mu}^{(b)})$ 

2) 
$$m{u}_i^{(b)} = \sum_{b'=1}^{B} \sum_{j=1}^{N} \mathbb{S}(m{x}_i^{(b)}, m{y}_j^{(b')}) m{\lambda}_j^{(b')}$$
  $i = 1, \dots, N, \ b = 1, \dots, B$  all-to-all

Stokes fast multipole method, linear cost in # sources+targets (Tornberg-Greengard '08)
Black-box software: FMM3D (Rachh et al), PVFMM (Malhotra), STKFMM (Wen et al)

Parallel throughput 10<sup>4</sup> to 10<sup>5</sup> pts/sec/core, depending on requested tolerance

3) 
$$oldsymbol{u}_i^{(b)} = oldsymbol{u}_i^{(b)} - G^{(bb)} oldsymbol{\lambda}^{(b)} + oldsymbol{\mu}^{(b)}, \quad b=1,\ldots,B$$
 replaces diag. blocks by  $I$ .

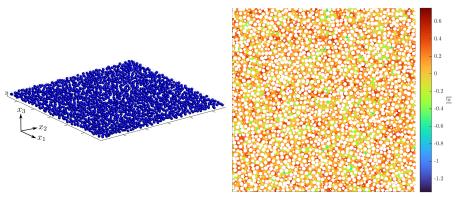
Once GMRES solved for  $\mu$ , get proxy strength vector  $\lambda$  by Step 1

Then use MFS rep. to evaluate Stokes flow  $(\boldsymbol{u},p)$  anywhere in  $\Omega$ 

Evaluate net forces & torques: easy, sum the sources 
$$\mathbf{F}_b = \sum_{j=1}^N \lambda_j^{(b)}$$
  $\tau_b = \sum_{j=1}^N (\mathbf{y}_j^{(b)} - \mathbf{c}_b) \times \lambda_j^{(b)}$ 

### Results: resistance problem via MFS

B=2000 monodisperse sphere layer given random motions  $\{\mathbf{v}_b, \boldsymbol{\omega}_b\}_{b=1}^B$ :

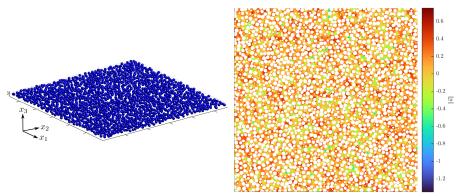


 $\delta_{\rm min} = 0.25$   $R_{\rm p} = 0.63$   $N \approx 700$   $M \approx 900$  solve time 5 hrs 12-core desktop



### Results: resistance problem via MFS

B=2000 monodisperse sphere layer given random motions  $\{m{v}_b, m{\omega}_b\}_{b=1}^B$ :



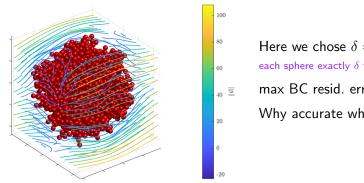
 $\delta_{\rm min} = 0.25$   $R_{\rm p} = 0.63$   $N \approx 700$   $M \approx 900$  solve time 5 hrs 12-core desktop

- FMM (step 2) is > 90% of cost good
- GMRES (rel. resid.  $10^{-7}$ ): 100 iters. weak growth w/ B
- $10^{-3}$  uniform residual in boundary condition  $m{u}|_{\partial\Omega} m{u}_{ exttt{BC}}$
- $10^{-5}$  in forces+torques by convergence study



### Results: cluster porosity problem via MFS

B = 2000 fixed spheres in background shear flow  $\mathbf{u}_0 = (0, -5x_1, 0)$ :



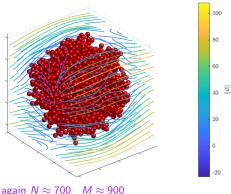
again  $N \approx 700$   $M \approx 900$ 

5 million unknowns 10 hrs desktop

Here we chose  $\delta = 10^{-3}$ each sphere exactly  $\delta$  from another max BC resid. error  $10^{-4}$ Why accurate when  $\delta$  so small?!

