Doubly-Periodic Algorithm for Stokes Flow

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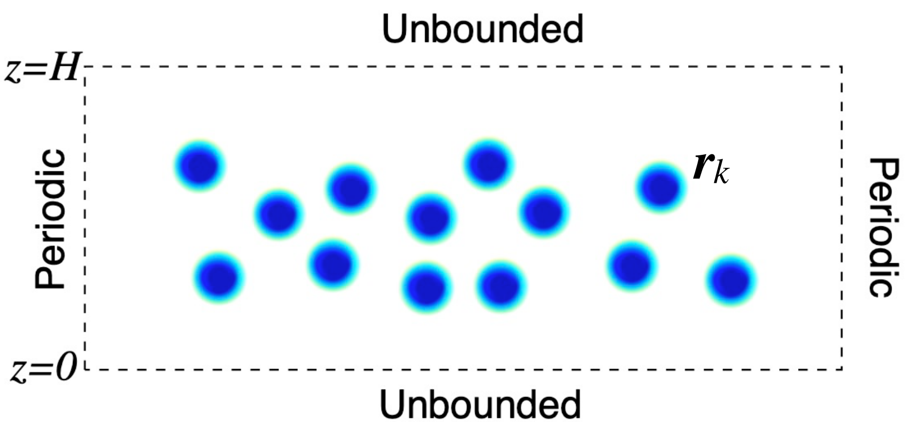
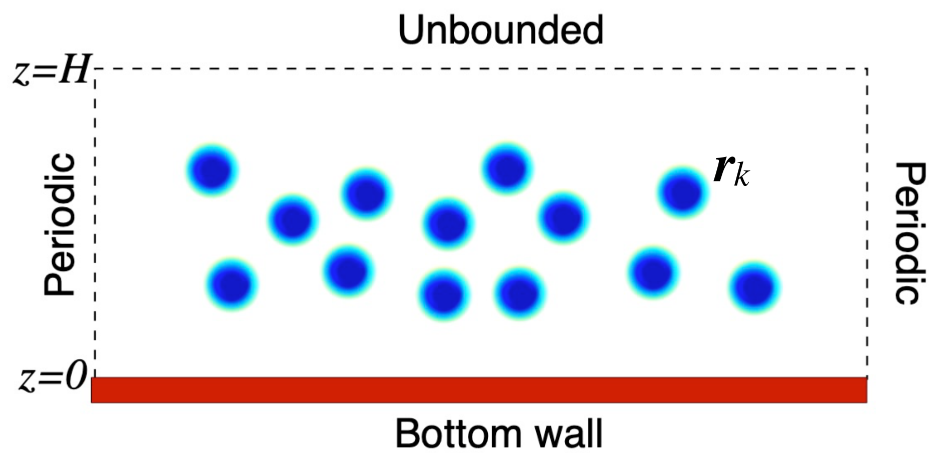
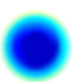
Doubly-Periodic Geometries





The Doubly-Periodic geometry (DP)
(done by Ondrej)

The bottom wall geometry
(goal)

 : Gaussians centered at $\boldsymbol{r}_k$ with effective hydrodynamic radius a.

- Dashed rectangle representing our actual domain of computation.
- Our method also applies to the slit channel geometry with both bottom & top walls; won't be today's topic for simplicity.

Bottom Wall Stokes Flow

We aim to solve the Stokes equations:

$$\eta\nabla^2\boldsymbol{u} - \nabla p = -\boldsymbol{f} \ ,$$
$$\nabla\cdot\boldsymbol{u} = 0 \ ,$$

on a doubly-periodic domain $[x, y]\in[-L, L]\times[-L, L]$ and $z\in[0, +\infty)$.

