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

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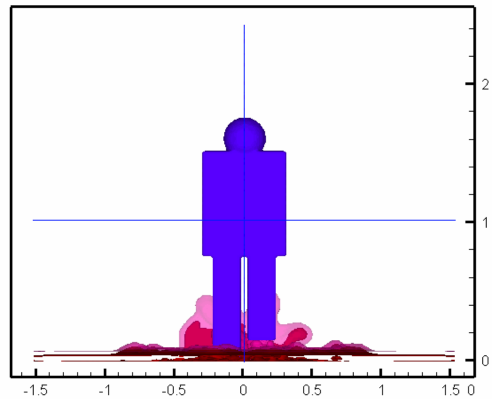
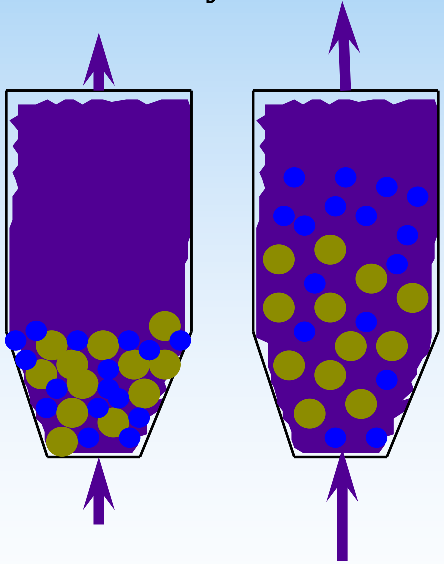
Background on Particulate Flows

- Particulate flows
  - Solid-gas flows, solid-liquid flows, liquid-gas flows, liquid-solid-gas flows
- Particle fluidization in a bed
  - Fluid injected from the bottom of the bed (distributor)
  - Particles remains packed if the fluid velocity is low (solid-like state, or packed bed)
  - Particles will be lifted when the flow velocity is high enough (fluid-like state)
- Advantages of particle fluidization
  - Large contact area between particles and fluid, better interaction: excellent for energy transfer, combustion and reactions between particles and fluid.
  - Low cost, easy to implement, suitable for continuous operation

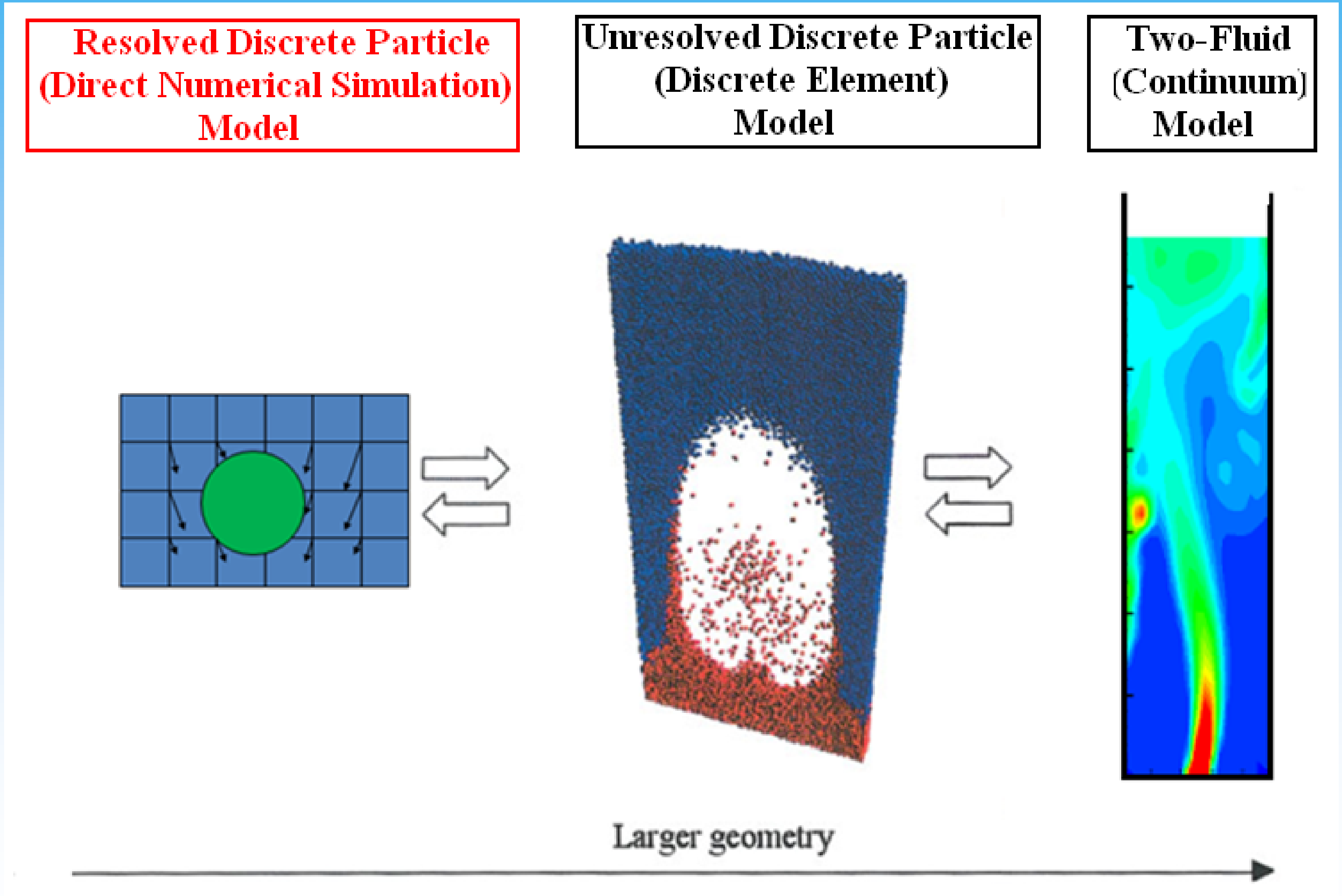


Dusty flow



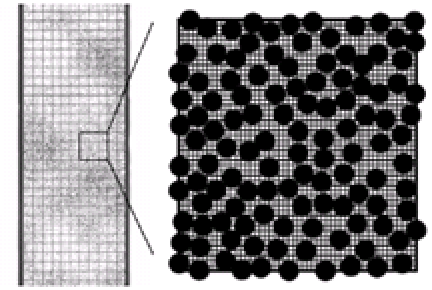
fluidization

Multiscale Modeling for Particlulate Flows



Direct Numerical Simulation (DNS)

Also called Resolved Discrete Particle Method *(RDPM)*



Fluid phase

$$\partial_t(\rho_f \vec{u}) + \vec{\nabla}\cdot(\rho_f \vec{u}\vec{u}) = -\vec{\nabla}P - \vec{\nabla}\cdot(\tau) + \boxed{\text{“boundary conditions”}}$$

Solid phase

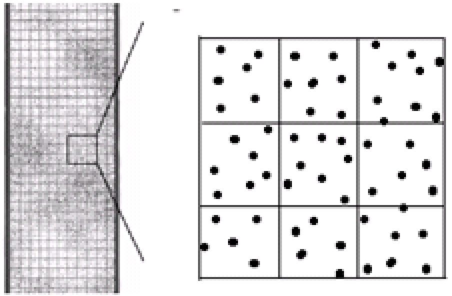
$$\frac{d}{dt}m\vec{v}_i = \sum_j \vec{F}_{ij} + \sum \vec{F}_b + \oint_{\partial S} \tilde{\sigma}\cdot d\vec{s}; \quad \tilde{I}_i \frac{d\vec{\omega}_i}{dt} = \oint_{\partial S} (\vec{x}-\vec{x}_i)\times(\tilde{\sigma}\cdot d\vec{s})$$

Particle-fluid interactions;
(Direct calculated)

Fluid: CFD (Eulerian) **Solid:** Particles tracking (Lagrangian)

Discrete Element Method (DEM)

Also called Unresolved Discrete Particle *(UDPM)*



Fluid phase

$$\partial_t(\rho_f \vec{u}) + \vec{\nabla}\cdot(\rho_f \vec{u}\vec{u}) = -\varepsilon\vec{\nabla}P - \vec{\nabla}\cdot(\varepsilon\tau) + \beta(\vec{v}-\vec{u})$$

Solid phase

$$\frac{d}{dt}m\vec{v}_i = \sum_j \vec{F}_{ij} + \frac{\beta V_i}{1-\varepsilon}(\vec{u}-\vec{v}_i)$$

Particle-particle interactions (Collision forces)

Particle-fluid interactions **(Estimated/Modeled)**

Fluid: CFD (Eulerian) **Solid:** Particles tracking (Lagrangian)

Two-Fluid Model (TFM)

Also called Continuum Model

Fluid phase

$$\partial_t(\rho_f \vec{u}) + \vec{\nabla}\cdot(\rho_f \vec{u}\vec{u}) = -\varepsilon\vec{\nabla}P - \vec{\nabla}\cdot(\varepsilon\tau) + \beta(\vec{v}-\vec{u})$$

Solid phase

$$\partial_t(\rho_s \vec{v}) + \vec{\nabla}\cdot(\rho_s \vec{v}\vec{v}) = -\varepsilon_s\vec{\nabla}P_s - \vec{\nabla}\cdot(\varepsilon_s\tau_s) - \beta(\vec{v}-\vec{u})$$

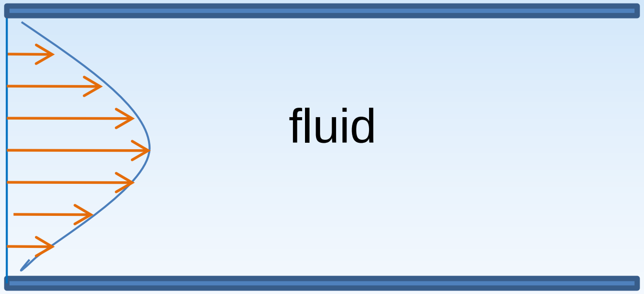
$$\tau_s = -\mu_s\left[(\vec{\nabla}\vec{v}) + (\vec{\nabla}\vec{v})^T - \frac{2}{3}(\vec{\nabla}\cdot\vec{v})I\right]$$

Fluid: CFD (Eulerian) **Solid**: CFD (Eulerian)

