FLATIRON INSTITUTE
Center for Computational Mathematics

Fast boundary integral solvers for Stokes flows: quadrature, periodization, adaptivity

Alex Barnett[1]

ShelleyFest, U. Michigan, 6/14/19

Main collaborators in work shown:
Jun Wang (CCM), Ehssan Nazockdast (UNC) - rheology
Bowie Wu, **Hai Zhu**, Shravan Veerapaneni (UMich) - quadrature, adaptivity
L. Zhao (INTECH), **G. Marple** (UMich), SV - periodic no-slip

[1]Center for Computational Mathematics, Flatiron Institute, Simons Foundation, NYC

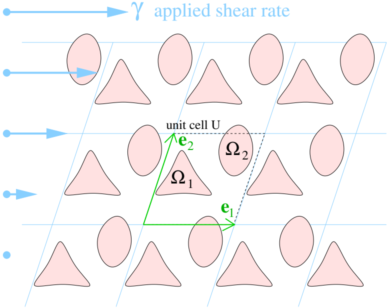
Rheology of spatially periodic suspensions

2D periodic mobility problem:

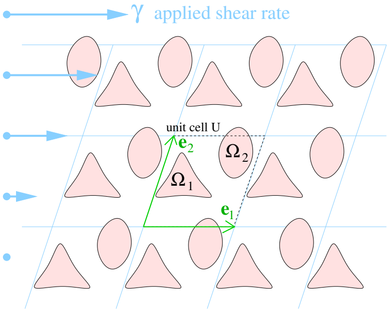
∞ lattice of neutrally buoyant, smooth rigid bodies in Stokes fluid   viscosity μ

"non-Brownian" (i.e. not microscopic)

given shear rate γ, skewing unit cell



Rheology of spatially periodic suspensions



2D periodic mobility problem:

∞ lattice of neutrally buoyant, smooth rigid bodies in Stokes fluid viscosity μ

"non-Brownian" (i.e. not microscopic)

given shear rate γ, skewing unit cell

What is bulk viscosity $\mu_{\text{eff}} := \frac{\text{mean force/length}}{\gamma}$?

i) quasi-static μ_{eff} at current configuration

ii) evolution of $\mu_{\text{eff}}(t)$ as bodies move under flow

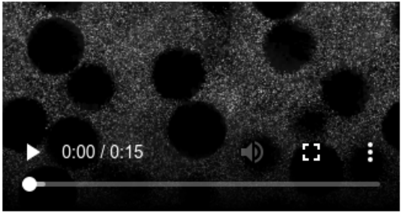
statistical moments $\langle \mu_{\text{eff}}^p \rangle_t$, correlation decay in t, dependence on shape, vol. frac?

A homogenization problem. Applications:

- industrial processes, complex fluids (e.g. lattice of fibers into page), modeling non-periodic random suspensions, electro-rheology devices

Motivations for sheared suspensions

PIV and dye imaging, 3D spheres   dia $\sim$ 2mm   vol. frac. $\phi = 0.35$ Re $\sim 10^{-4}$



(Souzy et al, '17)

observe: mixing, super-diffusion, turbulence, at Re ≈ 0

Questions:

- time-evolution, 2-pt correlations of bodies, mixing. . .

  transport: "rolling-coating" effect needs accurate numerical flow near surfaces

- effect of ϕ, validation of low-ϕ approx; shapes, jamming. . .

$\exists$ little accurate numerical simulation for general shapes   (even ellipses)

Goal: high-order solver, efficient, linear scaling w/ complexity in unit cell

FLATIRON INSTITUTE
Center for Computational Mathematics

Non-periodic mobility problem

Recall: at $\mathbf{x}$ on surface w/ normal $\mathbf{n_x}$, traction $\mathbf{T} = \mathbf{T}(\mathbf{u}, p) := \sigma \cdot \mathbf{n_x}$

where stress $\sigma(\mathbf{x}) := -p\boldsymbol{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$, $\quad$ $\boldsymbol{I}$ means 2×2 id. matrix

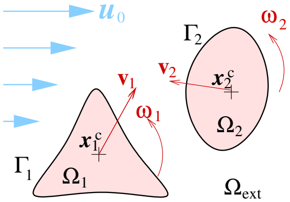
Non-periodic mobility problem

Recall: at $\mathbf{x}$ on surface w/ normal $\mathbf{n_x}$, traction $\mathbf{T} = \mathbf{T}(\mathbf{u}, p) := \sigma \cdot \mathbf{n_x}$

where stress $\sigma(\mathbf{x}) := -pI + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$, I means 2×2 id. matrix

Given background Stokes flow $(\mathbf{u}_0, p_0)$,
force- & torque-free bodies Ω_k, $k = 1, \ldots, n$

Find $(\mathbf{u}, p)$ change from bkgnd, and
$\mathbf{v}_k, \omega_k$ body velocities & rotation rates

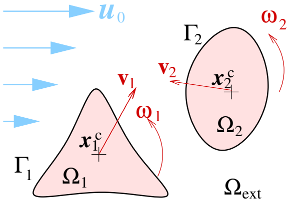


Non-periodic mobility problem

Recall: at $\mathbf{x}$ on surface w/ normal $\mathbf{n_x}$, traction $\mathbf{T} = \mathbf{T}(\mathbf{u}, p) := \sigma \cdot \mathbf{n_x}$

where stress $\sigma(\mathbf{x}) := -pI + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)$, I means 2×2 id. matrix

Given background Stokes flow $(\mathbf{u}_0, p_0)$,
force- & torque-free bodies Ω_k, $k = 1, \ldots, n$



Find $(\mathbf{u}, p)$ change from bkgnd, and
$\mathbf{v}_k, \omega_k$ body velocities & rotation rates

BVP: exists a unique solution to...

$$-\mu\Delta\mathbf{u} + \nabla p = \mathbf{0} \quad \text{in } \Omega_{\text{ext}} \qquad \text{fluid force balance}$$

$$\nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega_{\text{ext}} \qquad \text{incompressible}$$

$$\mathbf{u}(\mathbf{x}) + \mathbf{u}_0(\mathbf{x}) = \mathbf{v}_j + \omega_j(\mathbf{x} - \mathbf{x}_j^c)^\perp \quad \mathbf{x} \in \Gamma_k \qquad \text{rigid body motions}$$

$$\int_{\Gamma_k} \mathbf{T}\, ds = \mathbf{0} \qquad \text{zero net fluid force on bodies } k = 1, \ldots, n$$