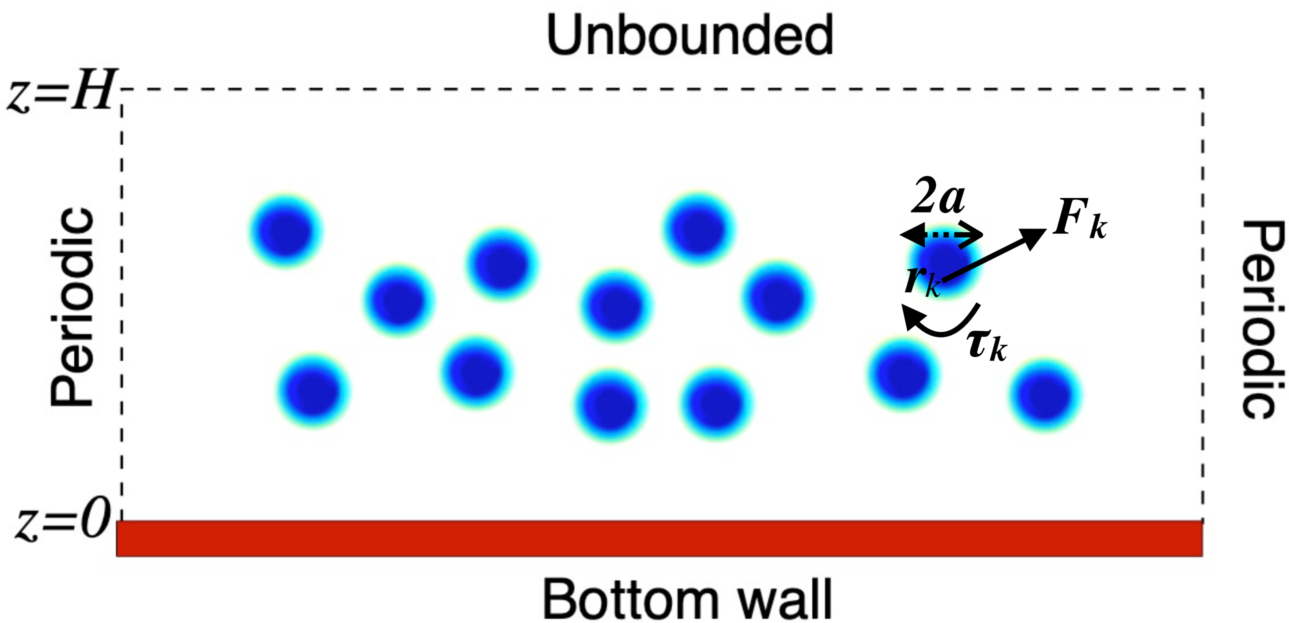
No-slip BCs on the bottom wall,

$$\boldsymbol{u}\big|_{z=0} = \boldsymbol{0} \ ,$$

where p is pressure, η is viscosity, $\boldsymbol{u}$ is fluid velocity.

- We will focus on the no-slip BCs case, our method can also be extended to bottom wall/slit channel with an active slip.

Clarifications for the model approximations



- The real system: actual particles (no fluid inside each sphere); BCs on each particle's surface. Particles will *not* overlap the wall. (Note: here we refer to particles as for colloids at mesoscopic scale; for ions the immersed particle picture is just a model.)
- The model: particles as Gaussians (fluid everywhere) with effective radii a (no point particle for Stokes). Particle velocities decided from averaging the fluid velocities near $\boldsymbol{r}_k$. Particle overlapping the wall is unavoidable in BD simulations.

Force-Coupling Method (FCM) Formulations

In the FCM (Maxey & Patel 2001; Lomholt & Maxey 2003), the surface traction on a spherical particle of radius *a* is replaced by finite, smoothly varying Gaussian and the multipole expansion truncated at dipole:

$$\boldsymbol{f}(\boldsymbol{x}) = \sum_{k=1}^{M} \left[\underbrace{\boldsymbol{F}_k}_{\text{Force}} \Delta_M(\boldsymbol{x} - \boldsymbol{r}_k) + \frac{1}{2} \nabla \times (\underbrace{\boldsymbol{\tau}_k}_{\text{Torque}} \Delta_D(\boldsymbol{x} - \boldsymbol{r}_k)) \right] ,$$

Δ_M and Δ_D 3D Gaussian envelopes, with standard deviations,

$$g_F = a/\sqrt{\pi} \text{ and } g_\tau = a/(6\sqrt{\pi})^{1/3}$$

- The standard deviations g_F and g_τ are decided from the Stokes' law for a sphere with radius *a* translating/rotating in free-space:

$$\boldsymbol{F} = 6\pi\eta a\boldsymbol{U} \text{ and } \boldsymbol{T} = 8\pi\eta a^3\boldsymbol{\Omega}$$

- FCM similar to IBM in modeling and simulation: both capture long-ranged hydrodynamic interactions.

