Use of a DNS Method to Reduce Uncertainties in Two-Fluid Models

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Principal Approaches for the Study of Particulate Flows

- Continuum model (two-fluid model)
  - Both the fluid phase and solid phase are treated as continuous media

$$\partial_t (\rho_s \vec{u}_s) + \vec{\nabla}\cdot(\rho_s \vec{u}_s \vec{u}_s) = -\epsilon_s \vec{\nabla} p - \vec{\nabla}\cdot(\epsilon_s \vec{\vec{\tau}}_s) + \beta(\vec{u}_g - \vec{u}_s) + \rho_s \vec{g}$$

$$\partial_t (\rho_g \vec{u}_g) + \vec{\nabla}\cdot(\rho_g \vec{u}_g \vec{u}_g) = -\epsilon \vec{\nabla} p - \vec{\nabla}\cdot(\epsilon \vec{\tau}_g) - \beta(\vec{u}_g - \vec{u}_s) + \rho_g \vec{g}$$

  - Need empirical inputs: $\varepsilon_{s,}$ β some of which cannot be measured directly;
  - Not very accurate at present, accuracy depends greatly on empirical inputs.
- Discrete particle model (one-way coupling)
  - The solid particles are treated as point particles; hydrodynamic drag force is given by closure equations.
  - The fluid phase is treated as continuous phase; the effect of solid particles to the fluid phase is modeled.
- Direct Numerical Simulation (DNS)
  - The Navier-Stokes equation for the fluid phase and the equations of motion for the solid particles are solved simultaneously.
  - Two-way coupling.
  - Exact method.

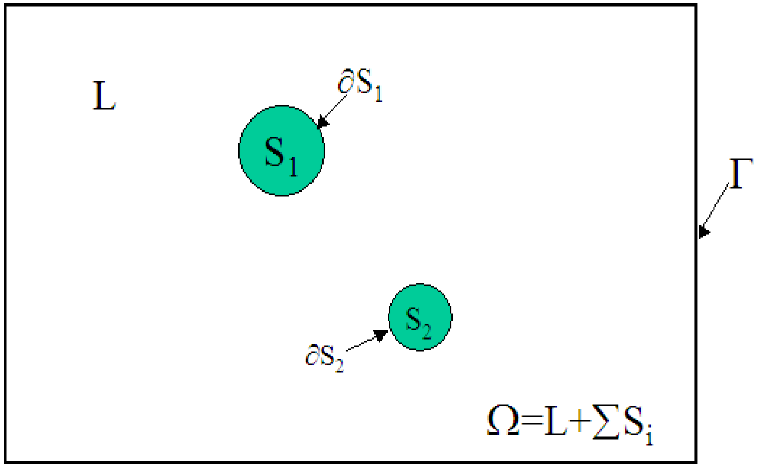
DNS Methods for Particulate Flow

- **Stokesian Dynamics** (Brady & Bossis, 1980s)
  - Valid for Stokes flow (Re<<1), spherical particles
- **Finite Element Method** (Dan Joseph's group, 1990s)
  - High Reynolds number, high accuracy, need mesh-adaptive, very expensive, two dimensional simulations.
- **Fictitious Domain Method** (Glowinski et al, 1998)
  - Low to medium Reynolds number, complicated to implement, computationally intensive.
- **Lattice Boltzmann Method** (Ladd, 1994 and after)
  - Low Reynolds number, high efficiency and fast, suitable for parallel computing
- ***Proteus* Method** (Feng and Michaelides, 2005)
  - Low to medium Reynolds number, easy to implement, improved accuracy compared to LBM.

Inclusion of Heat Transfer - Objectives

- Extend the DNS method to take into account the energy transfer to/from particles.
- Apply the Immersed Boundary Method (IBM) and the Direct Forcing (DF) scheme to momentum as well as the energy transfer problems.
- This is accomplished by substituting the surface of the particle with a series of forces and heat sources/sinks.

Conceptual Model and Governing Equations



Continuity, Momentum and Energy Equations

$$\vec{\nabla} \bullet \vec{u} = 0$$

$$\rho_f \frac{\partial \vec{u}}{\partial t} + \rho_f \vec{u} \bullet \nabla \vec{u} = -\vec{\nabla} p + \mu_f \nabla^2 \vec{u} + \beta_f (T - T_{fo}) \vec{g}$$

$$\rho_f c_f \frac{\partial T}{\partial t} + \rho_f c_f \vec{u} \bullet \nabla T = k_f \nabla^2 T + q$$

Modified Momentum and Energy Equations

$$\rho_{f0} \frac{\partial \vec{u}}{\partial t} + \rho_{f0} \vec{u} \bullet \nabla \vec{u} = -\vec{\nabla} p + \mu_f \nabla^2 \vec{u} + \beta_f (T - T_{fo}) \vec{g} + \vec{f}$$

$$\rho_f c_f \frac{\partial T}{\partial t} + \rho_f c_f \vec{u} \bullet \nabla T = k_f \nabla^2 T + q + \lambda$$