### Results: cluster porosity problem via MFS

B=2000 **fixed** spheres in background shear flow  $\boldsymbol{u}_0=(0,-5x_1,0)$ :



again  $N \approx 700$   $M \approx 900$ 5 million unknowns 10 hrs desktop

Here we chose  $\delta=10^{-3}$  each sphere exactly  $\delta$  from another max BC resid. error  $10^{-4}$  Why accurate when  $\delta$  so small?!

No rel. motion  $\rightarrow$  no lubrication sing. PDE analysis needed here! smooth u, plain MFS works well

Recall MFS discretization of resistance prob: (no backgnd, no slip, no precond.)  $G\lambda pprox oldsymbol{u}_{BC} =: K_M U$  motions vec.  $oldsymbol{U} := \{oldsymbol{v}_b, \omega_b\}_{b=1}^B$   $K_M$  tall:  $3MB \times 6B$ 

then extract 
$$m{F}:=\{m{F}_b,m{ au}_b\}_{b=1}^B=m{K}_N^Tm{\lambda}$$
 K<sub>N</sub> analogous 3NB  $imes$  6B

Recall MFS discretization of resistance prob: (no backgnd, no slip, no precond.)  $G\lambda \approx \textbf{\textit{u}}_{BC} =: K_M U \qquad \text{motions vec. } \textbf{\textit{U}} := \{\textbf{\textit{v}}_b, \omega_b\}_{b=1}^B \quad K_M \text{ tall: } 3MB \times 6B \text{ then extract } \textbf{\textit{F}} := \{\textbf{\textit{F}}_b, \tau_b\}_{b=1}^B = K_N^T \lambda \qquad K_N \text{ analogous } 3NB \times 6B \text{ And the substitute } G\lambda \approx K_M \textbf{\textit{U}} \quad \textbf{\textit{U}} \text{ unknown}$ 

Recall MFS discretization of resistance prob: (no backgnd, no slip, no precond.)  $G\lambda \approx \textbf{\textit{u}}_{BC} =: K_M U \qquad \text{motions vec. } \textbf{\textit{U}} := \{\textbf{\textit{v}}_b, \omega_b\}_{b=1}^B \quad K_M \text{ tall: } 3MB \times 6B \text{ then extract } \textbf{\textit{F}} := \{\textbf{\textit{F}}_b, \tau_b\}_{b=1}^B = K_N^T \lambda \qquad K_N \text{ analogous } 3NB \times 6B$ 

How solve mobility with linear cost, as resistance? abbrev. MFS rep.  $u = \mathbb{S}\lambda$ 

Let 
$$L :=$$
 orthog. proj. to Col  $K_N$ . Pick  $\lambda_0$  s.t.  $K_N^T \lambda_0 = F$ 

Idea: new rep. 
$$\boldsymbol{u} = \mathbb{S}[(I-L)\boldsymbol{\lambda} + \boldsymbol{\lambda}_0]$$
 has correct net  $\boldsymbol{F}$  since  $K_N^T(I-L) = 0$ 

Recall MFS discretization of resistance prob: (no backgnd, no slip, no precond.)  $G\lambda \approx \textbf{\textit{u}}_{BC} =: K_M U \qquad \text{motions vec. } \textbf{\textit{U}} := \{\textbf{\textit{v}}_b, \omega_b\}_{b=1}^B \quad K_M \text{ tall: } 3MB \times 6B \\ \text{then extract } \textbf{\textit{F}} := \{\textbf{\textit{F}}_b, \tau_b\}_{b=1}^B = K_N^T \lambda \qquad K_N \text{ analogous } 3NB \times 6B$ 

How solve mobility with linear cost, as resistance? abbrev. MFS rep.  $u = S\lambda$ 

Let L := orthog. proj. to Col  $K_N$ . Pick  $\lambda_0$  s.t.  $K_N^T \lambda_0 = \mathbf{F}$ 

