Immersed Boundary methods for DNS of gas-solid flows

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Training School "*Behaviour of Non-Spherical Particles in Flows*"
COST FP1005

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Outline

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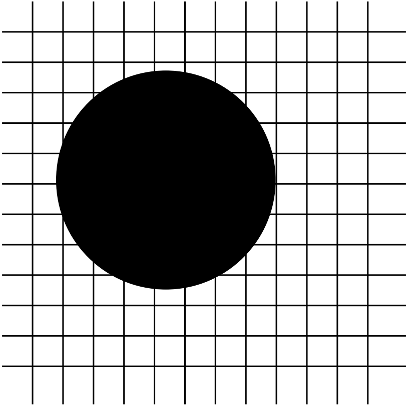

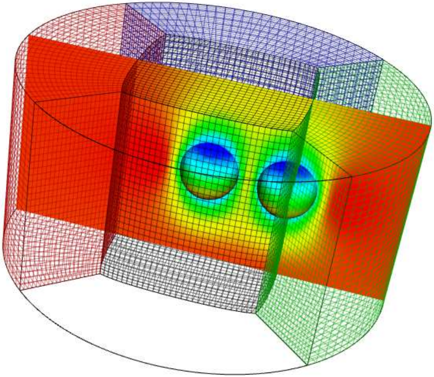

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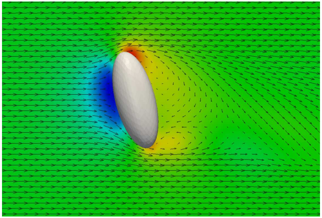
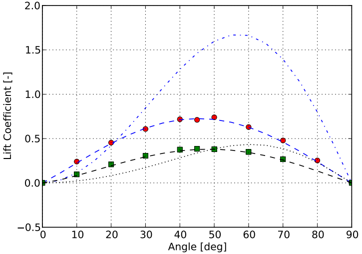
- Accurate flow solution
- Physical insight
  - Flow transition
  - Vortex structures
  - Accurate forces
- Too detailed to be "practical"
  - Can be used to derive engineering models for large scale simulations





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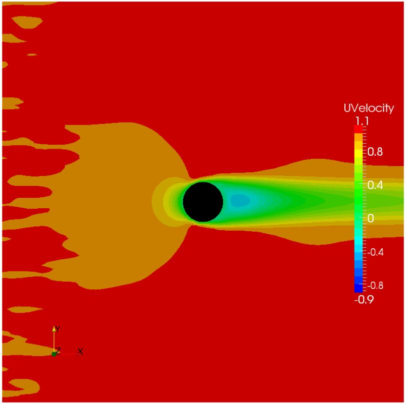
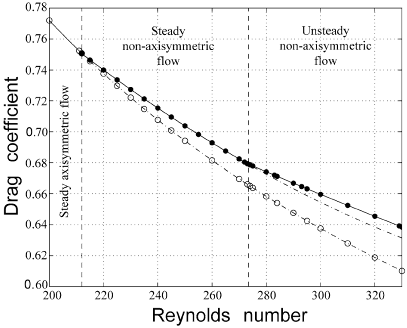
"TRUE" DNS METHODS





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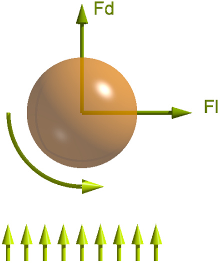
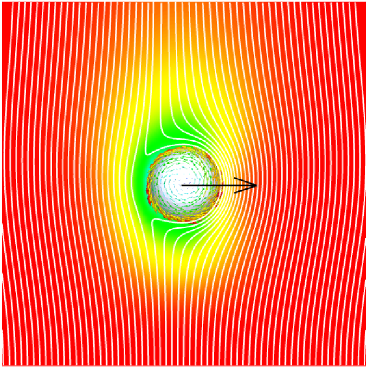
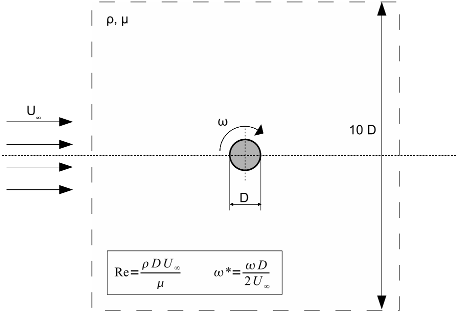
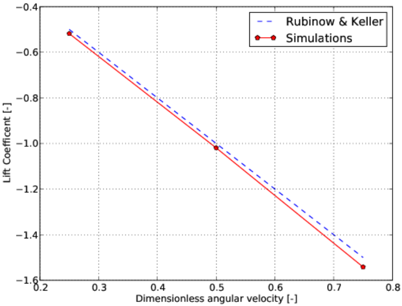
Velocity Field and Streamlines



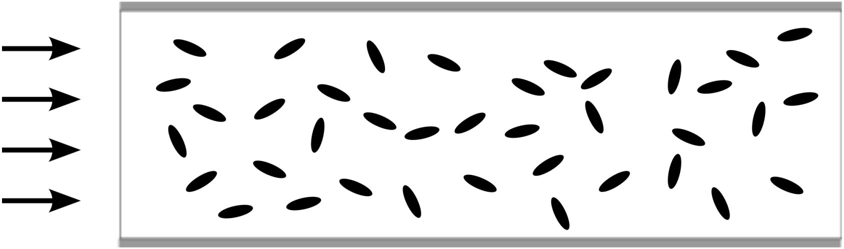






$Re_D < 1$, Rubinow & Keller (1961)

Example application - channel flow with particles



- Channel flow with non-spherical particles ($Re = 42'000$)
- Use DNS to model the forces on particles: $F_P = f(Re, \varphi)$
- Solve the problem using LES and point-particle approach

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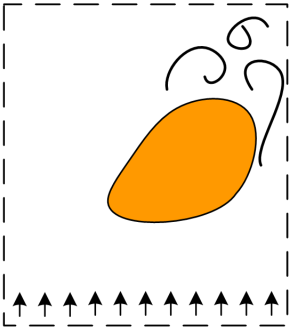
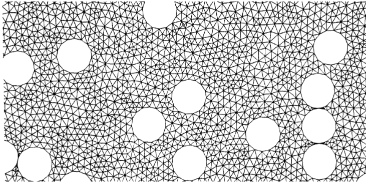


Strategies:

- Body fitting meshes (ALE formulation)
  - Particles are meshed
  - Accurate but expensive
  - Re-meshing required
  - Good when little movement is required.
- Alternative methods
  - Immersed Boundary
  - Cartesian Grid
  - Fictitious Domain
  - Lattice Boltzmann

Arbitrary Lagrangian Eulerian (ALE)



Hu (1996)

- The Lagrangian particles are meshed.
- Very accurate.
- Very expensive, difficult to have accurate interpolation.
- Remeshing required.
- Good for problems where little movement is required.

