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

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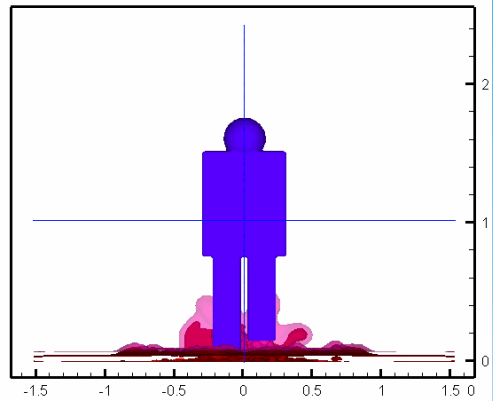
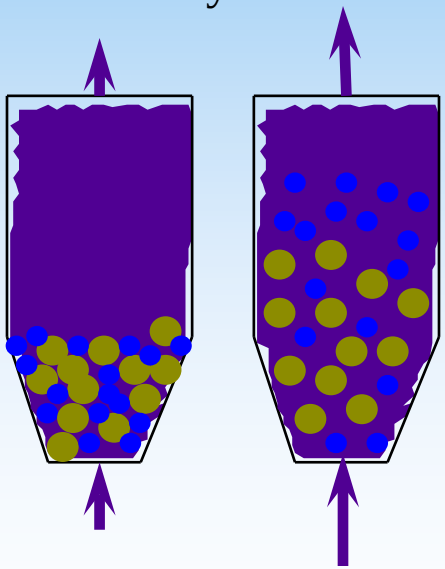
Background on Particulate Flows

- 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

Purification of Sea Sand Polluted by Heavy Oil with Fluidized Combustion Reactor

- Sand polluted with heavy oil could have large influence to ecosystem for long term
- To clean polluted sand can be very expensive
- A simple and very effective approach:
  - *fluidized bed combustion reactor*

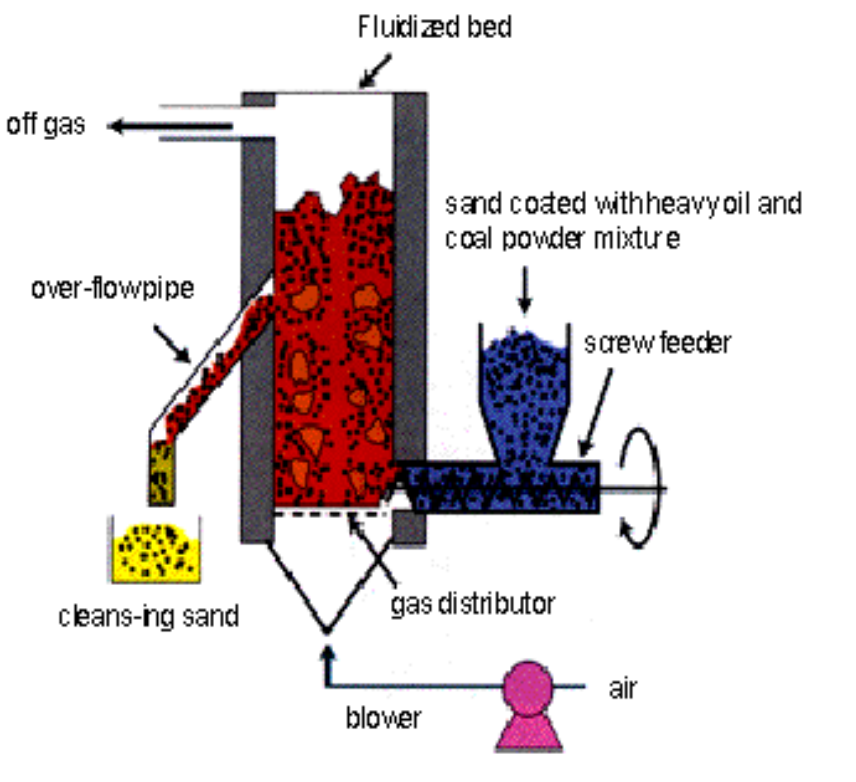
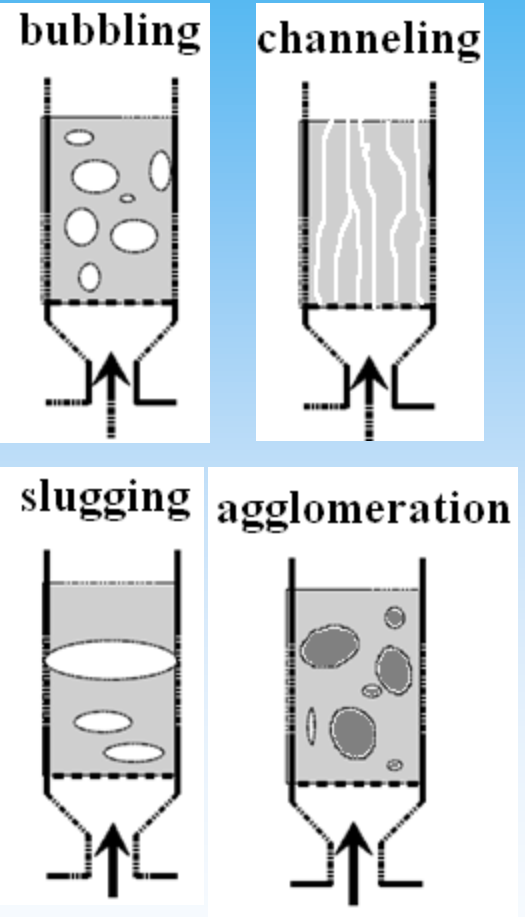