Importance of Boundary Conditions in CFD Simulations

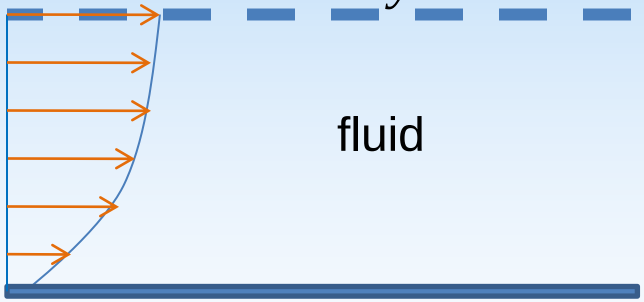
- Industrial scale simulations require two-fluid model
- Simulation results of two-fluid model strongly depend on the boundary conditions of solid phase
- Uncertainties on boundary conditions affect the accuracy of simulation results

$$v_f = v_w = 0$$



No-slip boundary condition on top

$$\frac{\partial v_f}{\partial y} = 0$$



free-slip boundary condition on top

Wall Boundary Condition of Solid Phase for Two-Fluid Model

- Uncertainties on velocity b.c. of solid phase
  - No slip condition $v_s = v_w$
  - Free slip condition $\frac{\partial v_s}{\partial n} = 0$
  - Johnson and Jackson boundary condition*

$$\frac{\boldsymbol{n} \cdot \sigma \cdot \mathbf{v}}{|\mathbf{v}|} + \sigma_{yy}^{f} \tan \delta' + \frac{\phi' \sqrt{3}\, \pi \rho_p \nu T^{1/2} |\mathbf{v}|}{6\nu_0 [1 - (\nu/\nu_0)^{1/3}]} = 0$$

    - Rarely used
  - Experimental results show that particles slip at wall
  - **Partial slip boundary condition**
    - $\frac{\partial v_s}{\partial n} + \beta (v_s - v_w) = 0$, β is the slip coefficient; effect of fluid field is not included
    - Need better partial slip model

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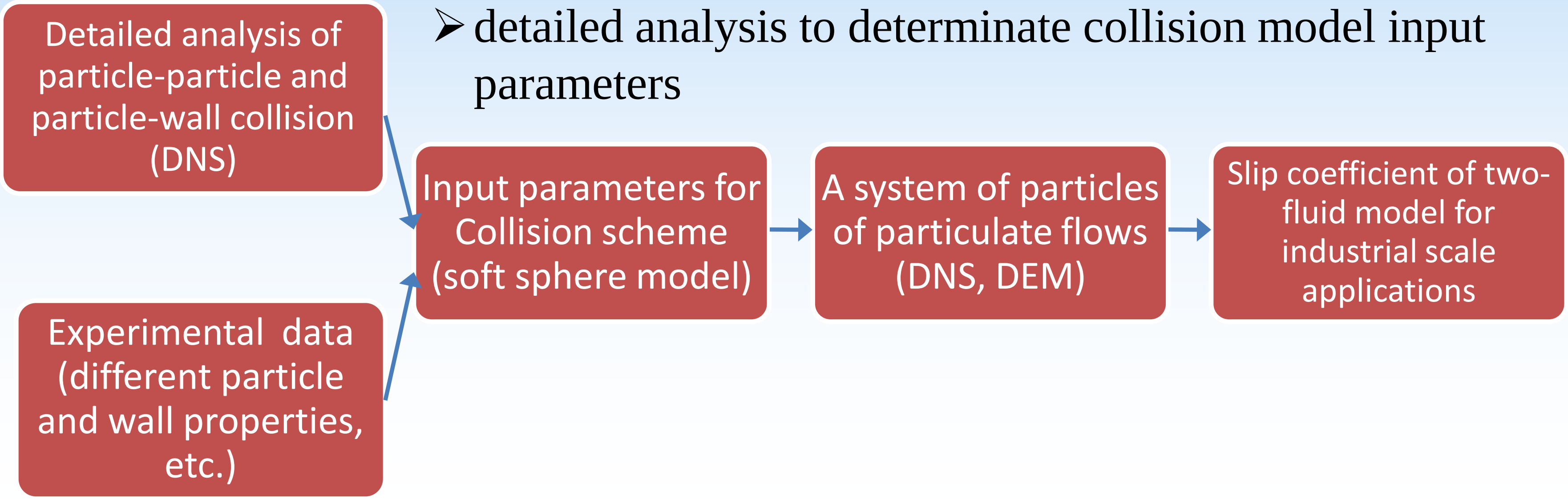
* Johnson, P.C., and Jackson, R. (1987), “Frictional-collisiional constitutive relations for granular materials, with application to plane shearing,” *J. Fluid Mech.*, vol.176, pp.67.

A Multi-scale Modeling Approach to Reduce Uncertainties on Wall B.C.

- two-fluid model simulations for industrial applications
    - reliable partial slip boundary condition for solid phase
        - solid phase velocity profile near wall
            - statistical average velocity of a large number of particles
                - **DNS +Collision Model** (resolved discrete particle method with the capability of handling particle-particle and particle-wall collisions)
                    - detailed analysis to determinate collision model input parameters



Detailed analysis of particle-particle and particle-wall collision (DNS)

Experimental data (different particle and wall properties, etc.)

Input parameters for Collision scheme (soft sphere model)

A system of particles of particulate flows (DNS, DEM)

Slip coefficient of two-fluid model for industrial scale applications

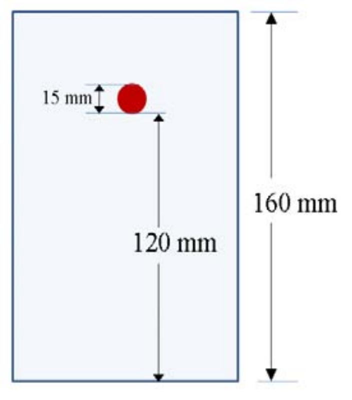
DNS simulation method: *Proteus**

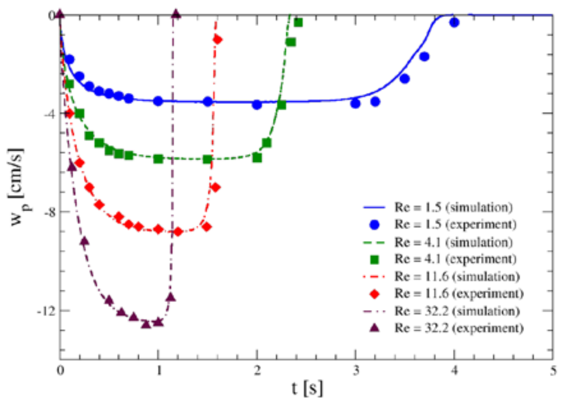
- Fluid velocity and pressure fields
  - Lattice-Boltzmann method or finite difference method based Navier-Stokes fluid solver; fixed regular grid.
- Particle-fluid interactions
  - Immersed boundary method; moving boundary nodes
- Particle-particle interactions
  - Soft-sphere collision scheme
  - Hybrid repulsive-force/lubrication scheme
- Particle dynamics
  - Newton's equations of motion (translational and rotational motions)

*Feng, Z.-G. and E. E. Michaelides, "***Proteus***: A direct forcing method in the simulations of particulate flow," *J. Comput. Phys.*, **202**: 20-51 (2005).

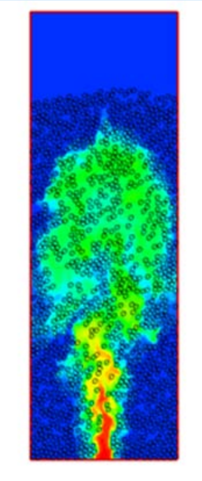
Validations of DNS

- Sedimentation of a spherical particle in a viscous fluid
  - Experiment measurement using PIV by ten Cate et al.*





- Fluidization of 3000 glass beads**



** Obuseh, C., Feng, Z.-G., and Paudel, B.D. (2012), “An experimental study of fluidization of bidisperse particulate flows,” *Journal of Dispersion Science Technology* .

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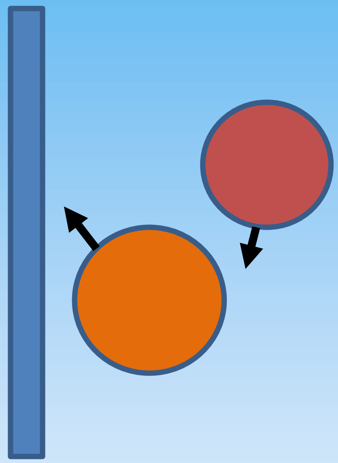
* A ten Cate, C. H. Nieuwstad, J. J. Derksen, and H. E. A. van den Akker(2002), “Particle imaging velocimetry experiments and lattice-Boltzmann simulations on a single sphere settling under gravity,” *Phys. Fluids*, **14**: 4012-4025 .

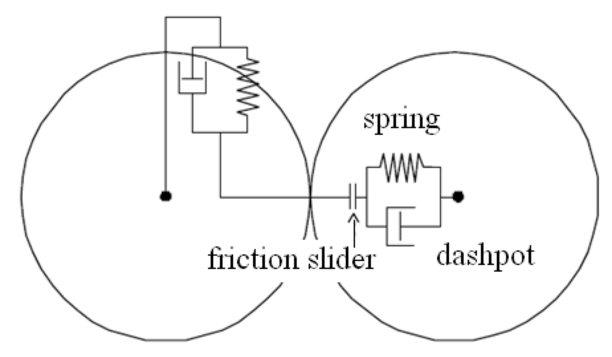
Determination of soft-sphere collision model parameters

Particle-Wall and Particle-Particle Collisions



- Collisions occur frequently, especially for dense particulate flows
- Collision models
  - Hard-sphere model
    - No overlap; inefficient for a large number of particles.
  - **Soft-sphere model**
    - Most widely used; allow small overlap; collision forces are computed based on overlap distance; need input parameters.
  - Lubrication force model
    - Not allow to contact; not applicable for high velocity and low viscosity flows

The Soft-Sphere Collision Model



- Collision force components*
  - normal $$f_{ij}{}^{n} = -k_n \delta^{n}{}_{ij} - \eta_n v^{n}{}_{ij}$$
  - tangential

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

- Model parameters
  - spring stiffness, k; cause the rebound off the colliding particles
  - damping coefficient, η; mimic the dissipation of kinetic energy due to inelastic collisions.
  - friction coefficient, μ; allow sliding.
- Collision model parameters depend on fluid and particle properties.
- How to choose the right model parameters?
  - matching numerical results with experimental data

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* Cundall, P.A. and O. D. L. Strack, “A discrete numerical model for granular assemblies,” *Géotechnique*, **29**:47 (1979).

Central Particle-Wall Collision (1)

- Experimental study*
  - Joseph et al. measured the particle rebounding velocity in various viscous fluids using spheres of different materials.