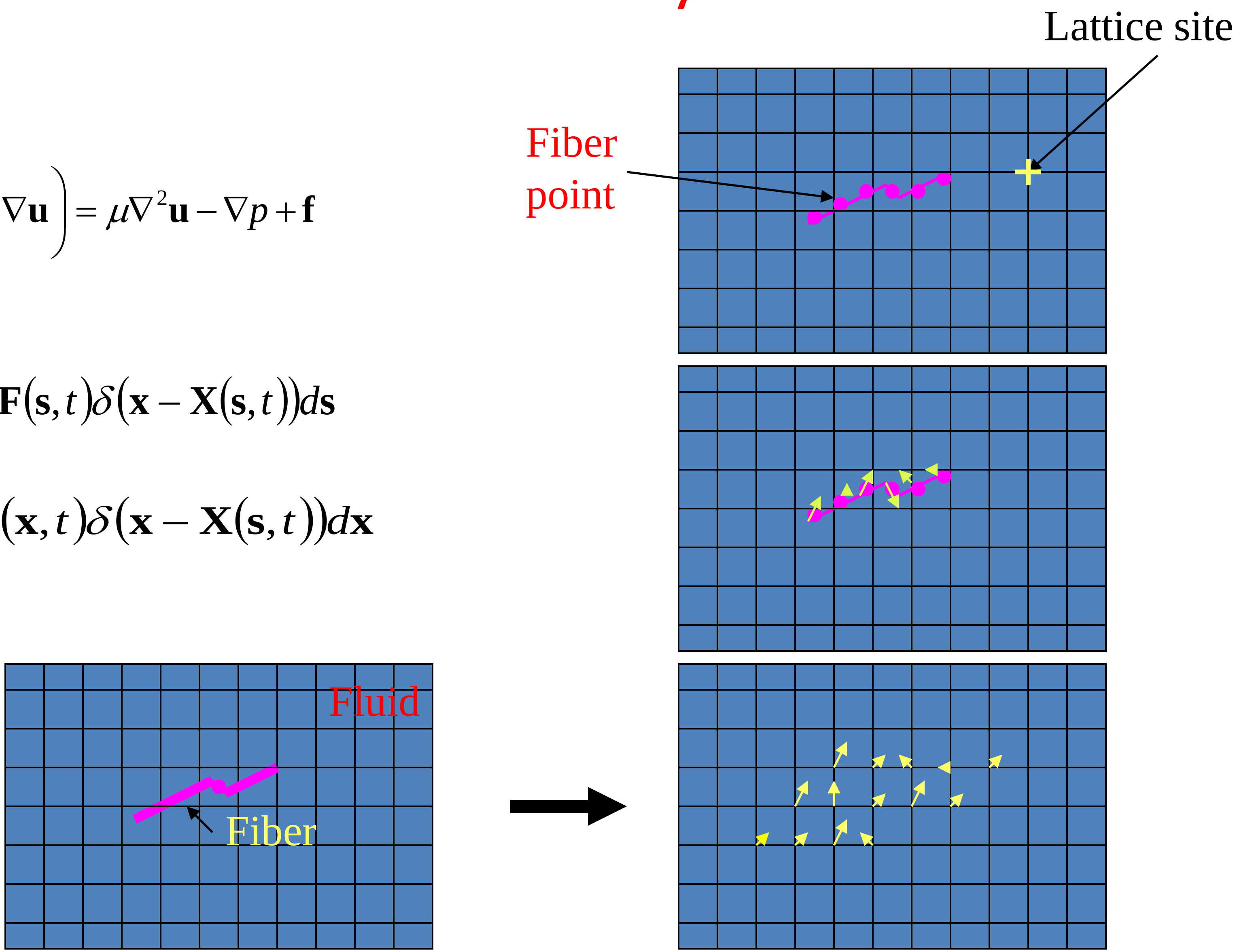
Immersed Boundary Method

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \bullet \nabla \mathbf{u}\right) = \mu \nabla^2 \mathbf{u} - \nabla p + \mathbf{f}$$

$$\nabla \bullet \mathbf{u} = 0$$

$$\mathbf{f}(\mathbf{x},t) = \int_\Gamma \mathbf{F}(\mathbf{s},t)\delta(\mathbf{x} - \mathbf{X}(\mathbf{s},t))ds$$

$$\frac{\partial \mathbf{X}}{\partial t} = \int_\Omega \mathbf{u}(\mathbf{x},t)\delta(\mathbf{x} - \mathbf{X}(\mathbf{s},t))d\mathbf{x}$$



Fluid + Solid / Fiber

Fluid with force distribution

Assumptions

- Boussinesq approximation on the effect of temperature on fluid properties.
- Particles have uniform temperature (Bi=0) that is, particles are very small or their conductivity is much higher than that of the fluid.
- No-slip at the particle surface.
- Equal temperatures (T_f=T_s) at the particle surface.

Momentum-side equations for the domain of particles

Translational motion

$$\left(\rho_p - \rho_f\right)V_P \frac{d\vec{U}_P}{dt} = \rho_f \int_S \vec{f} dv + \left(\rho_p - \rho_f\right)V_p \vec{g}$$

Rotational motion

$$I_P \left(1 - \frac{\rho_p}{\rho_f}\right)\frac{d\vec{\omega}_P}{dt} = -\rho_f \int_{Vp} \left(\vec{x} - \vec{x}_p\right) \times \vec{f} d\upsilon$$

Force density

$$\vec{f} = \rho_f \frac{\partial \vec{u}}{\partial t} + \rho_f \vec{u} \bullet \nabla \vec{u} + \vec{\nabla} p - \mu_f \nabla^2 \vec{u}$$

Particle interior motion
(rigid body rotation)

$$\vec{u} = \vec{U}_P + \vec{\omega}_P \times \left(\vec{x} - \vec{x}_P\right)$$

Heat transfer-side equations for the domain of particles

In analogy with the momentum forcing:

$$\rho_f c_f \frac{\partial T}{\partial t} + \rho_f c_f \vec{u} \bullet \nabla T = k_f \nabla^2 T + q + \lambda$$

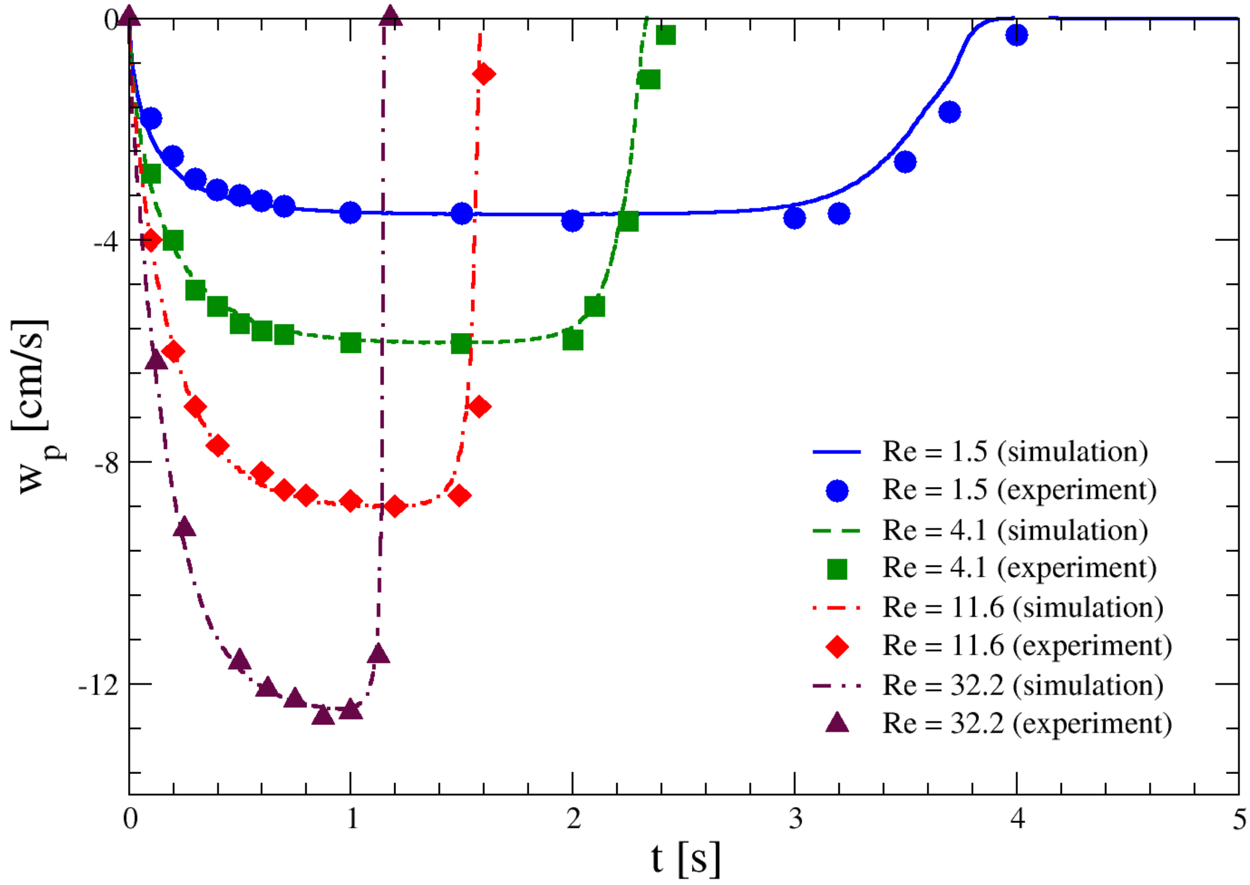
Or, in the solid region:

$$\lambda = \rho_f c_f \frac{\partial T}{\partial t} + \rho_f c_f \vec{u} \bullet \nabla T - k_f \nabla^2 T + q$$

