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Topic: Continuum-Particle Simulation Software (COPSS-Hydrodynamics)

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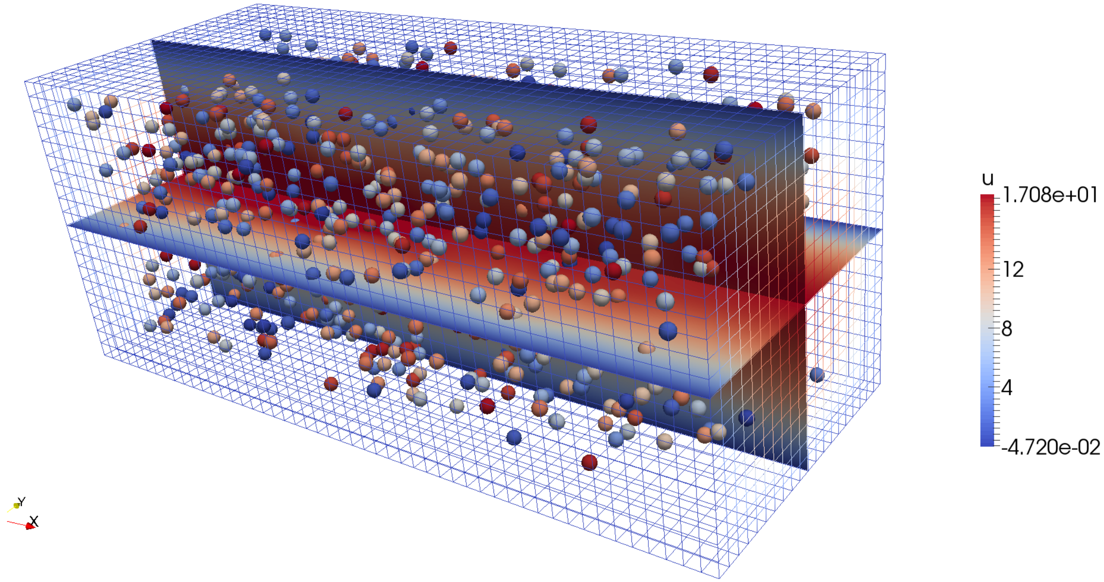
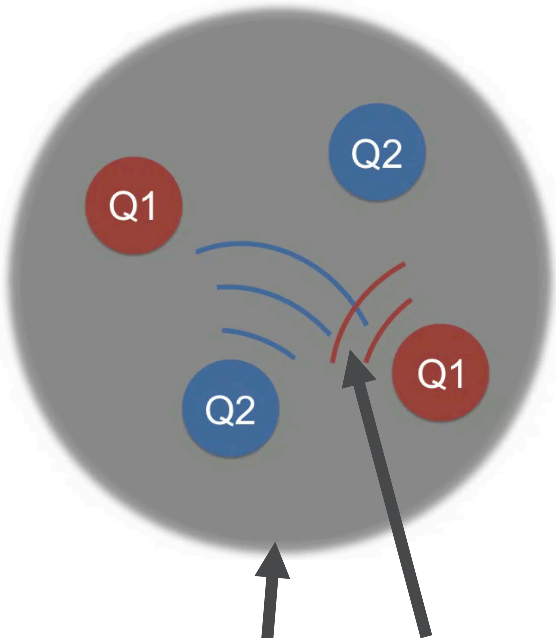
What is Continuum-Particle Simulation?

