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DNS modeling of fluid-particle systems with the Lattice-Boltzmann method

C. Tsigginos

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Manchester UK

ParaSolS

Particulate Solids Simulations

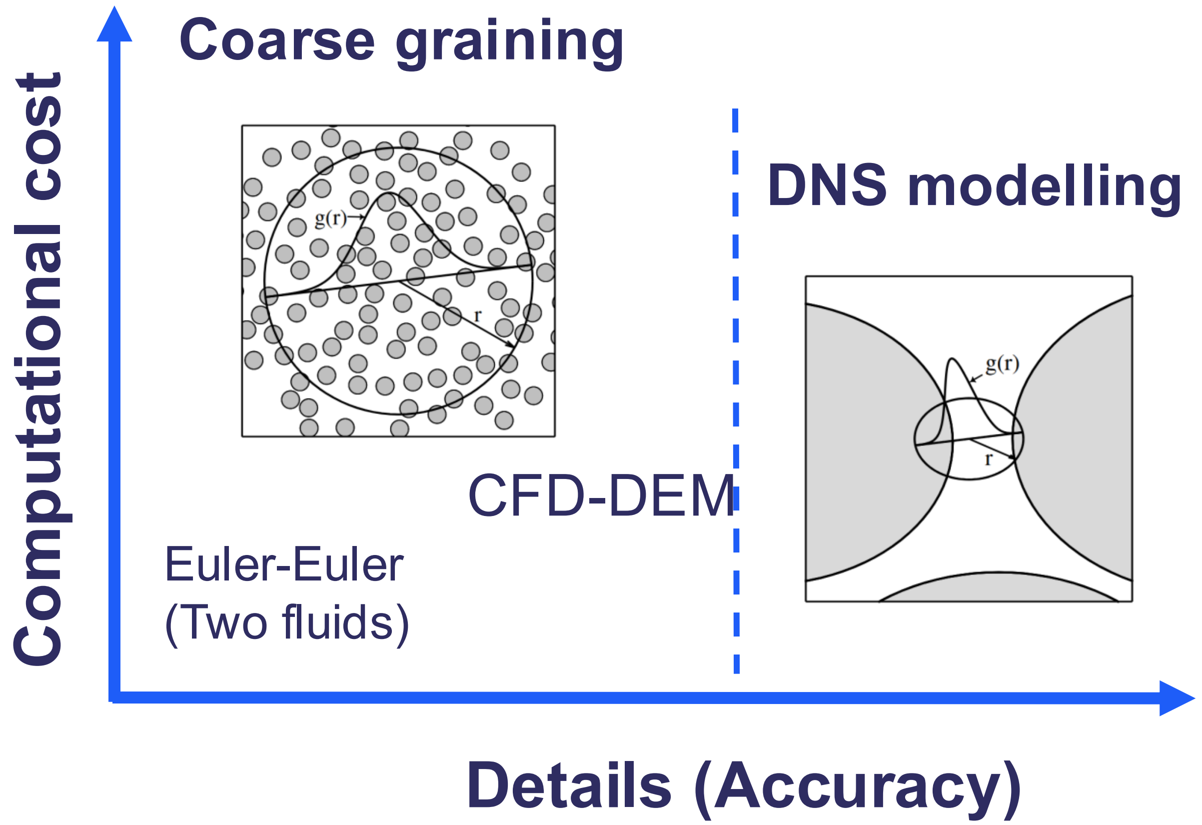
Introduction

Modeling approaches for fluid-particle systems

a) **Euler-Euler approach**
b) **CFD-DEM**
c) **DNS modeling of fluid-particle systems**

Why DNS modeling for fluid-particle systems?

- **No need for functional models to resolve the fluid-particle interactions**
- **Can provide expressions for the hydrodynamic force etc.**



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The Lattice Boltzmann method

The Lattice Boltzmann Method (LBM) in a nutshell

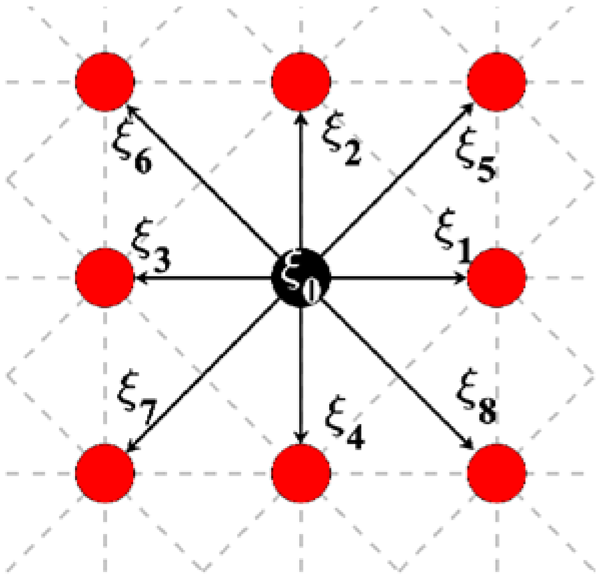
LBM is derived from the celebrated Boltzmann equation

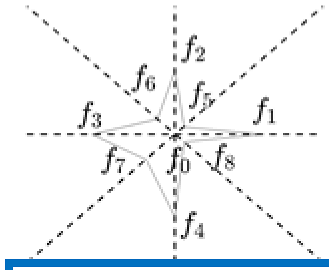
$$\frac{\partial f}{\partial t} + \xi_a \frac{\partial f}{\partial x_a} = Q(f)$$

Q(f): A collision operator

- **Unknowns**: The probable mass at point x with velocity ξ, f(x,ξ,t):
- Macroscopic fields obtained from moments of the distribution function
- LBM exploits a uniform grid

The Lattice Boltzmann method





Calculation (ρ, u)

$$\rho = \sum_i f_i$$

$$\rho u = \sum_i f_i \xi_i$$

$$f_i(x + \xi_i \Delta t, t + \Delta t) = f_i(x,t) - \frac{\Delta t}{\tau}\left(f_i(x,t) - f_i^{eq}(\rho, u)\right)$$