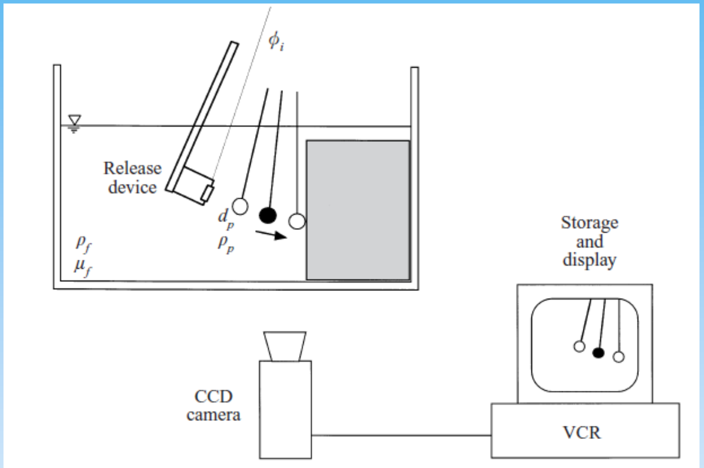

Image courtesy : Joesph et al. *

- DNS + Collision Model
  - fluid field is directly solved by DNS
  - collision is handled by soft-sphere model
    - select model parameters to match experimental data

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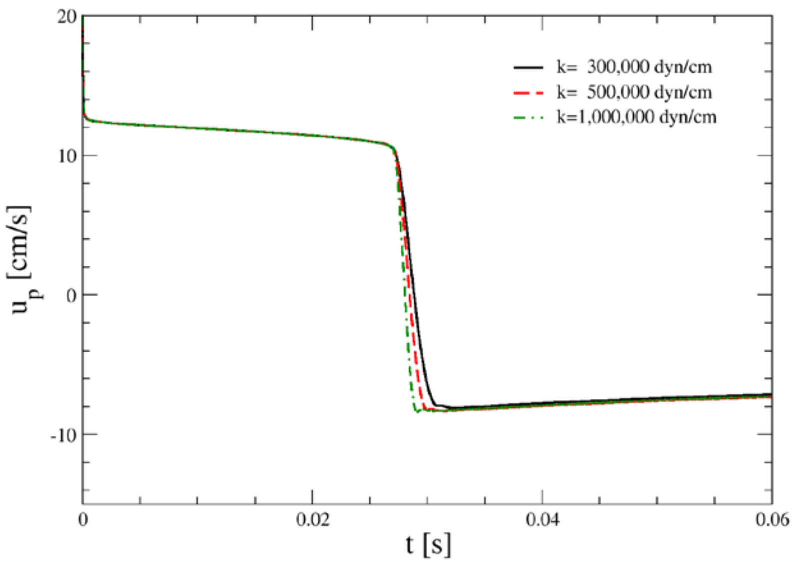
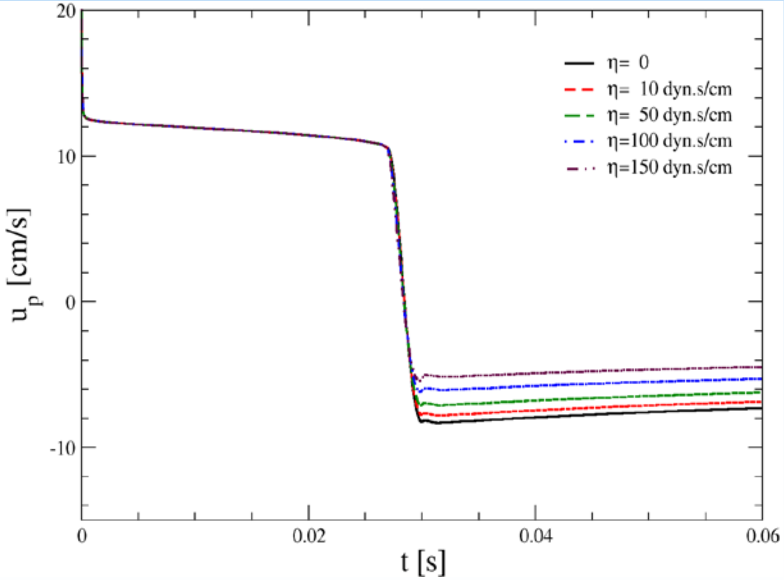
* Joseph, G. G.; R. Zenit, R., M. L. Hunt, and A. M. Rosenwinkel (2001), “Particle-wall collisions in a viscous fluid,” *J. Fluid Mech.*, **433**:329.

Central Particle-Wall Collision (2)

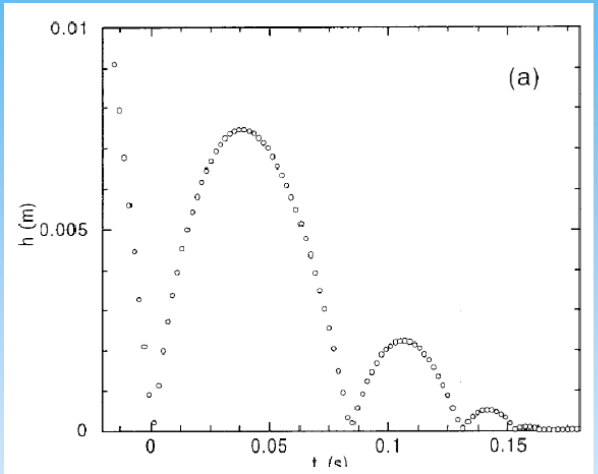
- Simulations are done using DNS combined with the soft-sphere collision model
- Study the effect of model parameters to the dynamics of particle in collision
  - Spring stiffness affects the duration time of collision
  - Damping coefficient affects the rebounding velocity

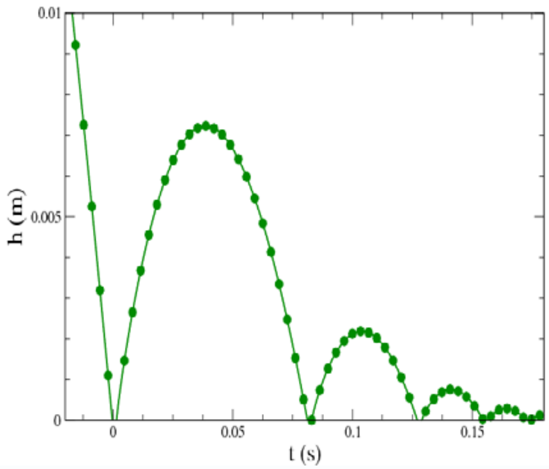




Bouncing Motion of a Sphere in a Viscous Fluid due to Gravity

- Experimental study[*]
  - Sphere falling onto a plate in viscous fluid (in silicon oil RV10).
  - trajectory of a sphere (diameter is 3mm) was recorded.
- DNS numerical simulation
  - k=317,000 dyn/cm,
  - η=140 dyn.s/cm





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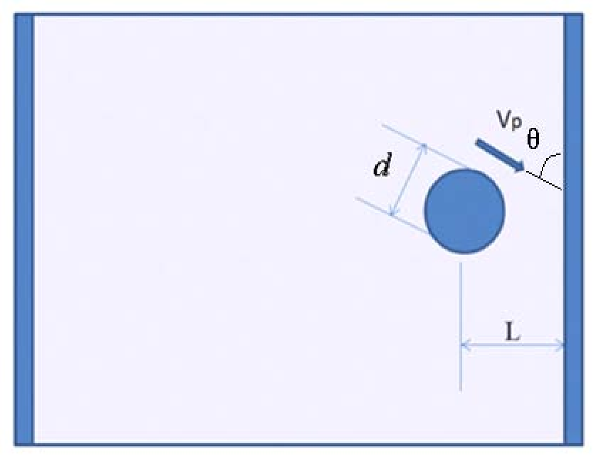
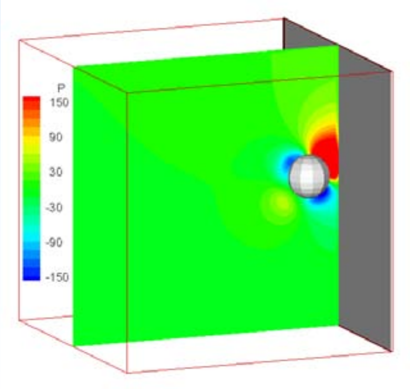
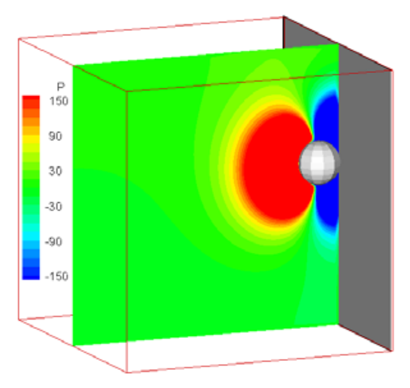
[*] Gondret, P.; M. Lance, & L. Petit (2002), “Bouncing motion of spherical particles in fluids,” *Phys. Fluids*, **14**:643-652 .

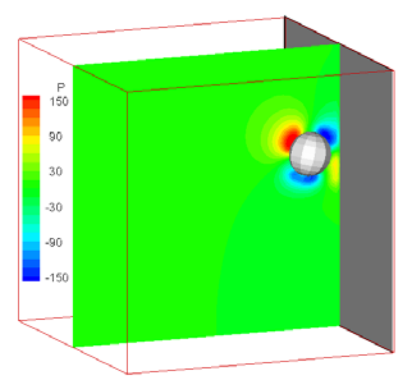
Oblique Particle-Wall Collision (1)

- A particle of diameter d=0.635 cm and density 2.54 g/cm^3 is given an initial velocity v_p≈10 cm/s; it then collides with a wall in water
- Collision angle Θ=45^o
- The soft-sphere model is applied