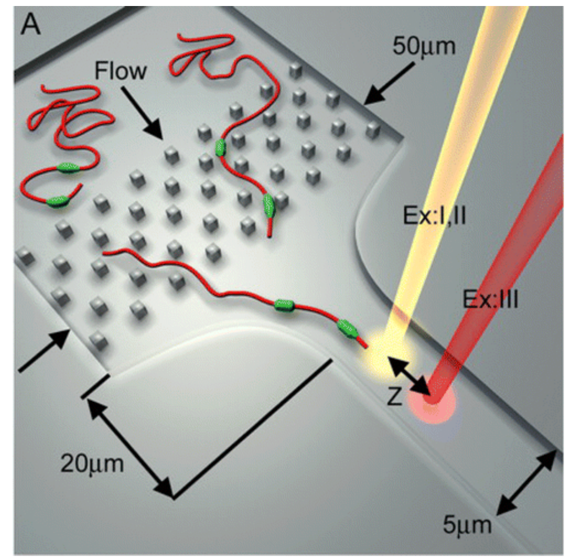


- Continuum simulation (Grid-based) solves Partial Differential Equations on discretized grids or meshes (Finite element method, Finite difference method, Boundary element method, *etc.*)
- Particle simulation (Particle-based) solves Equation of Motion, *e.g.,* Netwon 2nd law, to evolve positions and velocities of discrete particles (Molecular dynamics, Dissipative particle dynamics, *etc.*)
- *Continuum-particle coupling* aims solve complex materials/physics problems (multiple length-scales, phases, and physics)

Hydrodynamics



Confined walls   Hydrodynamics



Chan, EY et al.

- Moving particles in continuous fluid can disturb the flow field, which affects the motions of all the other particles within the field.
- Hydrodynamics: in-direct interactions mediated by fluid.

Many-body and long-range → expensive

Hydrodynamics

Stokes equations:

$$-\nabla p + \mu \nabla^2 \mathbf{u} = -\mathbf{f}$$
$$\nabla \cdot \mathbf{u} = 0$$

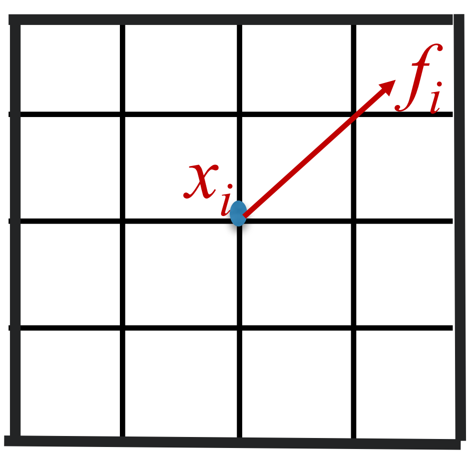
$$\mathbf{f} = \sum_{i=1}^{N_b} \mathbf{f}_i \delta(\mathbf{x} - \mathbf{x}_i)$$ (Point forces)

Unconfined space: Able to solve it analytically

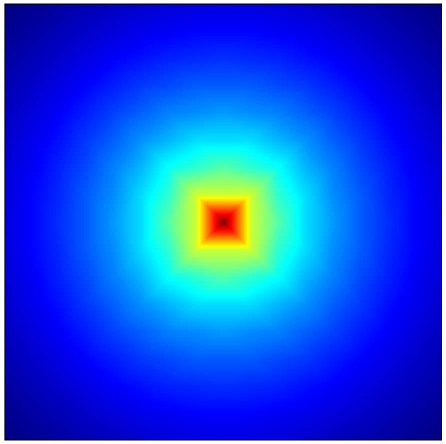
$$\mathbf{u}(\mathbf{x}) = \sum_\nu \mathbf{G}(\mathbf{x} - \mathbf{x}_\nu) \cdot \mathbf{f}_\nu$$

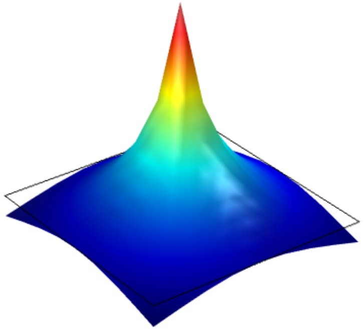
$$\mathbf{G}(\mathbf{x}) = \frac{1}{8\pi\eta r}\left[\boldsymbol{\delta} + \frac{\mathbf{xx}}{r^2}\right]$$ (free-space Green's function of Stokes equation)

Confined space: Directly FEM cause singularity



singularity





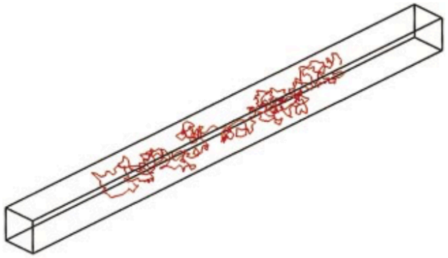
Hydrodynamics

- **Challenge 1: Confined space**

1. **Satisfy non-slip boundary conditions** → no analytic solution is available in complex geometries.
2. Directly using standard FEM will cause singularities in the solutions

- **Challenge 2: Brownian motions of particles**

1. **Conserve Fluctuation-dissipation theorem** : coupling dynamics of particles (Brownian dynamics) with dynamics of fluid (stokes flow).