τ linked to the viscosity via a Chapman-Enskog expansion

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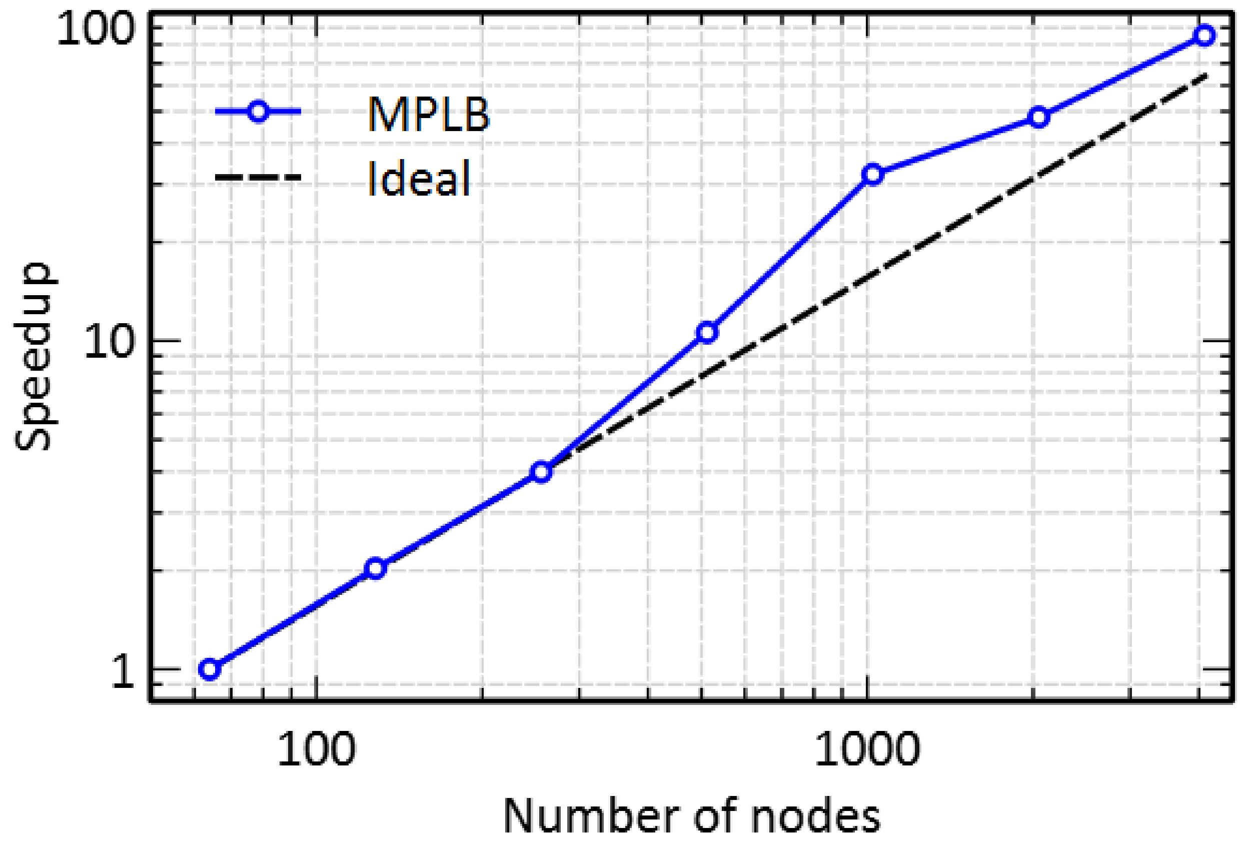
Why Lattice Boltzmann Method (LBM)?

Advantages
- Excellent parallel performance
- Simple evolution equation- No operation gradients
- No Poisson equation !

Disadvantages
- LBM is an explicit scheme -> Not suitable for steady-state problems
- Not intuitive (e.g., Difficulty in developing boundary conditions at the mesoscale)
- Larger memory footprint



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Challenges in coupling the DEM and LBM

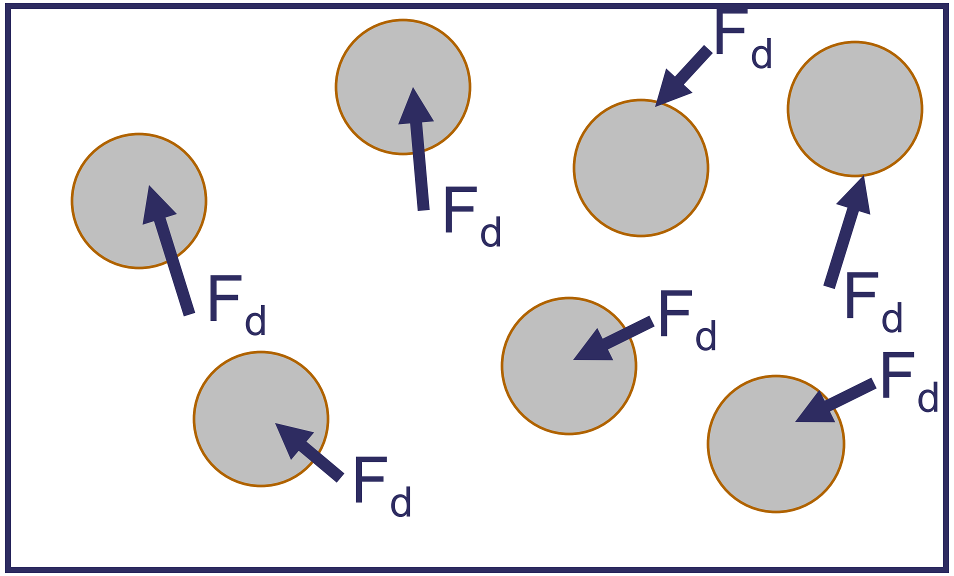
DEM

Challenge 1: Pick the proper model or ...