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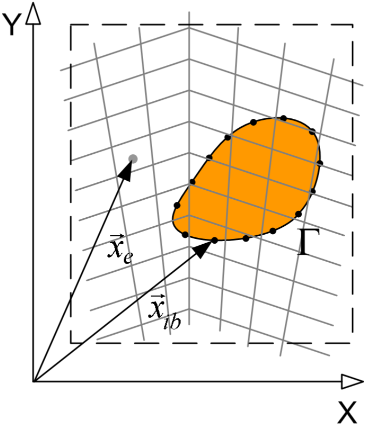

- Fluid domain is represented by an Eulerian grid
- A Lagrangian grid represents the solid-fluid interface
- Presented approach:
  - No-slip velocity boundary condition on the surface
  - Zero gradient pressure boundary condition on the surface
  - Force calculated from the resolved flow field

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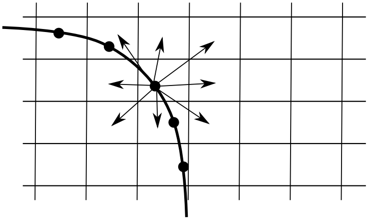
Distributed Immersed Boundary Method



- “Classic” IBM methods are distributed.
- A force is determined in the Lagrangian control points, so the fluid velocity matches the control point velocity.
- This force is distributed along the Eulerian neighbours of the control point.

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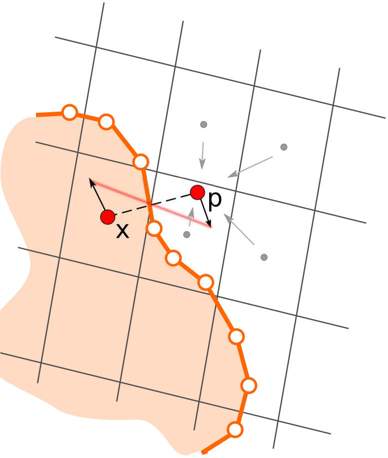

Mark and van Wachem, JCP 207, 2008

- Project (x) into the fluid domain to create p
- Internal point velocity is set to satisfy the no-slip boundary condition at the surface

$$u^i_{IB} = \frac{1}{2}\left(u^i_{IN} + \sum \beta_m u^i_m\right)$$

- Internal point pressure is set to obtain zero pressure gradient at the surface

$$\left(p^i_{IN} - \sum \beta_m p^i_m\right) = 0$$

- Coefficients β_m from geometric interpolation function.

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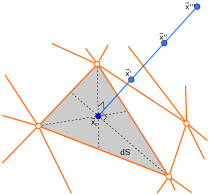
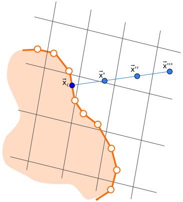
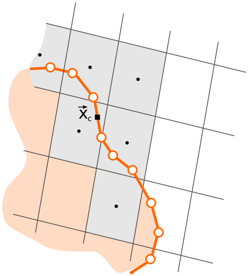
Force calculation







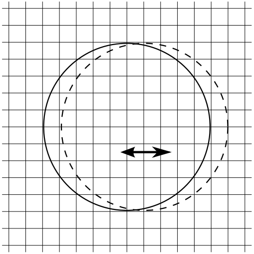
Force obtained from the resolved flow field:

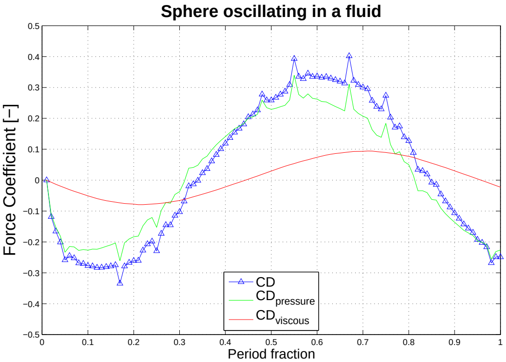
$$F_i = \int_{IB} \left(-p\delta_{ij} - \mu \left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right] \right) n_j dS$$

- Pressure:
  Quadratic extrapolation from auxiliary points
- Viscous Terms:
  Velocity gradients from least square fit of Taylor series

- Spurious pressure oscillation in simulations of moving bodies

$\Delta x/D = 0.1,$
$\Delta t/T = 0.01$





Oscillation scaling

$$2D \approx \frac{(\Delta x)^2}{(\Delta t)} \qquad 3D \approx \frac{(\Delta x)^3}{(\Delta t)}$$

SOURCE OF THE PRESSURE OSCILLATIONS - *Mittal, 2011*

MASS CONSERVATION LAW FOR IB SIMULATIONS

$$-\frac{\Delta V_{IB}}{\Delta t} + \int_{\sigma_{cv}} \vec{U}_f \cdot \vec{n} dA = \frac{\Delta V}{\Delta t}(q^{n+1} - q^n) + S_\sigma$$

$\frac{\Delta V}{\Delta t}(q^{n+1} - q^n)$ - changes in fluid volume around IB
q^n - total number of solid cells at time n
ΔV - cell volume
S_σ - "transpiration" error

- *RHS* represents the error in mass conservation
- Sudden changes in fluid volume around the body
- Experience high discontinuous variation in time

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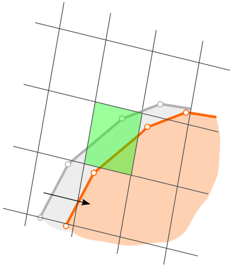
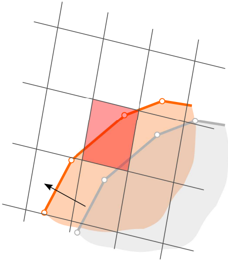
- Cells changing their behaviour:



fresh cells



dead cells

- Associated issues:
  - The “old” velocities and pressures in *fresh* and *dead* cells are not correct
  - Mass source error
  - Mirrored point change