Image courtesy: National Institute of Advanced Industrial Science and Technology (AIST), Japan.

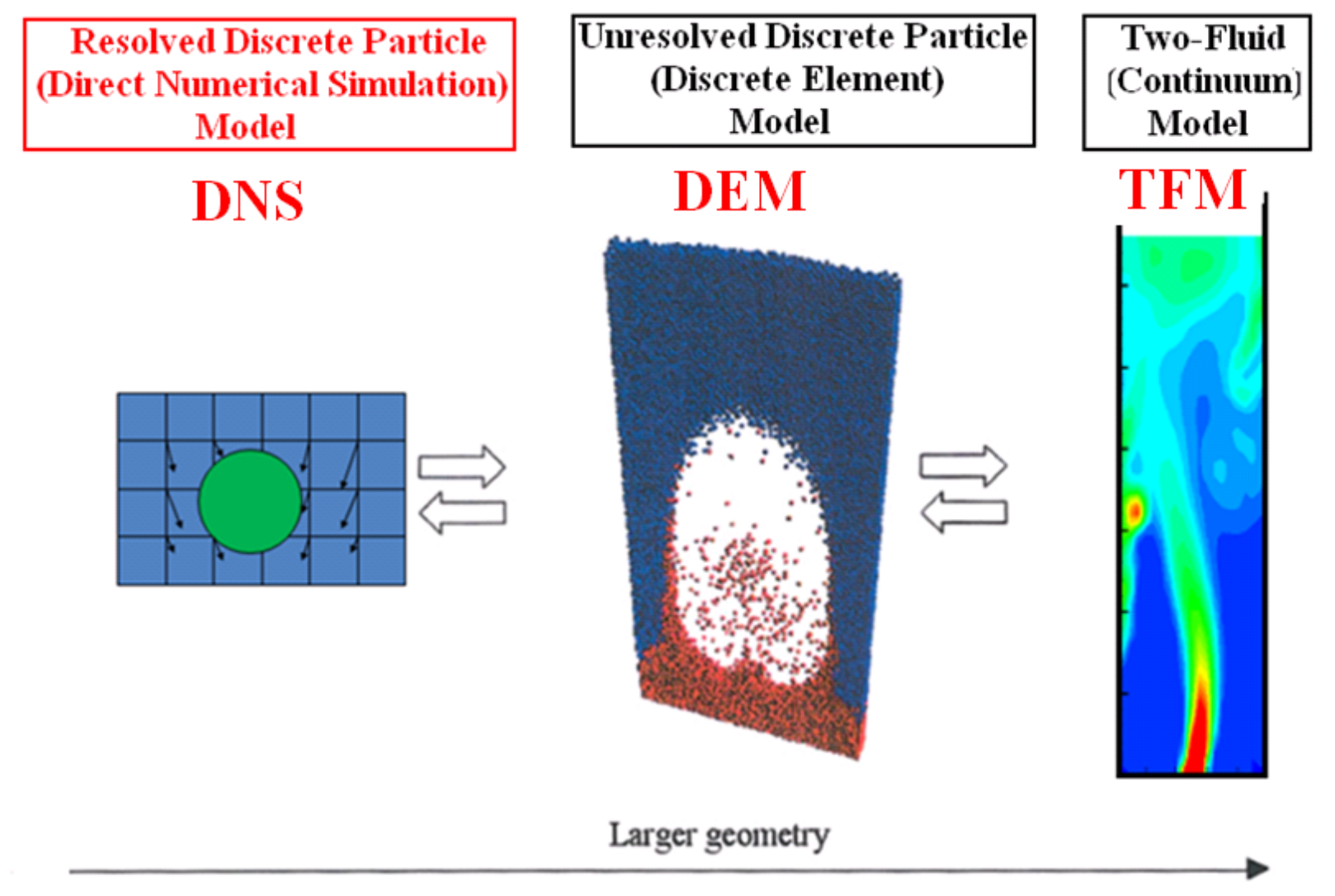
Main Problems in a Fluidized Bed

- Complex flow behavior
  - Bubbling: area with very few particles
  - Slugging: bubbles occupy entire cross section and divide the bed into layers
  - Channeling: channels through which most of the fluid passes
- Agglomeration
  - Sticky or wet particles agglomerated to form larger particles
- Segregation
  - Mainly due to particles' different sizes and properties
- Consequences
  - Defluidization, undesired variations in product quality, deterioration of the mixing efficiency, etc al.



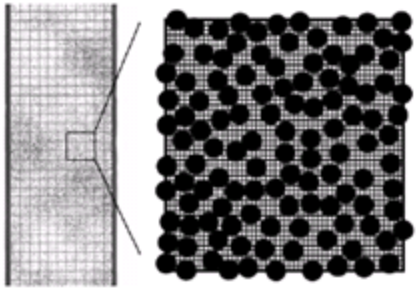