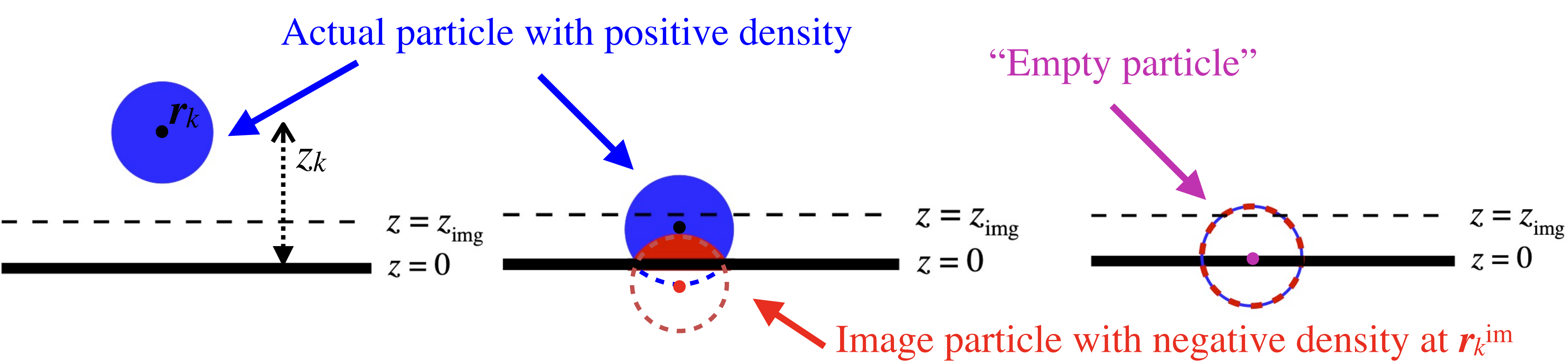
Wall Overlap

Modification of the Gaussian envelopes that overlap the wall

$$\Delta^W(\boldsymbol{x} - \boldsymbol{r}_k) = \Delta(\boldsymbol{x} - \boldsymbol{r}_k) - \Delta(\boldsymbol{x} - \boldsymbol{r}_k^{\text{im}}) \,, \quad \text{if } z_k < z_{\text{img}}$$

where $\boldsymbol{r}_k^{\text{im}}$ is the particle's point of reflection about the bottom wall.

2D illustrations:



- In a Brownian dynamic simulation, overlapping the wall is unavoidable
- Ensure particle mobility goes to zero as it approaches the no-slip wall

Mobility Matrix

Particle linear and angular velocities **interpolated** from fluid:

$$\boldsymbol{V}_k = \int_{\boldsymbol{x}} \boldsymbol{u}(\boldsymbol{x}) \Delta_M^W (\boldsymbol{x} - \boldsymbol{r}_k) d\boldsymbol{x} \ ,$$

$$\boldsymbol{\Omega}_k = \frac{1}{2} \int_{\boldsymbol{x}} \left(\nabla \times \boldsymbol{u}(\boldsymbol{x})\right) \Delta_D^W (\boldsymbol{x} - \boldsymbol{r}_k) d\boldsymbol{x} \ .$$

FCM provides a **far-field approximation** of the exact mobility problem:

$$\begin{pmatrix} \boldsymbol{V} \\ \boldsymbol{\Omega} \end{pmatrix} = \underbrace{\begin{pmatrix} \boldsymbol{M}^{tt} & \boldsymbol{M}^{tr} \\ \boldsymbol{M}^{rt} & \boldsymbol{M}^{rr} \end{pmatrix}^{FCM}}_{\boldsymbol{M}_{FCM}} \begin{pmatrix} \boldsymbol{F} \\ \boldsymbol{T} \end{pmatrix} ,$$

where $\boldsymbol{M}_{FCM}$ is the mobility matrix.

- Mobility matrix is symmetric and positive semidefinite (SPD)
- We will focus on the translation-translation mobilities (entries of $\boldsymbol{M}^{tt}$)

The DP + Correction Method

The Stokes problem under bottom wall geometry can be divided into two subproblems.

Subproblem #1: the "DP" problem

$$\eta\nabla^2\boldsymbol{u}_{DP} - \nabla p_{DP} = -\boldsymbol{f} \ ,$$
$$\nabla\cdot\boldsymbol{u}_{DP} = 0 \ .$$

with periodic BCs in *xy* directions and free-space BCs in *z*.