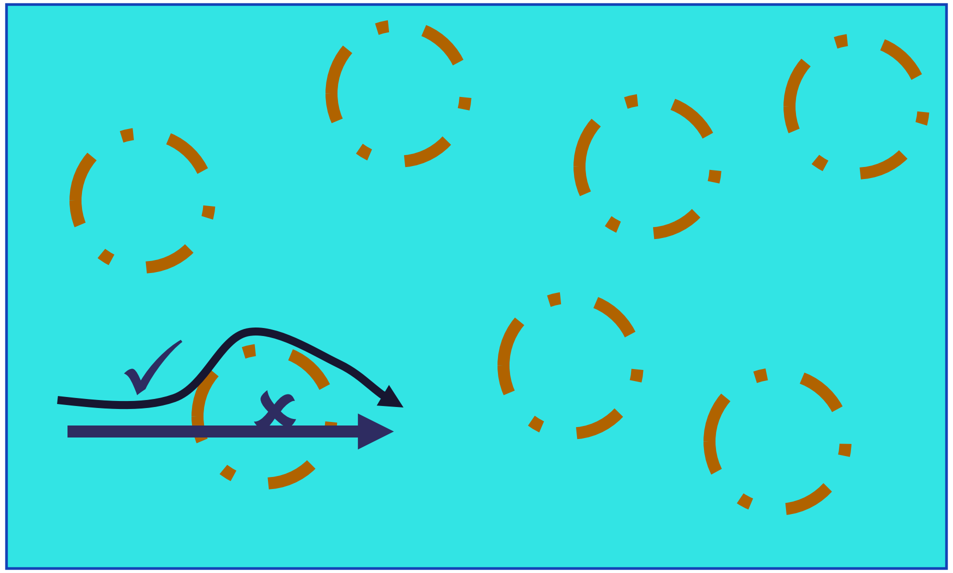
LBM

Update particle motion

Update fluid flow



Challenge 3: Develop an efficient coupling framework



Particle motion

$$m\,\ddot{u}_p = \sum_c f_c + f_b + f_d$$

Challenge 2: Benchmark cases

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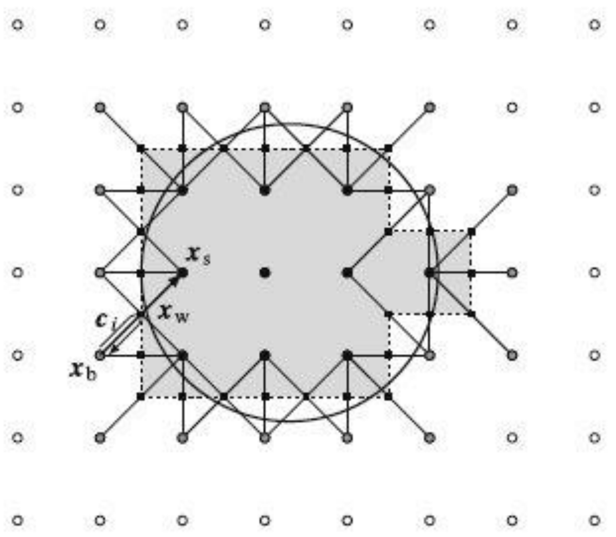
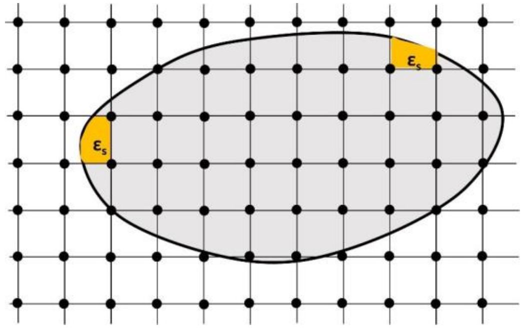
Fluid-particle interaction models

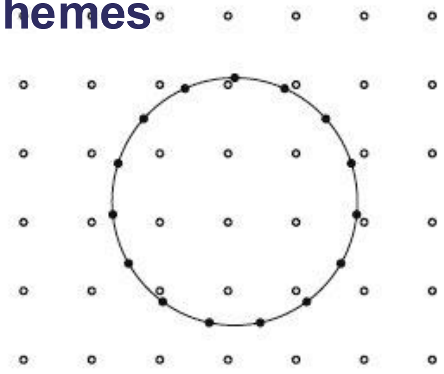
Interaction models for the DNS modeling of fluid-particle systems within the LBM-DEM framework



Bounce back type schemes



Interpolation based schemes

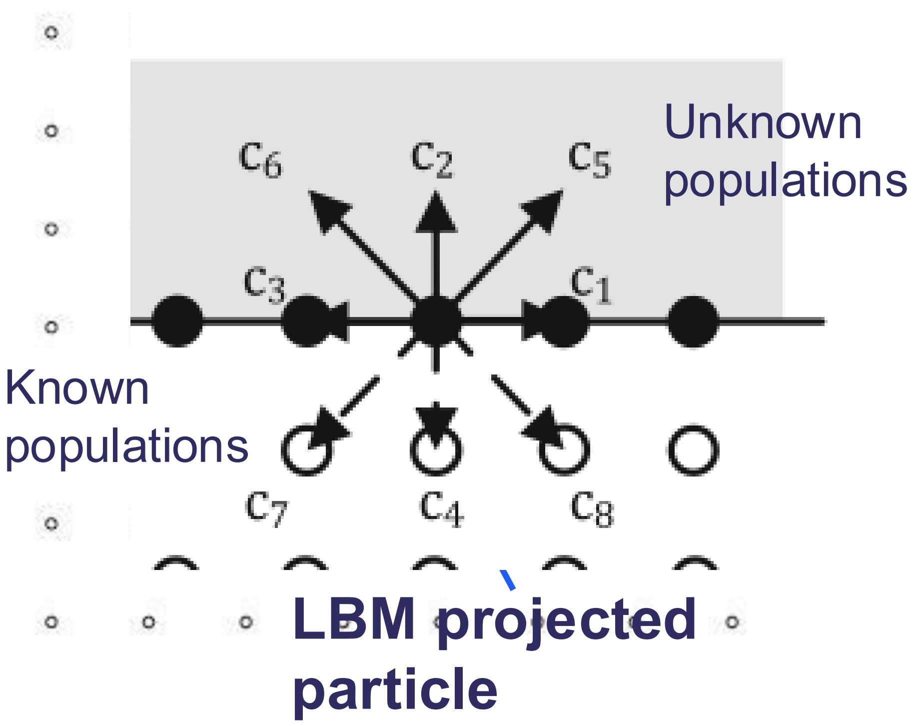


Immersed Boundary method

Three different types of models proposed over the years

Common characteristic:
Particle interior filled with fluid

Bounce-back methods



No-slip condition imposed by the bounce-back scheme

$$\boxed{f_i(\mathbf{x}, \xi_i, t) = f_{\bar{i}}(\mathbf{x}, \xi, t)} \pm \boxed{w_i \rho \frac{u_a^w \xi_{i_a}}{c_s^2}}$$

Bounce back **Velocity correction**

Computational complexities

- Inability to enforce the no-slip as τ increases.
- Particle shape sensitivity-especially for moving particles (Can be alleviated by interpolation based schemes)

Similarity to traditional boundary value problems

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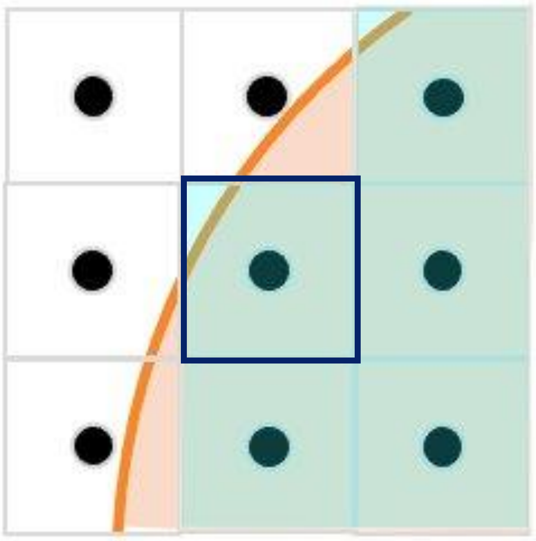
Interpolation based schemes: The PSM case

Computation cell assigned to each node



- Fluid & particles treated as dif. fluids composed by the same molecules (single distribution function)
- Solid fraction used as interpolation parameter
- $\Omega^{s,j}_i$ enforces the particle motion in the space filled by the particle

$$f_i(\mathbf{x} + \xi_i \Delta t) = f_i(\mathbf{x}, t) + \phi\Omega_i^f + \sum_j \varepsilon_j^s \Omega_i^{s,j}$$

Fluid collision operator $\phi\Omega_i^f = -\frac{\phi\beta\Delta t}{\tau + 0.5\Delta t}[f_i - f_i^{eq}(\rho, \mathbf{u}, T)]$