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Proposed Improvements

- *Fresh/dead* cell velocity and pressure interpolation
- Improving the mirroring interpolation
- Continuity equation modifications
  - Find the accurate cell areas and triangles in cells
  - Solve the continuity equation for the mirrored cells
  - Merge the mirrored cells with neighbouring fluid cells

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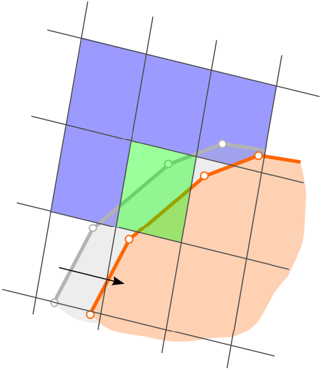
1. Interpolate **velocity** to *fresh* cells from surrounding fluid cells
2. Interpolate **pressure** to *fresh* cells from surrounding fluid cells
3. Use the flow velocity and mirroring principle to estimate the velocity and pressure of mirrored points
4. Re-calculate the explicit mass flux in the vicinity of the body



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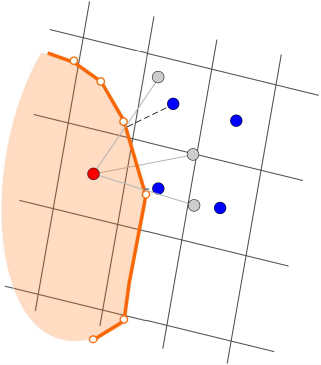
Mirroring interpolation coefficients

- Use multiple surface points for setting the boundary condition
- Calculate weighted average of the coefficients
- Cells close to the surface are more important (large ϕ_k)



Improved mirroring principle

$$\sum \phi_k u^i_{IB} = \sum \frac{1}{2} \phi_k \left(u^i_{IN} + \sum \beta_{m,k} u^i_m \right)$$

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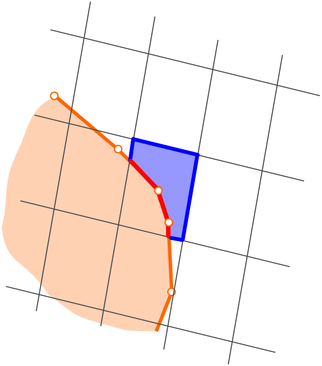
Continuity equation modifications

- Cut the fluid cells with the IB to get accurate flow areas and cell volumes
- Possible strategies:
  - Merge the mirrored cells with flow cells
  - Solve the continuity equation for mirrored cells

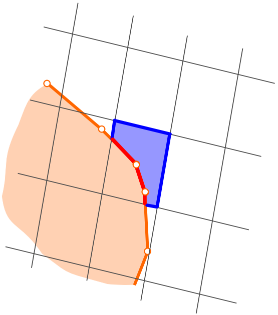


Gradient interpolation in cut cells

$$\frac{\delta\phi}{\delta x^i} = \sum\left(\phi_f a_f^{*i} + \phi_{IB}^i a_{IB}^{*i}\right)$$

SOLVE CONTINUITY IN MIRRORED CELLS

- Solve the continuity equation in mirrored cells
- Reduces mass error
- Flow between mirror cells needs special treatment
- Small cells may be inaccurate

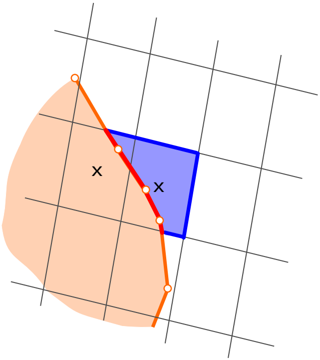


CONTINUITY EQUATION

$$\sum u_f^i a_f^{*i} + \sum u_{IB}^i a_{IB}^{*i} = \sum \left\langle \bar{u}_f^i + \hat{d}_f^{u^i} \left(\widetilde{\left[\frac{\delta p}{\delta x^i}\right]}_f - \overline{\left[\frac{\delta p}{\delta x^i}\right]}_f \right) \right\rangle + \sum u_{IB}^i a_{IB}^{*i} = 0$$

CELL MERGING

- Merge to fluid cell with largest flow area
- Find the interpolation coefficients for the continuity in mirrored cell
- Add the contribution of the body motion
- Input the coefficients to the continuity equation for merged cell



CONTINUITY EQUATION FOR MERGED CELL

$$\left(\sum u_f^i a_f^{*i} + \sum u_{IB}^i a_{IB}^{*i}\right)_{fluid} + \left(\sum u_f^i a_f^{*i} + \sum u_{IB}^i a_{IB}^{*i}\right)_{mirrored} = 0$$

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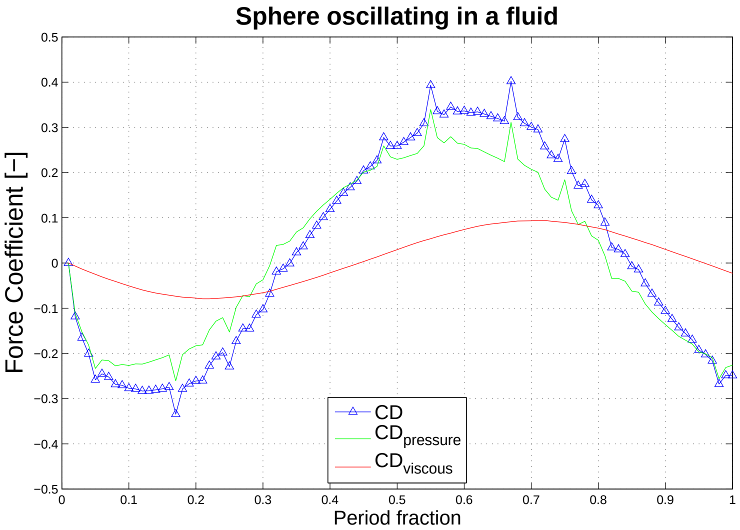
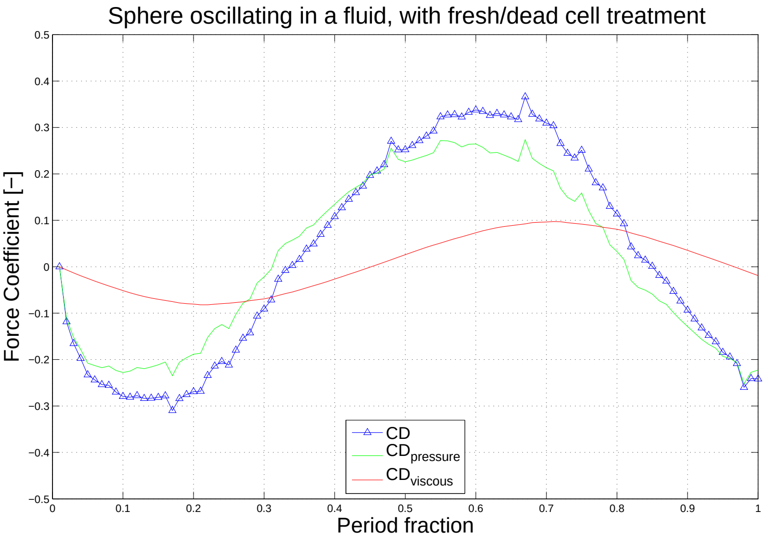
Oscillating sphere original approach