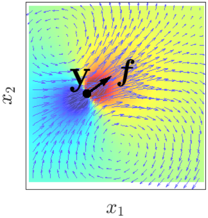
$$\int_{\Gamma_k} \mathbf{T}(\mathbf{x}) \cdot (\mathbf{x} - \mathbf{x}_k^c)^\perp ds_{\mathbf{x}} = 0 \qquad \text{zero net fluid torque, } k = 1, \ldots, n$$

$$|\mathbf{u}(\mathbf{x})| \to 0 \qquad |\mathbf{x}| \to \infty$$

FLATIRON INSTITUTE Center for Computational Mathematics

Boundary integral equations (BIE) for mobility

Re=0 (linear PDE) $\rightarrow$ BIE much more efficient than volume discr (FEM)



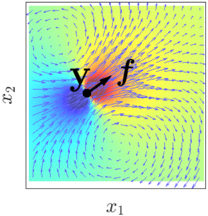
2D (free space) vel. Green's func, $\mathbf{r} := \mathbf{x} - \mathbf{y}$, $r := |\mathbf{r}|$

$$G(\mathbf{x}, \mathbf{y}) := \frac{1}{4\pi\mu}\left(I \log \frac{1}{r} + \frac{\mathbf{r}\otimes\mathbf{r}}{r^2}\right)$$

shown: $G(\mathbf{x}, \mathbf{y}) \cdot \mathbf{f}$ for some force vector $\mathbf{f}$

Boundary integral equations (BIE) for mobility

Re=0 (linear PDE) → BIE much more efficient than volume discr (FEM)



2D (free space) vel. Green's func, $\mathbf{r} := \mathbf{x} - \mathbf{y}$, $r := |\mathbf{r}|$

$G(\mathbf{x}, \mathbf{y}) := \frac{1}{4\pi\mu}\left(I \log \frac{1}{r} + \frac{\mathbf{r}\otimes\mathbf{r}}{r^2}\right)$

shown: $G(\mathbf{x}, \mathbf{y}) \cdot \mathbf{f}$ for some force vector $\mathbf{f}$

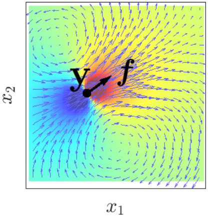
Simplest case, one body Ω (bdry Γ):

single-layer vel. potential $\mathbf{u}(\mathbf{x}) = (\mathcal{S}\varphi)(\mathbf{x}) := \int_\Gamma G(\mathbf{x}, \mathbf{y}) \cdot \varphi(\mathbf{y}) ds_\mathbf{y}$

force density "sprayed" onto Γ; $\exists$ sim. pressure pot. $p(\mathbf{x})$

Boundary integral equations (BIE) for mobility

Re=0 (linear PDE) → BIE much more efficient than volume discr (FEM)



2D (free space) vel. Green's func, $\mathbf{r} := \mathbf{x} - \mathbf{y}$, $r := |\mathbf{r}|$

$$G(\mathbf{x}, \mathbf{y}) := \frac{1}{4\pi\mu}\left(I \log \frac{1}{r} + \frac{\mathbf{r}\otimes\mathbf{r}}{r^2}\right)$$

shown: $G(\mathbf{x}, \mathbf{y}) \cdot \mathbf{f}$ for some force vector $\mathbf{f}$

Simplest case, one body Ω (bdry Γ):

single-layer vel. potential $\mathbf{u}(\mathbf{x}) = (\mathcal{S}\varphi)(\mathbf{x}) := \int_\Gamma G(\mathbf{x}, \mathbf{y}) \cdot \varphi(\mathbf{y}) ds_\mathbf{y}$

force density "sprayed" onto Γ; $\exists$ sim. pressure pot. $p(\mathbf{x})$

Combine 3 facts:

a) resulting $\mathbf{u}$ cont. & $(\mathbf{u}, p)$ obeys Stokes both in Ω_{ext} and *inside* Ω.

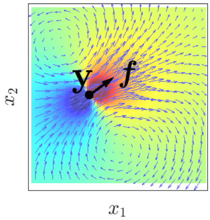
b) jump relations: on Γ_- (lim inside), $\mathbf{T}_-(\mathbf{u}, p) = ((\frac{1}{2}I + K)\varphi)(\mathbf{x})$

bdry integral operator $(K\varphi)(\mathbf{x}) := -\frac{1}{\pi} \int_\Gamma \frac{(\mathbf{n_x}\cdot\mathbf{r})(\mathbf{r}\cdot\varphi(\mathbf{y}))}{r^4} \mathbf{r}\, ds_\mathbf{y}$ "$\mathbf{n_x}$ · stresslet"

c) $\mathbf{T}(\mathbf{u} + \mathbf{u}_0, p + p_0) \equiv \mathbf{0}$ on Γ_- $\Rightarrow$ $\mathbf{u} + \mathbf{u}_0$ rigid body motion

Boundary integral equations (BIE) for mobility

Re=0 (linear PDE) $\to$ BIE much more efficient than volume discr (FEM)



2D (free space) vel. Green's func, $\mathbf{r} := \mathbf{x} - \mathbf{y}$, $r := |\mathbf{r}|$

$$G(\mathbf{x}, \mathbf{y}) := \frac{1}{4\pi\mu}\left(I \log \frac{1}{r} + \frac{\mathbf{r}\otimes\mathbf{r}}{r^2}\right)$$

shown: $G(\mathbf{x}, \mathbf{y}) \cdot \mathbf{f}$ for some force vector $\mathbf{f}$

Simplest case, one body Ω (bdry Γ):

single-layer vel. potential $\mathbf{u}(\mathbf{x}) = (\mathcal{S}\varphi)(\mathbf{x}) := \int_\Gamma G(\mathbf{x}, \mathbf{y}) \cdot \varphi(\mathbf{y}) ds_\mathbf{y}$