Particle temperature change:

$$\rho_p V_p c_p \frac{dT_p}{dt} = \oint_{\partial S} k_f \vec{\nabla} T_f \bullet \vec{n}\; ds + \int_S q_s dv$$

Model validation/verification



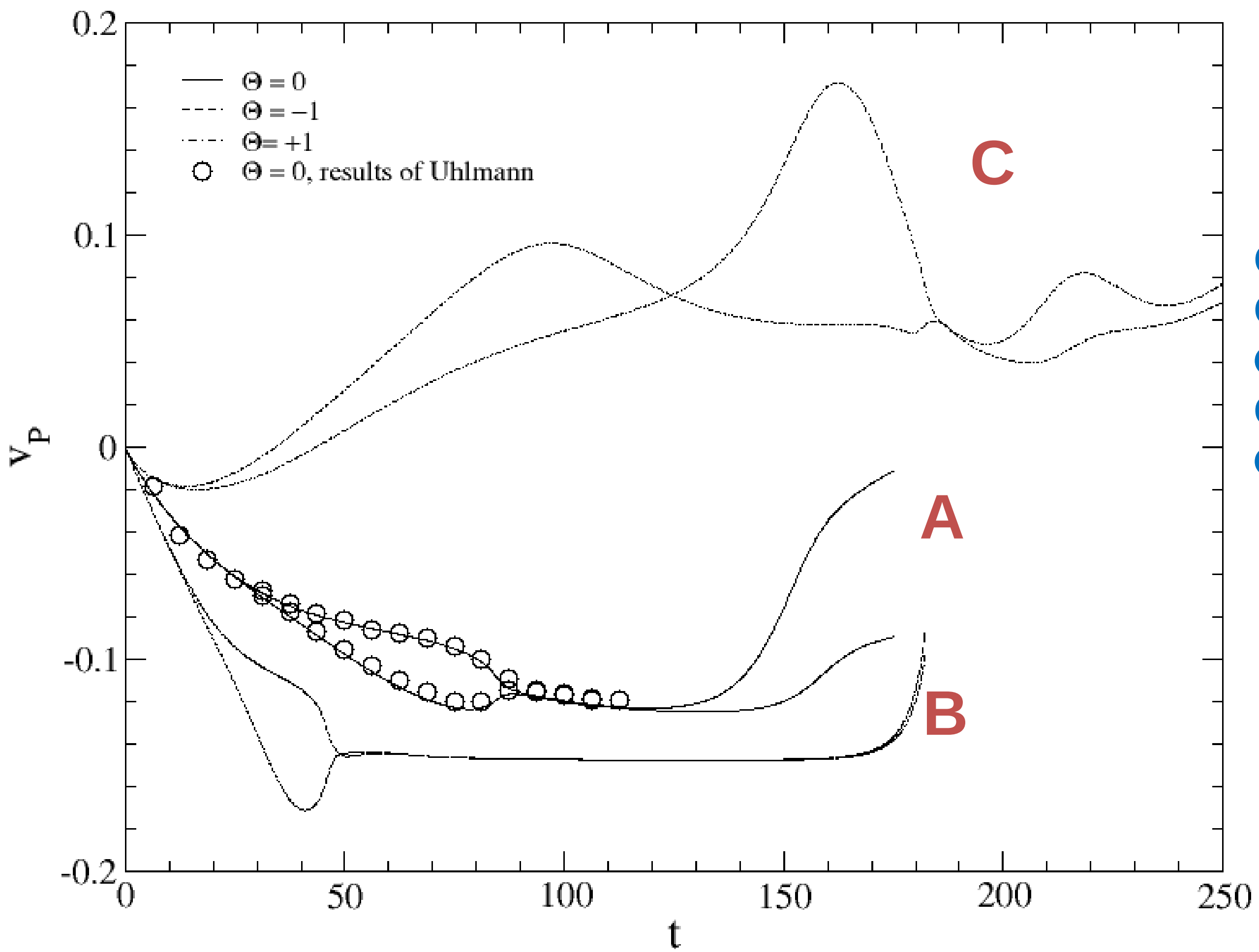
Comparison with falling particle data by ten Cate et al. (2002)

The Drafting-Kissing-Tumbling motion of two light particles – A

Physical parameters:

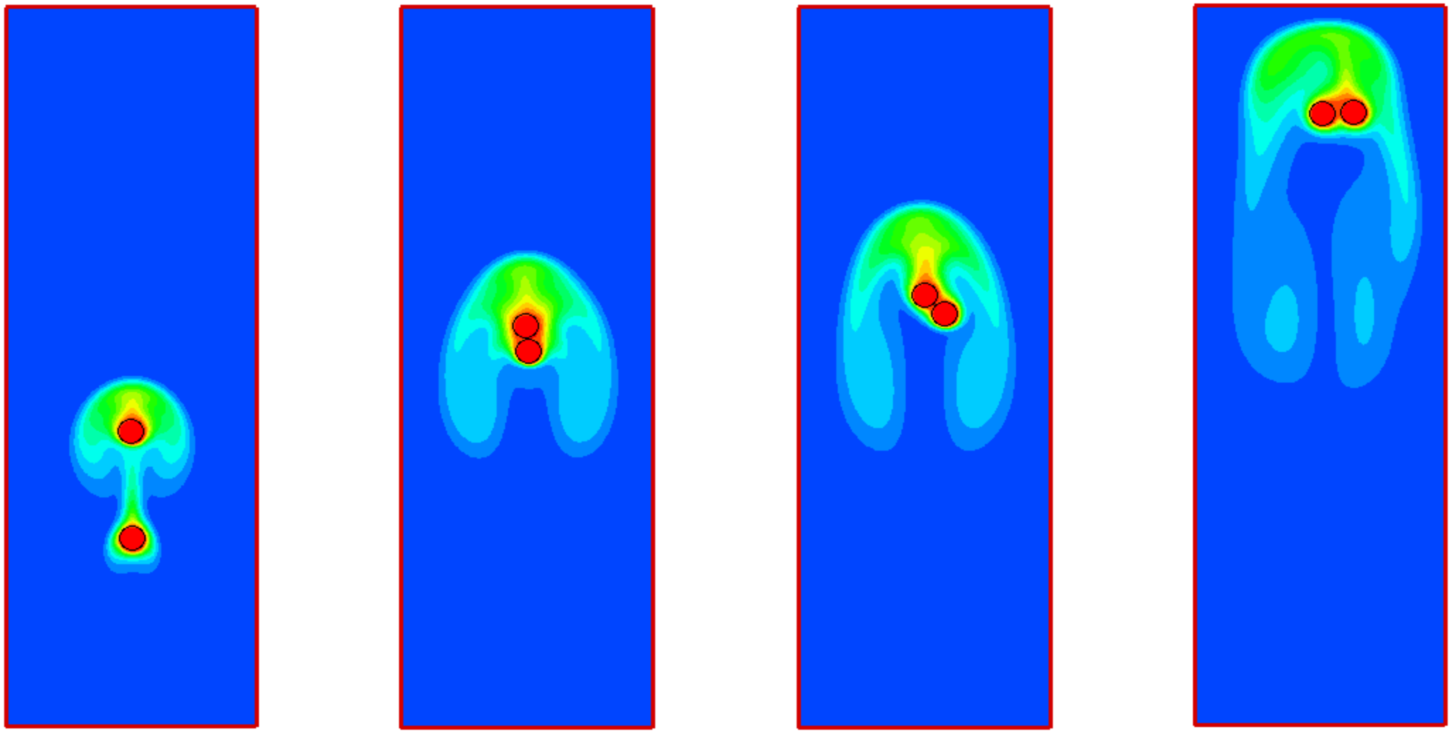
- Domain size: Ω = [-1,1]X[0,6];
- particle radius: r = 0.125;
- initial position of the two particles: $\boldsymbol{x}_{p1}$=[0, 5.2], and $\boldsymbol{x}_{p2}$=[0.001, 4.8];
- Particle/fluid density ratio: ρ_r=1.01.
- Fluid viscosity: ν=0.001.
- The grid is 200x600, and the dimensionless time step δt=0.005.