Note:

- same source term $\boldsymbol{f}$ as our original problem, i.e., only particles, no wall present.
- For bottom wall/slit channel geometries, the unbounded BCs in *z* can be reduced onto [*0*, *H*] through the *Dirichlet-to-Neumann map*, based on the fact that $\boldsymbol{f}$ is 0 outside [*0*, *H*].

The DP + Correction Method

Subproblem #2: the "Correction" problem (wall correction, no particle)

$$\eta \nabla^2 \boldsymbol{u}_{corr} - \nabla p_{corr} = 0 \,,$$
$$\nabla \cdot \boldsymbol{u}_{corr} = 0 \,,$$

with periodic BCs in *xy* directions and $z \in [0, +\infty)$, and with slip BCs on the bottom wall:

$$\boldsymbol{u}_{corr}\big|_{z=0} = -\boldsymbol{u}_{DP}\big|_{z=0} \,,$$

where $\boldsymbol{u}_{\mathrm{DP}}$ is the solution to the "DP" problem. By linearity,

$$\boldsymbol{u} = \boldsymbol{u}_{DP} + \boldsymbol{u}_{corr} \,, \quad \text{and} \quad p = p_{DP} + p_{corr} \,.$$

- The correction problem is homogeneous and can be solved analytically.
- The DP problem can be handled numerically through Fourier/ Chebyshev spectral method.

Boundary Value Problems

The DP solver (Ondrej):
Eliminating pressure p through a projection approach, take Fourier transforms in xy directions gives Four scalar BVPs for each ***k≠0***

$$\left(\partial_{zz} - k^2\right)\hat{p} = \iota k_x \hat{f}_x + \iota k_y \hat{f}_y + \partial_z \hat{f}_z \quad \text{and} \quad (\partial_z \pm k)\hat{p}|_{z=0(\text{or } H)} = 0, \quad \text{(solve first)}$$

$$\eta\left(\partial_{zz} - k^2\right)\hat{u} = \iota k_x \hat{p} - \hat{f}_x \quad \text{and} \quad (\partial_z \pm k)\hat{u}|_{z=0(\text{or } H)} = \pm \iota k_x \hat{p}|_{z=0(\text{or } H)}/(2\eta k),$$

$$\eta\left(\partial_{zz} - k^2\right)\hat{w} = \partial_z \hat{p} - \hat{f}_z \quad \text{and} \quad (\partial_z \pm k)\hat{w}|_{z=0(\text{or } H)} = \hat{p}|_{z=0(\text{or } H)}/(2\eta).$$

- One can solve the BVPs using the Chebyshev spectral integral BVP solver of Greengard [1], or a Galerkin approach (for Brownian Dynamics).
- Fourier/Chebyshev computations log-linear time using 3D FFTs.
- Main CPU cost in kernel spreading/interpolation to/from the grid.

[1] Leslie Greengard. Spectral integration and two-point boundary value problems. SIAM Journal on Numerical Analysis, 28(4):10711080, 1991.

Analytical Wall Correction

The correction solve (homogeneous Stokes + BCs):
solution in the form of plane wave expansion,

$$\boldsymbol{u}_{corr}(\boldsymbol{r}) = \frac{1}{2L^2}\sum_{\boldsymbol{k}=0}^{\infty}\hat{\boldsymbol{u}}_{corr}(\boldsymbol{k}, z)\cdot e^{i\boldsymbol{k}\cdot\boldsymbol{\nu}},$$

where $\boldsymbol{k}=[k_x, k_y]$, $\boldsymbol{\nu}=[x,y]$, and with slip BCs

$$\boldsymbol{u}_{corr}|_{z=0} = -\boldsymbol{u}_{DP}|_{z=0} = [u_0, v_0, w_0]$$

the analytical solution is,

$$\hat{u}_{corr}(\boldsymbol{k}, z) = -\frac{k_x}{k}(ik\hat{w}_0(\boldsymbol{k}) + k_x\hat{u}_0(\boldsymbol{k}) + k_y\hat{v}_0(\boldsymbol{k}))ze^{-kz} + \hat{u}_0(\boldsymbol{k})e^{-kz},$$