Combine 3 facts: force density "sprayed" onto Γ; $\exists$ sim. pressure pot. $p(\mathbf{x})$

a) resulting $\mathbf{u}$ cont. & $(\mathbf{u}, p)$ obeys Stokes both in Ω_{ext} and *inside* Ω.

b) jump relations: on Γ_- (lim inside), $\mathbf{T}_-(\mathbf{u}, p) = ((\frac{1}{2}I + K)\varphi)(\mathbf{x})$

bdry integral operator $(K\varphi)(\mathbf{x}) := -\frac{1}{\pi} \int_\Gamma \frac{(\mathbf{n_x}\cdot\mathbf{r})(\mathbf{r}\cdot\varphi(\mathbf{y}))}{r^4}\mathbf{r}\, ds_\mathbf{y}$ "$\mathbf{n_x}$ · stresslet"

c) $\mathbf{T}(\mathbf{u} + \mathbf{u}_0, p + p_0) \equiv \mathbf{0}$ on Γ_- $\Rightarrow$ $\mathbf{u} + \mathbf{u}_0$ rigid body motion

Gives BIE on Γ: $(\frac{1}{2}I + K)\varphi = -\mathbf{T}(\mathbf{u}_0, p_0)$

with constraints: $\int_\Gamma \varphi\, ds = \mathbf{0}$ zero net force from φ on fluid

$\int_\Gamma (\mathbf{x} - \mathbf{x}^c)^\perp \cdot \varphi(\mathbf{x})\, ds_\mathbf{x} = 0$ zero net torque

Mobility BIE formulation... (non-periodic)

But: BIE w/ 3 constraints $\begin{cases} (\frac{1}{2}I + K)\varphi &= -\mathbf{T}(\mathbf{u}_0, p_0) \\ \int_\Gamma \varphi \, ds &= \mathbf{0} \\ \int_\Gamma (\mathbf{x} - \mathbf{x}^c)^\perp \cdot \varphi(\mathbf{x}) \, ds_\mathbf{x} &= 0 \end{cases}$

is equivalent to:

BIE on Γ $\quad (\frac{1}{2}I + K + L)\varphi = -\mathbf{T}(\mathbf{u}_0, p_0)$ $\quad L =$ rank-3, applies constraints

(Karrila–Kim '89; Rachh–Greengard '16)

What about $n > 1$ bodies Ω_k? $\quad \varphi = \{\varphi_k\}_{k=1}^n$, $n \times n$ blocks $\{K_{k,k'}\}$, L block-diag.

Mobility BIE formulation... (non-periodic)

But: BIE w/ 3 constraints $\begin{cases} (\frac{1}{2}I + K)\varphi &= -\mathbf{T}(\mathbf{u}_0, p_0) \\ \int_\Gamma \varphi\, ds &= \mathbf{0} \\ \int_\Gamma (\mathbf{x}-\mathbf{x}^c)^\perp \cdot \varphi(\mathbf{x})\, ds_\mathbf{x} &= 0 \end{cases}$

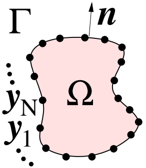
is equivalent to:

BIE on Γ $\quad (\frac{1}{2}I + K + L)\varphi = -\mathbf{T}(\mathbf{u}_0, p_0)$ $\quad L =$ rank-3, applies constraints

(Karrila–Kim '89; Rachh–Greengard '16)

What about $n > 1$ bodies Ω_k? $\quad \boldsymbol{\varphi} = \{\varphi_k\}_{k=1}^n$, $n \times n$ blocks $\{K_{k,k'}\}$, L block-diag.

Nyström discretization (one body): $\quad \mathbf{z}(t)$, 2π-periodic global parameterization of Γ



quadr. rule: $\int_\Gamma g\, ds \approx \sum_{j=1}^N w_j g(\mathbf{y}_j)$ $\quad$ nodes $\mathbf{y}_j = \mathbf{z}(\frac{2\pi j}{N})$

weights $w_j = \frac{2\pi}{N} |\mathbf{z}'(\frac{2\pi j}{N})|$

Mobility BIE formulation... (non-periodic)

But: BIE w/ 3 constraints
$$\begin{cases} (\tfrac{1}{2}I + K)\varphi &= -\mathbf{T}(\mathbf{u}_0, p_0) \\ \int_\Gamma \varphi\, ds &= \mathbf{0} \\ \int_\Gamma (\mathbf{x}-\mathbf{x}^c)^\perp \cdot \varphi(\mathbf{x})\, ds_{\mathbf{x}} &= 0 \end{cases}$$

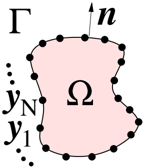
is equivalent to:

BIE on Γ $\quad (\tfrac{1}{2}I + K + L)\varphi = -\mathbf{T}(\mathbf{u}_0, p_0)$ $\quad L =$ rank-3, applies constraints

(Karrila–Kim '89; Rachh–Greengard '16)

What about $n > 1$ bodies Ω_k? $\quad \varphi = \{\varphi_k\}_{k=1}^n$, $n \times n$ blocks $\{K_{k,k'}\}$, L block-diag.

Nyström discretization (one body): $\quad \mathbf{z}(t)$, 2π-periodic global parameterization of Γ



quadr. rule: $\int_\Gamma g\, ds \approx \sum_{j=1}^N w_j g(\mathbf{y}_j)$ $\quad$ nodes $\mathbf{y}_j = \mathbf{z}(\frac{2\pi j}{N})$

weights $w_j = \frac{2\pi}{N}|\mathbf{z}'(\frac{2\pi j}{N})|$

enforce BIE at each node & apply quad. rule to integral

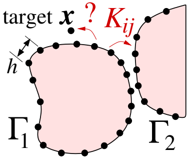
get $N \times N$ linear system $\quad A\varphi = \mathbf{f}$ $\quad A = \frac{1}{2}I + K + L$

matrix els. ptwise samples of kernels, e.g. $K_{ij} = K(\mathbf{y}_i, \mathbf{y}_j)w_j$, $i \neq j$