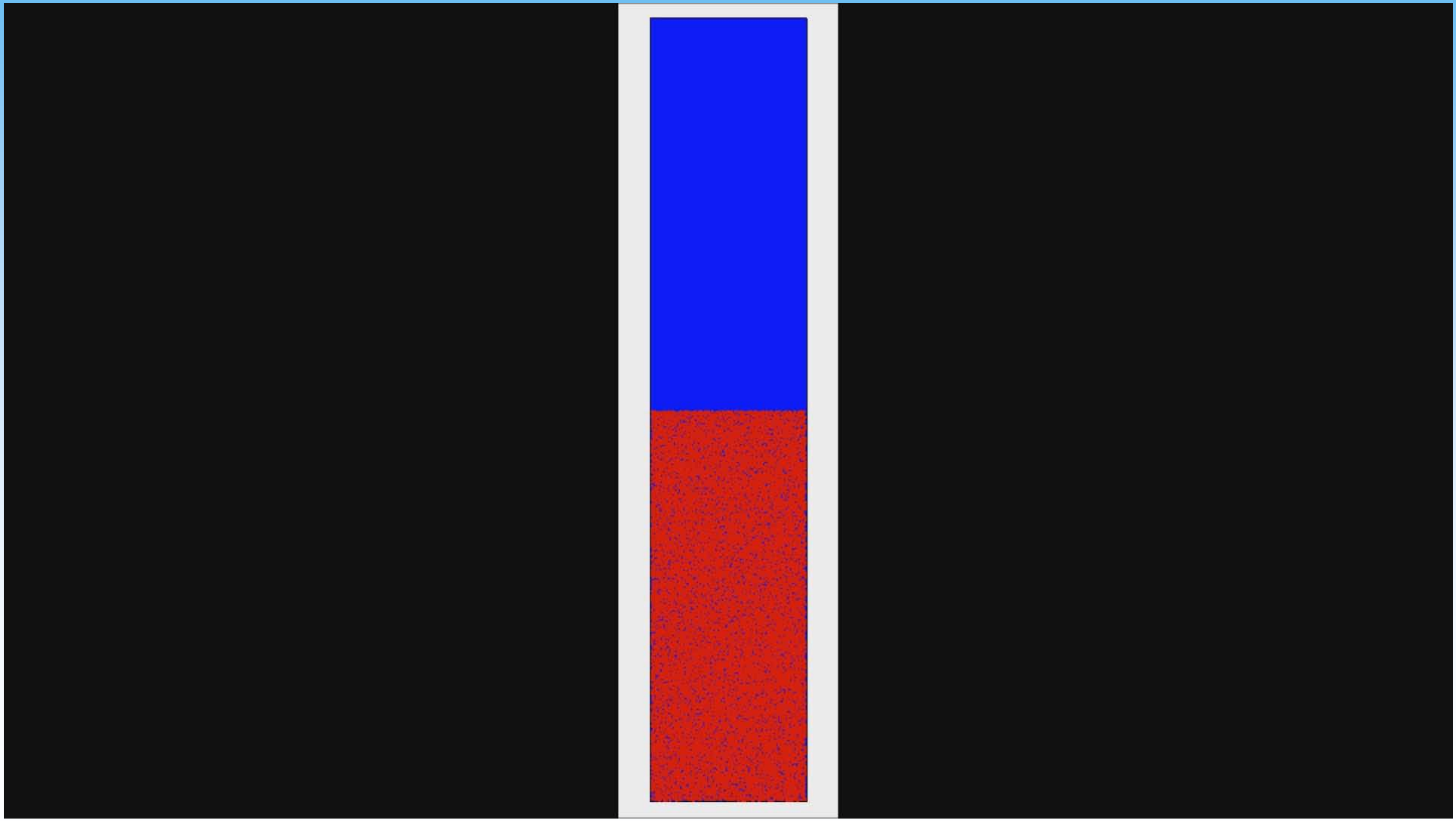






Derivation of velocity profile of solid phase at a wall

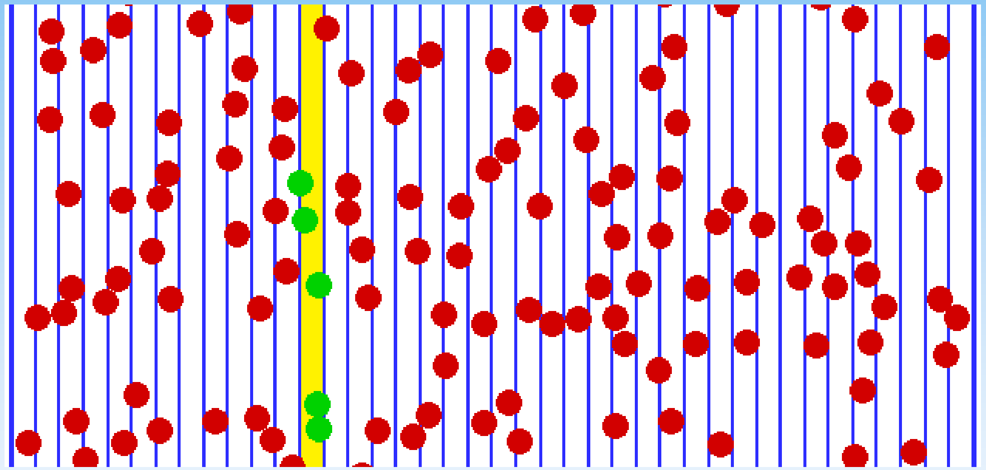
Particles fluidization by a jet



Decomposition domain

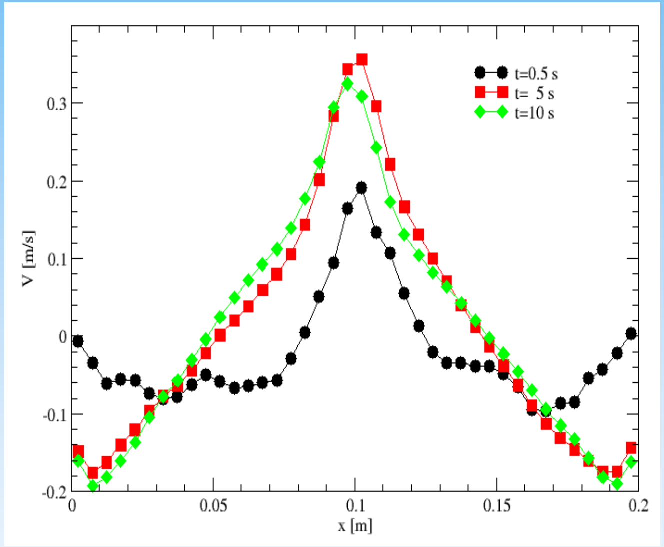
- The width of each section equals to the diameter of the particle
- Statistical velocity
  - Velocity at ith column

$$V_i = \frac{1}{N_{\delta t}} \sum_k \left(\frac{\sum_j V_j(t_k)}{N_i(t_k)} \right)$$

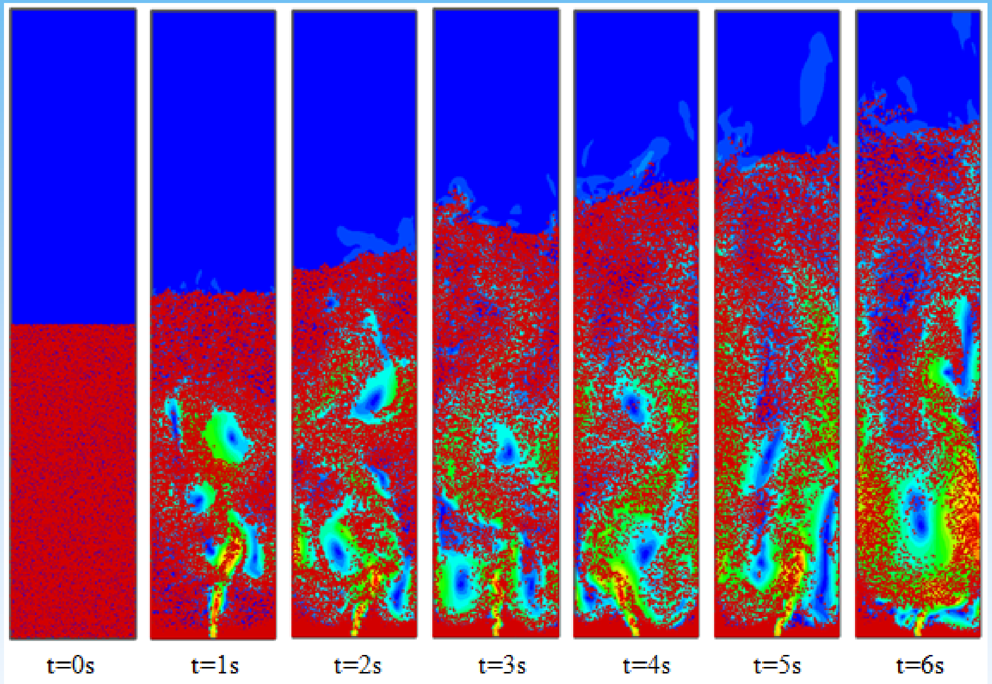


  - Ndt is the total time steps
  - N*i* is the total number of particles within the ith column.

Slip velocity of solid particles at a solid wall



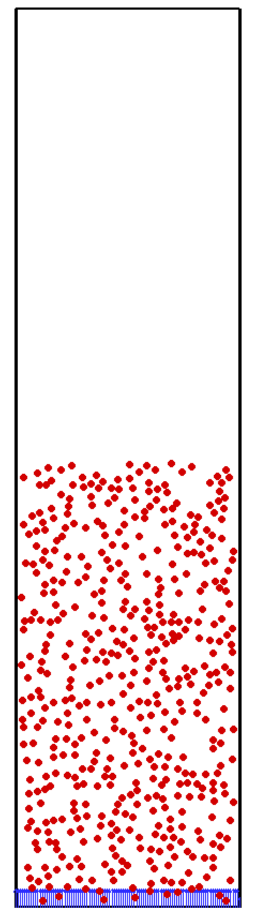
Time-space averaged velocity



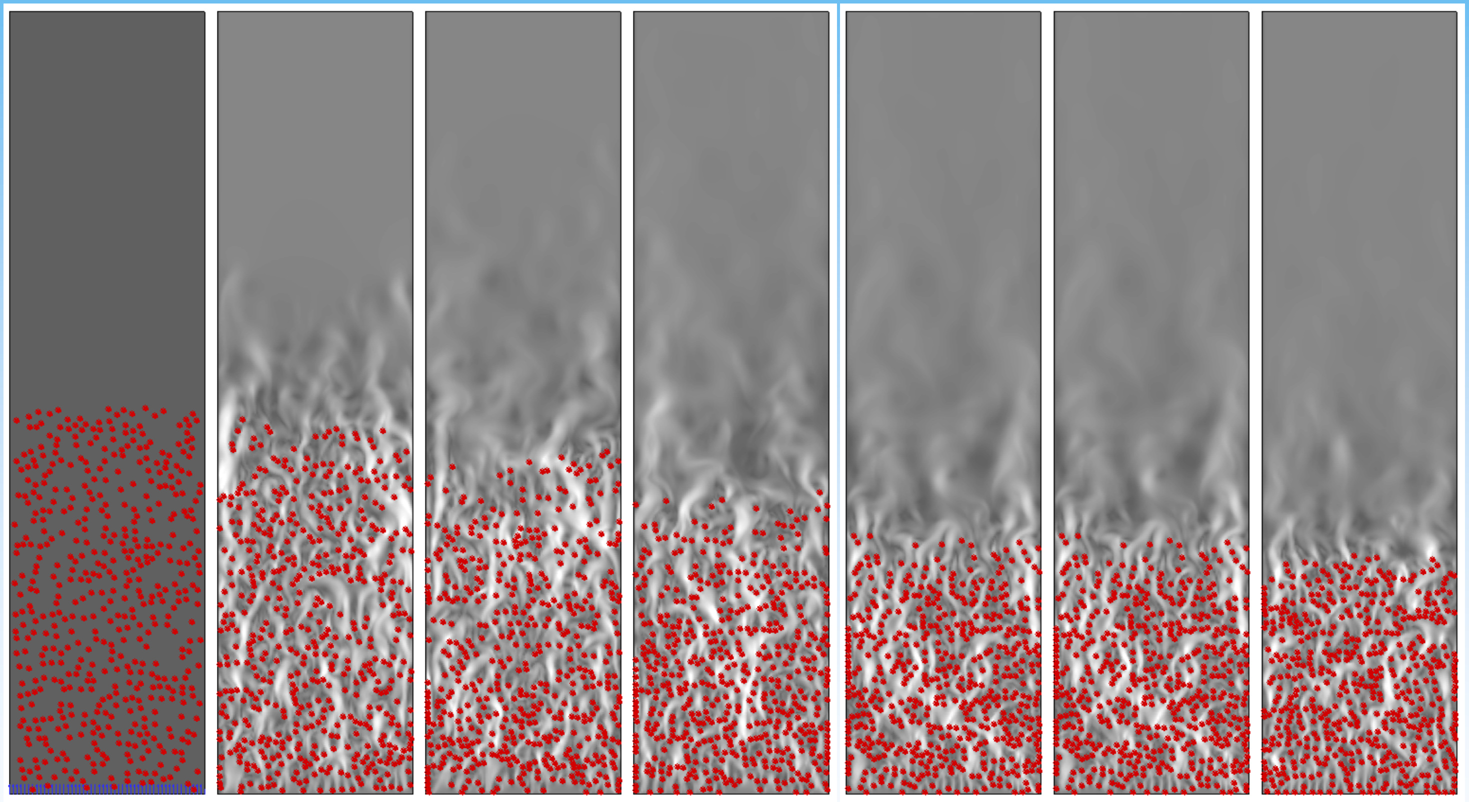
10,000 spherical particles in a jet fluidized bed