Solid collision operator $\varepsilon_j^s\Omega_i^{s,j} = \varepsilon_j^s a_j \left[f_{\bar{i}} - f_{\bar{i}}^{eq}(\rho, \mathbf{u}, T) + f_i^{eq}(\rho, \mathbf{u}_j^s, T_j^s) - f_i\right]$

Hydro. drag & torque $\mathbf{F}_d^j = -\frac{\Delta x^{nsd}}{\Delta t}\sum_k \varepsilon_{j,k}^s a_{j,k} \sum_i \Omega_i^{s,j}\xi \mathbf{T}_d^j = -\frac{\Delta x^{nsd}}{\Delta t}\sum_k \varepsilon_{j,k}^s a_{j,k} (\mathbf{x}_k - \mathbf{x}_p) \times \sum_i \Omega_i^{s,j}\xi_i$

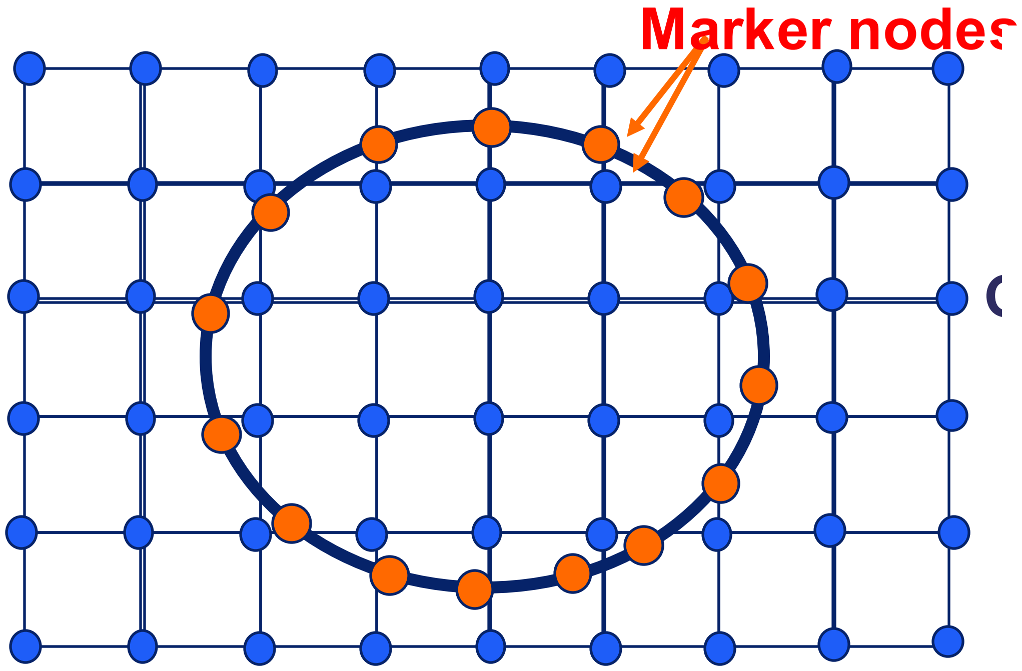
Advantages

- Easy to implement (Local operations)

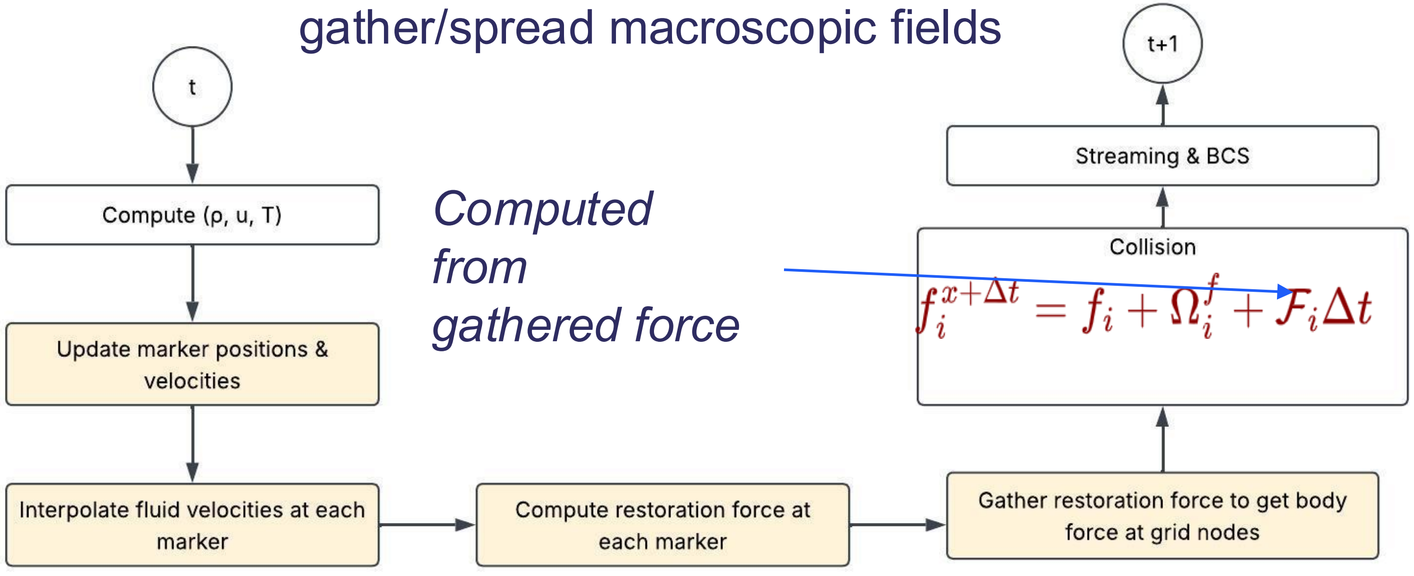
Disadvantages

- Sensitivity to correction factors and solid fraction calculations
- 1st order scheme

The immersed boundary method



g(r): Interpolation function to gather/spread macroscopic fields



Computed from gathered force

$$\mathbf{u}^f = \sum_m \mathbf{u}_m g(\mathbf{r}) \Delta x_s$$

$$f_d = \rho \frac{u_f - u_s}{\Delta t}$$

- **Fluid-particle interface treated as a collection of markers**
- **No slip condition imposed by the so-called restoration force**

Advantages

- Easy to extent to complex geometries & different boundary conditions

Disadvantages

- Complex extension to parallel universe
- Difficulties in modeling dense-fluid particle systems