- Γ smooth $\to$ kernels smooth $\to$ spectrally accurate $\quad$ (Anselone, Kress)
- 2nd-kind BIE $\Rightarrow$ well-cond. $\Rightarrow$ rapid convergence of GMRES

So, for $N \gtrsim 10^3$ use FMM to apply A in iter. solver $\to$ scaling $\mathcal{O}(N)$

Evaluating potentials close to source curve

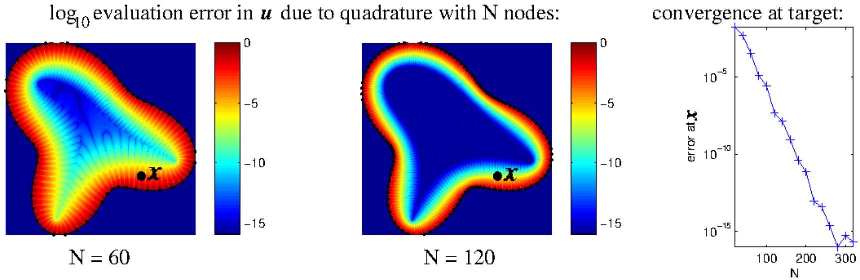


Now have samples $\{\varphi(\mathbf{y}_j)\}_{j=1}^N$, how eval $\mathbf{u}(\mathbf{x})$ near Γ ?
Similarly, how fill matrix els. K_{ij} between close curves?

Naive: same quadr. rule $u(\mathbf{x}) \approx \sum_{j=1}^N w_j G(\mathbf{x}, \mathbf{y}_j) \cdot \varphi(\mathbf{y}_j)$

$\#$ correct digits $\approx 2.7 \frac{\text{dist}(\mathbf{x},\Gamma)}{h}$ dist. $\lesssim h$ bad

Demo: naive potential eval. interior to curve Γ



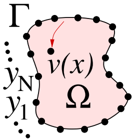
Thm: analytic Γ, exp. rate = imag. part of preimage $\mathbf{z}^{-1}(\mathbf{x})$ of complexified param. (B '14)

Better: Stokes pots. in terms of Laplace pots, in terms of Cauchy ints. . .

Beautiful quadrature idea: barycentric Cauchy in $\mathbb{C}$

Interior potential task: given samples $v_j = v(y_j)$,

eval. Cauchy $\quad v(x) = \frac{i}{2\pi}\int_\Gamma \frac{v(y)}{x-y}dy, \quad x \in \Omega \subset \mathbb{C}$

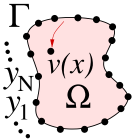


- plain quadr. rule fails close to Γ, as before

Beautiful quadrature idea: barycentric Cauchy in $\mathbb{C}$

Interior potential task: given samples $v_j = v(y_j)$,

eval. Cauchy $\quad v(x) = \frac{i}{2\pi} \int_\Gamma \frac{v(y)}{x-y} dy, \quad x \in \Omega \subset \mathbb{C}$



- plain quadr. rule fails close to Γ, as before

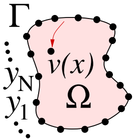
Subtract the above from $v(x)$ times the special case $1 = \frac{i}{2\pi} \int_\Gamma \frac{1}{x-y} dy$:

$0 \;=\; \int_\Gamma \frac{v(x)-v(y)}{x-y} dy$ cancels singularity; integrand smooth even as $x \to \Gamma$

Beautiful quadrature idea: barycentric Cauchy in $\mathbb{C}$

Interior potential task: given samples $v_j = v(y_j)$,

eval. Cauchy $\quad v(x) = \frac{i}{2\pi} \int_\Gamma \frac{v(y)}{x-y} dy, \qquad x \in \Omega \subset \mathbb{C}$



- plain quadr. rule fails close to Γ, as before

Subtract the above from $v(x)$ times the special case $1 = \frac{i}{2\pi} \int_\Gamma \frac{1}{x-y} dy$:

$0 \;=\; \int_\Gamma \frac{v(x)-v(y)}{x-y} dy$ cancels singularity; integrand smooth even as $x \to \Gamma$

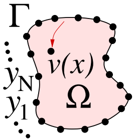
Apply periodic trap. rule... spectrally accurate for smooth integrands

$0 \;\approx\; \sum_{j=1}^N \frac{v(x)-v_j}{x-y_j} w_j$ now rearrange...

Beautiful quadrature idea: barycentric Cauchy in $\mathbb{C}$

Interior potential task: given samples $v_j = v(y_j)$,

eval. Cauchy $\quad v(x) = \frac{i}{2\pi}\int_\Gamma \frac{v(y)}{x-y}dy, \qquad x \in \Omega \subset \mathbb{C}$



- plain quadr. rule fails close to Γ, as before

Subtract the above from $v(x)$ times the special case $1 = \frac{i}{2\pi}\int_\Gamma \frac{1}{x-y}dy$:

$$0 \;=\; \int_\Gamma \frac{v(x)-v(y)}{x-y}dy$$

cancels singularity; integrand smooth even as $x \to \Gamma$

Apply periodic trap. rule... spectrally accurate for smooth integrands

$$0 \;\approx\; \sum_{j=1}^N \frac{v(x)-v_j}{x-y_j}w_j$$

now rearrange...

Gives $\quad v(x) \;\approx\; \dfrac{\sum_{j=1}^N \frac{v_j}{x-y_j}w_j}{\sum_{j=1}^N \frac{1}{x-y_j}w_j}$ 2nd form barycentric interp, but *complex* nodes

uniformly accurate in $\overline{\Omega}$, if nodes resolved v on Γ (Ioakimidis '91, Helsing '08)

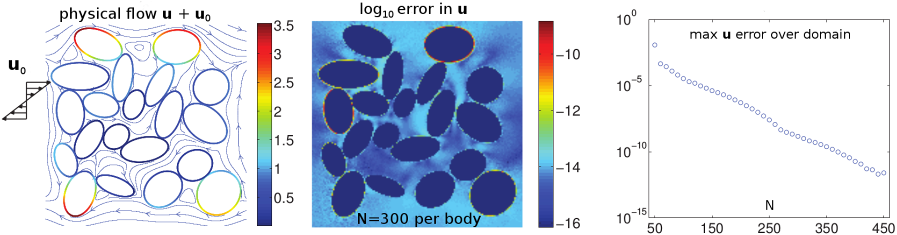
- no such trick in 3D :($\quad\exists$ schemes: radial patches, QBX, adaptive...