DNS Simulation of particle fluidization by a uniform flow

- Simulation Parameters
  - Width w=0.2 m; height h=0.8 m
  - Particle radius r=0.002 m;
  - Fluid density 1000 kg/m3; viscosity 0.001
  - Particle density 2300 kg/m3
  - Uniform fluid velocity at inlet, v=0.12 m/s
  - Dx=0.0004, CFL=1.2
  - Total particles 1274, randomly distributed



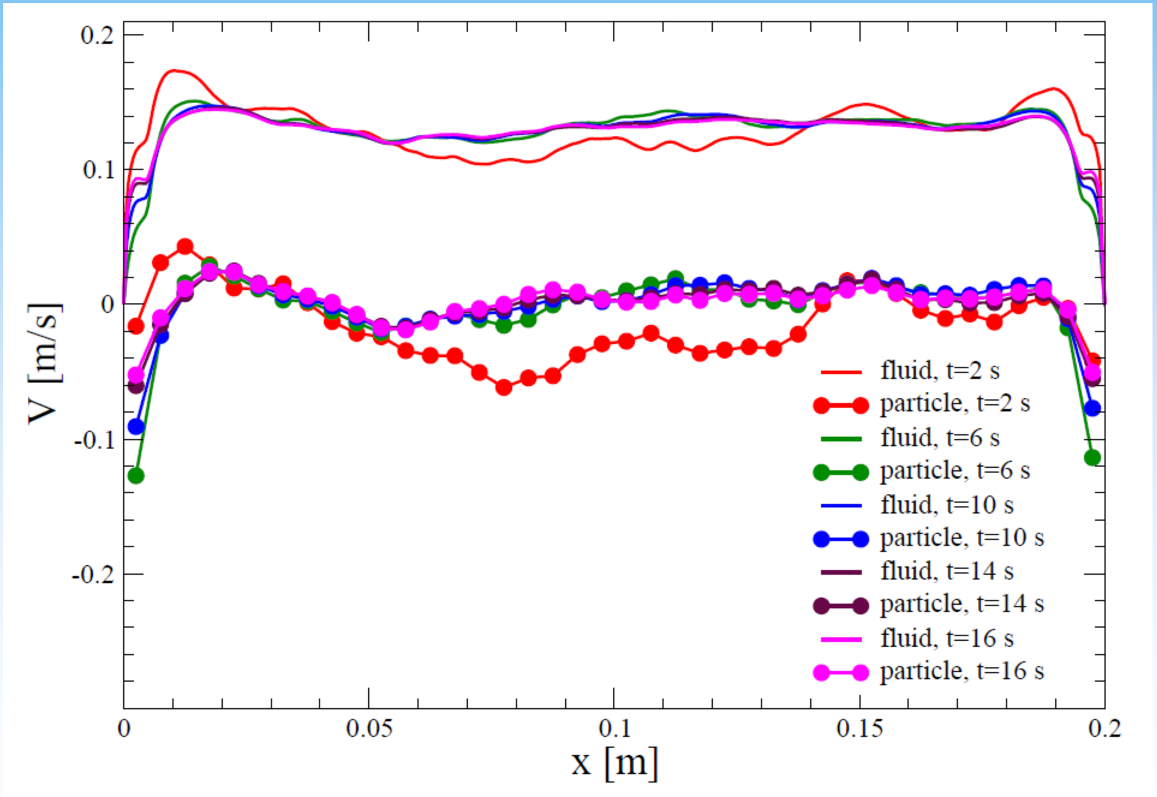
Uniform Fluidization velocity V=12 cm/s



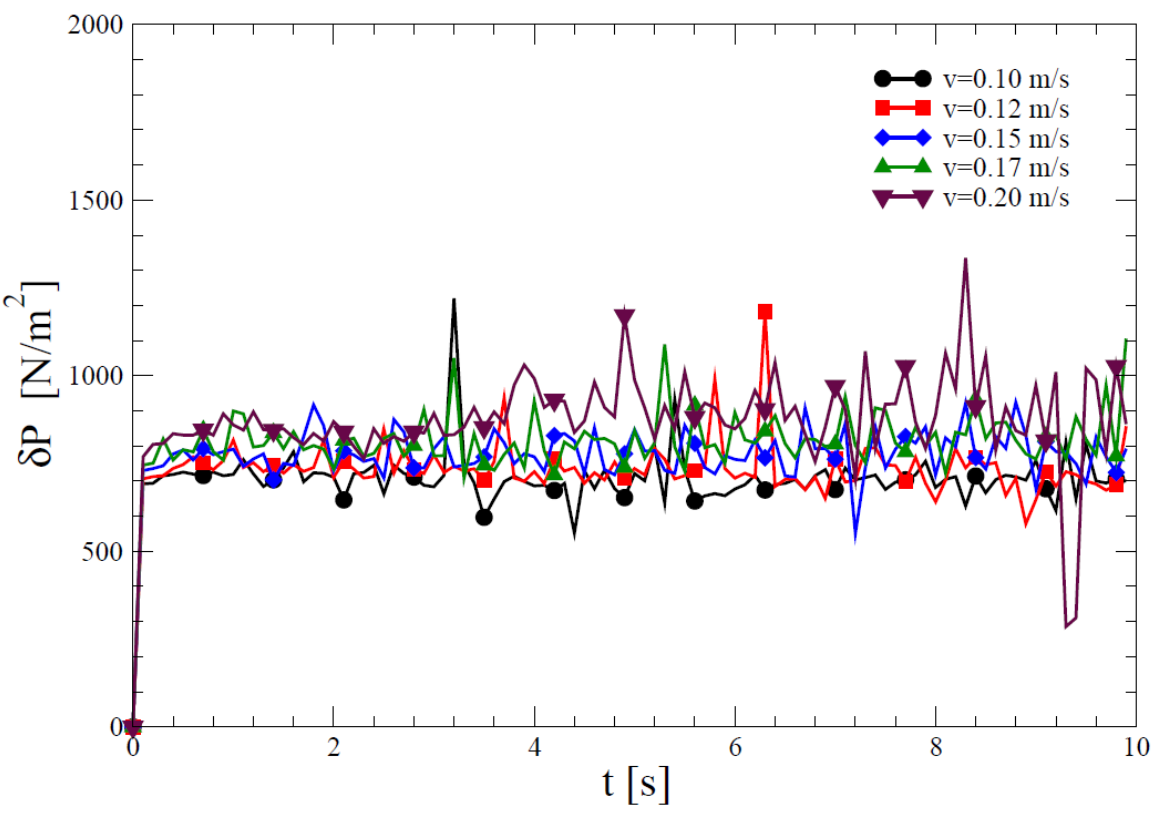
Snapshot at time t=0, 1s, 2s, 3s, 4s, 6s, and 10s.