The Drafting-Kissing-Tumbling motion of two light particles – B



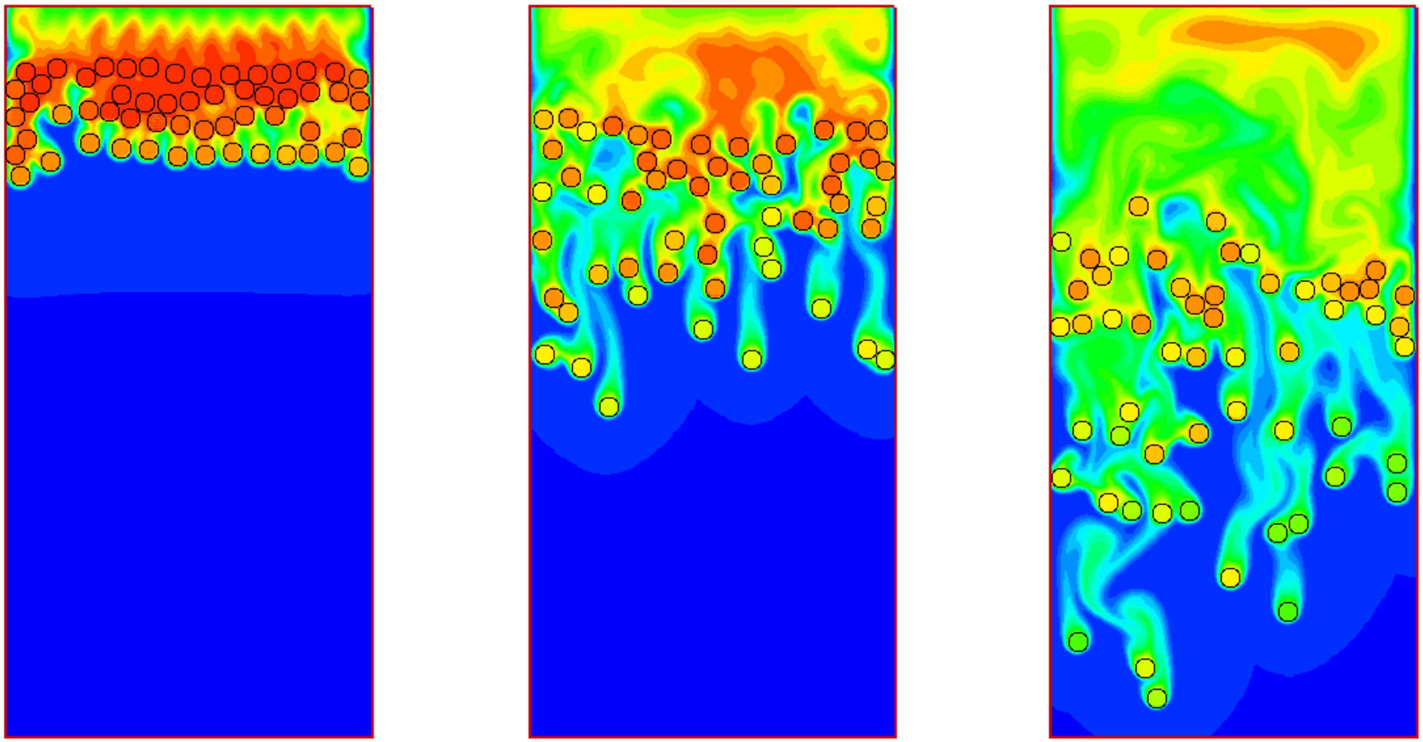
Case A: Θp=Θf=0; Gr=0;
Case B: ambient fluid Θf = 0; Θp = -1; Gr=1000;
Case C: ambient fluid Θf = 0; Θp = 1; Gr=1000.

The Drafting-Kissing-Tumbling motion of two light particles – C



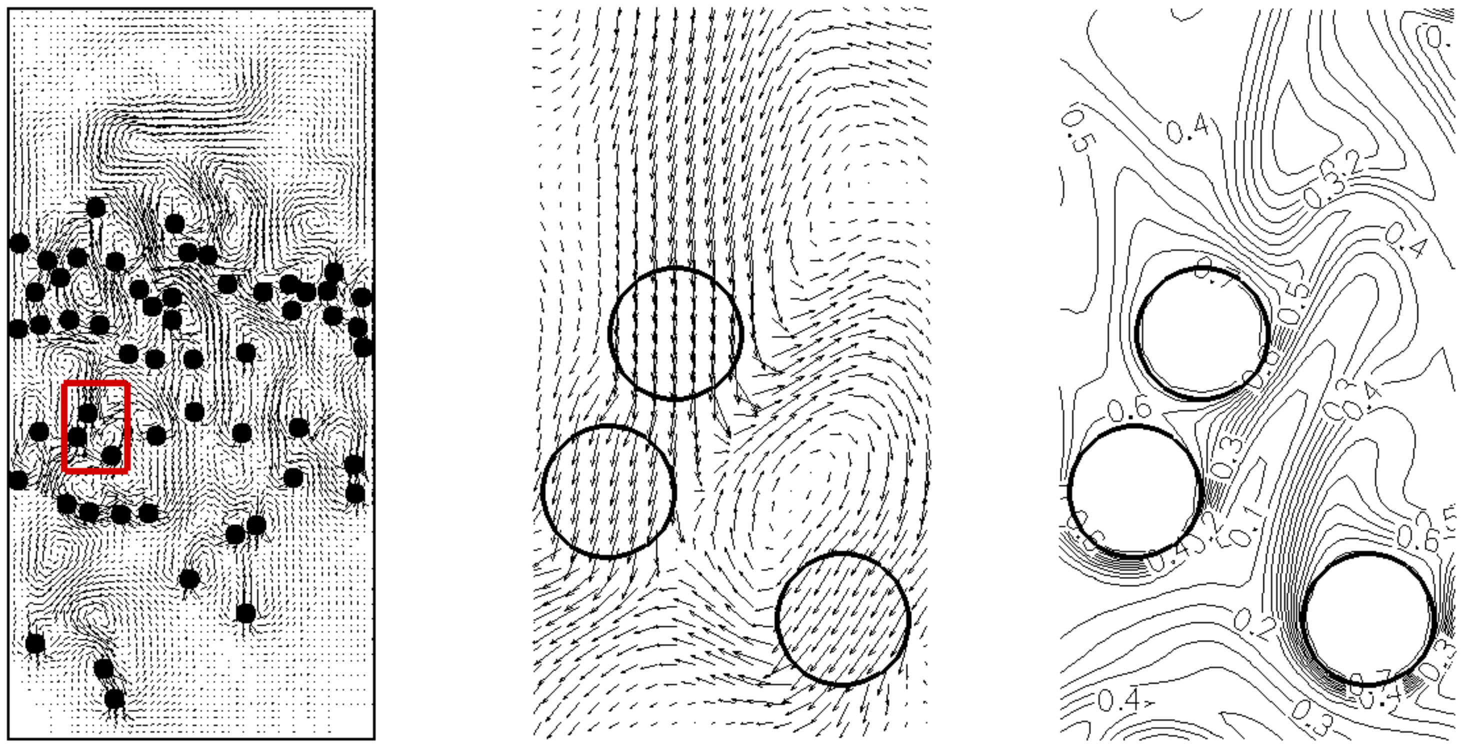
T=112 T=185 T=210 T=315

Sedimentation of 56 “hot” particles – A



t=3 t=6 t=9

Sedimentation of 56 “hot” particles – B



Use of the DNS model to determine the behavior of the particulate phase(s) near walls

- Use a physically meaningful wall-particle interaction model.
- Observe the behavior of a statistically large number of particles in the wall region.
- Determine the average behavior of the particles.
- Deduce the appropriate "boundary condition."