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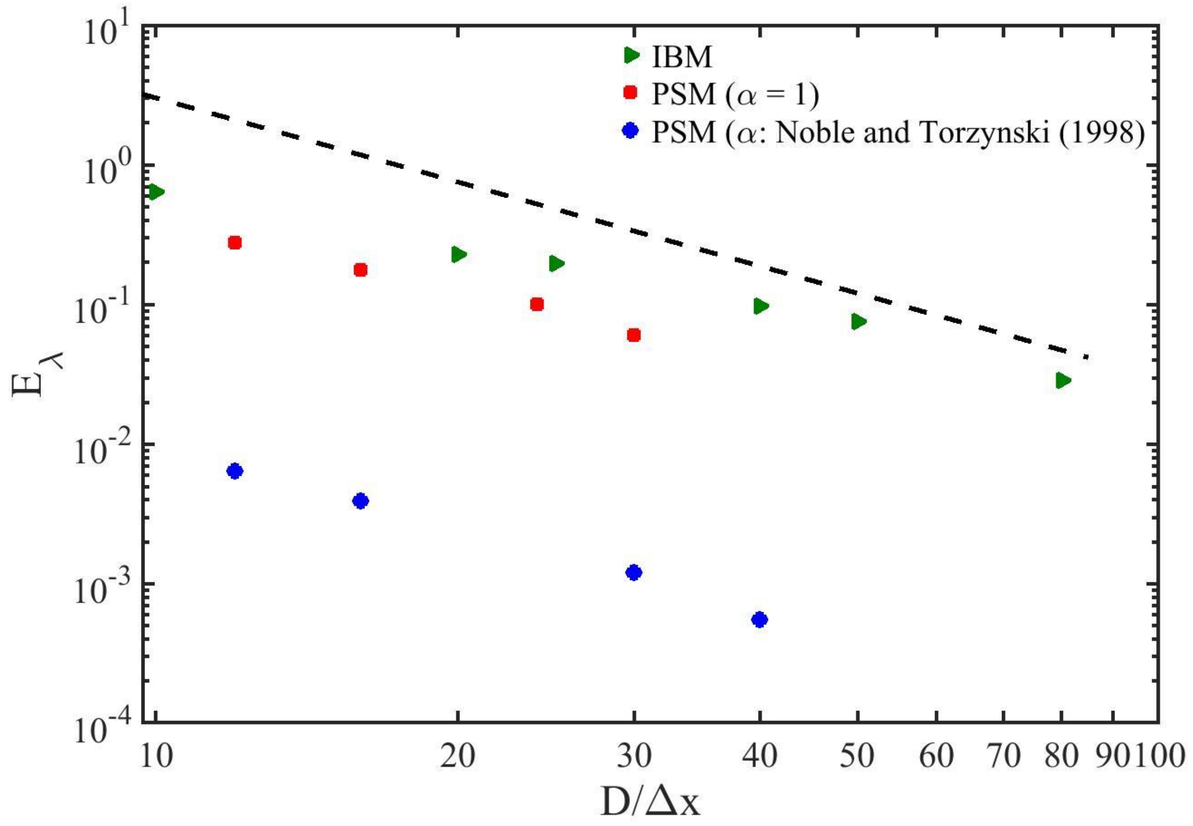
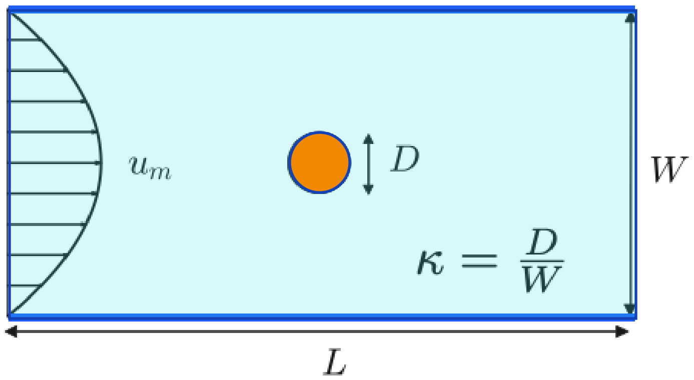
Benchmark cases for model validation

Benchmark Case I: Stationary cylinders





Wall correction factor $\lambda = \frac{F_h}{\mu u_m} = \frac{4\pi}{h_1(k)+g_{1(k)}}$ [1]

- For Stokesian flows, an analytical solution exists[1]
- PSM performs better than IBM due to better assumptions
- N&T coefficient (αj) allows a quite accurate approximation of fluid and solid collision operators

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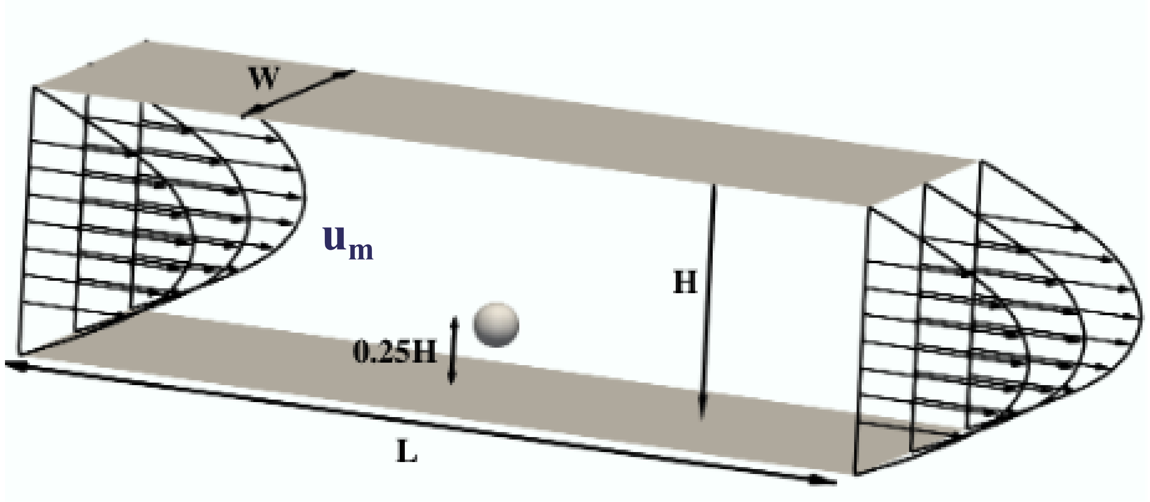
[1] Faxen, O.H “Forces exerted on a rigid cylinder in a viscous fluid between two parallel fixed planes”, Proc. Royal Swedish Acad. Eng. Science 187 (1946), 1-13.