Velocity profiles of solid phase and fluid phase

- Time and space averaged

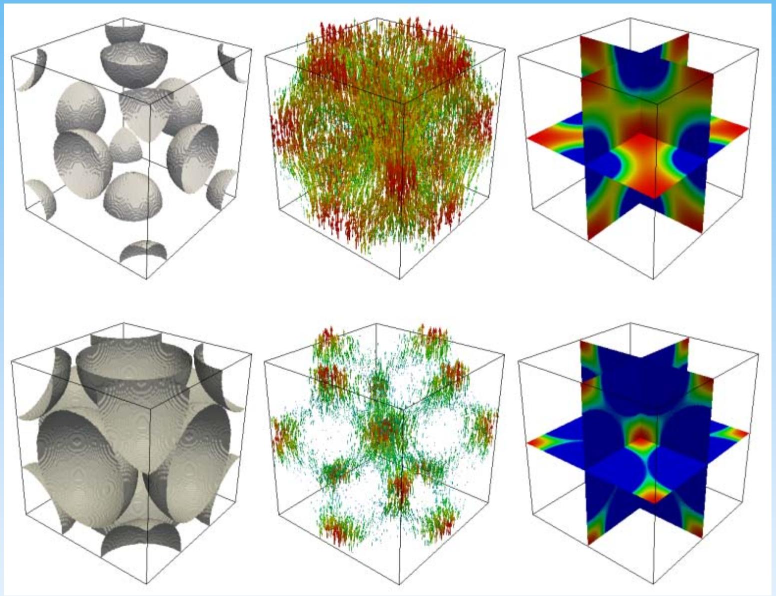


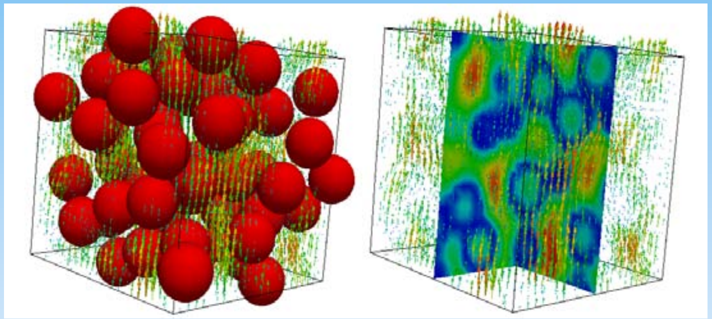
Pressure drop over the bed



Influence of neighboring particles

Flow over arrays of fixed spheres





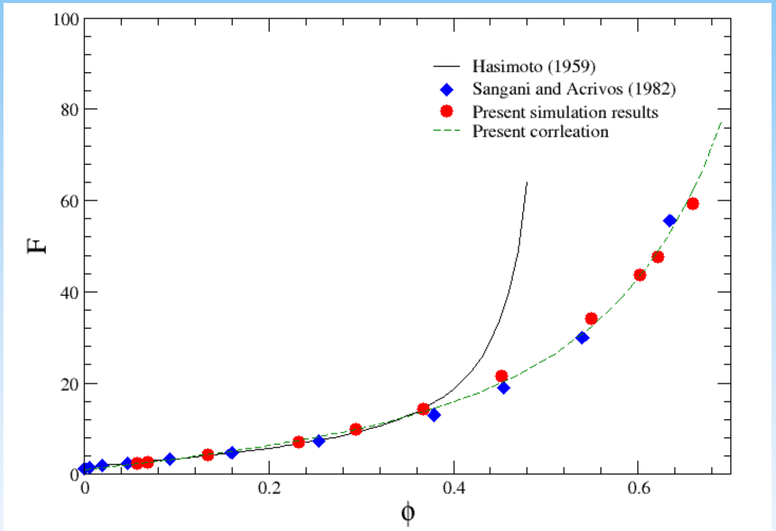
Random arrays of spheres

Face centered arrays of spheres

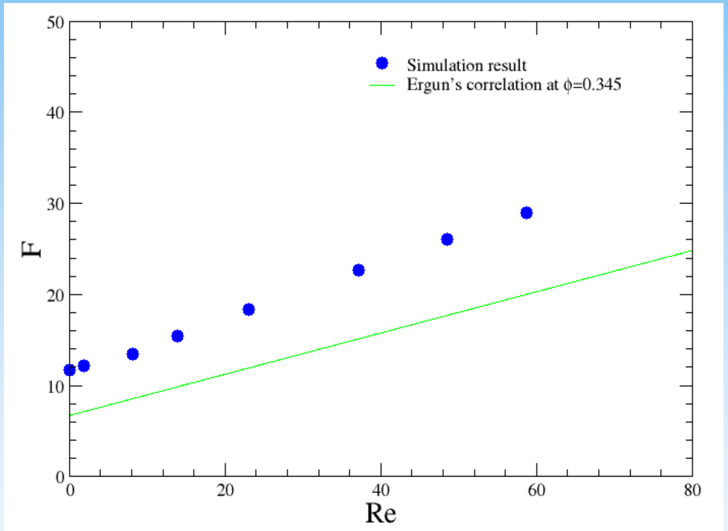
Affect of drag laws due to the neighboring particles

Define dimensionless drag force

$$F = \frac{F_d(\phi)}{6\pi\mu a U}$$



Stoke flows



Flows of different Reynolds number at volume fraction 0.35.

Influence of neighboring particles when particles are in motion

- Physical properties (*)
  - Settling particle diameter d=15mm,density ρ_p=1500kg/m3;
  - Fluid viscosity 0.058 kg/m.s, density=960 kg/m3.
- Simulation parameters:
  - $\delta x = d/16$; $\delta t = 2.5\times10^{-4}$ s;
  - Flow domain: regular grid 96x96x480;
  - Particle: 789 surface nodes for one particle
  - Periodic boundary conditions
  - At zero solid fraction, $U_\infty = 0.27 m/s$; flow Reynolds number ~68.

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*A ten Cate, C. H. Nieuwstad, J. J. Derksen, and H. E. A. van den Akker(2002), “Particle imaging velocimetry experiments and lattice-Boltzmann simulations on a single sphere settling under gravity,” *Phys. Fluids*, **14**: 4012-4025 .

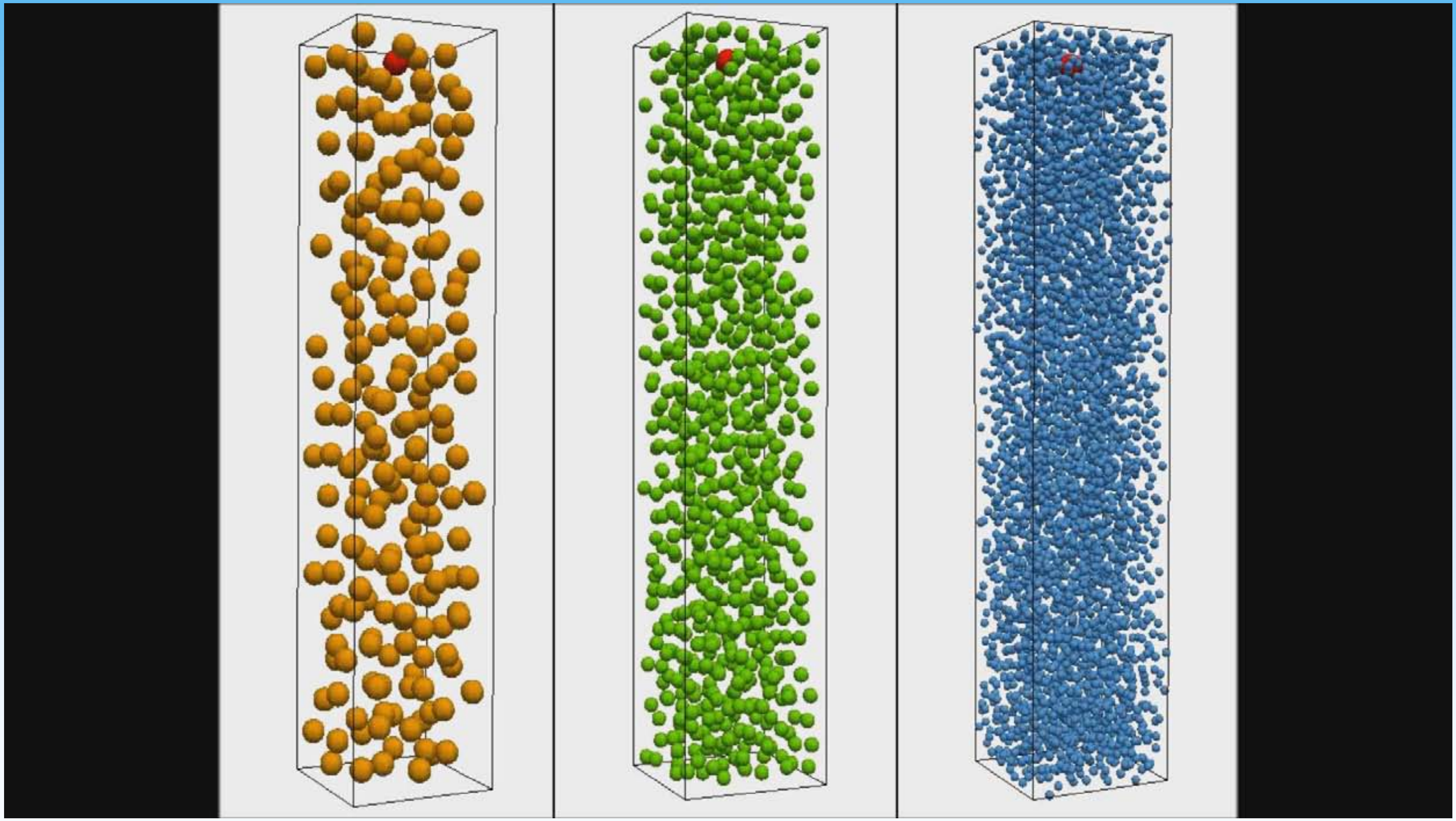
Effect of the size of neighboring particles

- Consider three cases at the same solid volume fraction ϕ=10%

Case No.	Diameter of neighboring particles	Number of neighboring particles
1	1d	200
2	0.625d	819
3	0.375d	3793

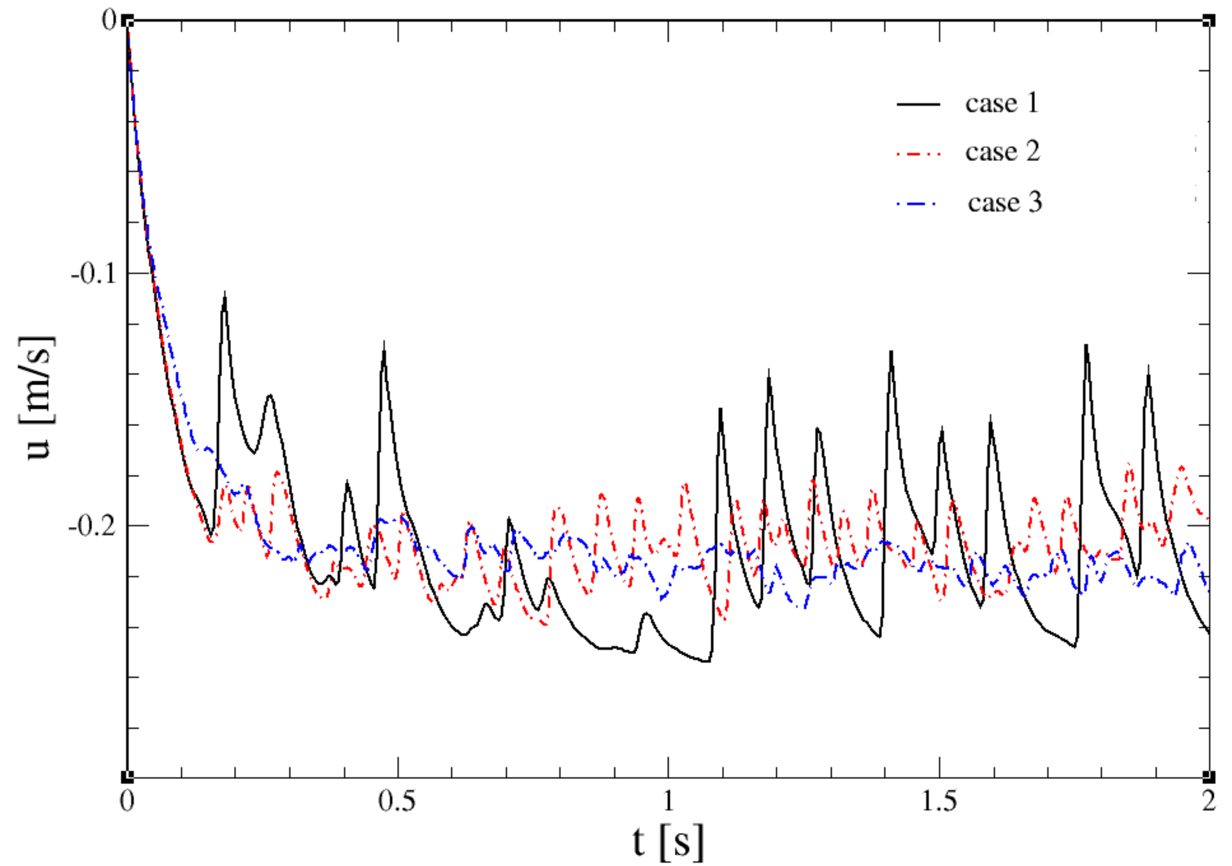
- Question:
  - – Which case the heavy particle falls the fastest?