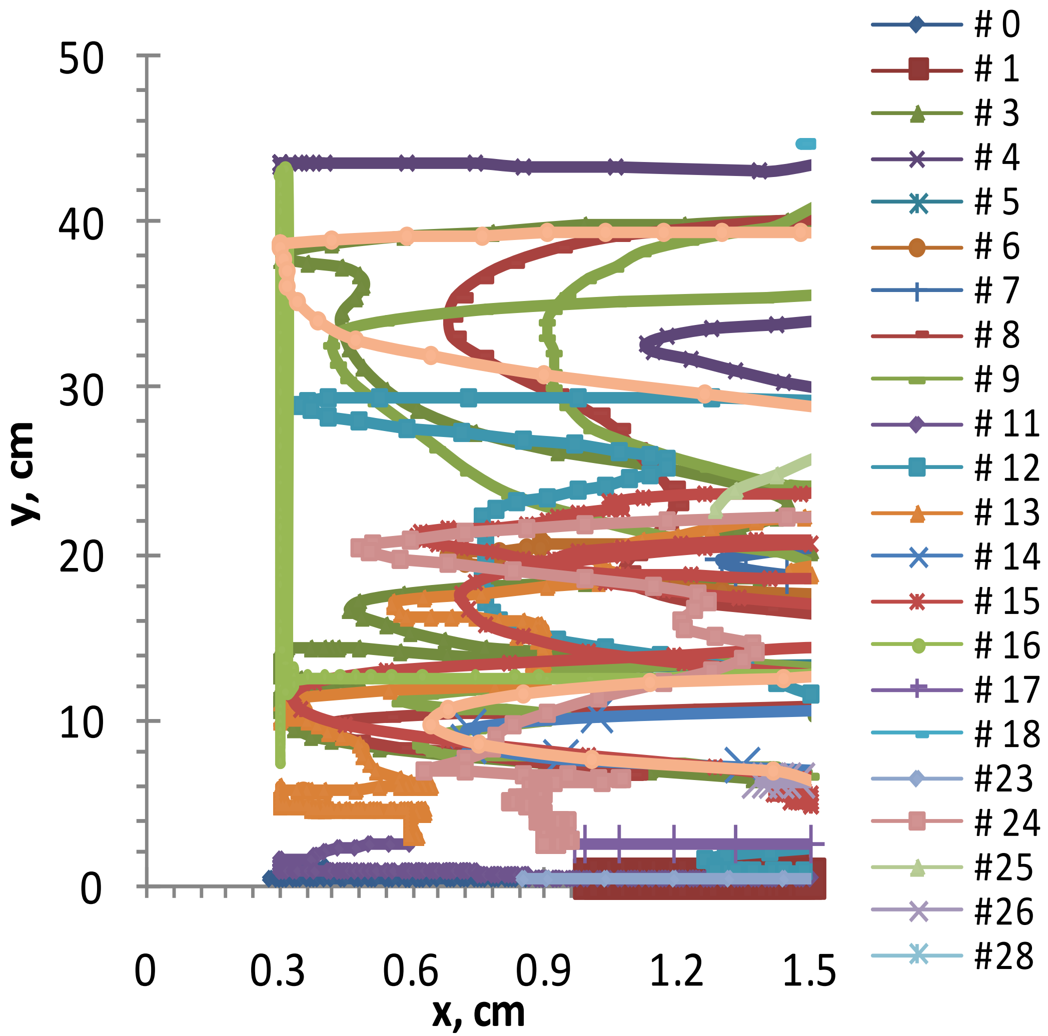
Collision Model with the Wall – reflection method (Glowinski et al. (2001)

When the gap between a particle and the wall is less than a given threshold, ζ, a repulsive force is applied to the particle, which is added to a total force the particle experiences.

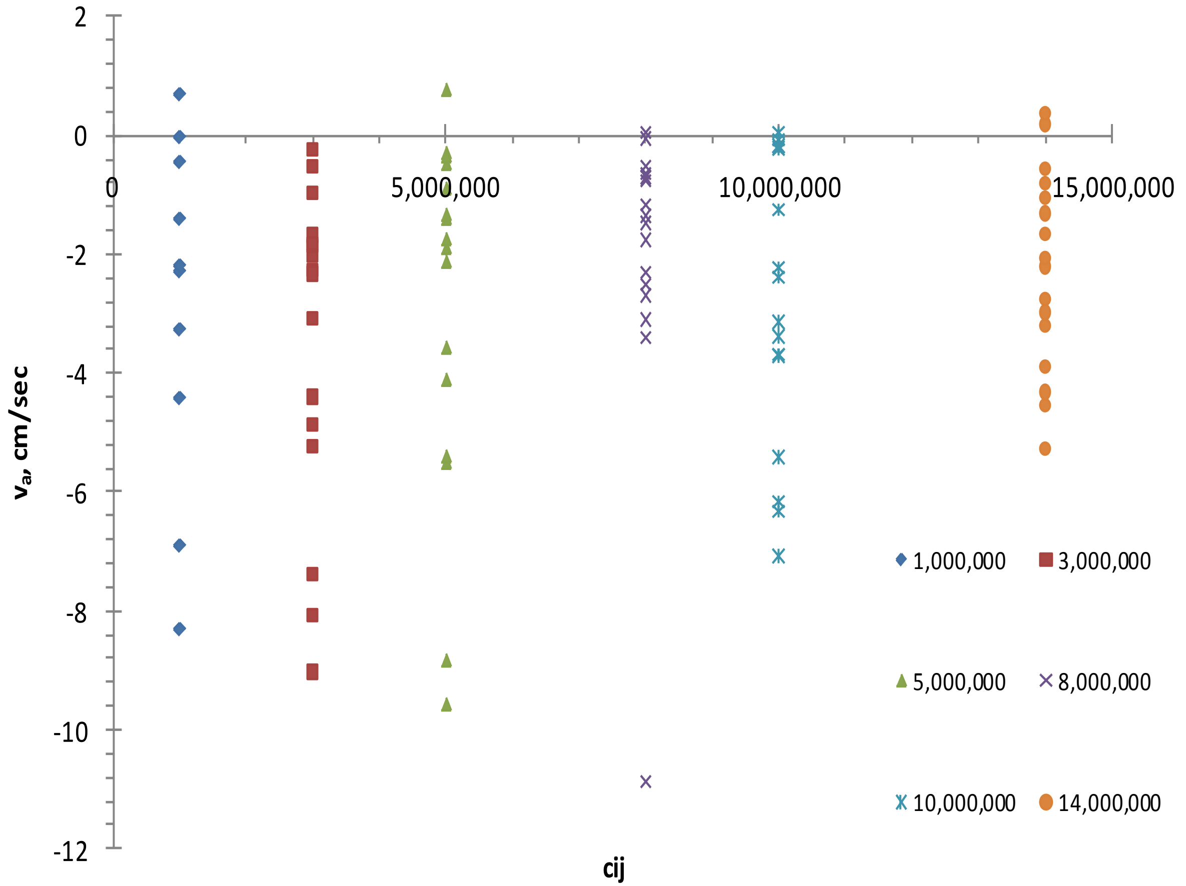
$$F_{ij}^{W} = \begin{cases} 0, & \left\| x_i - x_{i,j} \right\| > 2R_i + \zeta \\ \dfrac{c_{ij}}{\varepsilon_w}\left(\dfrac{\left\| x_i - x_{i,j} \right\| - 2R_i - \xi}{\zeta}\right)^2 \left(\dfrac{x_i - x_j}{\left\| x_i - x_j \right\|}\right), & \left\| x_i - x_{i,j} \right\| \le 2R_i + \zeta \end{cases}$$