DNA diffusion within confined channel

Parallel Finite Element – Generalized Geometry Ewald-like method (pFE-GgEm)

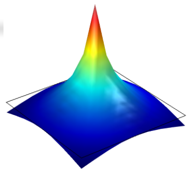
- Step 1. Solve Stokes flow using GgEm (O(N)), satisfying non-slip boundary conditions and avoid singularity.

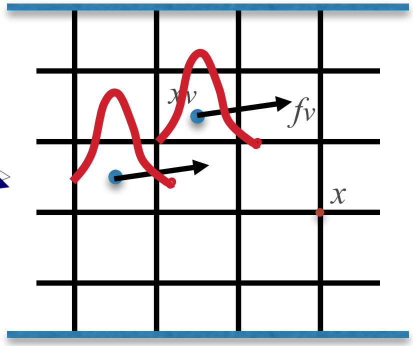
- Step 2. Evolving particle motions using stochastic PDE.

Step 1: solve stokes flow using GgEM

$$-\nabla p + \mu \nabla^2 \mathbf{u} = -\mathbf{f}$$
$$\nabla \cdot \mathbf{u} = 0$$

$$\mathbf{f} = \sum_{i=1}^{N_b} \mathbf{f}_i \delta(\mathbf{x} - \mathbf{x}_i) \quad \text{(Point forces)}$$





$$\mathbf{f}(\mathbf{x}) = \mathbf{f}_l(\mathbf{x}) + \mathbf{f}_g(\mathbf{x})$$

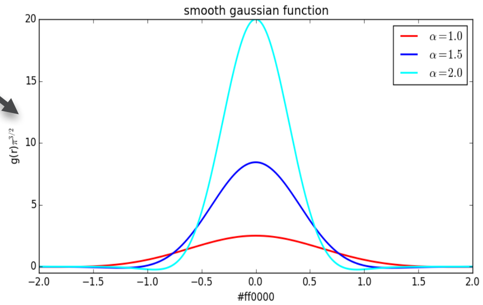
$$\mathbf{f}_l = \sum_{i=1}^{N_b} \mathbf{f}_i [\delta(\mathbf{x} - \mathbf{x}_i) - g(\mathbf{x} - \mathbf{x}_i)]$$ Local

$$\mathbf{u}_l(\mathbf{x}) = \sum_{i=1}^{N_b} \mathbf{G}_l(\mathbf{x} - \mathbf{x}_i) \cdot \mathbf{f}_i$$

$$\mathbf{f}_g = \sum_{i=1}^{N_b} \mathbf{f}_i g(\mathbf{x} - \mathbf{x}_i)$$ global

$$g(r) = \frac{\alpha^3}{\pi^{3/2}} e^{-\alpha^2 r^2} \left(\frac{5}{2} - \alpha^2 r^2 \right)$$

$$\mathbf{f}_g = \sum_{i=1}^{N_b} \mathbf{f}_i g(\mathbf{x} - \mathbf{x}_i) \xrightarrow{\text{Numerical solution}} \mathbf{u}_g(\mathbf{x})$$



Step 2: Evolving particle motion using Stochastic PDE

$$d\mathbf{R} = \left[\mathbf{U}_0 + \mathbf{M}\cdot\mathbf{F} + k_B T \frac{\partial}{\partial \mathbf{R}}\cdot\mathbf{M}\right]dt + \sqrt{2}\mathbf{B}\cdot d\mathbf{w}$$

$$\mathbf{B}\cdot\mathbf{B}^T = k_B T\mathbf{M} = \mathbf{D}$$

$$M * F = U$$

R: the positions of particles
U_0: undisturbed velocities of particles (induced by pressure driven flow, shear, etc)
M: mobility tensor (cannot be explicitly built)
F: non-hydrodynamic and non-Brownian force (electrostatic, spring force, etc.)
dw: random vector with mean zero and variance dt