Oscillating sphere with fresh/dead cell treatment



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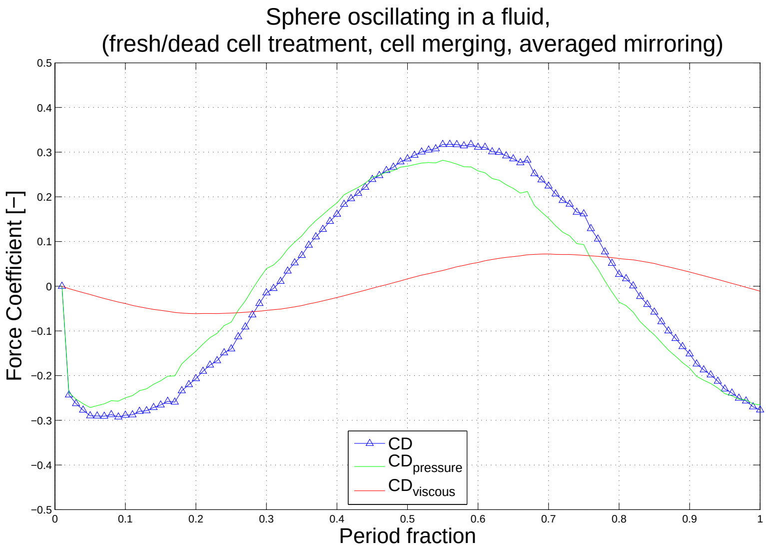
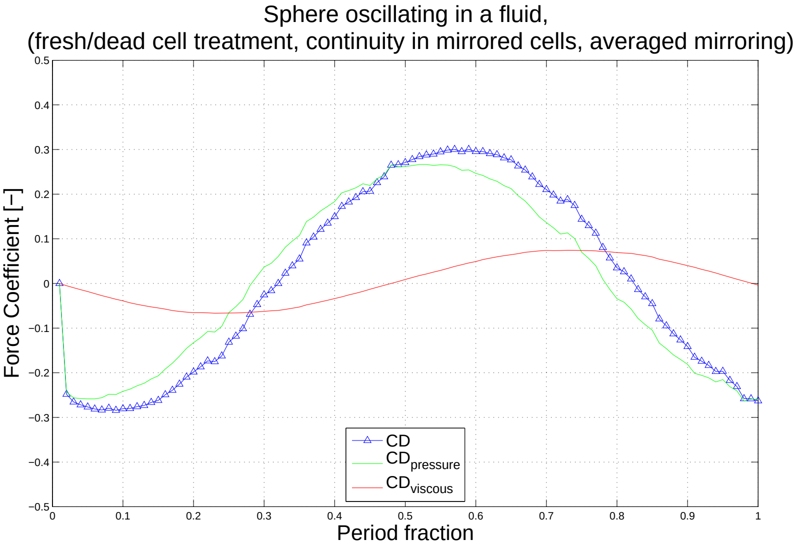
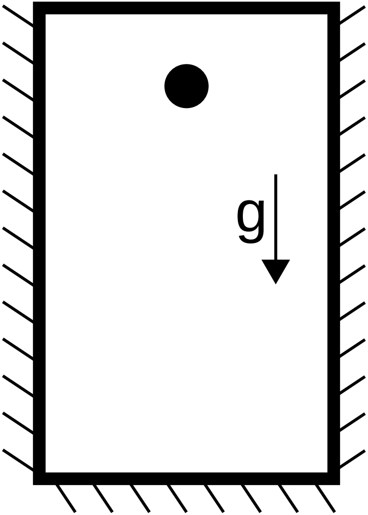

Sphere oscillating in a fluid,
(fresh/dead cell treatment, cell merging, averaged mirroring)
Force Coefficient [−]
Period fraction
0.5
0.4
0.3
0.2
0.1
0
−0.1
−0.2
−0.3
−0.4
−0.5
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
CD
CDpressure
CDviscous