Settling of a heavy particle in suspension flows with different size of particles



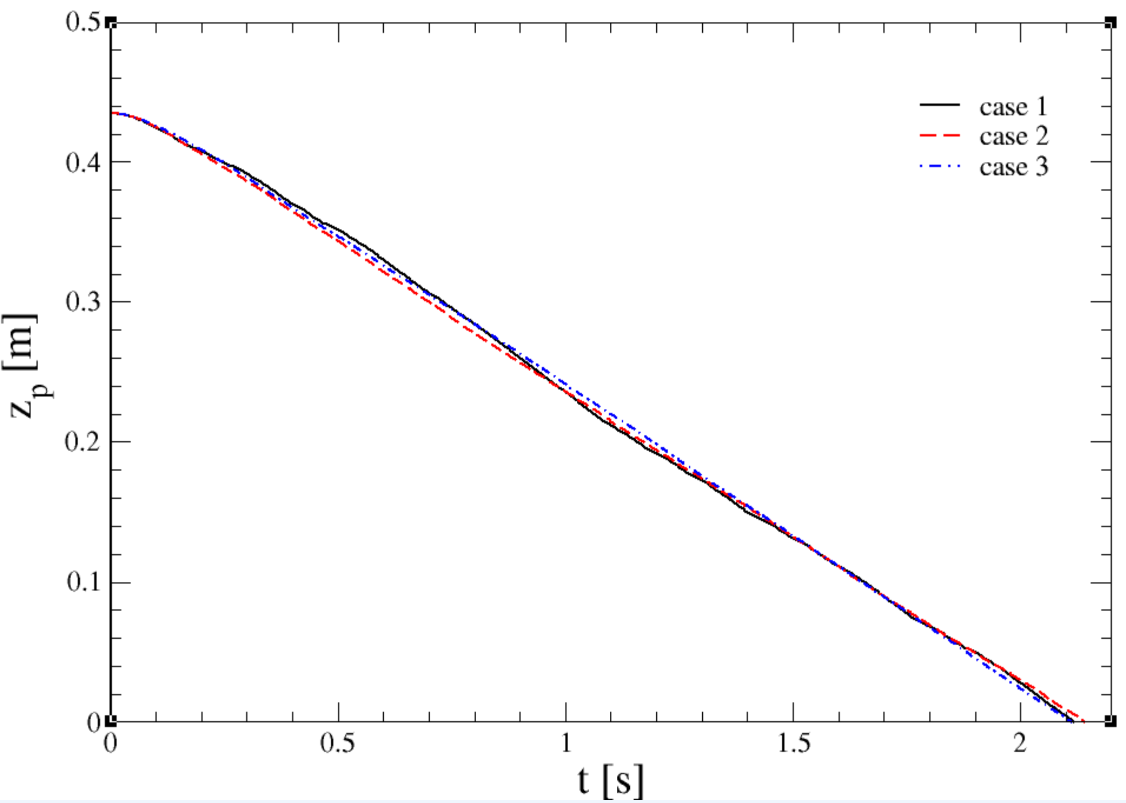
Case 1: N=200   case 2: N=819   case 3: N=3793

Settling velocity of the heavy particle



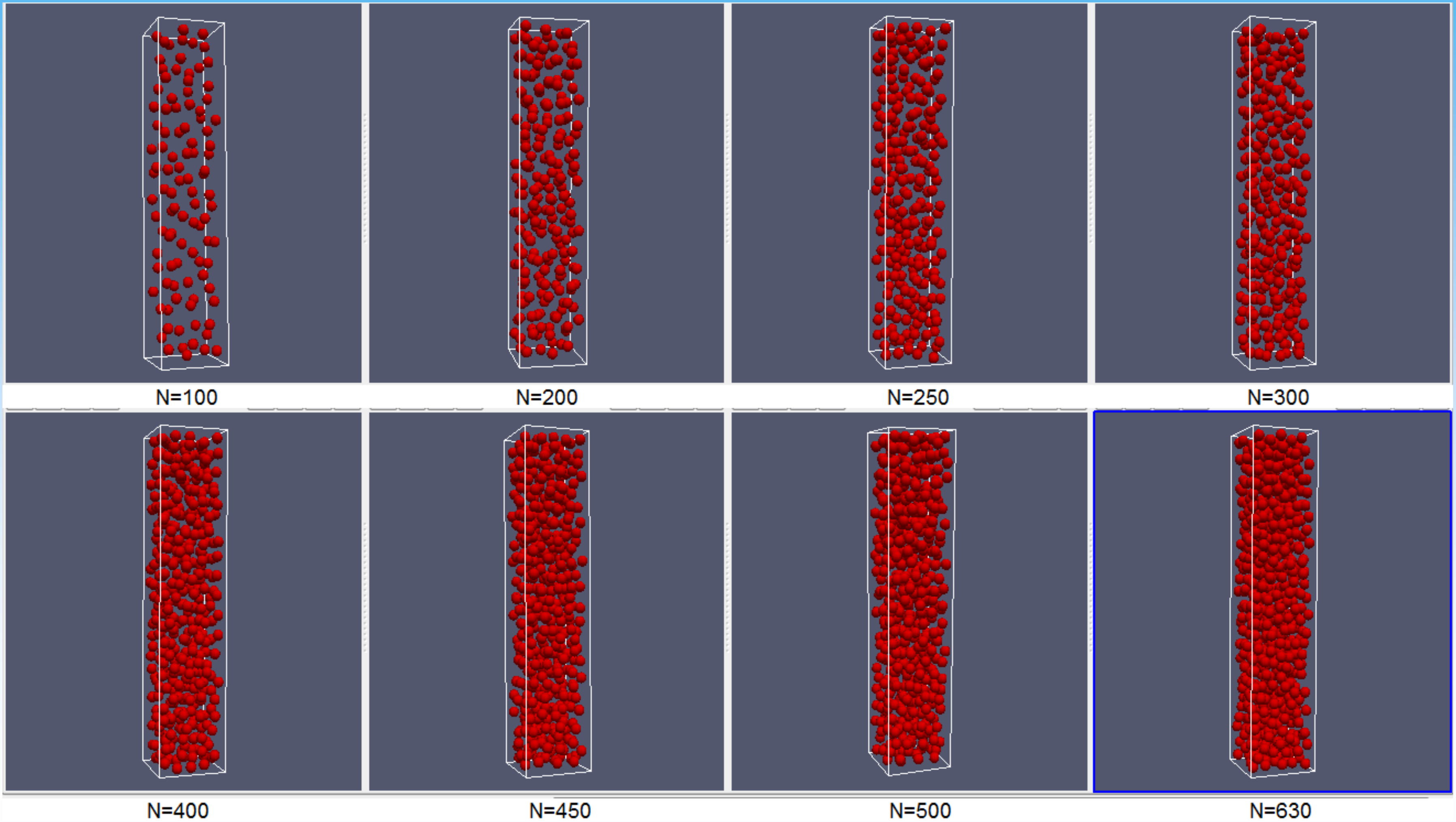
Resistance: drag force + collision force

Vertical position of the heavy particle



Almost the same slope in *z*-*t* graph. The mean settling velocity=slope=0.21 m/s.

Initial distributions of particles at eight different solid fractions



N=100

N=200

N=250

N=300

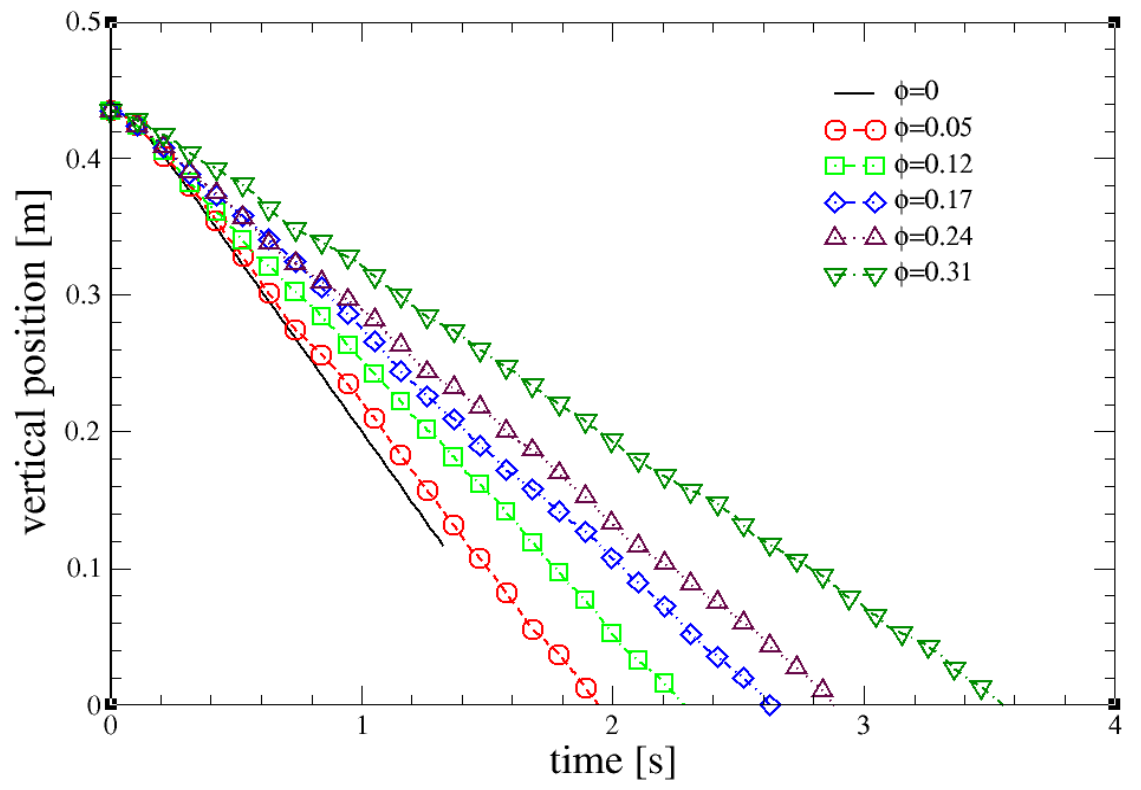
N=400

N=450

N=500

N=630

Vertical position of the settling particle at different solid fractions



After a brief unsteady transition at the beginning, the slope in *z*-*t* graph is nearly a const for each case.