Idea: new rep. 
$$\boldsymbol{u} = \mathbb{S}[(I-L)\boldsymbol{\lambda} + \boldsymbol{\lambda}_0]$$
 has correct net  $\boldsymbol{F}$  since  $K_N^T(I-L) = 0$ 

Idea: couple  $\boldsymbol{U}$  to unused 6B-dim  $\boldsymbol{\lambda}$  subspace: Ansatz  $\boldsymbol{U} = -K_{N}^{T}\boldsymbol{\lambda}$ 

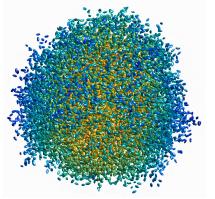
Get lin. sys: 
$$[G(I-L) + K_M K_N^T] \lambda = -G \lambda_0$$
 known RHS, eval. by FMM

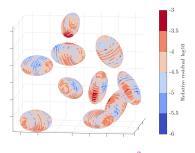
once solved, extract motions vec. **U** using Ansatz

- new; related to "completed double-layer" formulation (Power–Miranda '87)
- modified blocks, can apply 1-body precond, GMRES+FMM iter. solve

### Large scale mobility via MFS

B=10000 ellipsoids, random forces+torques:  $\delta_{min}=0.2$ , semiaxes (0.4,0.6,1)





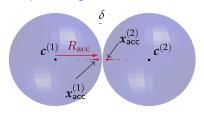
zoom of surface resid. err.  $10^{-3}$  proxy sources displaced along n

- $10^{-5}$  errors in *U*, total degrees of freedom  $3MB \approx 2.6 \times 10^7$
- solution time 2 hrs 8-core desktop, only 7 iters needed
- for mobility we see # iters. does not grow with B for resistance it grows already observed (Ichiki '02, Usabiaga '16); explanation needed!
- usually mobility of this scale needs MPI (2k cores for 80k spheres: Yan et al. '20)

### Close-touching spheres with relative motion

Laplace Dirichlet BVP: 2 charged conducting spheres has analytic soln

a point charge c at radius r reflects in 1 unit sphere: inversion  $r \mapsto 1/r$ , strength -c/r



Alternating sphere reflections:  $\infty$  series (electrostatics, Lord Kelvin 1853)

Limit (accumulation) point:

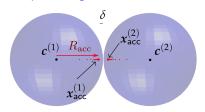
$$R_{
m acc} = 1 + rac{\delta}{2} - \sqrt{\delta + rac{\delta^2}{4}} = 1 - \mathcal{O}(\delta^{1/2})$$

limit singularity lies dist  $\mathcal{O}(\delta^{1/2})$  under surface

### Close-touching spheres with relative motion

Laplace Dirichlet BVP: 2 charged conducting spheres has analytic soln

a point charge c at radius r reflects in 1 unit sphere: inversion  $r \mapsto 1/r$ , strength -c/r



Alternating sphere reflections:  $\infty$  series (electrostatics, Lord Kelvin 1853)

Limit (accumulation) point:

$$R_{ ext{acc}} = 1 + rac{\delta}{2} - \sqrt{\delta + rac{\delta^2}{4}} = 1 - \mathcal{O}(\delta^{1/2})$$

limit singularity lies dist  $\mathcal{O}(\delta^{1/2})$  under surface

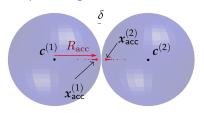
#### Stokes BVP is more elaborate:

- Stokeslet reflecting in 1 sphere already gives line density  $r \mapsto [0, 1/r]$
- no known 2-sphere images, but expect line singularity only on [0, R<sub>acc</sub>]
  matches decay rate of bipolar-coords series soln for 2 squeezing spheres (Brenner '61)

### Close-touching spheres with relative motion

Laplace Dirichlet BVP: 2 charged conducting spheres has analytic soln

a point charge c at radius r reflects in 1 unit sphere: inversion  $r \mapsto 1/r$ , strength -c/r