Apply barycentric to 2D Stokes potentials

Built close-evaluation Stokes global quadratures on Laplace on Cauchy

- Cauchy enables double-layer; we generalized to single-layer

Use close-eval. for mat. els. K_{ij} and for flow eval: (B–Wu–Veerapaneni '14)



ext. Stokes, no-slip BCs, SLP+DLP formulation, $n = 20$ bodies, body separation $\delta \sim 10^{-4}$

- density φ peak width $\mathcal{O}(\delta^{1/2})$ (e.g. Sangani–Mo '94), good for $\delta \gtrsim h^2$
- for mobility prob: also traction of SLP (needs v'') (Wang–B, in prep.)

`github: ahbarnett/BIE2D, dstein/pyBIE2D`

- for $\delta \to 0$, global quadr. scheme bad $\to$ need adaptive (later!)

Issues periodizing the BIE

recall discretized BIE on Γ: $A\varphi := (\frac{1}{2}I + K + L)\varphi = -\mathbf{T}(\mathbf{u}_0, p_0)$

FLATIRON INSTITUTE
Center for Computational Mathematics

Issues periodizing the BIE

recall discretized BIE on Γ: $A\varphi := (\frac{1}{2}I + K + L)\varphi = -\mathbf{T}(\mathbf{u}_0, p_0)$

could simply replace G by $G_{\text{per}}(\mathbf{x},\mathbf{y}) := \sum_{m,n\in\mathbb{Z}} G(\mathbf{x}, \mathbf{y} + m\mathbf{e}_1 + n\mathbf{e}_2)$?
minor problem: $G_{\text{per}} = \infty$ $(\log r \to \infty)$

but *can* periodize stokeslets when sum $= \mathbf{0}$: true since $\int_\Gamma \varphi = \mathbf{0}$

Issues periodizing the BIE

recall discretized BIE on Γ: $A\varphi := (\frac{1}{2}I + K + L)\varphi = -\mathbf{T}(\mathbf{u}_0, p_0)$

could simply replace G by $G_{\text{per}}(\mathbf{x},\mathbf{y}) := \sum_{m,n\in\mathbb{Z}} G(\mathbf{x}, \mathbf{y} + m\mathbf{e}_1 + n\mathbf{e}_2)$?
minor problem: $G_{\text{per}} = \infty$ ($\log r \to \infty$)

but *can* periodize stokeslets when sum $= \mathbf{0}$: true since $\int_\Gamma \varphi = \mathbf{0}$

Two common ways to periodize (compatible with FMM to apply A):

A) Lattice sums $\approx$ Taylor coeffs of *smooth* sum $\sum_{(m,n)\neq(0,0)} G(\mathbf{x}, \mathbf{y} + m, n))$

(Rayleigh 1892; Hasimoto, Helsing, Greengard–Kropinski '04)

issues:
- regularization: setting divergent sums to opaque values
- spherically symm. expansions $\to$ high aspect/skew, bad

B) Particle-Mesh Ewald can be spectrally accurate (Lindbo–Tornberg '10, '11)

split G_{per}: local (spatial) + decaying in Fourier (spectral) (Ewald '21)
issue:
- non-adaptive FFT grid to apply spectral part

Issues periodizing the BIE

recall discretized BIE on Γ: $A\varphi := (\frac{1}{2}I + K + L)\varphi = -\mathbf{T}(\mathbf{u}_0, p_0)$

could simply replace G by $G_{\text{per}}(\mathbf{x},\mathbf{y}) := \sum_{m,n\in\mathbb{Z}} G(\mathbf{x}, \mathbf{y} + m\mathbf{e}_1 + n\mathbf{e}_2)$?

minor problem: $G_{\text{per}} = \infty$ ($\log r \to \infty$)

but *can* periodize stokeslets when sum $= \mathbf{0}$: true since $\int_\Gamma \varphi = \mathbf{0}$

Two common ways to periodize (compatible with FMM to apply A):

A) Lattice sums $\approx$ Taylor coeffs of *smooth* sum $\sum_{(m,n)\neq(0,0)} G(\mathbf{x}, \mathbf{y} + m, n))$

(Rayleigh 1892; Hasimoto, Helsing, Greengard–Kropinski '04)

issues:
- regularization: setting divergent sums to opaque values
- spherically symm. expansions $\to$ high aspect/skew, bad

B) Particle-Mesh Ewald can be spectrally accurate (Lindbo–Tornberg '10, '11)

split G_{per}: local (spatial) + decaying in Fourier (spectral) (Ewald '21)

issue:
- non-adaptive FFT grid to apply spectral part

Issues periodizing the BIE

recall discretized BIE on Γ: $A\varphi := (\frac{1}{2}I + K + L)\varphi = -\mathbf{T}(\mathbf{u}_0, p_0)$

could simply replace G by $G_{\text{per}}(\mathbf{x},\mathbf{y}) := \sum_{m,n\in\mathbb{Z}} G(\mathbf{x},\mathbf{y} + m\mathbf{e}_1 + n\mathbf{e}_2)$?

minor problem: $G_{\text{per}} = \infty$ ($\log r \to \infty$)

but *can* periodize stokeslets when sum $= \mathbf{0}$: true since $\int_\Gamma \varphi = \mathbf{0}$

Two common ways to periodize (compatible with FMM to apply A):

A) Lattice sums $\approx$ Taylor coeffs of *smooth* sum $\sum_{(m,n)\neq(0,0)} G(\mathbf{x},\mathbf{y} + m,n))$

(Rayleigh 1892; Hasimoto, Helsing, Greengard–Kropinski '04)

issues:
- regularization: setting divergent sums to opaque values
- spherically symm. expansions $\to$ high aspect/skew, bad

B) Particle-Mesh Ewald can be spectrally accurate (Lindbo–Tornberg '10, '11)

split G_{per}: local (spatial) + decaying in Fourier (spectral) (Ewald '21)

issue:
- non-adaptive FFT grid to apply spectral part

We believe have simpler general approach fixing issues ...