Mixture theory

- Effective density and viscosity of solid-liquid suspension:

$$\rho_m = \rho_f, \quad \mu_m \approx \mu_f \left(1 + 2.5\phi + 5.2\phi^2 + \ldots\right) \quad \text{(Batchelor*)}$$

or $$\mu_m \approx \mu_f \left(1 + 2.5\phi + 10.05\phi^2 + \ldots\right) \quad \text{(Thomas**)}$$

Force balance:

$$C_d(\phi)\frac{1}{2}\rho_m V_t^2(\phi)\frac{\pi d^2}{4} = \left(\rho_p - \rho_f\right)\frac{1}{6}\pi d^3$$

Empirical drag law: $C_d(\phi) = (0.63 + \frac{4.8}{\sqrt{\mathrm{Re}(\phi)}})^2$

Only unknown: $V_t(\phi)$

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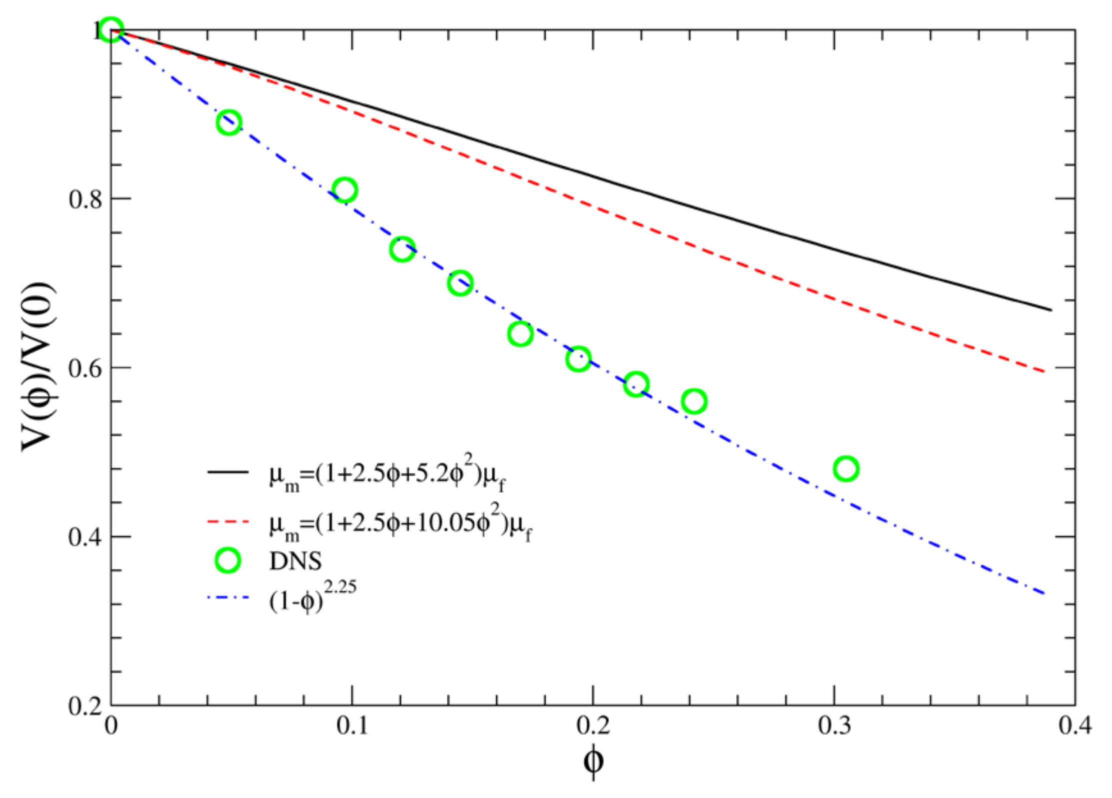
*G.K. Bachelor, 1967, *An Introduction to Fluid Dynamics, Cambridge University Press, Cambridge*

** Thomas, D., Transport characteristics of suspensions: VIII. A note on the viscosity of Newtonian suspensions of uniform spherical particles, *J. Colloid Sci., 20, 267–277, 1965.*

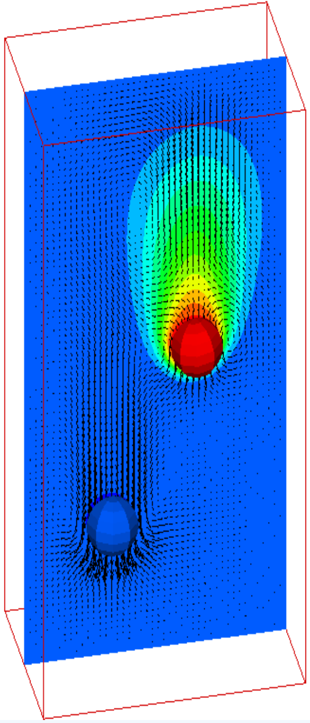
Theory and simulation results

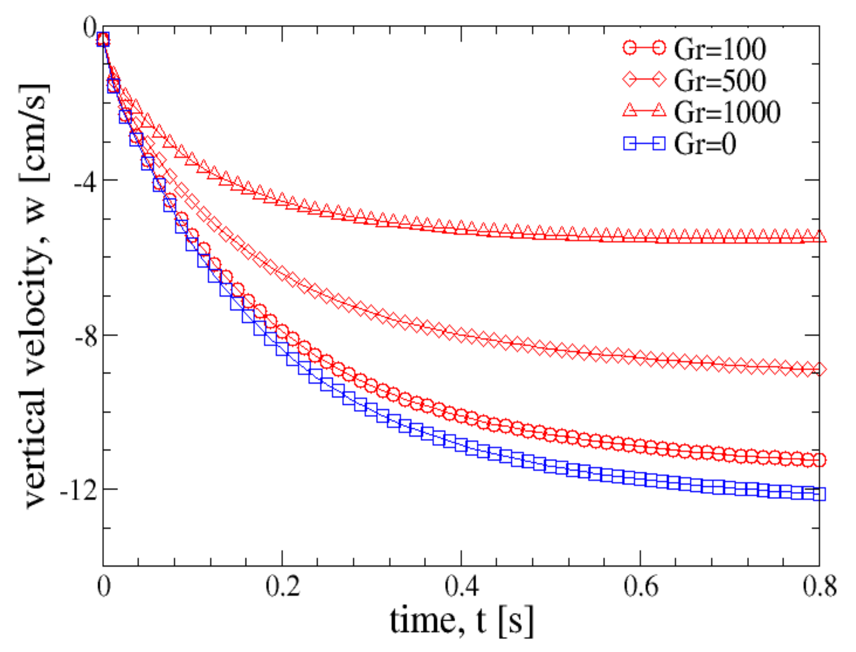


Possible cause: the mixture theory doesn't account for the particle-particle collisions which are critical when particles have comparable sizes.

DNS for heat transfer between particles and fluid

Effect of thermal buoyancy effect to the motion of particles





Falling of spheres of different temperatures

Particle clustering

Summary

- A *Direct Numerical Simulation (DNS)* method has been successfully developed and extensively validated.
- *DNS* is able to produce detailed information of particles and fluid dynamics in particulate flows.
- *DNS* combined with the soft-sphere collision model (with proper input parameters) is able to capture the dynamics of particle-wall collisions.
- DNS has been used to study particles slip velocity at a solid wall.
- The drag force on a particle is strongly influenced by its neighboring particles.
- DNS can be used to predict particles clustering/agglomeration in particulate flows.
- DNS has been used to investigate the influence of a particle temperature to its motion.

Papers Published

- **Peer Reviewed Journal Papers:**
  - Feng, Z.G., Michaelides, E. E. and Mao, S.L., 2010, “A Three-Dimensional Resolved Discrete Particle Method for Studying Particle-Wall Collision in a Viscous Fluid,” *J. of Fluids Eng.*, vol. 132, number 091302, 2010.
  - Feng, Z.-G., Michaelides, E. E. and Mao, S.-L., 2012, “On the drag force of a viscous sphere with interfacial slip at small but finite Reynolds numbers,” *Fluid Dynamics Research*, *Fluid Dyn. Res.* 44 025502 doi:10.1088/0169-5983/44/2/025502.
  - Buseh, C., Feng, Z.-G., and Paudel, B.D. (2010), “An experimental study of fluidization of bidisperse particulate flows,” *Journal of Dispersion Science Technology* (accepted).
  - Kartushinski, A., Michaelides, E. E., Rudi, Y., and Graham, N. (2010), “RANS Modeling of a particulate turbulent round jet,” *J. of Chem.Eng Sci.*, in print, doi:10.1016/j.physletb.2003.10.071.
  - Yang, B. J., Mao, S. L., Altin, O., Feng, Z. G. and Michaelides, E. E., 2011, “Condensation Analysis of Exhaust Gas Recirculation (EGR) Cooler for Heavy-Duty Trucks,” *Applied Thermal Engineering*, volume 3, doi:10.1115/1.4004745.
  - Michaelides, E. E., and Roig, A., 2010, “A Reinterpretation of the Odar and Hamilton Data on the Unsteady Equation of Motion of Particles,” A.I. Ch. E. Journal, DOI 10.1002/aic.12498, 2010.
  - A.P. Davis, et al., 2011, Particle velocity near vertical boundaries — A source of uncertainty in two-fluid models, Powder Technol., doi:10.1016/j.powtec.2011.09.031
  - Michaelides, E. E., 2012, “Entropy Production and Optimization of Geothermal Power Plants,” *J. of Non-Equilibrium Thermodynamics*, Accepted for publication.

- **Conference Papers:**
  - Feng, Z-G, Michaelides, E. E., and S-L Mao (2010), “Investigation of Particle-Wall Collisions in a Viscous Fluid using a Resolved Discrete Particle Method,” August 1-5, 2010, Montreal, Canada.
  - Feng, Z-G, X. Zhang and Basu D. Paudel (2010), "An immersed boundary based method for studying thermal interaction of a solid in a viscous fluid, "ASME 3rd Joint US-Europen Fluids Engineering Summer Meeting, August 1-5, 2010, Montreal, Canada.
  - Davis, A. P., Michaelides, E. E., and Feng, Z.-G. (2010), “Particle velocity near vertical boundary - a source of uncertainty in two-fluid models,” 7th International Conference on Multiphase Flow, FL. May 30-June 4, 2010.
  - A. P. Davis, Z-G Feng and E. E. Michaelides, “Application of the Immersed Boundary Method and Direct Numerical Simulation for the Heat Transfer from Particles,” Proceedings of the 2009 ASME-FEDSM, meeting of the Division of Fluids Engineering at Veil, CO.
  - Roig, A. and Michaelides, E.E., “A re-interpretation of the Odar and Hamilton data on the history terms of the equation of motion,” ICMF-2010, May 2010, Tampa, FL.
  - (keynote presentation) Michaelides, E. E. and Feng, Z.-G., “Direct Numerical Simulations of Particulate Flows that Include Momentum, Heat and Mass Exchanges” ICMF-2010, May 2010, Tampa, FL.
  - Alexander Kartushinsky and Efstathios E. Michaelides, “RANS Modeling of a Particulate Turbulent Downward Jet,” 7th International Conference on Multiphase Flow, ICMF 2010, Tampa, FL, May 30 – June 4, 2010.
  - Feng, Z.-G. and Michaelides, E. E., 2010, "Simulation Of The Particle-Wall Collisions In A Viscous Fluid Using A Resolved Discrete Particle Method," Proceedings of the ASME 3rd Joint US-European Fluids Engineering Summer Meeting, FEDSM-ICNMM 2010, August 1-5, 2010, Montreal, Canada.
  - Feng, Z-G, Michaelides, E. E., and Mao, Shaolin, 2011,“A multilevel simulation approach to derive the slip boundary condition of the solid phase in two-fluid models,” 64th Annual Meeting of the APS Division of Fluid Dynamics, Baltimore, Maryland. November, 2011.
  - Feng, Z-G, and Samuel, G.M., “The Effect of Neighboring Particles on the Dynamics of a Particle in a Viscous Fluid,” NETL 2012 Conference on Multiphase Flow Science, NRCCE, Morgantown, WV. May 22-24.
  - Feng Z-G, Musong, S.G. and Michaelides, E.E., “Effect of Model Parameters of Soft-Sphere Collision Scheme to the Particle-Particle Collision in a Viscous Fluid,” NETL 2012 Conference on Multiphase Flow Science, NRCCE, Morgantown, WV. May 22-24.

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