where c_{ij} is the force scale factor, ε_w is the stiffness parameter of the collision, R_i is the radius of the particle, ζ is the threshold or the "safe zone, and $x_{i,j}$ is the position of the fictitious particle $P_{i,j}$, which is located symmetrically on the other side of the wall.

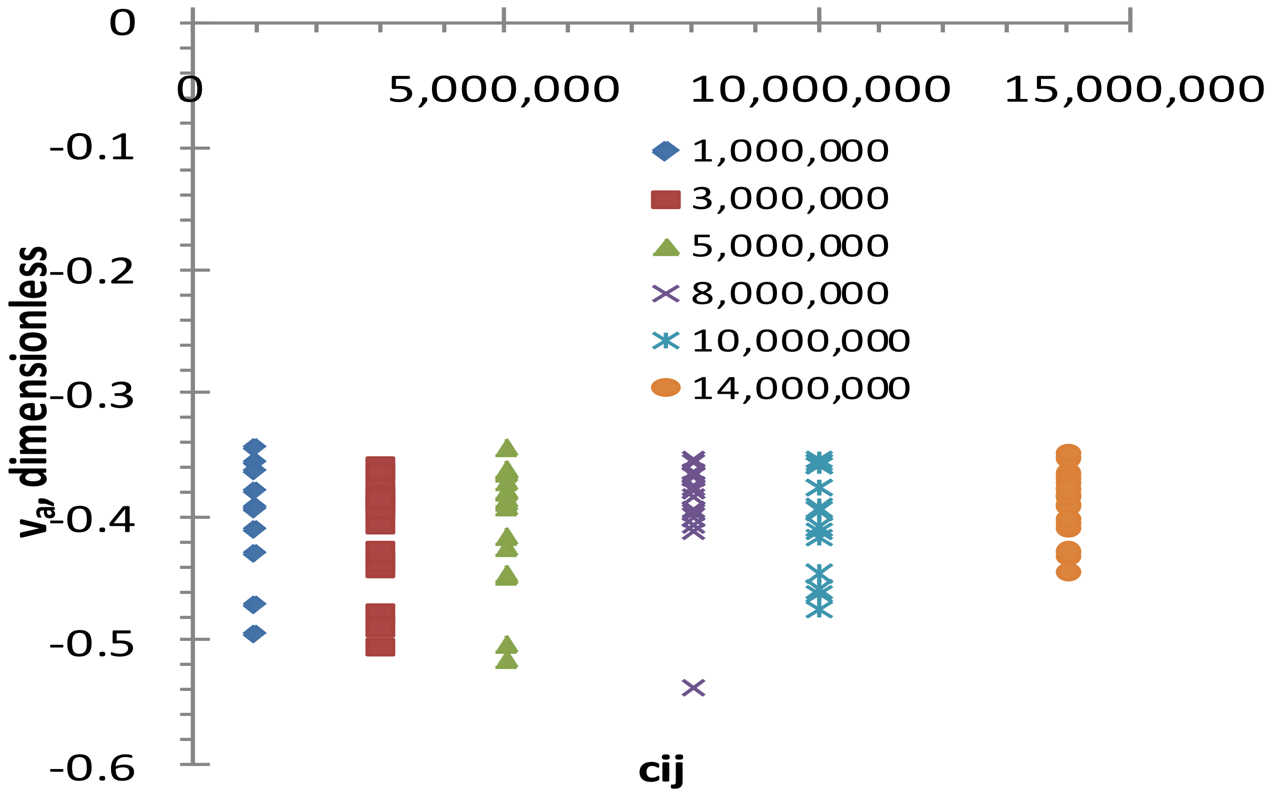
Near-wall particle trajectories – 264 particles of d=0.6 cm