Alternating sphere reflections:  $\infty$  series (electrostatics, Lord Kelvin 1853)

Limit (accumulation) point:

$$R_{ ext{acc}} = 1 + rac{\delta}{2} - \sqrt{\delta + rac{\delta^2}{4}} = 1 - \mathcal{O}(\delta^{1/2})$$

limit singularity lies dist  $\mathcal{O}(\delta^{1/2})$  under surface

#### Stokes BVP is more elaborate:

- Stokeslet reflecting in 1 sphere already gives line density  $r \mapsto [0, 1/r]$
- no known 2-sphere images, but expect line singularity only on [0, R<sub>acc</sub>]
  matches decay rate of bipolar-coords series soln for 2 squeezing spheres (Brenner '61)

Concept: exterior PDE soln may continue inside as PDE soln for some dist.

"analytic continuation": holomorphic theory of PDE for analytic data and boundary  $\partial\Omega$ 

Upshot: for 2 unit Stokes spheres,  ${\it u}$  continues in to radius  $R_{ ext{acc}} < 1$ 

### MFS theory: stability & convergence rate

Unit spheres sep. by  $\delta$ : PDE soln continues inside to  $R_{acc}(\delta) < 1$ 

2D MFS theorems (Katsurada '89, B-Betcke '08) then suggest in 3D...

- stable i.e.  $\|\lambda\|_{\infty} = \mathcal{O}(1)$  iff  $R_n > R_{\text{acc}}$ proxy surface must enclose singularities
- $R_p = R_{acc}$  decent choice:



 MFS conv. rate is then set by R<sub>acc</sub>: error =  $\mathcal{O}(R_{\rm acc}^{\sqrt{N}})$ 

This explains dashed lines in convergence plot...

### MFS theory: stability & convergence rate

Unit spheres sep. by  $\delta$ : PDE soln continues inside to  $R_{ ext{acc}}(\delta) < 1$ 

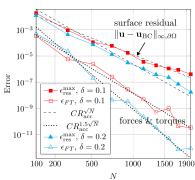
2D MFS theorems (Katsurada '89, B-Betcke '08) then suggest in 3D...

- stable i.e.  $\|\lambda\|_{\infty}=\mathcal{O}(1)$  iff  $R_{p}\geq R_{\mathrm{acc}}$  proxy surface must enclose singularities
- $R_p = R_{acc}$  decent choice:



• MFS conv. rate is then set by  $R_{\rm acc}$ : error =  $\mathcal{O}(R_{\rm acc}^{\sqrt{N}})$ 

This explains dashed lines in convergence plot...



### MFS theory: stability & convergence rate

Unit spheres sep. by  $\delta$ : PDE soln continues inside to  $R_{ ext{acc}}(\delta) < 1$ 

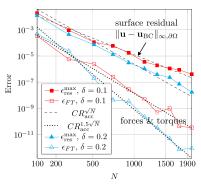
2D MFS theorems (Katsurada '89, B-Betcke '08) then suggest in 3D...

- stable i.e.  $\|\lambda\|_{\infty}=\mathcal{O}(1)$  iff  $R_p\geq R_{\mathrm{acc}}$  proxy surface must enclose singularities
- $R_p = R_{acc}$  decent choice:



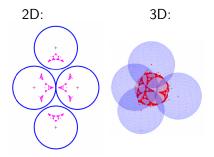
• MFS conv. rate is then set by  $R_{\rm acc}$ : error =  $\mathcal{O}(R_{\rm acc}^{\sqrt{N}})$ 

This explains dashed lines in convergence plot...



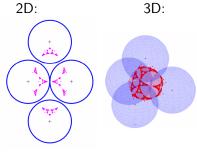
Problem: close spheres makes  $R_{\rm acc} \to 1^-$ , means convergence grinds to halt to maintain fixed error demands huge  $N \gtrsim \mathcal{O}(\delta^{-1})$   $\mathcal{O}(N^3)$  cost would be impractical for  $\delta \lesssim 0.05$  We now fix that...

