An accurate method of fundamental solutions for large and dense particle systems in Stokes flow

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Joint work with
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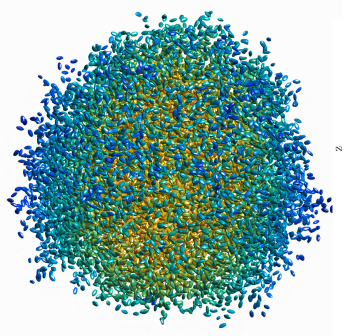
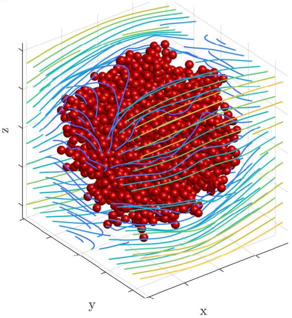
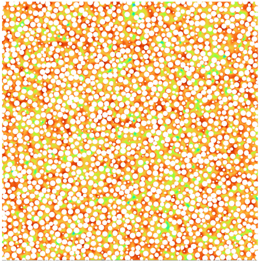






Setting: tiny rigid particles in a viscous fluid

On the scale of bacteria or red blood cells (nm-μm)

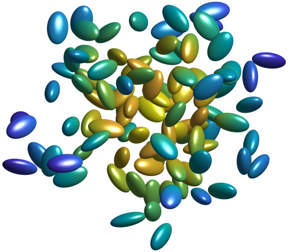
Motivated by studies of rheology, transport or diffusion processes

The Stokes model for the fluid:

- A linear and viscous-dominant version of Navier-Stokes, valid in the limit of small Reynolds numbers

$$\text{Re} = UL/\nu$$

- No inertia (no acceleration!)



Force balance on the particles:

- Particles interact hydrodynamically (via the fluid) and are also affected by external forces (e.g. gravity, electrostatics)

Two Stokes boundary value problems

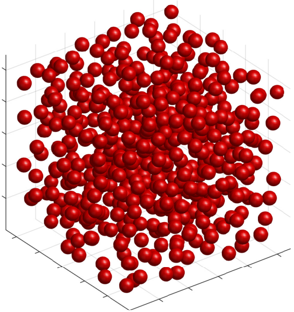
- At a snapshot in time, the Stokes PDEs determine flow velocity $\boldsymbol{u}$ and pressure P in the fluid domain
- No-slip bc: Flow velocity at particle surface $=$ rigid body motion of the particle
- Solution pair $(\boldsymbol{u}, P)$ relates to hydrodynamic forces and torques ($=$ external forces and torques)

The resistance problem:

- Given rigid body motion
- Solve for external forces and torques

The mobility problem:

- The inverse problem
- To be solved to study dynamics



Two Stokes boundary value problems

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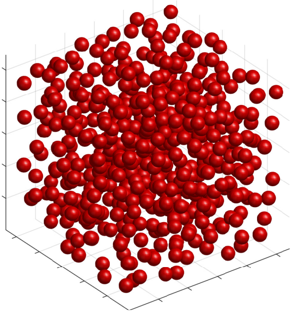
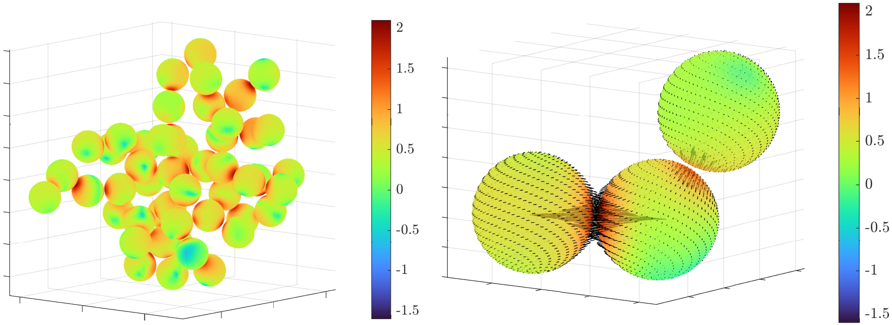
Challenges:

- Hydrodynamic interactions are long-ranged!
- Close interactions are hard to resolve!