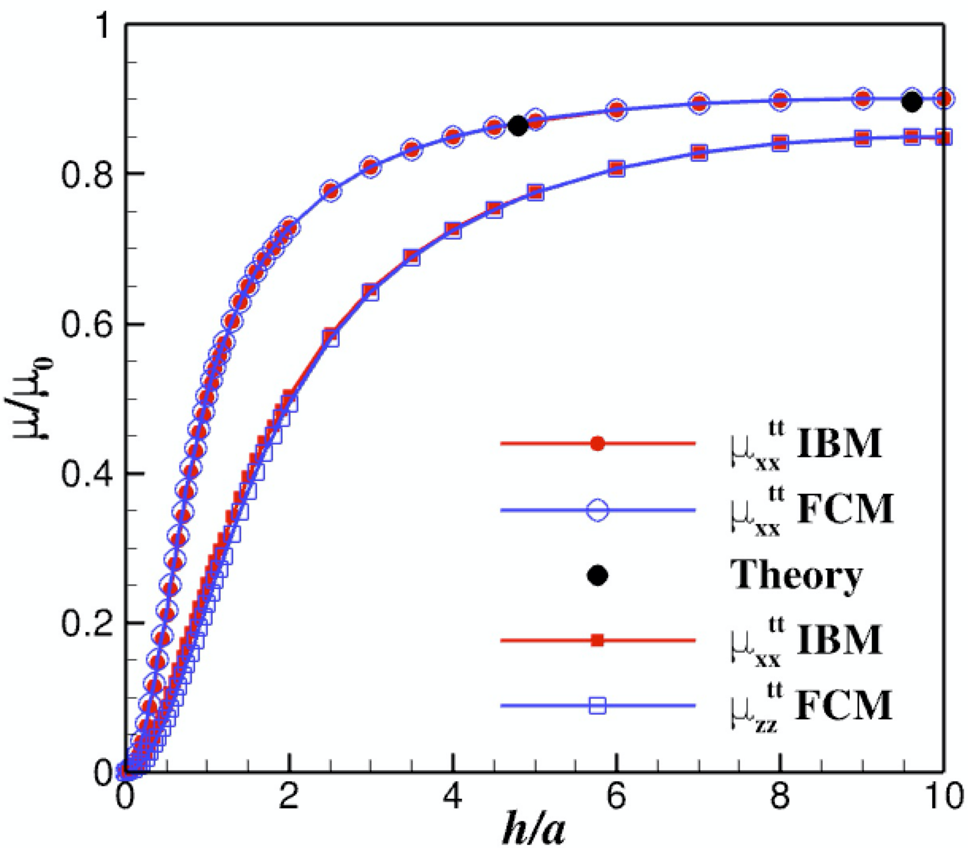
$$\hat{v}_{corr}(\boldsymbol{k}, z) = -\frac{k_y}{k}(ik\hat{w}_0(\boldsymbol{k}) + k_x\hat{u}_0(\boldsymbol{k}) + k_y\hat{v}_0(\boldsymbol{k}))ze^{-kz} + \hat{v}_0(\boldsymbol{k})e^{-kz},$$

$$\hat{w}_{corr}(\boldsymbol{k}, z) = (k\hat{w}_0(\boldsymbol{k}) - ik_x\hat{u}_0(\boldsymbol{k}) - ik_y\hat{v}_0(\boldsymbol{k}))ze^{-kz} + \hat{w}_0(\boldsymbol{k})e^{-kz}.$$

u_0, v_0 and w_0 are from the numerical solution of DP so known in $\boldsymbol{k}$-space.