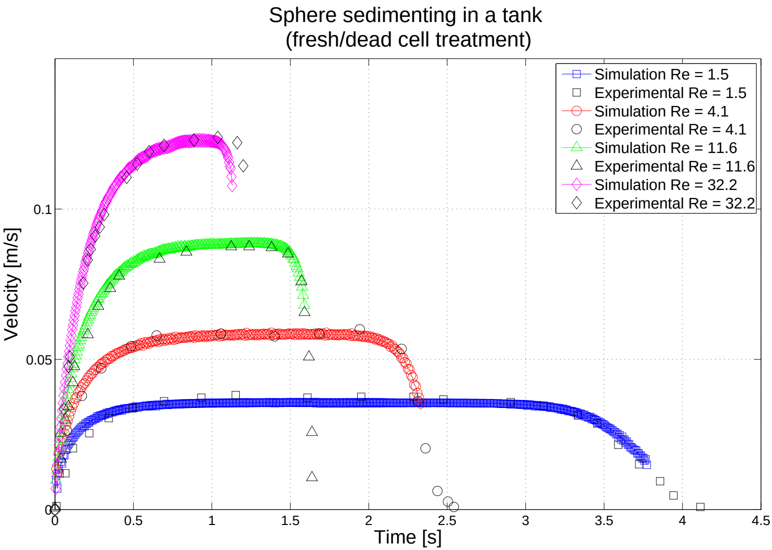
CONTINUITY IN MIRRORED CELLS



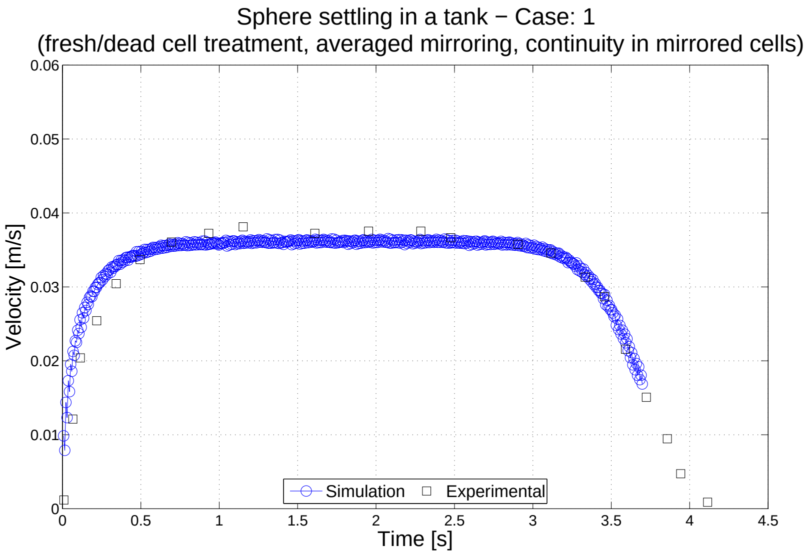
- Experimental setup: *Ten Cate, 2002*
- $D/\Delta x = 8$
- 4 cases considered (adjustment of fluid density and viscosity):

Case	u_t	Re_T
1	0.038	1.5
2	0.060	4.1
3	0.091	11.6
4	0.128	31.9

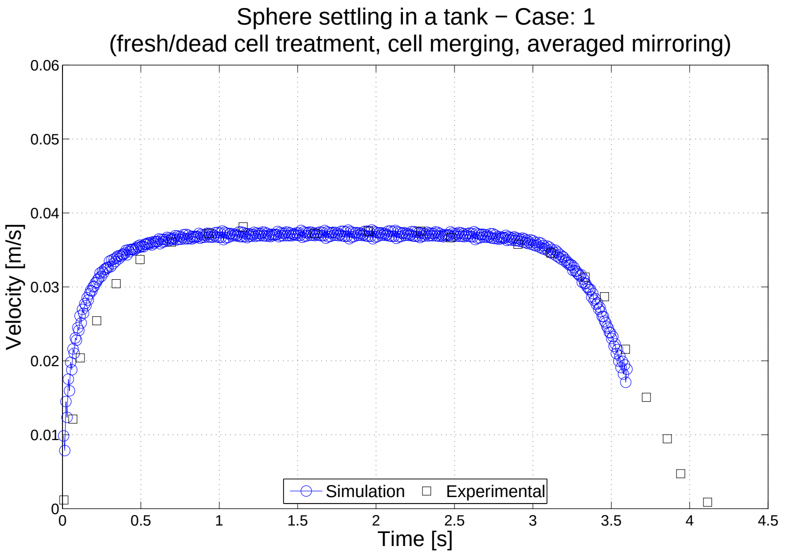



Sphere sedimenting in a tank
(fresh/dead cell treatment)
Simulation Re = 1.5
Experimental Re = 1.5
Simulation Re = 4.1
Experimental Re = 4.1
Simulation Re = 11.6
Experimental Re = 11.6
Simulation Re = 32.2
Experimental Re = 32.2
Velocity [m/s]
0.1
0.05
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
Time [s]

Continuity in mirrored cells



Cell merging



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Improvements to standard IBM methods

- Decreasing the oscillations:
  - Interpolation of flow between mirrored cells
  - Fresh/dead cell treatment
  - Mirroring technique
- Functionality of the method:
  - Force calculation improvement
  - Multiple particles
  - Particle-wall, particle-particle collisions

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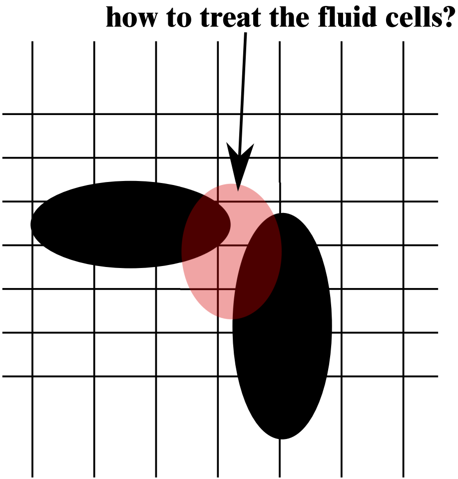
Multiple particles

When 2 particles come close there are complications:

1. The fluid between the particles cannot be resolved.
2. The force from the fluid on the particles cannot be resolved.
3. The particles may collide.



Particle collisions

Difficulty to describe collisions of particles with arbitrary shape:

- No canonical centre or contact direction.
- May have multiple contact areas.
- May be that a single contact point does not describe the contact, for example can have no net force, but a torque.
- During contact, the particle no longer has a closed surface with the fluid.

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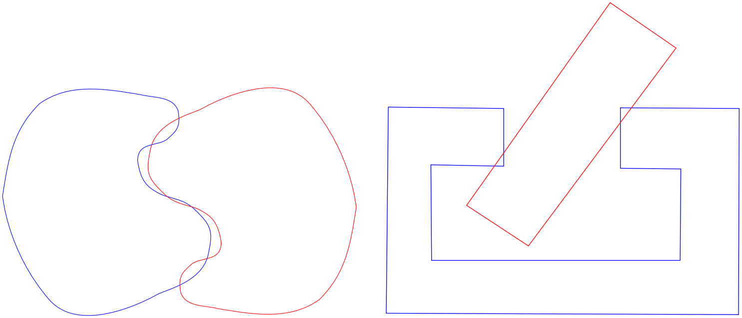
PARTICLE COLLISIONS



(a) No obvious contact position and direction

(b) Mutiple contact patches cannot be seen as one

FIGURE : Two dimensional represention of contacts that have not got a simple parameterisation

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Proposed Discretisation Scheme

- Breakdown overlap of particles into simple pieces
- Each piece bounded by only two triangles (one from each body)
- Each piece easily parameterised
    - Total volume
    - Centre of volume
    - Contact area
    - Contact direction
    - Effective curvature
- Easy to recombine to produce complex contact behaviour
- Closed surface for pressure re-obtained by using an additional internal pressure, calculated by smoothing the external pressure.