Periodize by solving BVP in one unit cell

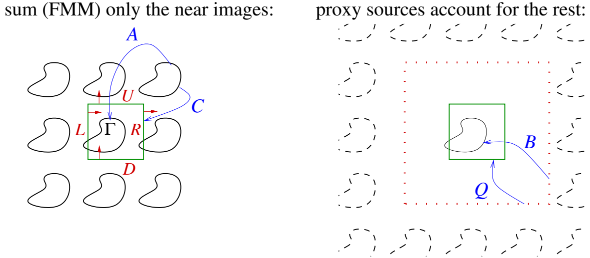
Never think about sums! (technical, conditionally convergent, Ewald formulae. . . yuk)

Just augment lin. sys. with BCs you'd like on walls of single unit cell:

Periodize by solving BVP in one unit cell

Never think about sums! (technical, conditionally convergent, Ewald formulae. . . yuk)

Just augment lin. sys. with BCs you'd like on walls of single unit cell:



Here A is as before, but also sums nearby images to make proxies accurate

Get "extended lin. sys:" $\begin{bmatrix} A & B \\ C & Q \end{bmatrix} \begin{bmatrix} \text{density } \varphi \\ \text{proxy strengths} \end{bmatrix} = \begin{bmatrix} \text{BC on } \Gamma \\ \text{mismatch btw 4 walls} \end{bmatrix}$

stable & FMM-compat: tricky rank-2-pert. Schur compl. (B–Marple–Veerapaneni–Zhao '18)

- idea from Helmholtz (B–Greengard '10); implicit in (Larson–Higdon '80s)
- inspired cubical-unit-cell periodization of PVFMM (Yan–Shelley '18)

2D porous medium Stokes flow

given pressure drop

doubly-periodic
shown: one unit cell

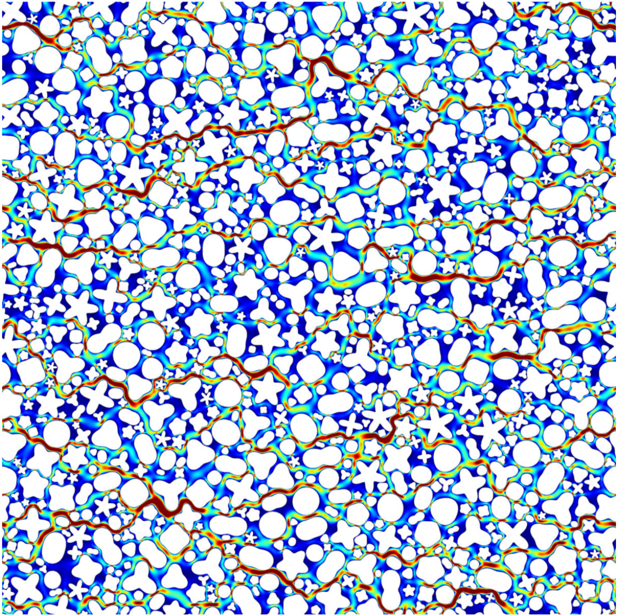
$n = 10^3$
close-to-touching
no-slip islands

error 10^{-8}

1 day CPU

$2N = 7 \times 10^5$

(B–Marple–Veerapaneni–Zhao '18)



Back to periodic mobility: quasi-static BVP

Fix bkgnd shear flow $\mathbf{u}_0(\mathbf{x}) = (\gamma x_2, 0)$ physical flow will be $\mathbf{u}_0 + \mathbf{u}$

At time t: find $\{\mathbf{v}_k, \omega_k\}$, and $(\mathbf{u}, p)$ periodic in current unit cell $\mathcal{U}(t)$, s.t.

$$-\mu\Delta\mathbf{u} + \nabla p = \mathbf{0} \qquad \text{in } \mathcal{U}\backslash\{\overline{\Omega_k}\}$$

$$\nabla \cdot \mathbf{u} = 0 \qquad \text{in } \mathcal{U}\backslash\{\overline{\Omega_k}\}$$

$$\mathbf{u}(\mathbf{x}) + \mathbf{u}_0(\mathbf{x}) = \mathbf{v}_j + \omega_j(\mathbf{x} - \mathbf{x}_j^c)^\perp \qquad \mathbf{x} \in \Gamma_k$$

rigid body motions

$$\int_{\Gamma_k} \mathbf{T} ds = \mathbf{0}$$

zero net fluid force on bodies $k = 1, \ldots, n$

$$\int_{\Gamma_k} \mathbf{T}(\mathbf{x}) \cdot (\mathbf{x} - \mathbf{x}_k^c)^\perp ds_\mathbf{x} = 0$$

zero net fluid torque, $k = 1, \ldots, n$

Then extract: $\mu_{\text{eff}}(t) = \frac{1}{\gamma|\mathbf{e}_1|}\int_D \mathbf{T}(\mathbf{u}_0 + \mathbf{u}, p) \cdot \mathbf{t}\, ds$

horiz. force on bottom wall; avoids cell avg $\langle\sigma\rangle_\mathcal{U}$ of (Brady, etc)

Other new ingredients

- G_{per} issue: stokeslet force $\neq \mathbf{0}$, but periodic BCs $\Rightarrow$ net traction $= \mathbf{0}$

Propose generalized $G_{\text{per}}^{\text{Neu}}(\mathbf{x},\mathbf{y}) := [\mathbf{w}_{(1,0)}(\mathbf{x}),\ \mathbf{w}_{(0,1)}(\mathbf{x})]$, where $\mathbf{w}_{\mathbf{f}}$ solves:

$$
\begin{aligned}
-\mu\Delta\mathbf{w} + \nabla q &= \mathbf{f}\delta_{\mathbf{y}} && \text{in } \mathcal{U}\backslash\{\overline{\Omega_k}\} \\
\nabla\cdot\mathbf{w} &= 0 && \text{in } \mathcal{U}\backslash\{\overline{\Omega_k}\} \\
\mathbf{w}_R - \mathbf{w}_L &= \mathbf{0} && \text{periodic} \\
\mathbf{T}(\mathbf{w},q)_R - \mathbf{T}(\mathbf{w},q)_L &= \mathbf{f}/2|\mathbf{e}_2| && \text{const leakage of net force} \\
\mathbf{w}_U - \mathbf{w}_D &= \mathbf{0} && \text{periodic} \\
\mathbf{T}(\mathbf{w},q)_U - \mathbf{T}(\mathbf{w},q)_D &= \mathbf{f}/2|\mathbf{e}_1| && \text{const leakage of net force}
\end{aligned}
$$

unique up to consts; $\mathcal{S}_{\text{per}}^{\text{Neu}}\varphi$ *not periodic* unless $\int_\Gamma \varphi ds = \mathbf{0}$ "Neumann function"