Single particle trans-trans mobility in slit channel

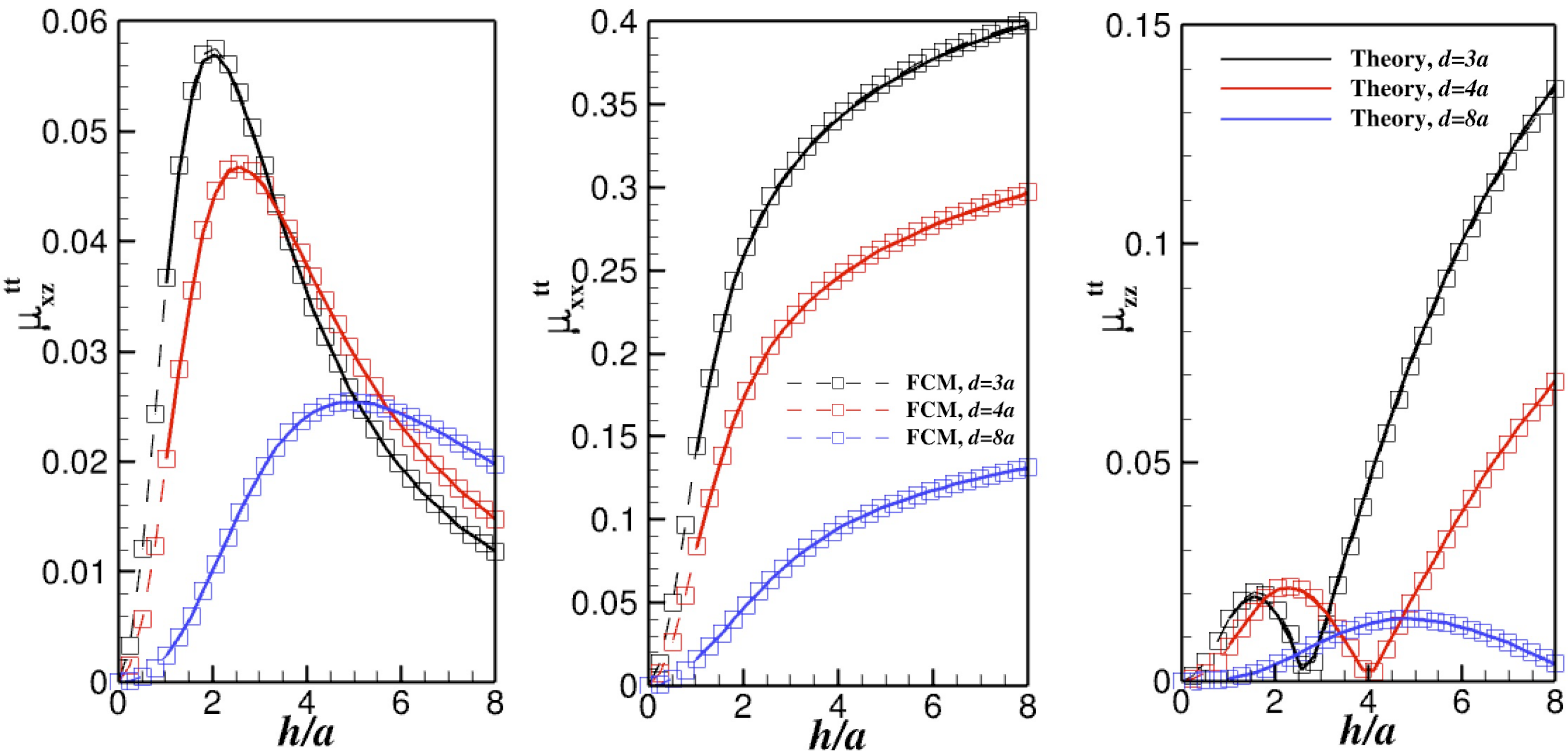
Parallel and perpendicular normalized trans-trans mobilities for a single particle in slit channel of width *H=19.2a*



Our results in good agreement with theory by Faxen, and also matches well with the immersed boundary method.

Trans-trans coupling above a wall

Trans-trans coupling for two particles above a no-slip wall



The solid lines correspond to the direct formulas of Swan and Brady. We are in reasonable agreement with the theoretical predictions for $h>a$.

Switching to ES kernel

The "Exponential of a Semicircle" (ES) kernel is given by,

$$\phi_\beta(z;\alpha) = \frac{1}{\int_{-\alpha}^{\alpha} e^{\beta(\sqrt{1-(\frac{z}{\alpha})^2}-1)} dz} \begin{cases} e^{\beta(\sqrt{1-(\frac{z}{\alpha})^2}-1)}, & |\frac{z}{\alpha}| \le 1 \\ 0, & \text{otherwise.} \end{cases}$$

where $\alpha = wh/2$, where h is the grid spacing in xy, w is the number of grid points to which we spread in each direction.

- Almost optimal convergence in w in terms of spreading/interpolation [2]
- However, it is not isotropic in 3D, loss of translation/rotation invariance