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Discretisation scheme continued

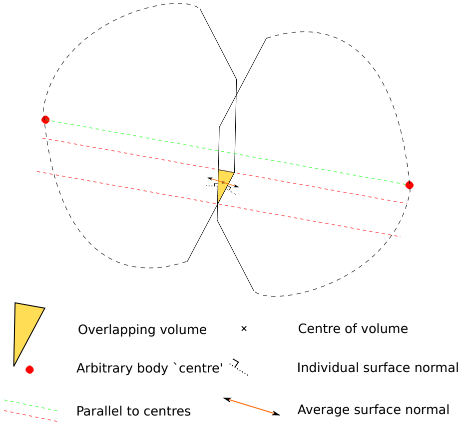

Figure : Decomposing of contact overlap into sections bounded by only two triangles

The curvature for each triangle is calculated in a Lagrangian framework:

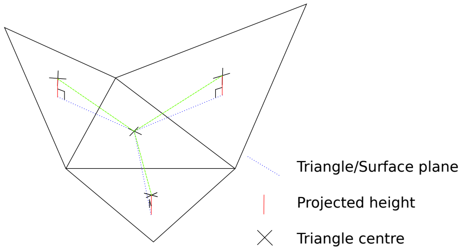

FIGURE : Decomposing of neighbouring triangle cell centres in in and out of plane components, in order to estimate curvature.

Curvature estimation continued

Curvature is fitted by comparing the in-triangle plane and out-of-plane components of the relative position of adjacent triangles. The in-triangle plane can be considered as is or fitted to account for skewness in the surrounding triangles.

And overall 'effective' curvature ($C_{\text{effective}}$) for the contact volume is considered by combining the curvatures of the two triangles that make it (C_A and C_B). This is done in the usual way.

$$C_{\text{effective}} = \frac{1}{\frac{1}{C_A} + \frac{1}{C_B}} \tag{1}$$

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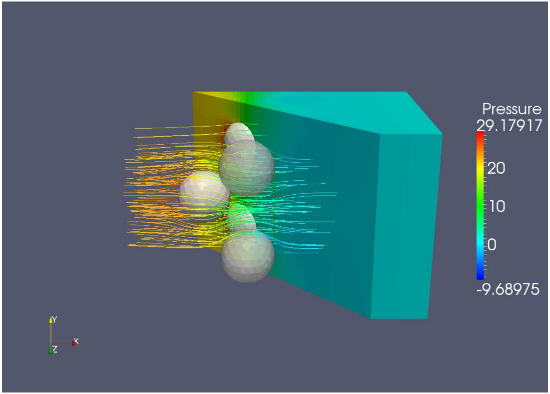

FIGURE : Flow past an array of 5 spheres

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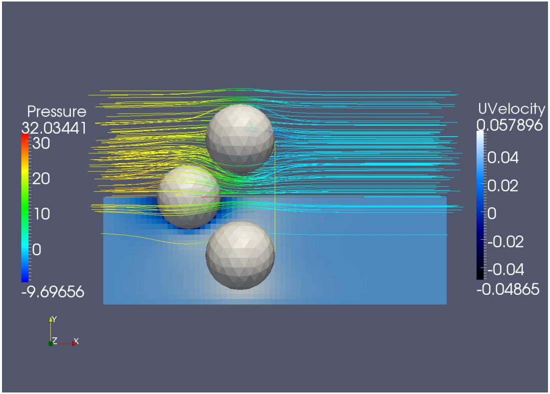
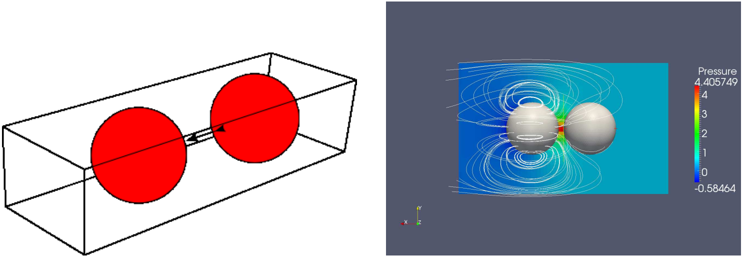


FIGURE : Flow past an array of 5 spheres



(a) Setup (b) Flow around particles

FIGURE : Setup and flow field used to determine the lubrication force between two particles

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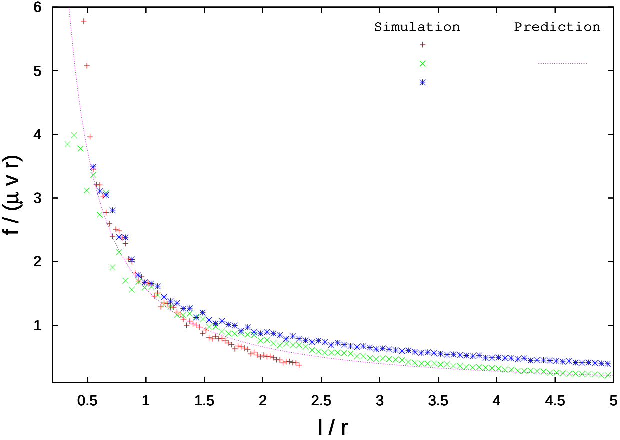

FIGURE : A plot of the non-dimensionalised lubrication force along with the proposed law, assuming low Reynolds number

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Non-dimensional lubrication force prediction.

$$\frac{F}{\mu \cdot v \cdot r} = \frac{\pi}{2} \times \left(\frac{r}{l}\right)^{1.25}$$
$$F = \frac{\pi \cdot \mu \cdot v \cdot r}{2} \times \left(\frac{r}{l}\right)^{1.25}$$

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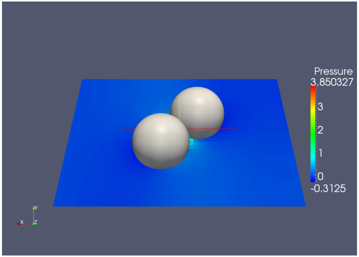
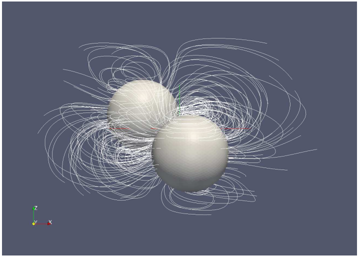