Multi-sphere reflection images:



2D: "Indra's pearls" (Klein 1897)

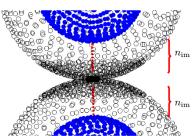
*Multi*-sphere reflection images:

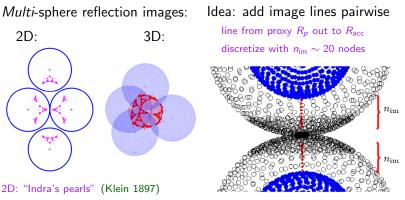


2D: "Indra's pearls" (Klein 1897)

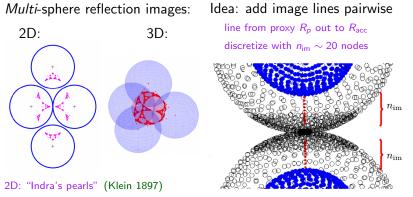
### Idea: add image lines pairwise

line from proxy  $R_p$  out to  $R_{\rm acc}$  discretize with  $n_{\rm im} \sim 20$  nodes





- Indra's singularity "dust" ⇒ not obvious that pairwise lines enough!
   but suggested by 2D success of elaborate pairwise image sums (Cheng-Greengard '98)
- true singularity unknown: Stokeslets + rotlets + doublets needed
- must increase collocation node density near singularity



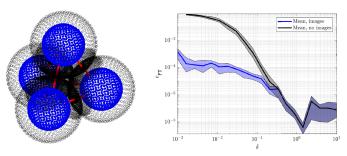
- Indra's singularity "dust" ⇒ not obvious that pairwise lines enough!
   but suggested by 2D success of elaborate pairwise image sums (Cheng-Greengard '98)
- true singularity unknown: Stokeslets + rotlets + doublets needed
- must increase collocation node density near singularity

Philosophy: be *inspired* by elaborate analytic formulae .... but instead make the *computer* solve for the coeffs!

### Results: resistance for B = 4 close spheres

We target 3-digit accuracy for separations down to  $\delta = 10^{-3}$ :

in  $\mu \mathrm{m}$  particles, surface roughness breaks the model at that scale

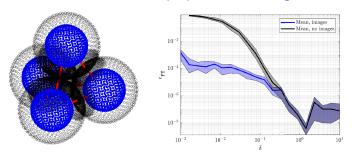


 $N \approx 700$   $n_{\rm im} = 20$ , equiv to 60 extra sources per near-contact

### Results: resistance for B = 4 close spheres

We target 3-digit accuracy for separations down to  $\delta = 10^{-3}$ :

in  $\mu m$  particles, surface roughness breaks the model at that scale



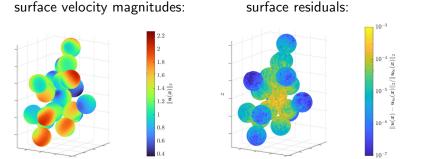
 $N \approx 700$   $n_{\rm im} = 20$ , equiv to 60 extra sources per near-contact

- ullet With a few extra unknowns we've extended the  $\delta$  by factor  $10^2$
- Compared against (non-adaptive) BIE scheme, impractical for  $\delta \leq 10^{-2}$
- GMRES iter. count grows badly, like  $\sim \delta^{-1/2}$

### Results: resistance for B = 20 close spheres

Random cluster of spheres with separations  $\delta = 10^{-3}$ . Target error  $10^{-3}$ :

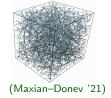
Random motions  $\boldsymbol{U}$  excites generic lubrication singularities



- here we used dense (slow) matvecs; drop-in of FMM in progress
- emphasize Broms ran all numerical expts and invented many ideas

# Convergent BIE for slender rigid bodies (quick sketch)

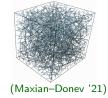




Fibers in Stokes regime: cilia, flagellae, actin, cytoskeleton, nematic fluids, cellulose pulp We tackle the rigid fiber case