Challenging close interactions

Relative motion results in strong ***lubrication forces*** for closely interacting particles and peaked force densities on their surfaces.



(a) Force density magnitude ($\log_{10}$)

(b) Force density direction (black)

How?

Technique: The method of fundamental solutions (MFS)

Wish list for solver:

- Controllable accuracy, also for close interactions
- Coarse particle representations
- Scalable

Roadmap:

- Problems with *weak* lubrication forces: basic algorithms for
  1. Resistance
  2. Mobility
- Problems with close interactions and strong lubrication forces:
  3. Image enhancement
  4. Preconditioning

Fundamental solutions

The Stokes equations are given by

$$\begin{cases} \nabla P - \nabla^2 \boldsymbol{u} = \boldsymbol{0}, & \text{in fluid domain} \\ \nabla \cdot \boldsymbol{u} = 0, & \text{in fluid domain} \\ \boldsymbol{u}_{\mathsf{bc}} = \text{rigid body motion}, & \text{on any particle surface} \end{cases}$$

$\boldsymbol{u}$ flow velocity, P pressure.

Stokes fundamental solutions

- The Stokeslet, $\mathbb{S}$, gives velocity solution due to a point force $\boldsymbol{f} = \boldsymbol{f}^* \delta(\boldsymbol{x} - \boldsymbol{y})$:

$$\boldsymbol{u}(\boldsymbol{x}) = \mathbb{S}(\boldsymbol{x} - \boldsymbol{y}) \boldsymbol{f}^*, \quad \boldsymbol{x} \in \mathbb{R}^3 \backslash \{\boldsymbol{y}\}$$

- Other fundamental solutions exist too, called the rotlet, stresslet and potential dipole
- All are singular at $\boldsymbol{x} = \boldsymbol{y}$

Basic MFS algorithm for the resistance problem

- The linear combination $\boldsymbol{u}(\boldsymbol{x}) = \sum_{j=1}^{N} \mathbb{S}(\boldsymbol{x} - \boldsymbol{y}_j)\boldsymbol{\lambda}_j$ solves the set of PDEs, with **strategically** picked source locations $\boldsymbol{y}_j$ and **if** $\boldsymbol{\lambda}_j \in \mathbb{R}^3$ can be chosen to match the boundary conditions.

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MFS has long history:

Katsurada (1989), Götz (2003), Fairweather et al. (2005), Betcke & Barnett (2008), Alves (2009), Liu & Barnett (2016)...

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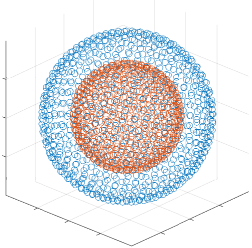
- Let the N source points $\boldsymbol{y}_j$ lie on a **proxy-surface** in the particle interior.
- Impose bc in a set of $M > N$ target (collocation) points $\boldsymbol{x}_i$ at the particle surface.



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- Let the N source points $\boldsymbol{y}_j$ lie on a **proxy-surface** in the particle interior.
- Impose bc in a set of $M > N$ target (collocation) points $\boldsymbol{x}_i$ at the particle surface.
- As surfaces are **different**, singularities in $\mathbb{S}$ are avoided!
- Let $\boldsymbol{G}$ be the target-from-source matrix, with $G_{ij} := \mathbb{S}(\boldsymbol{x}_i - \boldsymbol{y}_j)$, such that

$$\boldsymbol{G}\boldsymbol{\lambda} = \sum_{j=1}^{N} \mathbb{S}(\boldsymbol{x} - \boldsymbol{y}_j)\boldsymbol{\lambda}_j.$$

Solving for MFS coefficients (Part 1)