CFD provides a tool that predicts performance at a much higher level of details

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

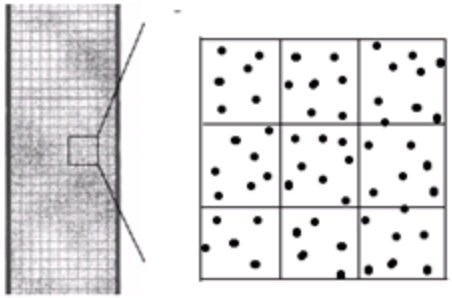
$$\frac{d}{dt} m\vec{v}_i = \sum_j \vec{F}_{ij} + \sum \vec{F}_b + \oint_{\partial S} \tilde{\sigma}\cdot d\vec{s}; \quad \tilde{I}_i \frac{d\vec{\omega}_i}{dt} = \oint_{\partial S} (\vec{x} - \vec{x}_i) \times (\tilde{\sigma}\cdot d\vec{s})$$

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

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

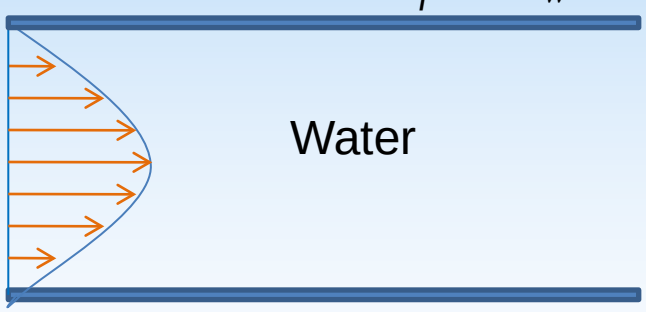
$$\tau_s = -\mu_s\left[(\vec{\nabla}\vec{v}) + (\vec{\nabla}\vec{v})^T - \frac{2}{3}(\vec{\nabla}\cdot\vec{v})I\right]$$