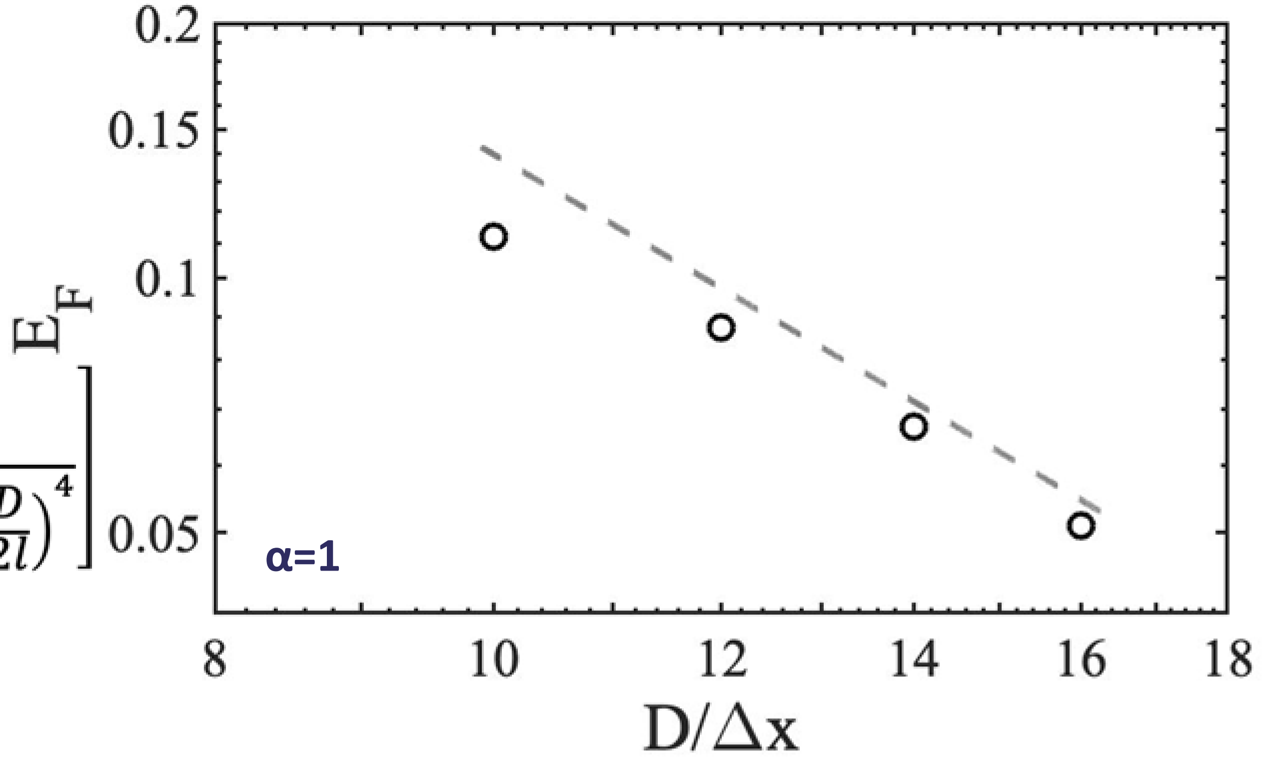
Benchmark Case II: A stationary sphere in Poiseuille flow



H = 8D	W = 30 D	L = 60D
$\nu = 0.001\ c_s\ D$	$u_m = 10^{-7}\ c_s$	

Comparison of the numerical F_d with the analytical solution[1]

$$F_d = 3\pi\rho\nu U_l\left[\frac{1-\frac{1}{9}\left(\frac{D}{2l}\right)^2}{1-0.6526\left(\frac{D}{2l}\right)+0.316\left(\frac{D}{2l}\right)^3-0.242\left(\frac{D}{2l}\right)^4}\right]$$



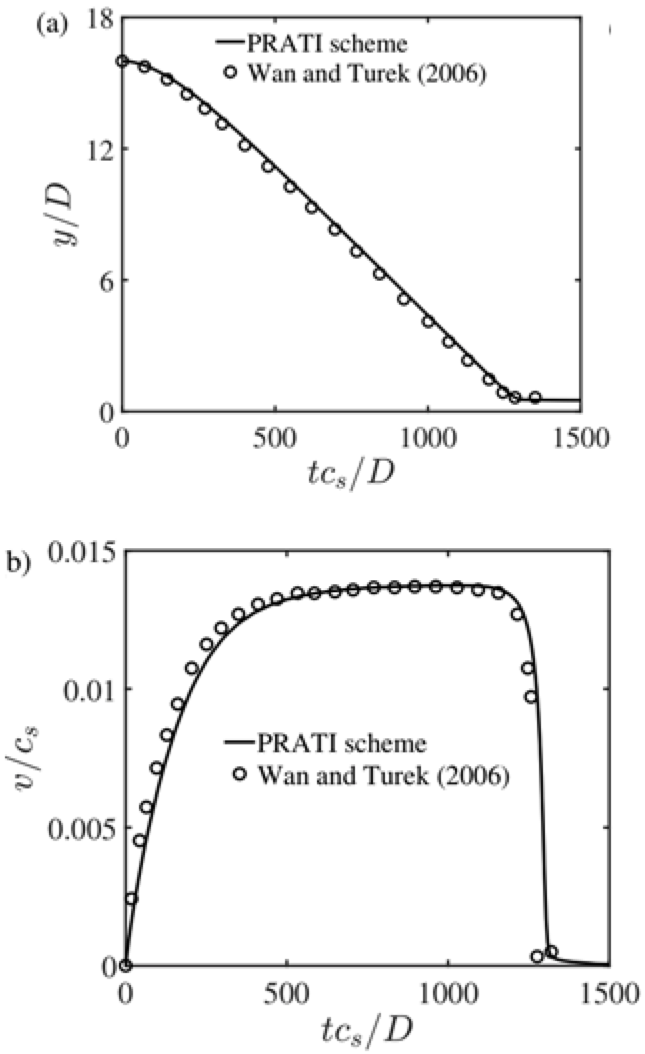
PSM convergence rate close to the theoretical convergence rate of the LBM

[1]Happel, H. Brenner, Low Reynolds number hydrodynamics: with special applications to particulate media, Springer Science & Business Media, 2012

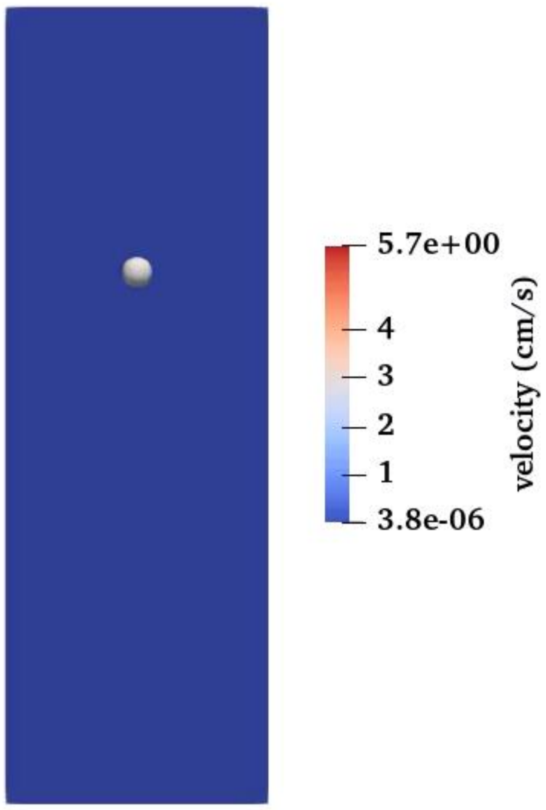
Benchmark Case III: Cylinder settling in a 2D channel