Vertical Velocities at the Wall



The effect of the parameter c_{ij}



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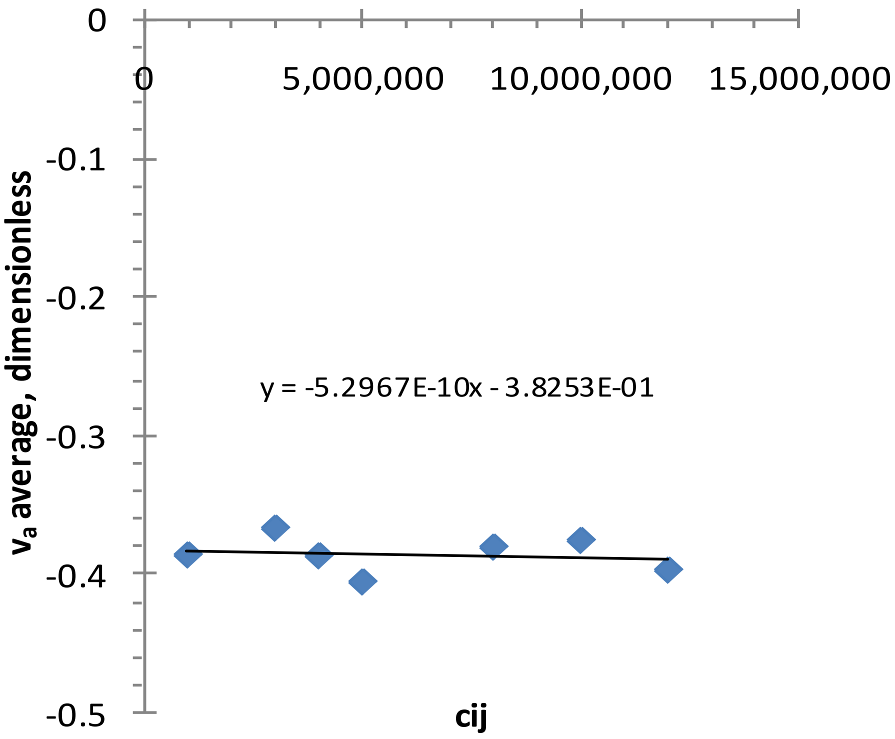
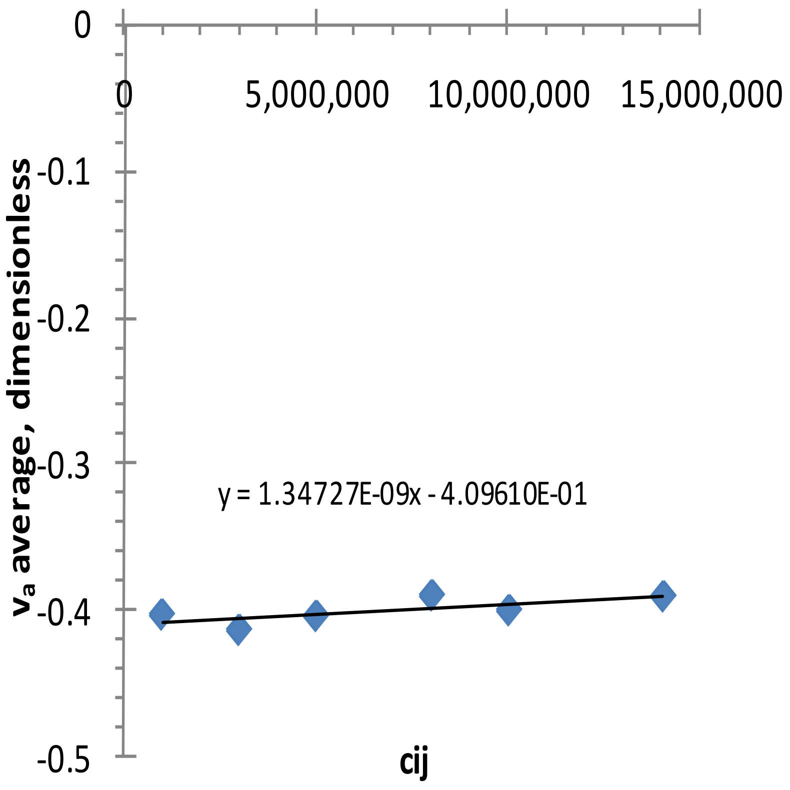
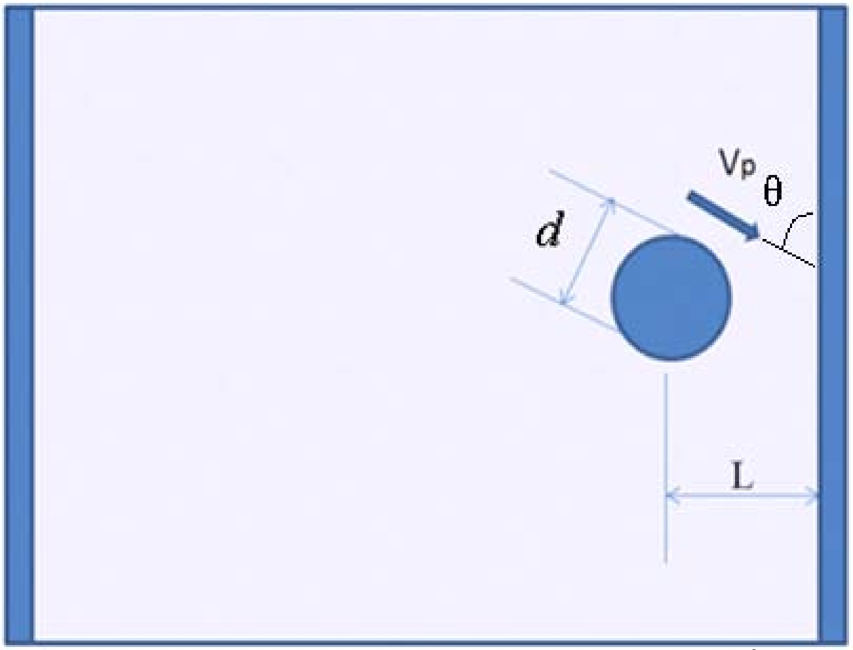
The effect of the parameter c_{ij} – all averaged results for d=0.4 and 0.6 cm





Single-sphere collision with walls – the soft sphere collision scheme



Spring-dashpot model with normal and tangential forces

$$f_{ij}{}^{n} = -k_n \delta^n{}_{ij} - \eta_n v^n{}_{ij}$$

$$f_{ij}{}^{t} = -k_t \delta^t{}_{ij} - \eta_t v^t{}_{ij}$$

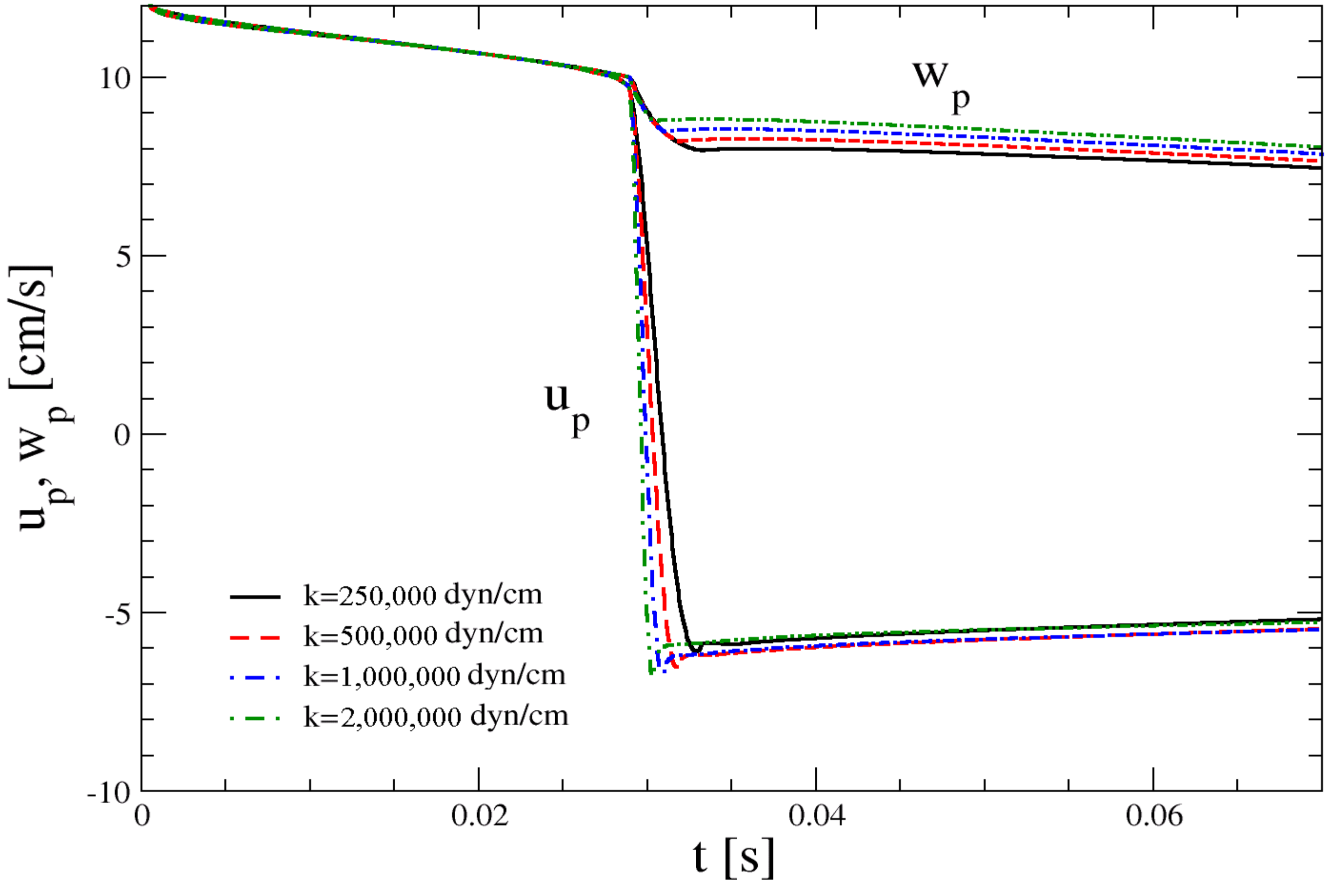
The relative tangential velocity component at the contact point may be computed as follows

$$\vec{v}_{ij}^{\,t} = \vec{v}_{ij} - \left(\vec{v}_{ij} \cdot \hat{n}_{ij}\right)\hat{n}_{ij} + \left[\vec{\omega}_i \times r_i \vec{n}_{ij} - \vec{\omega}_j \times r_j\left(-\vec{n}_{ij}\right)\right]$$