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

Importance of Boundary Conditions in CFD Simulations

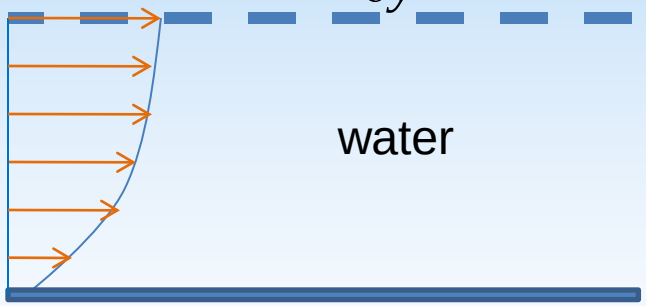
- Industrial scale simulations require two-fluid model
- Simulation results of two-fluid model strongly depend on the boundary conditions of solid phase
- Uncertainties on boundary conditions affect the accuracy of simulation results

$$v_f = v_w = 0$$



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*

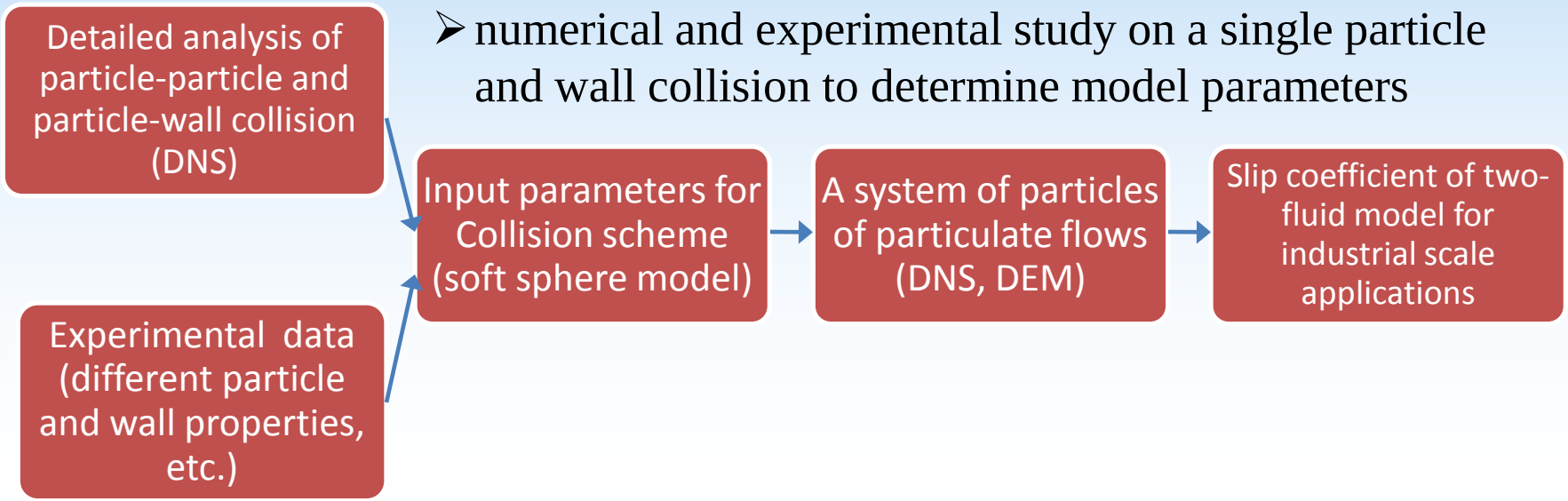
$$\frac{\boldsymbol{n}\cdot\sigma\cdot\mathbf{v}}{|\mathbf{v}|} + \sigma^f_{yy}\tan\delta' + \frac{\phi'\sqrt{3}\,\pi\rho_p\nu T^{1/2}|\mathbf{v}|}{6\nu_0[1-(\nu/\nu_0)^{1/3}]} = 0$$