(a) Interstitial pressure



(b) Streamlines of the fluid phase

FIGURE : Flow field around two obliquely colliding spheres

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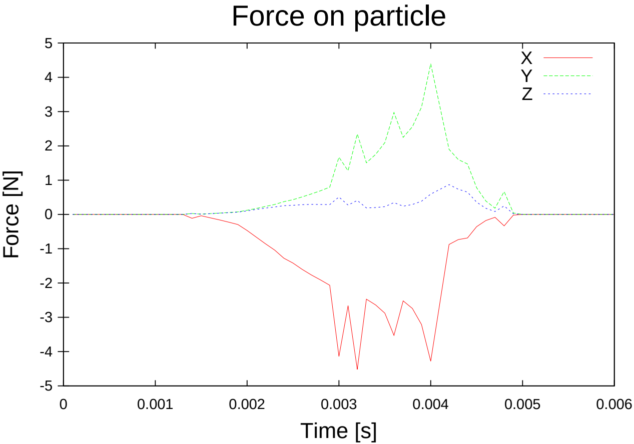
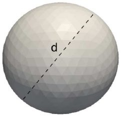
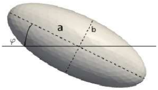
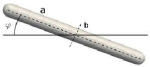
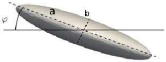


FIGURE : A plot of the components of collision forces between the particles

- Disc falling in a fluid
- Disc falling in a fluid
- Disc falling in a fluid
- Collision of two particles
- Interacting particles
- Comparison of shape on settling
- Collision of two particles
- Interaction of bubble with particle
- Interaction of disc with free surface

PARTICLE SHAPES

shape	sphericity	proportions	size
sphere	1		$d = 200\,\mu m$
			
ellipsoid	0.88	$\frac{a}{b} = \frac{5}{2}$	$a = 368\,\mu m$ $b = 147\,\mu m$
			
fiber	0.70	$\frac{a}{b} = 5$	$a = 510\,\mu m$ $b = 102\,\mu m$
			
disc	0.88	$\frac{a}{b} = 5$	$a = 350\,\mu m$ $b = 70\,\mu m$
			

Forces and Torques on a particle

Drag Force

$$F_d = C_D(\ldots)\frac{1}{2}\rho_g\frac{\pi}{4}d_p^2\left(\tilde{\mathbf{v}}_f - \mathbf{v}_p\right)^2$$

Lift Force

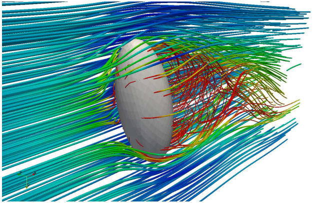
$$F_l = C_L(\ldots)\frac{1}{2}\rho_g\frac{\pi}{4}d_p^2\left(\tilde{\mathbf{v}}_f - \mathbf{v}_p\right)^2$$

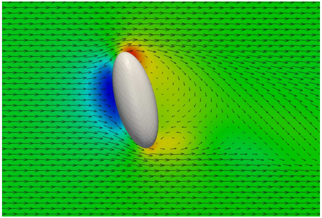
Aerodynamic Torque

$$T_{aero} = C_T(\ldots)\frac{1}{2}\rho_g\frac{\pi}{8}d_p^3\left(\tilde{\mathbf{v}}_f - \mathbf{v}_p\right)^2$$

Rotational Torque

$$\mathbf{T}_{rot} = C_R(\ldots)\frac{\rho}{2}\left(\frac{d_p}{2}\right)^5|\omega_p|\omega_p$$





$$C_D(\varphi) = C_{D,\varphi=0^o} + (C_{D,\varphi=90^o} - C_{D,\varphi=0^o}) sin^{a_0}\varphi$$

$$C_{D,\varphi=0^o} = \frac{a_1}{Re^{a_2}} + \frac{a_3}{Re^{a_4}}$$

$$C_{D,\varphi=90^o} = \frac{a_5}{Re^{a_6}} + \frac{a_7}{Re^{a_8}}$$

$$C_L = \left(\frac{b_1}{Re^{b_2}} + \frac{b_3}{Re^{b_4}}\right) sin(\varphi)^{b_5+b_6 Re^{b_7}} cos(\varphi)^{b_8+b_9 Re^{b_{10}}}$$

$$C_T = \left(\frac{c_1}{Re^{c_2}} + \frac{c_3}{Re^{c_4}}\right) sin(\varphi)^{c_5+c_6 Re^{c_7}} cos(\varphi)^{c_8+c_9 Re^{c_{10}}}$$

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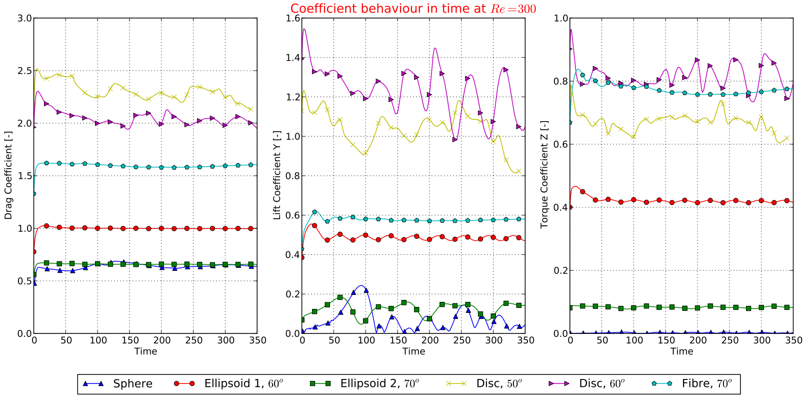
Zastawny et al. (2012) Int. J. Multiphase Flows 39, pp 227