- The rectangular matrix $\boldsymbol{G}$ is ill-conditioned! Impose bc in the least-squares sense as

$$\min_{\boldsymbol{\lambda}} \|\boldsymbol{G}(\boldsymbol{x}, \boldsymbol{y})\boldsymbol{\lambda} - \boldsymbol{u}(\boldsymbol{x})\|_2^2. \quad (1)$$

- With $\boldsymbol{G} = \boldsymbol{U\Sigma V}$, the pseudo-inverse is $\boldsymbol{G}^\dagger = \boldsymbol{V\Sigma}^\dagger \boldsymbol{U}^T$, where singular values are truncated below a threshold to form $\boldsymbol{\Sigma}^\dagger$.
- Solve (1), backward-stably as

$$\boldsymbol{\lambda} = \boldsymbol{V\Sigma}^\dagger \left(\boldsymbol{U}^T \boldsymbol{u}(\boldsymbol{x})\right).$$ Order of multiplication matters!

Stein & Barnett (2022), Lai, Kobayashi & Barnett (2015), Malhotra & Biros (2015)

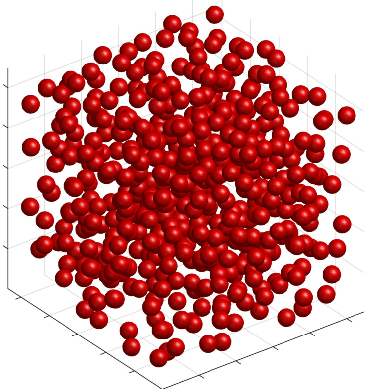
- Evaluate flow in new set of points $\widetilde{\boldsymbol{x}}$ as

$$\boldsymbol{u}(\widetilde{\boldsymbol{x}}) = \sum_{j=1}^{N} \mathbb{S}(\widetilde{\boldsymbol{x}} - \boldsymbol{y}_j)\boldsymbol{\lambda}_j.$$

Solving for MFS coefficients (Part 2)

Assume that the system consists of many particles.

- Cannot do a dense SVD globally!
- Scales as $\mathcal{O}\left(3MP \cdot (3NP)^2\right)$ for P particles, with $M > N$.

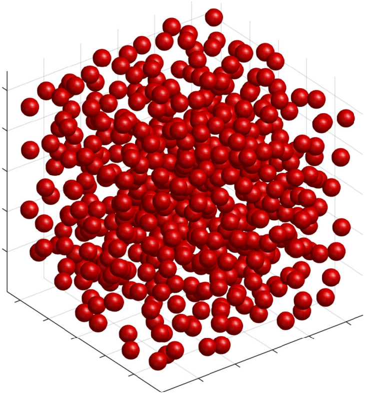


Solving for MFS coefficients (Part 2)

Assume that the system consists of many particles.

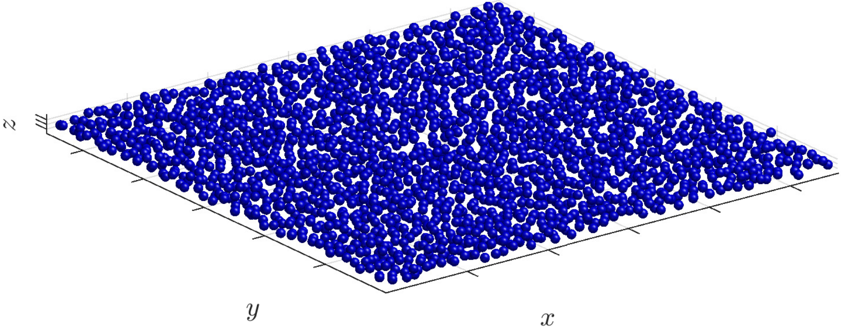
We construct an $\mathcal{O}(P)$ algorithm for P particles via

- GMRES
- A fast summation technique (FMM)
- Use of the block structure of the target-from-source matrix G
- **One-body preconditioning:** Only a small SVD needed to create well-conditioned system