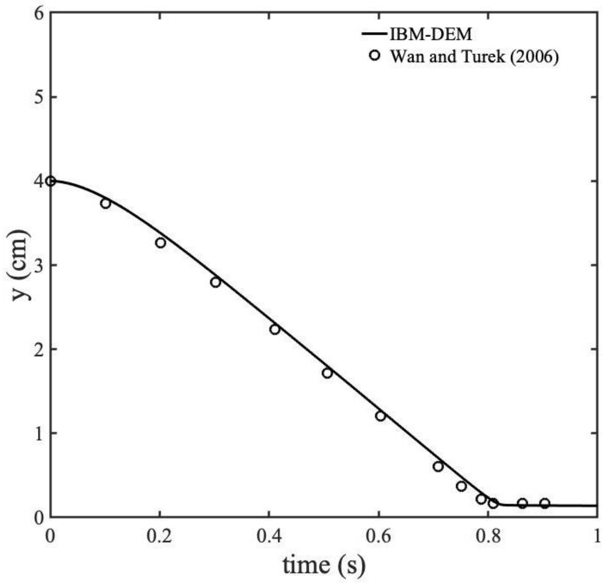
PSM

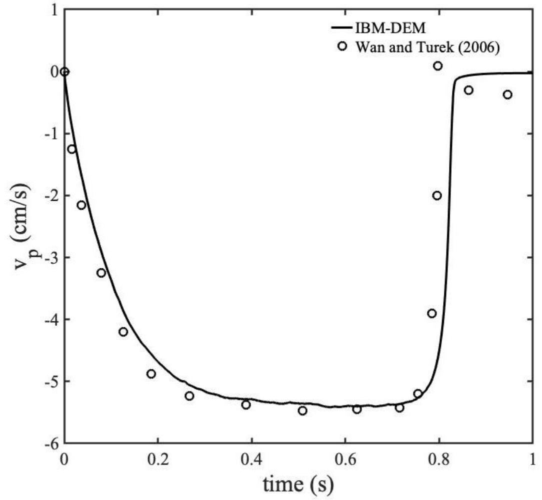
Simulation details
ρ_s= 1.25 g/cm^3
ρ = 1 g/cm^3
ν = 0.1 cm^2/s
D/Δx = 30



IBM







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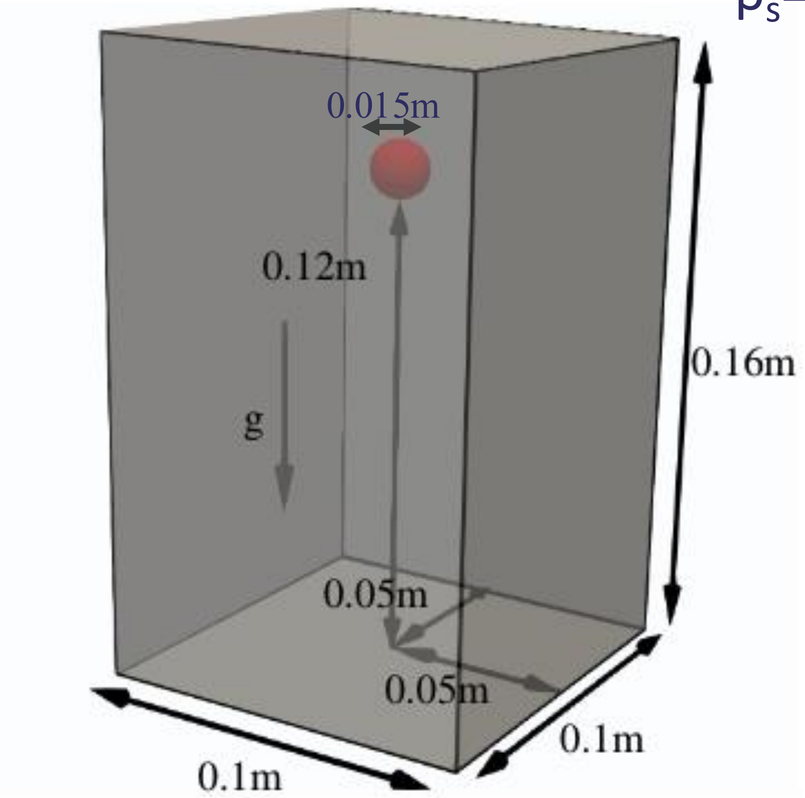
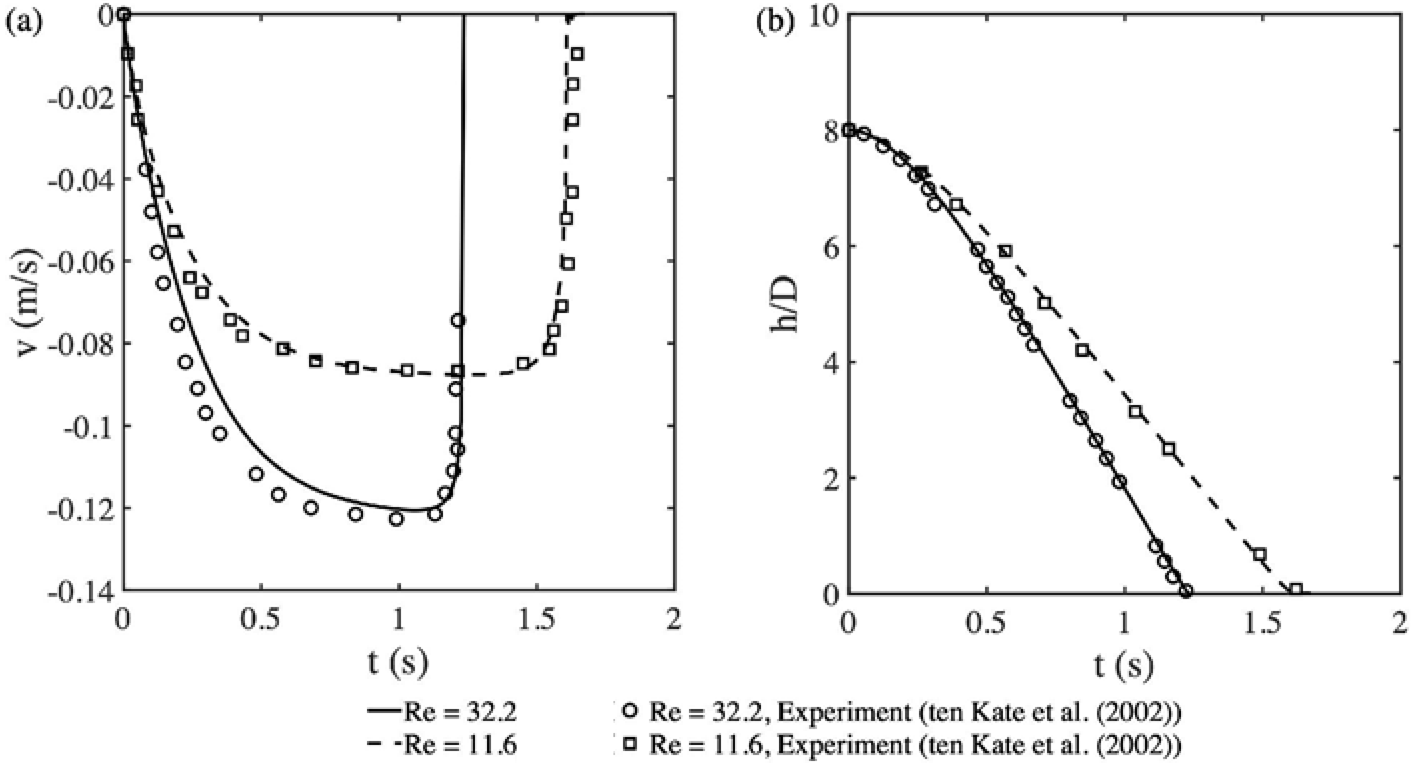
Benchmark Case IV: A sphere settling in a 3-D box