Other new ingredients

- G_{per} issue: stokeslet force $\neq \mathbf{0}$, but periodic BCs $\Rightarrow$ net traction $= \mathbf{0}$

Propose generalized $G^{\text{Neu}}_{\text{per}}(\mathbf{x},\mathbf{y}) := [\mathbf{w}_{(1,0)}(\mathbf{x}),\ \mathbf{w}_{(0,1)}(\mathbf{x})]$, where $\mathbf{w}_{\mathbf{f}}$ solves:

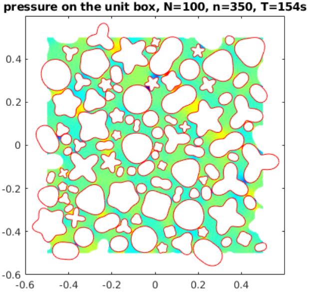
$$
\begin{aligned}
-\mu\Delta\mathbf{w} + \nabla q &= \mathbf{f}\delta_{\mathbf{y}} && \text{in } \mathcal{U}\backslash\{\overline{\Omega_k}\} \\
\nabla\cdot\mathbf{w} &= 0 && \text{in } \mathcal{U}\backslash\{\overline{\Omega_k}\} \\
\mathbf{w}_R - \mathbf{w}_L &= \mathbf{0} && \text{periodic} \\
\mathbf{T}(\mathbf{w},q)_R - \mathbf{T}(\mathbf{w},q)_L &= \mathbf{f}/2|\mathbf{e}_2| && \text{const leakage of net force} \\
\mathbf{w}_U - \mathbf{w}_D &= \mathbf{0} && \text{periodic} \\
\mathbf{T}(\mathbf{w},q)_U - \mathbf{T}(\mathbf{w},q)_D &= \mathbf{f}/2|\mathbf{e}_1| && \text{const leakage of net force}
\end{aligned}
$$

unique up to consts; $\mathcal{S}^{\text{Neu}}_{\text{per}}\varphi$ *not periodic* unless $\int_\Gamma \varphi ds = \mathbf{0}$ "Neumann function"

- eval. traction of $G^{\text{Neu}}_{\text{per}}$ fast, gives a stable mat-vec for GMRES:
  - FMM for near images + correction of wall mismatch via cheap "empty unit cell" BVP
  - "empty" BVP solved to 10^{-14} via method of fundamental solutions (proxy pts)
- kd-tree to find close targets needing special quadratures
- extract μ_{eff} via cheap far-field contour integral

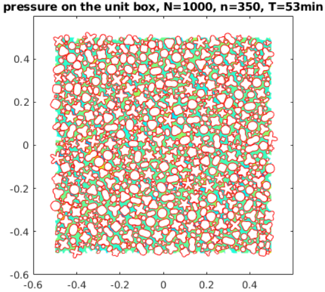
Results: quasi-static solve

$n = 10^2$ bodies, close-touching



$2N = 7 \times 10^4$ unknowns, 2.5 mins

$n = 10^3$ bodies, close-touching:

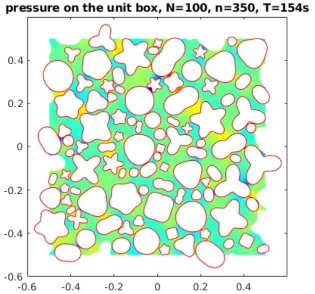


$2N = 7 \times 10^5$ unknowns, 1 hr

8-digit accuracy $\quad N = 350$ per body $\quad$ typ. < 100 GMRES iters.

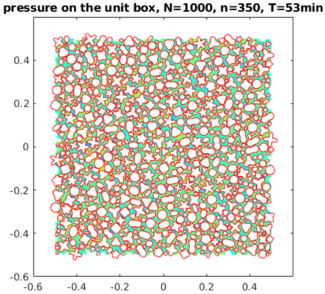
Results: quasi-static solve

$n = 10^2$ bodies, close-touching



$2N = 7 \times 10^4$ unknowns, 2.5 mins

$n = 10^3$ bodies, close-touching:



$2N = 7 \times 10^5$ unknowns, 1 hr

8-digit accuracy $N = 350$ per body   typ. < 100 GMRES iters.

Evolution: define body state vector $\mathbf{z}(t) := \{\mathbf{x}_k^c, \theta_k\} \in \mathbb{R}^{3n}$

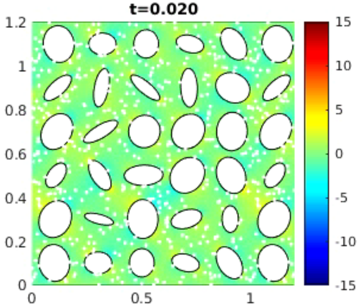
wrap the quasi-static solve as evaluating $\{\mathbf{v}_k, \omega_k\} = \frac{d\mathbf{z}}{dt} = \mathbf{F}(\mathbf{z}(t))$

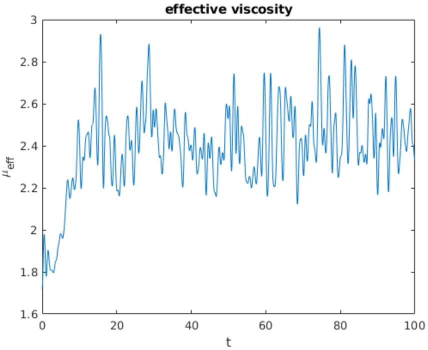
autonomous ODE system

Feed to favorite t-stepper: fixed-Δt Euler, or high-order adaptive

Results: time-evolution

$n = 25$ ellipses, run for 100 shear-times, apparently equilbrium...