Results from DNS



Zastawny et al. (2012) Int. J. Multiphase Flows 39, pp 227

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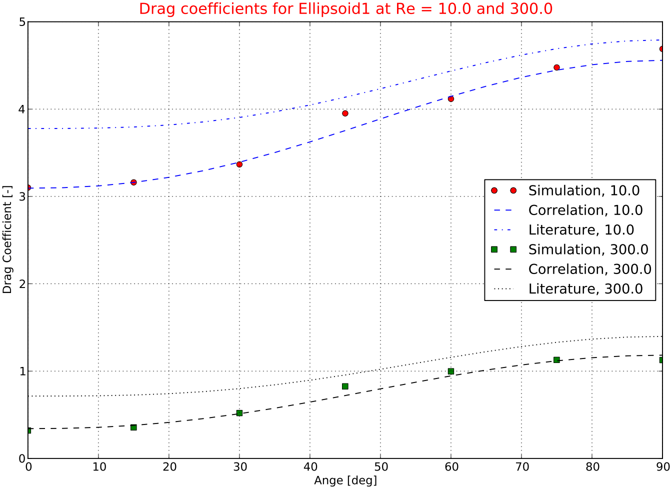
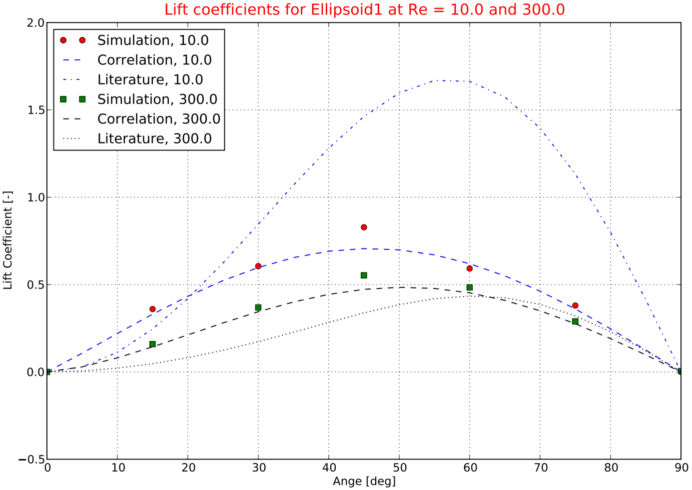
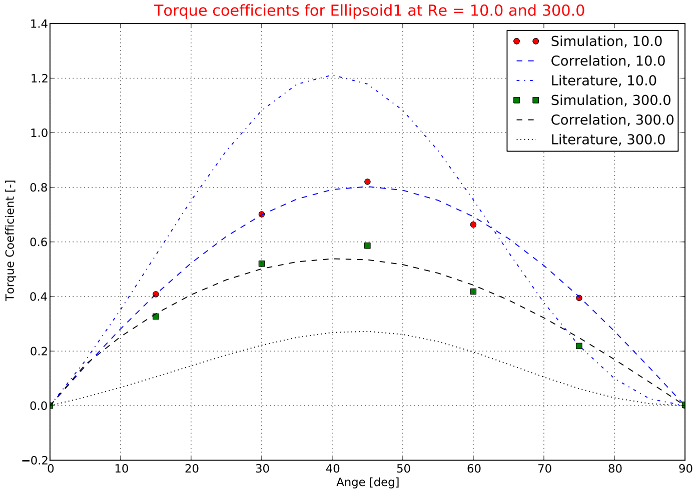

Drag coefficients for Ellipsoid1 at Re = 10.0 and 300.0
Drag Coefficient [-]
Ange [deg]
0
1
2
3
4
5
0
10
20
30
40
50
60
70
80
90
Simulation, 10.0
Correlation, 10.0
Literature, 10.0
Simulation, 300.0
Correlation, 300.0
Literature, 300.0

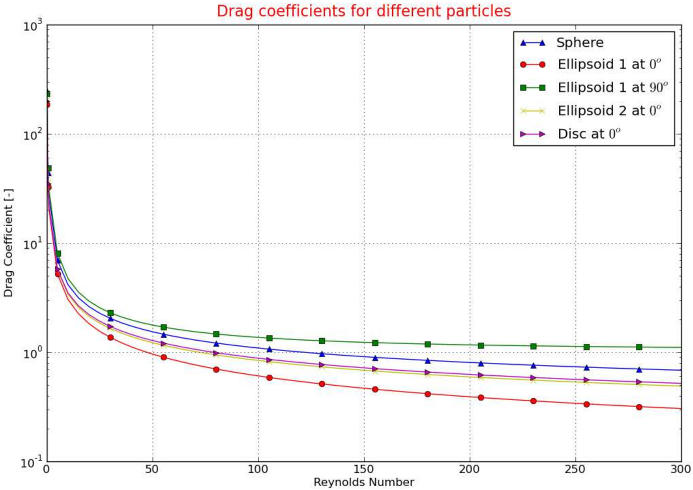


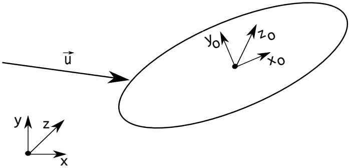
Hoerner (1965)

Results from DNS

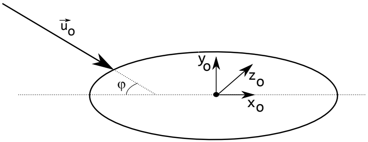


Rosendahl (2000)


Drag coefficients for different particles
Sphere
Ellipsoid 1 at 0^o
Ellipsoid 1 at 90^o
Ellipsoid 2 at 0^o
Disc at 0^o
Drag Coefficient [-]
10^3
10^2
10^1
10^0
10^{-1}
0
50
100
150
200
250
300
Reynolds Number



world space



body space

$$\varphi = \left| \arctan\left(\frac{u_{o,sh}}{u_{o,ln}}\right) \right|$$

$$F_o, x = \frac{1}{2} \cdot \rho \cdot A_{eq} \cdot C_D(\varphi, Re) \cdot |\boldsymbol{u}_o| u_{o,x} + F_L \cdot \sin\varphi \cdot sign(-u_{o,x})$$

$$F_o, y = \frac{1}{2} \cdot \rho \cdot A_{eq} \cdot C_D(\varphi, Re) \cdot |\boldsymbol{u}_o| u_{o,y} + F_L \cdot \cos\varphi \cdot \frac{u_{o,y}}{\sqrt{u_{o,y}^2 + u_{o,z}^2}}$$

$$F_o, z = \frac{1}{2} \cdot \rho \cdot A_{eq} \cdot C_D(\varphi, Re) \cdot |\boldsymbol{u}_o| u_{o,z} + F_L \cdot \cos\varphi \cdot \frac{u_{o,z}}{\sqrt{u_{o,y}^2 + u_{o,z}^2}}$$

Example Zhao and van Wachem, Acta Mechanica 224, 2013

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Conclusions

- Discussion of Immersed Boundary Methods
- Shortcomings/treatments in IBM
- Particle-Particle interactions in IBM
- Deriving force/torque model from IBM

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