## Convergent BIE for slender rigid bodies (quick sketch)





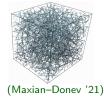
Fibers in Stokes regime: cilia, flagellae, actin, cytoskeleton, nematic fluids, cellulose pulp We tackle the rigid fiber case

Standard tool "slender body theory": rep.  $\pmb{u}$  as center-line integral matched asymptotics in radius  $\epsilon \ll 1$  (Keller–Rubinow '76, Johnson '80; Tornberg et al)

Error? classical  $\mathcal{O}(\epsilon^2 \log \epsilon^{-1})$ ; recent rigorous analysis  $\mathcal{O}(\epsilon \log^{3/2} \epsilon^{-1})$  (Mori–Ohm–Spirn '19)

## Convergent BIE for slender rigid bodies (quick sketch)

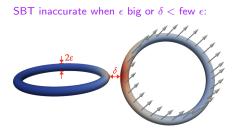


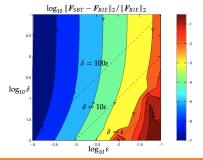


Fibers in Stokes regime: cilia, flagellae, actin, cytoskeleton, nematic fluids, cellulose pulp We tackle the rigid fiber case

Standard tool "slender body theory": rep.  $\pmb{u}$  as center-line integral matched asymptotics in radius  $\epsilon \ll 1$  (Keller–Rubinow '76, Johnson '80; Tornberg et al)

Error? classical  $\mathcal{O}(\epsilon^2 \log \epsilon^{-1})$ ; recent rigorous analysis  $\mathcal{O}(\epsilon \log^{3/2} \epsilon^{-1})$  (Mori–Ohm–Spirn '19)





### Layer potentials and surface quadrature

Goal: high-order accurate BIE for resistance & mobility BVPs with cost independent of  $\epsilon$  user sets  $\epsilon = 0.1$  or  $10^{-5}$ , dials in accuracy, e.g.  $10^{-6}$ 

### Layer potentials and surface quadrature

Goal: high-order accurate BIE for resistance & mobility BVPs with cost independent of  $\epsilon$  user sets  $\epsilon=0.1$  or  $10^{-5}$ , dials in accuracy, e.g.  $10^{-6}$ 

We needed new layer potential combined representations:

$$\mathbf{u} = (\mathcal{D} + \frac{1}{2\epsilon \log \epsilon^{-1}} \mathcal{S})[(I - L)\sigma] + \mathcal{S}\sigma_0 \qquad \text{mobility, stays well cond. as } \epsilon \to 0$$
 single-layer  $\mathcal{S}[\sigma](x) := \int_{\partial \Omega} \mathbb{S}(x, y)\sigma(y)dS_y$ , double-layer  $\mathcal{D}[\sigma](x) := -\frac{3}{4\sigma} \int_{\partial \Omega} \frac{(x-y)\cdot n(x-y)(x-y)^T}{\|x-y\|_{X=0}^{1/2}} \sigma(y)dS_y$ ,

### Layer potentials and surface quadrature

Goal: high-order accurate BIE for resistance & mobility BVPs with cost independent of  $\epsilon$  user sets  $\epsilon=0.1$  or  $10^{-5}$ , dials in accuracy, e.g.  $10^{-6}$ 

We needed new layer potential combined representations:

$$oldsymbol{u} = ig(\mathcal{D} + rac{1}{2\epsilon \log \epsilon^{-1}} \mathcal{S}ig) ig[ (I - L) \sigma ig] + \mathcal{S} \sigma_0$$
 mobility, stays well cond. as  $\epsilon \to 0$  single-layer  $\mathcal{S}[\sigma](x) := \int_{\partial \Omega} \mathbb{S}(x,y) \sigma(y) dS_y$ , double-layer  $\mathcal{D}[\sigma](x) := -rac{3}{4\sigma} \int_{\partial \Omega} rac{(x-y) \cdot n (x-y) (x-y)^T}{\|x-y\|_{\Sigma}^5} \sigma(y) dS_y$ ,

Discretize surface  $\partial\Omega$ : 2nd kind ( $\mathit{I} + \mathsf{cpt} \ \mathsf{op.}) o \mathsf{well-cond.}$  square linear system

Chebyshev panels, adaptive in arclength,  $\theta ext{-}$ Fourier modes adaptive per panel

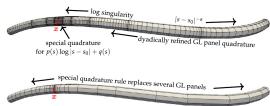


### Nyström quadrature for integral operator

Integral operator on-surface is weakly singular  $\mathcal{O}(1/\|\mathbf{x}-\mathbf{y}\|)$  Standard triangle/patch based BIE quadratures would die as  $\epsilon \to 0$ 

We developed...