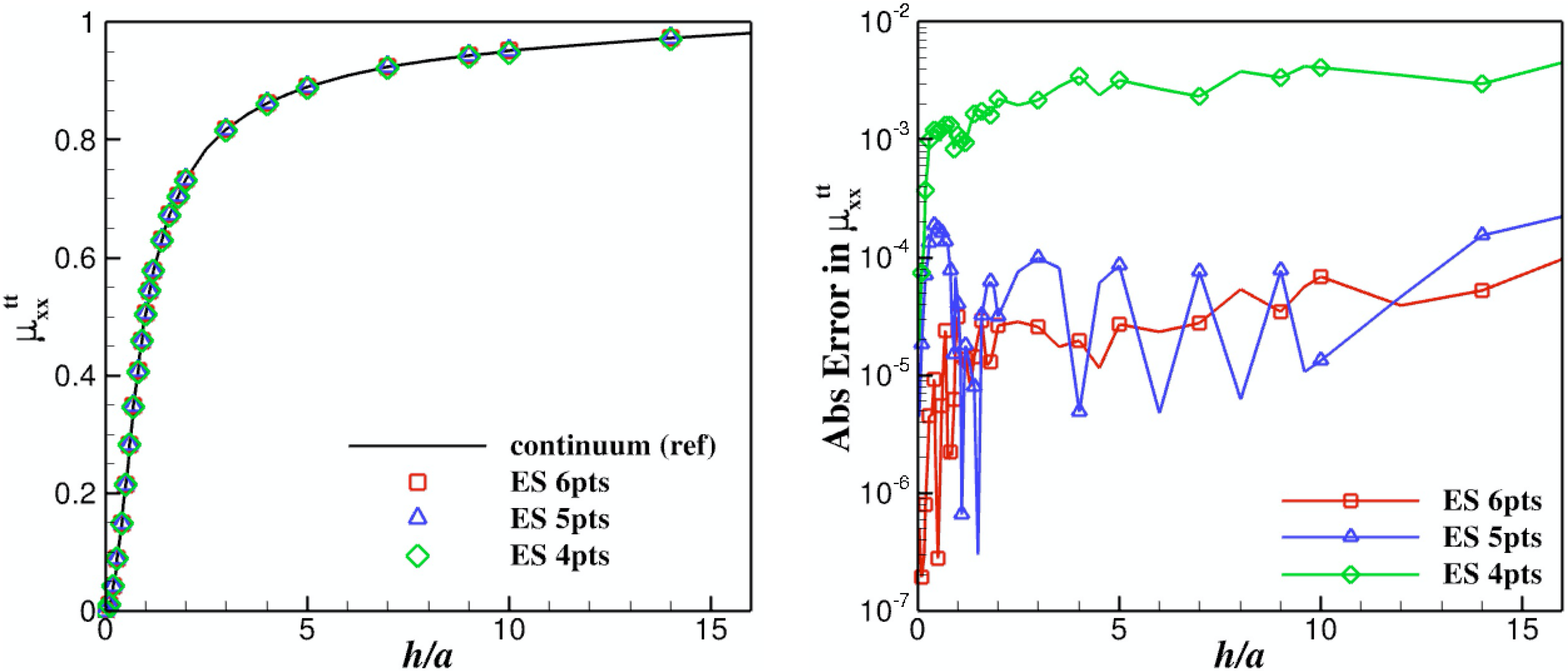
Optimal combinations of w_F and β_F along with optimal errors and effective radii

w_F	4	5	6
β_F/w_F	1.785	1.886	1.714
%-error$_F$	0.3695	0.0554	0.0214
a/h_{xy}	1.2047	1.3437	1.5539

[2] Alex Barnett, et, al. A parallel non-uniform fast Fourier Transform library based on an "Exponential of Semicircle" kernel, SIAM Journal on Scientific Computing. 2019;41(5):C479-504.