Large scale example

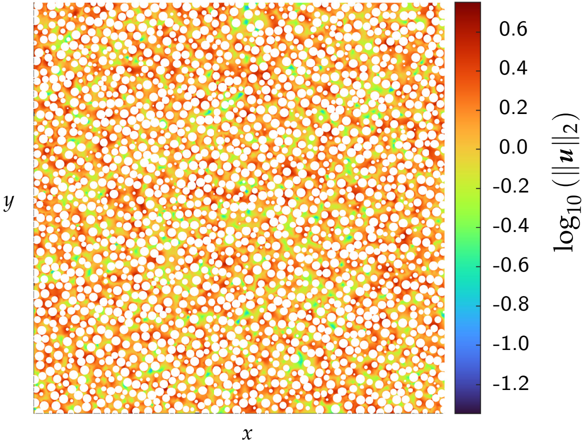
- Example: Dilute suspension of 2000 spheres in a layer.
- No-slip bc with randomly sampled angular and translational velocity on every sphere.



Large scale example

- Max relative residual 10^{-3}, with target tolerance 10^{-3}.

  Residual = difference from boundary condition in new set of points on the surface of every particle.



Mobility formulation

The resistance problem (1 particle):

- Solve
$$G\lambda \approx K_M U,$$
for λ, with $K_M U$ the **known** rigid body motion at the surface.
- Compute forces and torques in post-processing step:
$$f = \sum_{j=1}^{N} \lambda_j, \; t = \sum_{j=1}^{N} (y_j - c) \times \lambda_j \qquad (*)$$

The mobility problem (1 particle):

- Solve
$$G\lambda \approx K_M U,$$
with **unknown** U subject to
$$K_N^T \lambda = F$$
Compact notation for $(*)$

Mobility formulation

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$$(*)$$

Cost for P particles?

Resistance: $\mathcal{O}(P)$
Mobility: Constrained LSQ...

The mobility problem (1 particle):

- Solve
$$G\lambda \approx K_M U,$$
with **unknown** U subject to
$$K_N^T \lambda = F$$
Compact notation for $(*)$

Mobility algorithm with linear cost

Ideas:

1. Create source vector $\boldsymbol{\lambda}$ that automatically satisfies constraints:
2. Split $\boldsymbol{\lambda} = (\boldsymbol{I} - \boldsymbol{L})\hat{\boldsymbol{\lambda}} + \boldsymbol{\lambda}_0$, so that $\boldsymbol{K}_N^T \boldsymbol{\lambda}_0 = \boldsymbol{F}$ ($\boldsymbol{\lambda}_0$ satisfies the constraints) and $(\boldsymbol{I} - \boldsymbol{L})\hat{\boldsymbol{\lambda}} \in \mathcal{N}(\boldsymbol{K}_N^T)$ via projection matrix $\boldsymbol{L}$

Proposed representation:

$$\boldsymbol{u}(\boldsymbol{x}) = \sum_{j=1}^{N} \mathbb{S}(\boldsymbol{x} - \boldsymbol{y}_j)(\boldsymbol{I} - \boldsymbol{L})\hat{\boldsymbol{\lambda}}_j + \sum_{j=1}^{N} \mathbb{S}(\boldsymbol{x} - \boldsymbol{y}_j)\boldsymbol{\lambda}_{0,j}$$

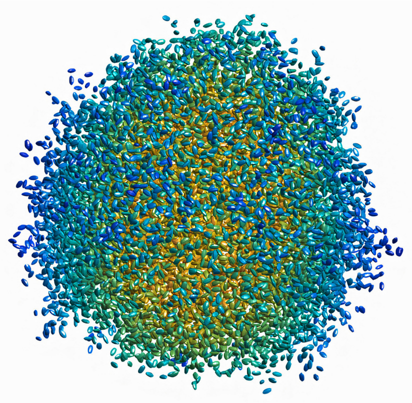
3. Impose relation between source vector and unknown velocities: $\boldsymbol{U} = -\boldsymbol{K}_N^T \hat{\boldsymbol{\lambda}}$ (utilize unused subspace)