Midpoint time integration scheme. –Fixman, J. Chem. Phys, 69, 1527 (1978)

$$\mathbf{R}^* = \mathbf{R} + \frac{1}{2}\left[\mathbf{U}_0(\mathbf{R}) + \mathbf{M}(\mathbf{R})\cdot\mathbf{F}(\mathbf{R})\right]\Delta t + \frac{1}{2}\sqrt{2}\mathbf{D}(\mathbf{R})\mathbf{B}^{-1}(\mathbf{R})\cdot d\mathbf{w}(t)$$

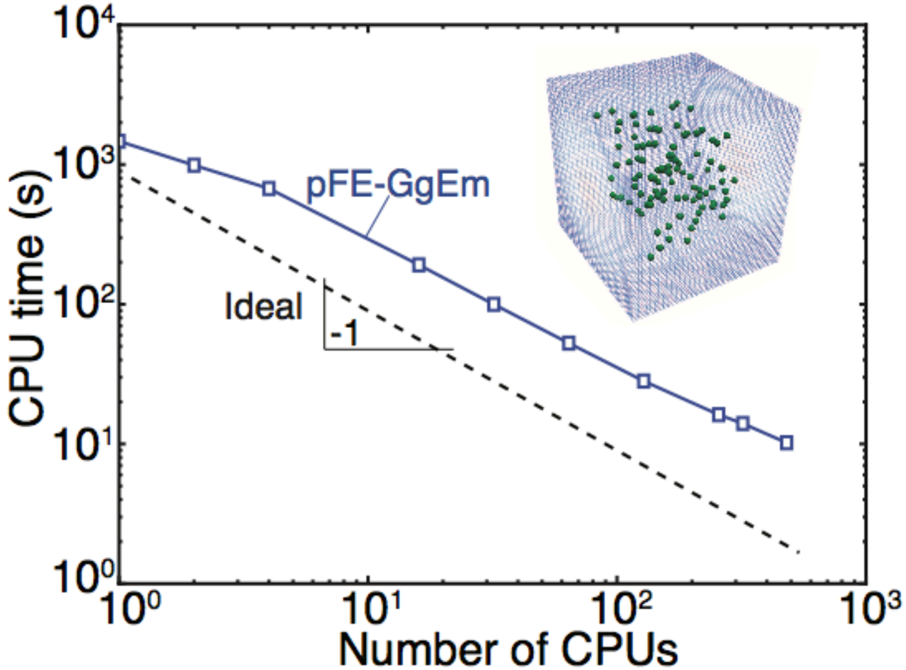
$$\mathbf{R}(t+\Delta t) = \mathbf{R}(t) + \left[\mathbf{U}_0(\mathbf{R}^*) + \mathbf{M}(\mathbf{R}^*)\cdot\mathbf{F}(\mathbf{R}^*)\right]\Delta t + \sqrt{2}\mathbf{D}(\mathbf{R}^*)\mathbf{B}^{-1}(\mathbf{R})\cdot d\mathbf{w}(t)$$

GGEM ← Chebyshev polynomial **~ M*Vec**

M*_Vec_ = solution of Stokes induced by _Vec_

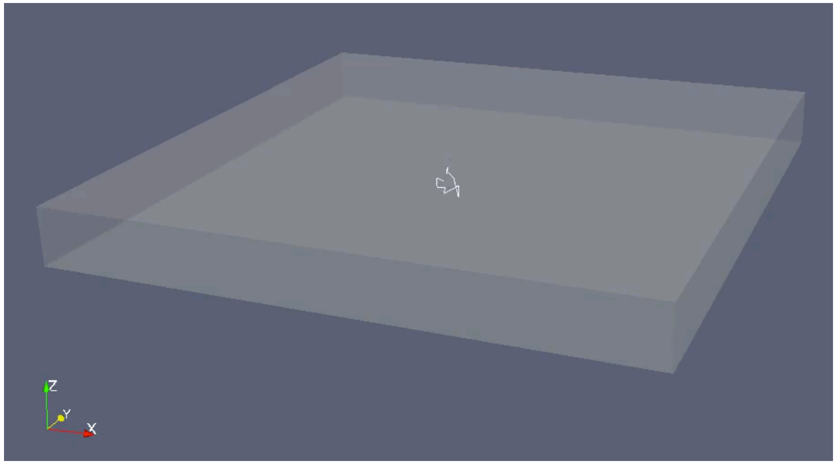
COPSS-Hydrodynamics: parallel performance

Each time step requires multiple solves of Stokes equation, thus an efficient and parallel Stokes solver is necessary.