With friction at contact, the tangential contact force becomes:

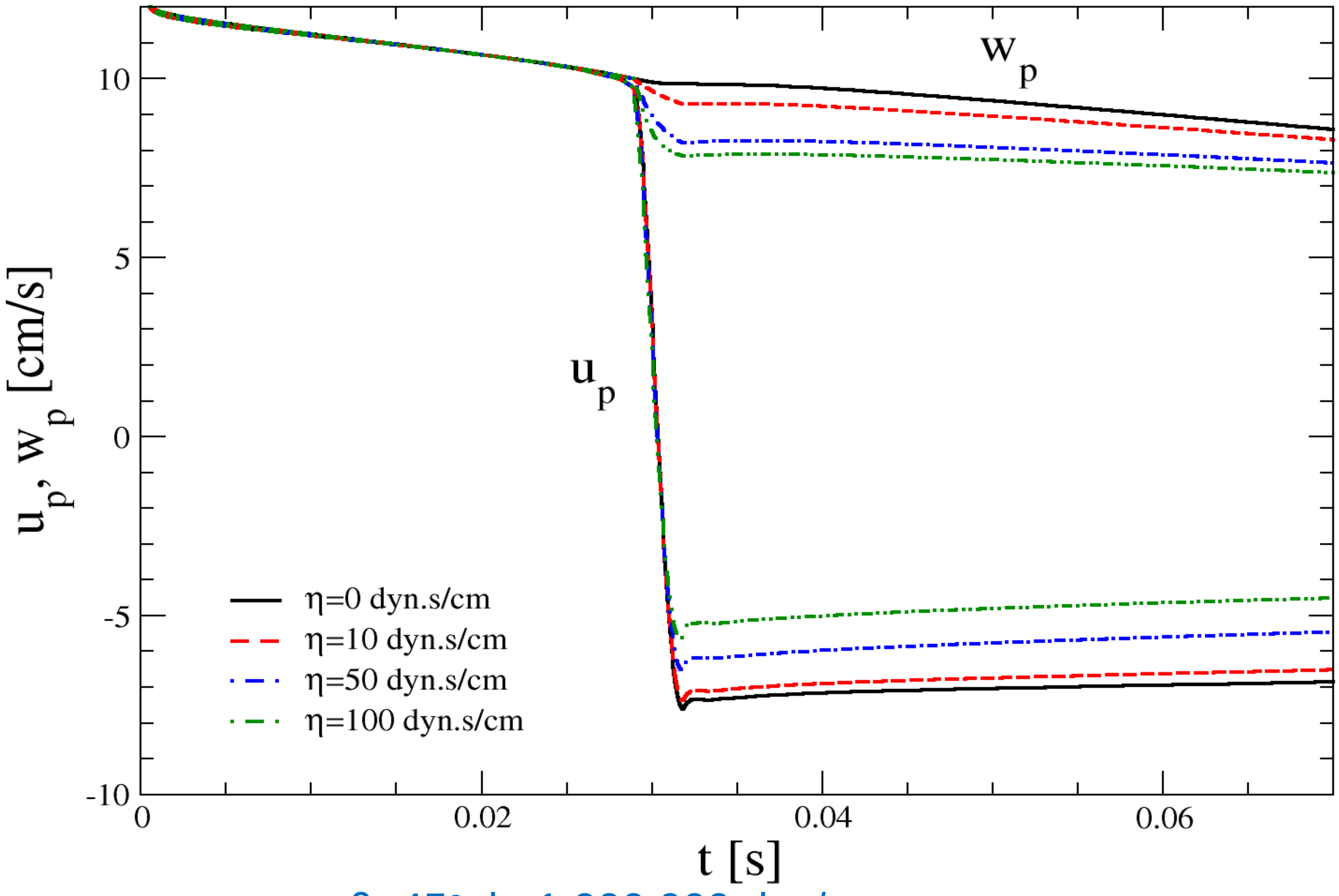
$$f_{ij}{}^{t} = \begin{cases} -k\delta^t{}_{ij} - \eta v^t{}_{ij}, & if \ \left|f_{ij}{}^{t}\right| \le \mu_s \left|f_{ij}{}^{t}\right| \\ \mu_k \left|f_{ij}{}^{t}\right| \dfrac{\delta^t{}_{ij}}{\left|\delta^t{}_{ij}\right|}, & if \ \left|f_{ij}{}^{t}\right| > \mu_s \left|f_{ij}{}^{t}\right| \end{cases}$$

Results of the soft-sphere collision scheme – A



θ=45º, η=50 dyn.s/cm
r≈0.65

Results of the soft-sphere collision scheme – B



θ=45°, k=1,000,000 dyn/cm
0.54<r<0.76

Summary – Conclusions

- A DNS with a forcing scheme, used to ensure rigid body motion, has been developed for the motion of the particles. In analogy with the momentum forcing scheme, a heat transfer forcing scheme was developed for the determination of the temperature field in the fluid.
- The collision parameters affect significantly the behavior of particles close to the wall. Having an accurate collision model is paramount for accuracy.
- Particle interactions close to the wall influence the trajectories, the wall collisions and, hence, the boundary conditions at the wall.
- There is significant evidence that particles "slip" near a vertical wall with a velocity close to 0.4 of their terminal velocity.
- The single-particle collision model with viscous fluids may be used more extensively to analyzed better single-particle collisions with a wall.

Publications and Acknowledgements

On the DNS model:

Feng, Z.G. and Michaelides, E. E., "The Immersed Boundary - Lattice Boltzmann Method for solving fluid-particles interaction problems," *J. Computational Physics,* vol. 195, pp.602-628, 2004.

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Feng, Z.-G. and Michaelides, E. E., 2008, "Inclusion of heat transfer computations for particle laden flows," *Phys. Fluids,* vol. **20**, #040604.

Feng, Z.-G. and Michaelides, E. E., 2008, "Heat Transfer in Particulate Flows with Direct Numerical Simulation (DNS)" *Int. J. Heat Mass Transf.,* doi:10.1016/j.ijheatmasstransfer.2008.07.023.

On the particle-wall interactions:

Feng, Z.-G. Michaelides, E. E. and Mao, S.-L. 2010, "Numerical Simulation of Particle-wall Collision in a Viscous Fluid using a Resolved Discrete Particle Method with the Soft-Sphere Collision Model," J. Fluids Engineering, accepted for publication,.

Davis, A., Michaeldes, E. E. and Feng, Z.-G., 2010, "Particle Velocity near Vertical Boundaries – A Source of Uncertainty in Two-Fluid Models, In proceedings of the ICMF-2010,.

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