System to solve without explicit constraints (1 particle):

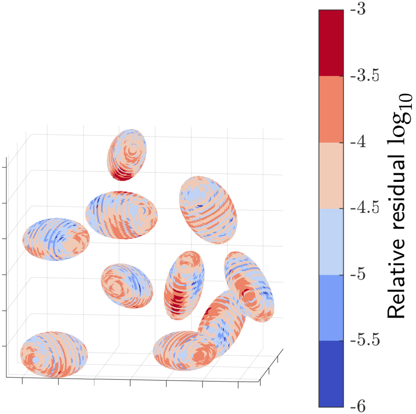
$$\left(\boldsymbol{G}(\boldsymbol{I} - \boldsymbol{L}) + \boldsymbol{K}_M \boldsymbol{K}_N^T\right) \hat{\boldsymbol{\lambda}} = -\boldsymbol{G}\boldsymbol{\lambda}_0$$

4. Apply one-body preconditioning

Example: 10000 ellipsoids



(a) Surface velocities

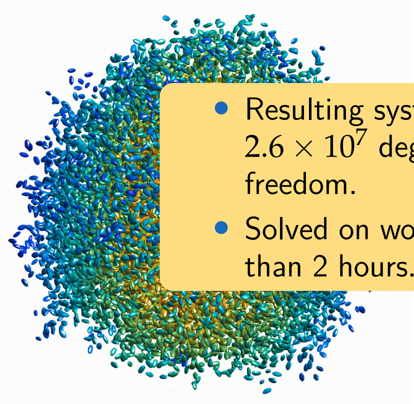


(b) Relative surface error

Figure: Minimum separation $\delta_{\min} = 0.2$, semi-axes: 0.4,0.6,1

Example: 10000 ellipsoids

- Resulting system has 2.6×10^7 degrees of freedom.
- Solved on workstation in less than 2 hours.



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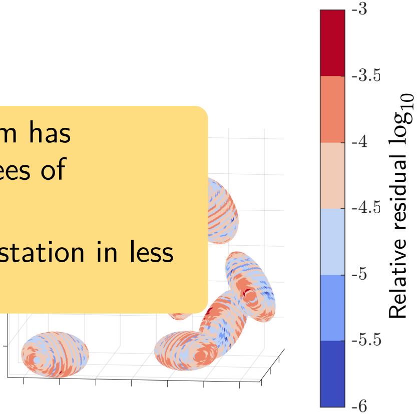


(b) Relative surface error

Figure: Minimum separation $\delta_{\min} = 0.2$, semi-axes: 0.4,0.6,1

Accuracy in MFS with coarse grids: Image points

Idea: Introduce extra sources at image points, with a combination of different types of fundamental solutions at each point.

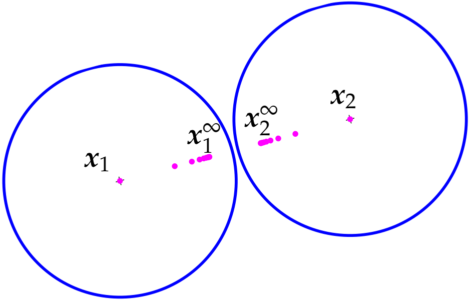
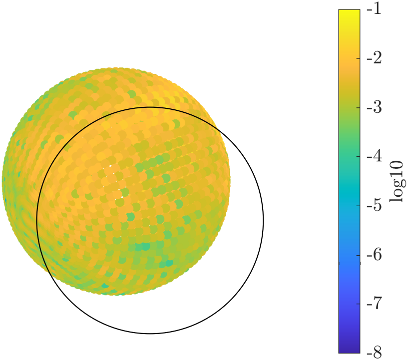


Image systems: Lord Kelvin (1853), Cheng & Greengard (1998), Cheng (2000).