X., Zhao, J., Li, X. Jiang, J. Hernandez-Ortiz, J. J de Pablo. JCP, 2017

COPSS-Hydrodynamics: correct diffusion behavior



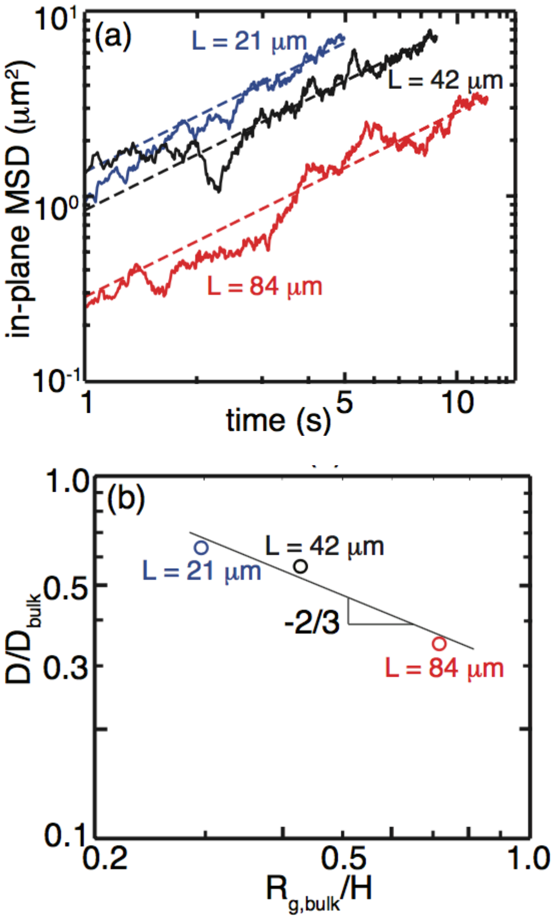


FIG. 3. (a) Typical in-plane MSD for DNA molecules with contour length of 21 μm, 42 μm and 84 μm confined in a slit. (b) Confined chain diffusion coefficient as a function of the confinement $R_{g,\mathrm{bulk}}/H$

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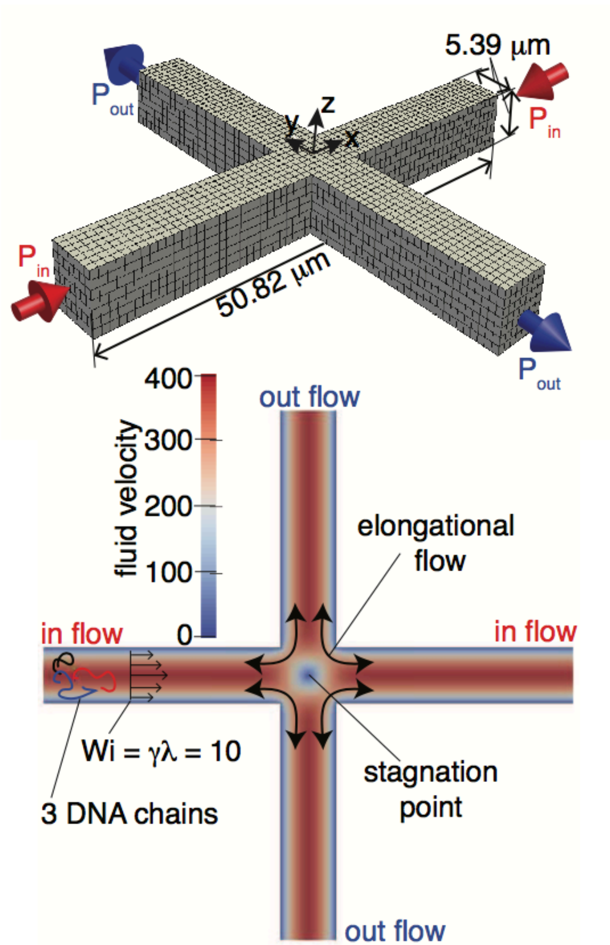
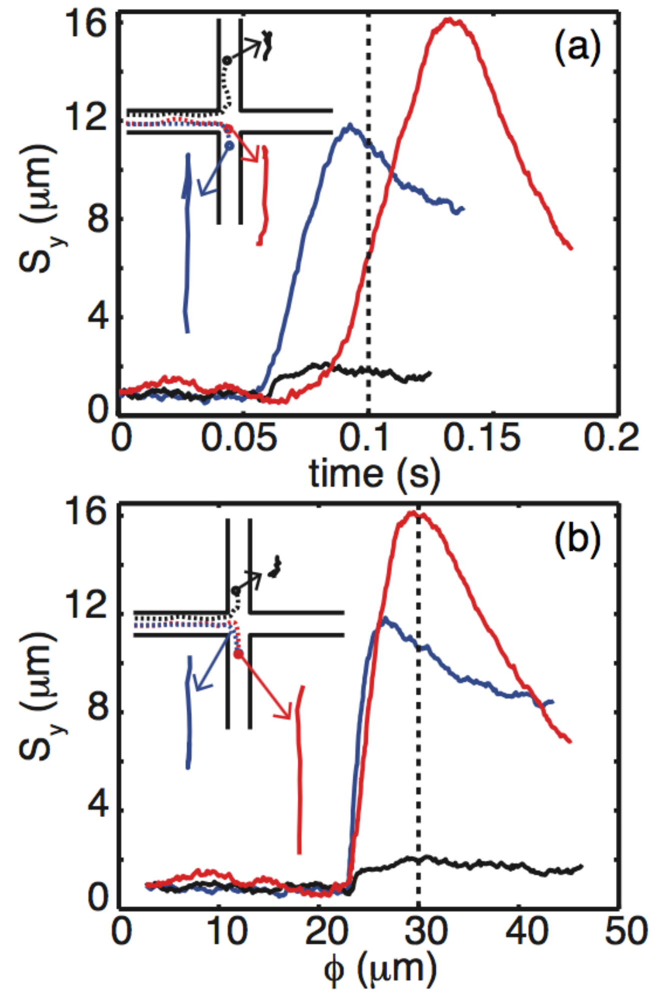
COPSS-Hydrodynamics: complex geometry