ρ_s=1120 kg/m^3



Re	ρ_f (kg/m^3)	μ_f (10^{-3} N s/m^2)	τ/Δt
11.6	962	113	0.8
32.2	960	58	0.65



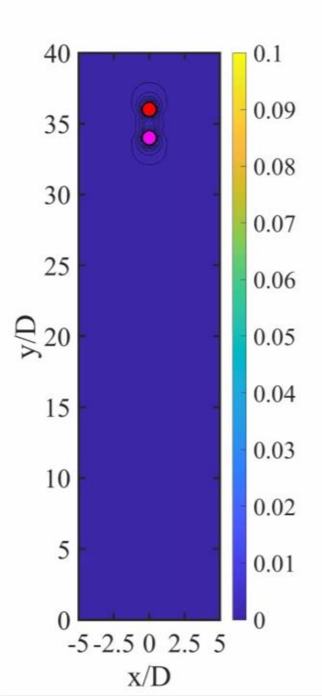
PSM predictions agree well with the experimental results of Ten Kate et al.[1]

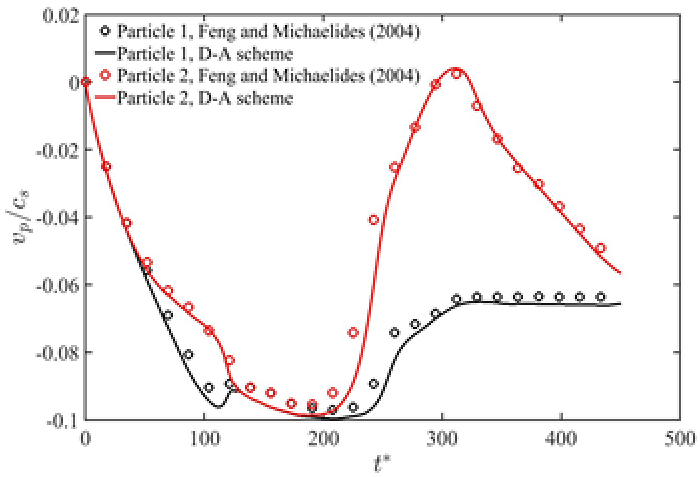
[1]A. Ten Cate, C. Nieuwstad, J. Derksen, H. Van den Akker, Particle imaging velocimetry experiments and lattice-Boltzmann simulations on a single sphere settling under gravity, Phys. Fluids 14 (2002) 4012–4025.

Benchmark Case V: Cylinders settling in a 2D channel

Particle 1, Feng and Michaelides (2004)
Particle 1, PRATI
Particle 2, Feng and Michaelides (2004)
Particle 2, PRATI

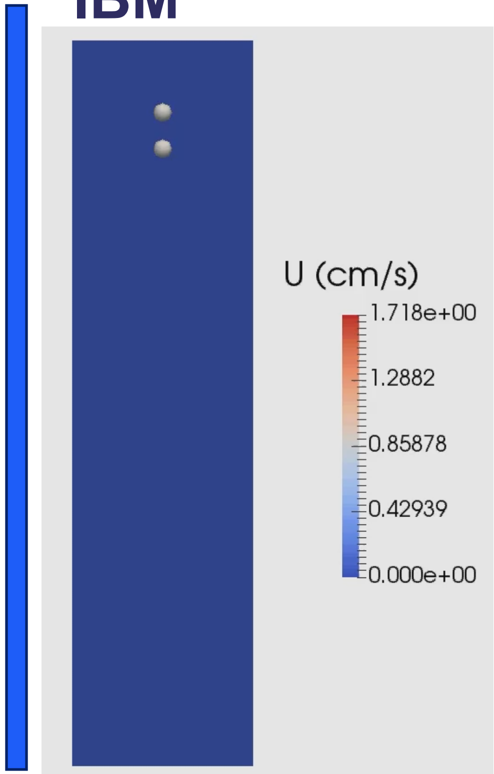
PSM

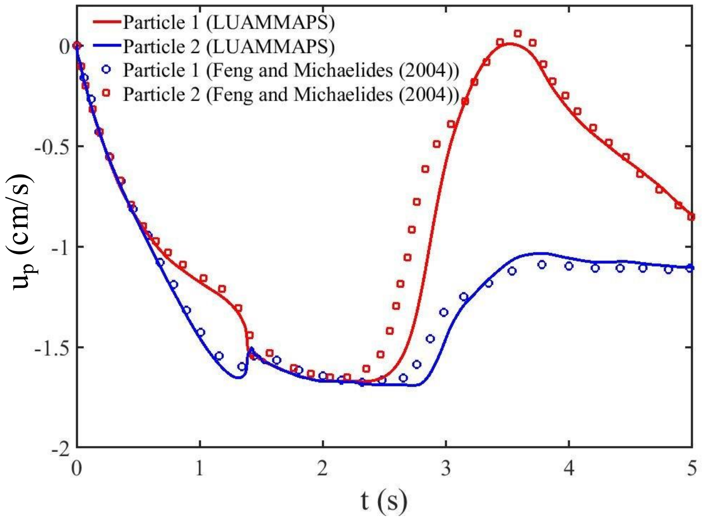




- $\rho_1 = \rho_2 = 1.01\ \rho$
- $D/\Delta x = 30$

IBM





Observed differences after kissing stage attributed to contact model

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Z.-G. Feng, E. E. Michaelides, The immersed boundary-lattice Boltzmann method for solving fluid–particles interaction problems, J. of Comput. Phys.195 (2) (2004) 602–628.

Conclusions

- LBM is a good candidate for DNS modeling of fluid-particle systems
- Three different families of fluid-particle models
- LBM-DEM frameworks provide good parallel performance
- Method expensive for 3D simulations
- Unable to capture lubrication phenomena w/o grid refinement

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Thank you

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