    - 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 slip boundary condition model

* 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 Multiscale 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)
          - numerical and experimental study on a single particle and wall collision to determine model parameters

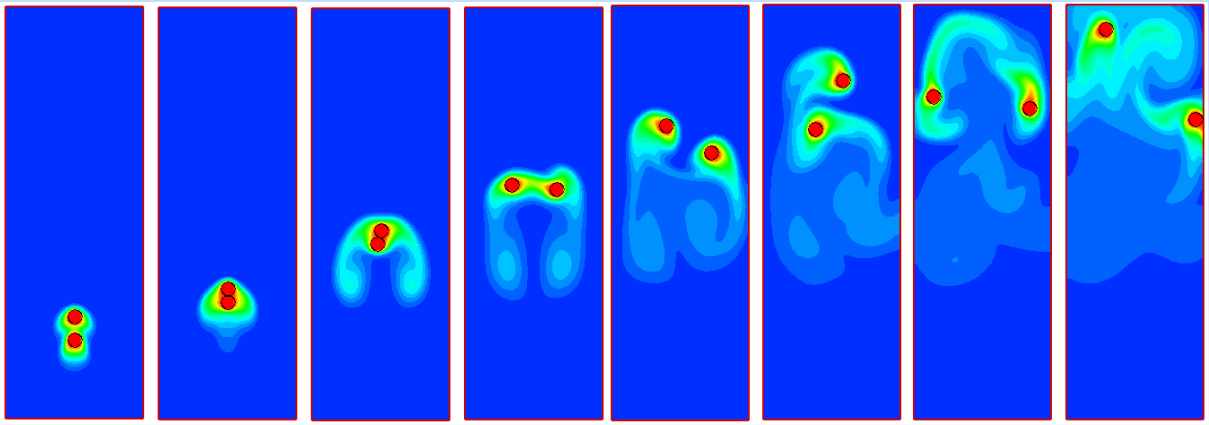


DNS (RDPM) Methods for Particulate Flows

- **Stokesian Dynamics** (Brady, 1980s)
  - Valid for Stokes flow (Re<<1), spherical particles
- **Finite Element Method** (Joseph 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, moderate efficient, complicated to implement
- **Lattice Boltzmann Method** (Ladd, 1994)
  - Low Reynolds number, high efficient and fast, suitable for parallel computing
- ***Proteus* Method** (Feng & Michaelides, 2005)
  - Low to medium Reynolds number, easy to implement, improved accuracy compared to LBM
- ***Inclusion of Heat Transfer in DNS*** (Feng and Michaelides, 2008)
  - Extend ***Proteus*** method to solve heat transfer in particulate flows

Inclusion of Heat Transfer in DNS

- *Direct Forcing Scheme* for treating solid boundary
  - Compute force density function directly from fluid and particle velocities
  - Eliminate the need of reference points and spring constant
- *DNS* for heat and mass transfer
  - Introduce the concept of thermal energy density function

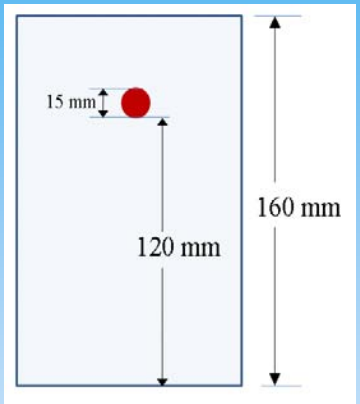


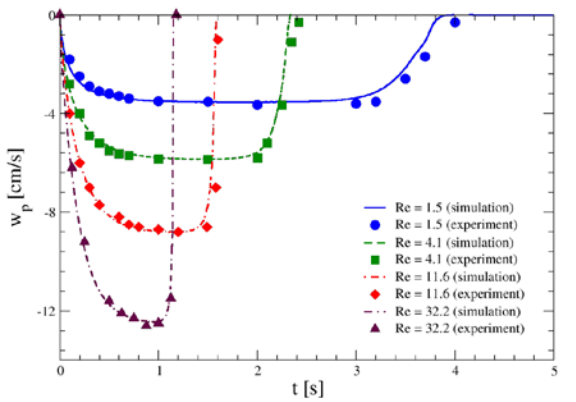
Rising of two hot particles in a channel*

Feng, Z.-G. and Michaelides, E. E. (2008), "Inclusion of heat transfer computations for particle laden flows," *Phys. Fluids*, vol. **20**:675-684.