Outer quadrature in arclength s:



### Nyström quadrature for integral operator

Integral operator on-surface is weakly singular  $\mathcal{O}(1/\|x-y\|)$  Standard triangle/patch based BIE quadratures would die as  $\epsilon \to 0$ 

Both use "generalized Chebyshev quadrature": (Bremer–Gimbutas–Rokhlin '10) precompute custom nodes & weights to integrate a family of functions

Get up to 10-digit accuracy, down to separations  $\delta=\epsilon/20$  omit many details

HPC implementation SIMD kernels, OpenMP; far-field done by PVFMM (MPI) quadrature setup rate: 20k unknowns/sec/core @ 7-digit accuracy

### A large-scale result: sedimentation of 512 rigid tori

time-evolve  $\dot{\pmb{X}} = \pmb{U}(\pmb{X})$ 

where  ${\it U}$  is mobility BVP solve at config.  ${\it X}$ 

gravity force, no inertia

ODE t-step: 5th-order SDC

1-body preconditioning

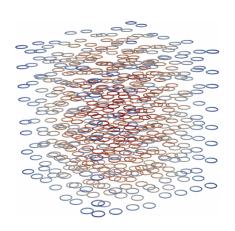
1.6 million unknowns

7-digit accuracy

 $\sim 1$  day on 160 cores

all Dhairya's HPC C++ codebase plus many inventions

my job was to code SBT and prove theorems:)





### **Conclusions**

- Linear-cost solvers for Stokes flows with many simple rigid particles
  - getting the right answer when close-to-touching is hard
  - preconditioned fundamental solutions (MFS), pair image lines

High-aspect-ratio rigid fibers: boundary integral equations (BIE)

- new representation, high-order quadratures, HPC
- replace slender body theory in close-fiber simulations
- A. Broms, A. H. Barnett, A.-K. Tornberg, J. Comput. Phys. 523 (2025)
- A. Broms, A. H. Barnett, A.-K. Tornberg, accepted, Adv. Comput. Math.
- D. Malhotra, A. H. Barnett, *J. Comput. Phys.* **503** (2024)
- https://github.com/dmalhotra/CSBQ

In progress/future in this area:

- 2-body precond. for 3D mobility w/ images + FMM
- collision-handling; flexible fiber BVP
- Brownian? sampling U from Gaussian with covariance the mobility matrix



#### **EXTRAS**



## Preliminary results: "2-body" preconditioning

recall 1-body precond: GMRES iteration count grows as  $\delta o 0$ 

Idea: direct solution of a fine discretization for each near **pair** of bodies "compress" (factorize) to an effective coarse proxy representation; GMRES sees only that

### Preliminary results: "2-body" preconditioning

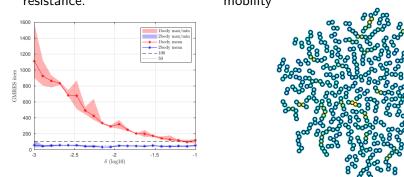
recall 1-body precond: GMRES iteration count grows as  $\delta o 0$ 

ldea: direct solution of a fine discretization for each near  $\boldsymbol{pair}$  of bodies

"compress" (factorize) to an effective coarse proxy representation; GMRES sees only that

2D monodisperse disks, shows huge reduction in iteration count:

resistance: mobility.



 $\delta=10^{-3}$ . Generalizes ideas of (Cheng–Greengard '98) to local pairwise BVP solves