Numerical Results: Trans-trans Mobilities with ES kernel

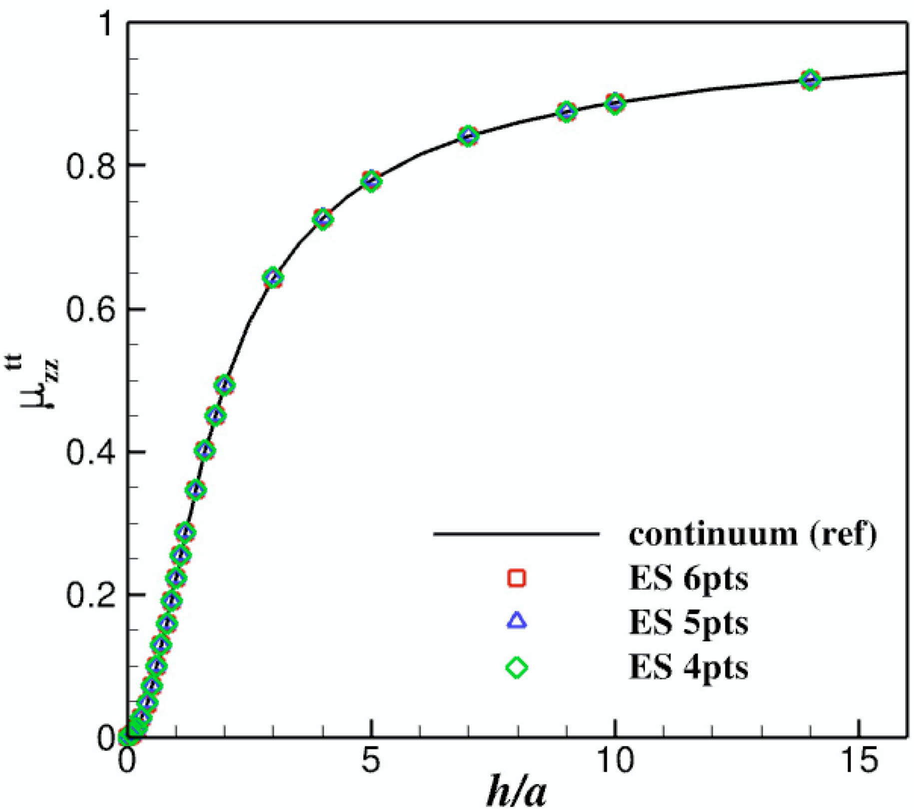
Normalized parallel trans-trans mobilities with ES kernel

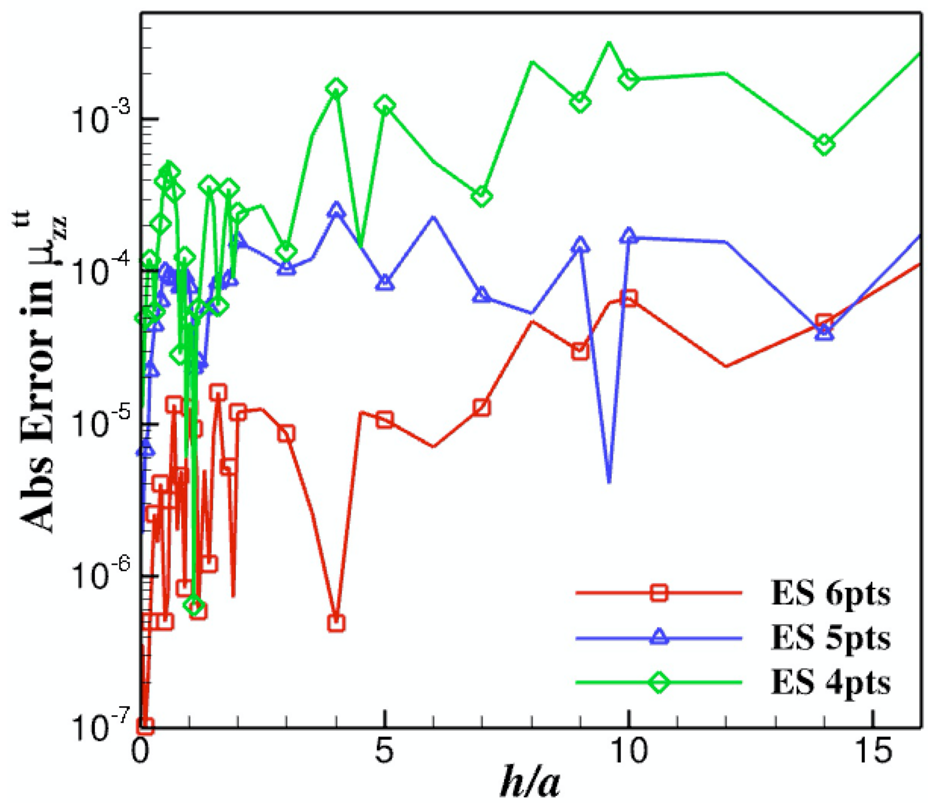


Gaussian needs ~10 pts in each direction to obtain 3~4 digits accuracy. Reference calculated using ES ($w_F = 12$) with refined mesh (for $w_F = 6$), so that the hydrodynamic radius a remains the same.

Numerical Results: Trans-trans Mobilities with ES kernel

Normalized perpendicular trans-trans mobilities with ES kernel





Reference calculated using ES ($w_F = 12$) with refined mesh (for $w_F = 6$), so that the hydrodynamic radius a remains the same.

Thank you!