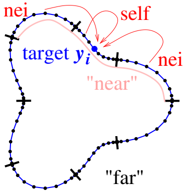


- spatial solve error 10^{-10}, evolution typ. 10^{-4} $\sim$ 1 s / step, FMM+GMRES
- we can run fwd-Euler, or adaptive RK4 (slows down)
- add short-range repulsive force, needed for higher ϕ; in progress

FLATIRON INSTITUTE Center for Computational Mathematics

Panel quadratures and adaptivity

To best handle arbitrary geometries: need composite quadr. rules

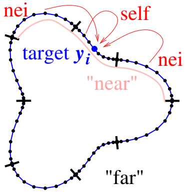


Gauss–Legendre

rule on each panel

Panel quadratures and adaptivity

To best handle arbitrary geometries: need composite quadr. rules



Gauss–Legendre

rule on each panel

far: Nyström rule

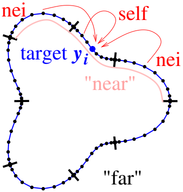
$K_{ij} = K(\mathbf{y}_i, \mathbf{y}_j) w_j$

nei + self + close-eval: complex interpolatory rules

(Helsing '08, Ojala–Tornberg '15)

Panel quadratures and adaptivity

To best handle arbitrary geometries: need composite quadr. rules



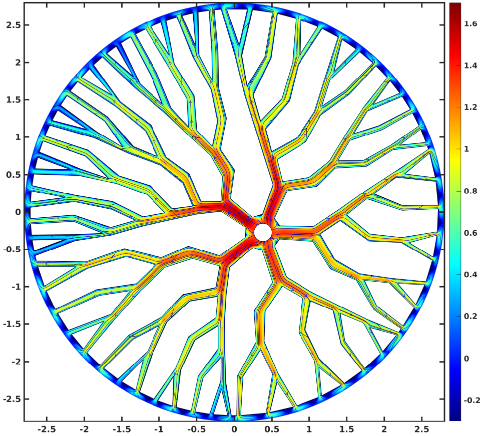
Gauss–Legendre rule on each panel

far: Nyström rule

$K_{ij} = K(\mathbf{y}_i, \mathbf{y}_j) w_j$

nei + self + close-eval: complex interpolatory rules

(Helsing '08, Ojala–Tornberg '15)



378 corners $2N = 3 \times 10^5$ 10 digits 2 hours

- No-slip Stokes flow in 2D vascular network model:

  (Wu–Zhu–B–Veerapaneni, in prep.)

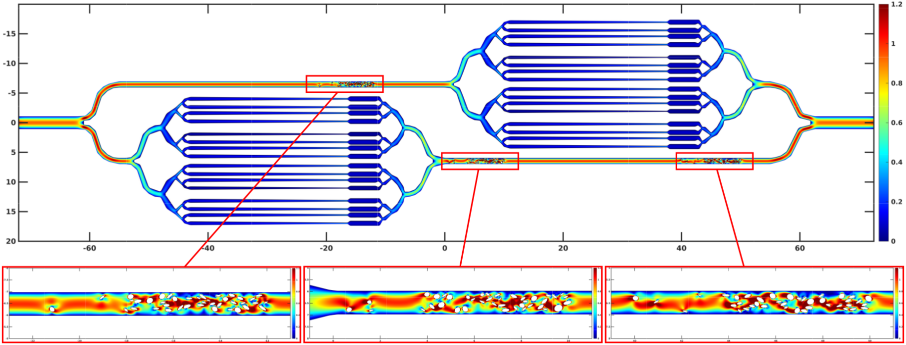
adaptivity: panels split until resolve geom to user-requested tolerance ε

panel order $p \approx \log_{10}(1/\epsilon)$

FLATIRON INSTITUTE
Center for Computational Mathematics

Panel quadratures and adaptivity II

microfluidic device design: "worm clamps" plus nearby particles



flow speed shown $2N = 1.2 \times 10^6$ 120 swimmer particles 6 digits 8 hrs

(Wu–Zhu–B–Veerapaneni, in prep.)

- could factorize fixed walls via *fast direct solver*, cheap t-steps

(Marple–B–Gillman–Veerapaneni '16)

Conclusions

Flavor of efficient & accurate Stokes solvers, which need:

- special quadratures for close-evaluation
- new periodization tools for skewing unit cells
- adaptivity for complex devices

Numerical analysis philosophy: solve the actual BVP, to many digits

Software is harder, in progress at Flatiron for BIE in 2D, 3D

(Stein/Yan (CCB), Racch/Greengard/B (CCM), O'Neil/Malhotra (NYU). . .)

$*$ Special issue of Adv. Comput. Math. on BIE, submissions due 8/31/20

Although I haven't yet modeled swimming fish (Re $\gg 1$), thanks Mike for help over the years and helping guide me into fun fluids!

EXTRA SLIDES

Jamming?

Two 4-pointed smooth stars per unit cell:

jamming stars 1

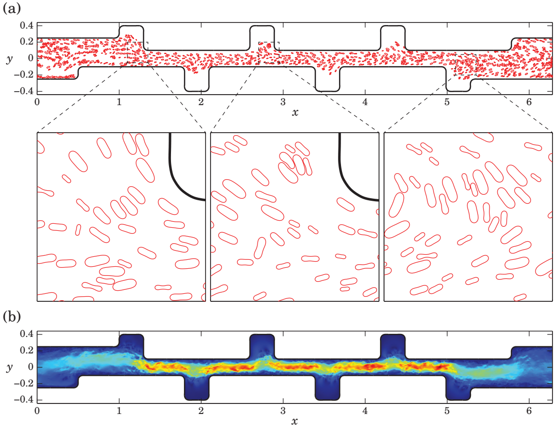
jamming stars 2

jamming stars 3

(we don't understand jamming yet. . .)

Singly-periodic pipe with vesicles

Fast direct solver factorizes pipe solve once and for all, cheap to apply:



1000 vesicles $N = 128000$ 1 min/timestep (Marple–B–Gillman–Veerapaneni '16)

FLATIRON INSTITUTE Center for Computational Mathematics