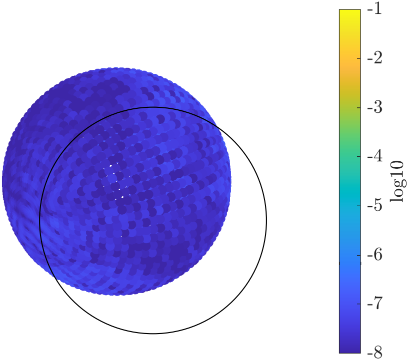
Fundamental solutions for reflection in a plane: Blake (1971), Greengard, Gimbutas & Veerapaneni (2015), Yan & Shelley (2018), *Fundamental solutions for reflection of point in a sphere:* Wróbel, Cortez, Varela & Fauci (2016), Maul & Kim (1996)

Example: two spheres with images, separation 10^{-2}

Residual without image points



Residual with 10 image points



Example: adaptive use of images

- Adaptive number of image points per close particle pair
- Each sphere has random translational and angular velocity
- Target accuracy of 10^{-3} reached everywhere

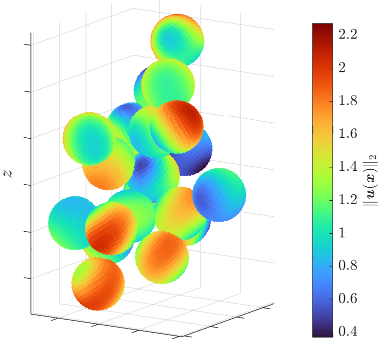


Figure: Surface velocities.

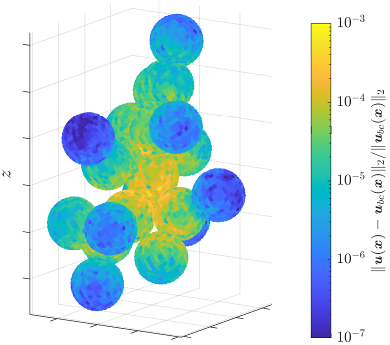


Figure: Relative residual at particle surfaces.

Preconditioning for close contacts

One-body preconditioning

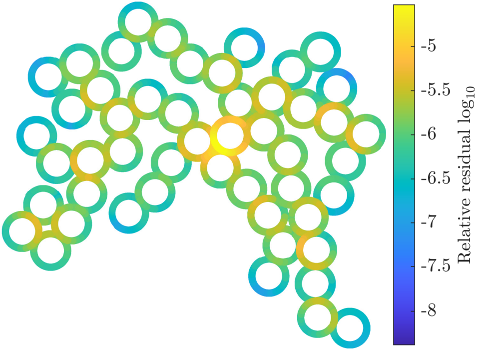
- Works well if lubrication forces are weak!
- **Slow** GMRES convergence if lubrication forces are strong...
- True in both 2D and 3D

New idea:

- Use a pair corrected basis inspired by
  - Cheng & Greengard (1998)
- Flavour of a fast direct solver: solve a BVP with a fine grid only locally for each close pair of particles
- Global solve only needs coarse grid

Preconditioning mobility example in 2D

- Each unit circle $\delta = 10^{-3}$ from at least one neighbour, random net forces and torques (very challenging)
- 297 iterations with one-body preconditioning, 57 with the new idea to reach GMRES tol 10^{-6}
- 60 points per particle in coarse grid



Summary

The method of fundamental solutions

- Singularity free technique
- Additional sources at approximate image locations improve accuracy for closely interacting particles
- Controllable accuracy obtained for all separations $> 10^{-3}$
- Well-conditioned solvers for both resistance and mobility (work in progress for close contacts – talk to me!)
- Coarse representations and scalable to many particles

Accurate Stokes flow for closely interacting spheres using lubrication-adapted image systems, A. Broms, A. H. Barnett and A.-K. Tornberg, JCP, 113636 (2025)

A method of fundamental solutions for large-scale 3D elastance and mobility problems, A. Broms, A. H. Barnett and A.-K. Tornberg, Preprint (2024) – on arXiv, submitted to ACOM, under review

– Thank you! – annabrom@kth.se