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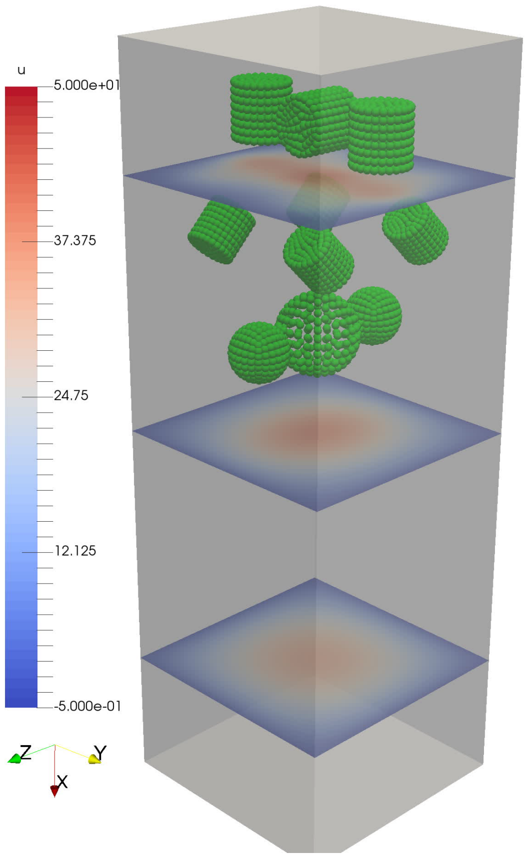
COPSS-Hydrodynamics: rigid particles

Particle sedimentation under gravity within a confined channel. Particle shapes can be arbitrary in COPSS-Hydrodynamics.



- 10 particles with different shapes/sizes
- 2600 tracking points
- P2-P1 mixed element (Hex20)
- 10125 elements
- 145,696 degrees of freedom
- 2580 time steps

Summary:

- COPSS-hydrodynamics relies on Stochastic PDE for trajectory integration.
- Each integration step requires multiple solves of Stokes equation using a parallel O(N) algorithm, **pFE-GgEm.**
- COPSS-Hydrodynamics can work with complex confined geometries.
- COPSS-Hydrodynamics can work with rigid-particles with arbitrary shapes.
- Implement of user-defined features, force fields, geometries, etc., is straight--forward.