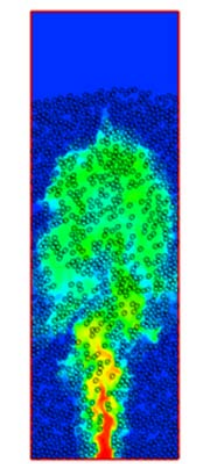
Validations of DNS

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





- Fluidization of 3000 glass beads**

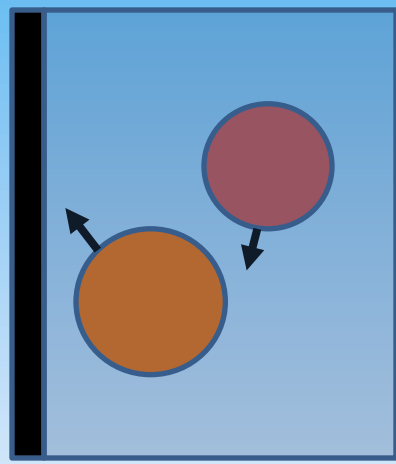


** Obuseh, C., Feng, Z.-G., and Paudel, B.D. (2010), "An experimental study of fluidization of bidisperse particulate flows," *Journal of Dispersion Science Technology* (accepted).

* 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 .

Particle-Wall and Particle-Particle Collisions

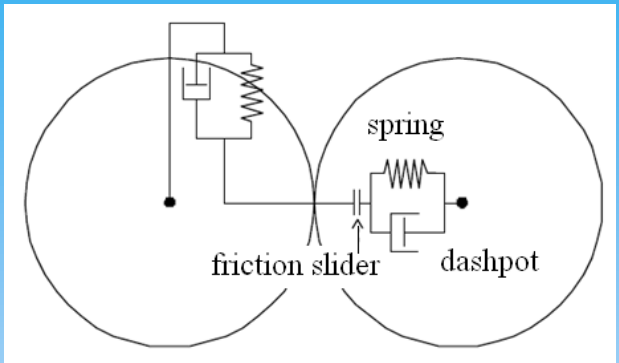
- Collisions occur frequently, especially for dense particulate flows
- Collision models
  - Hard-sphere model
    - No overlap; inefficient for a large number of particles.
  - Soft-sphere model
    - Widely used; allow small overlap; collision forces are computed based on overlap distance; need input 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

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



- 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

* 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.

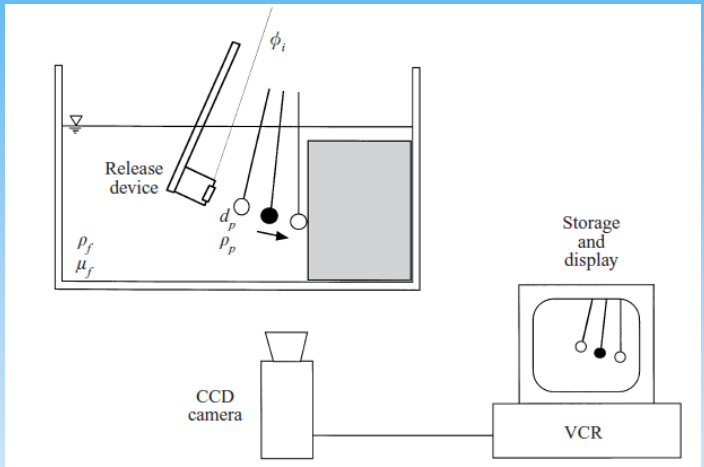


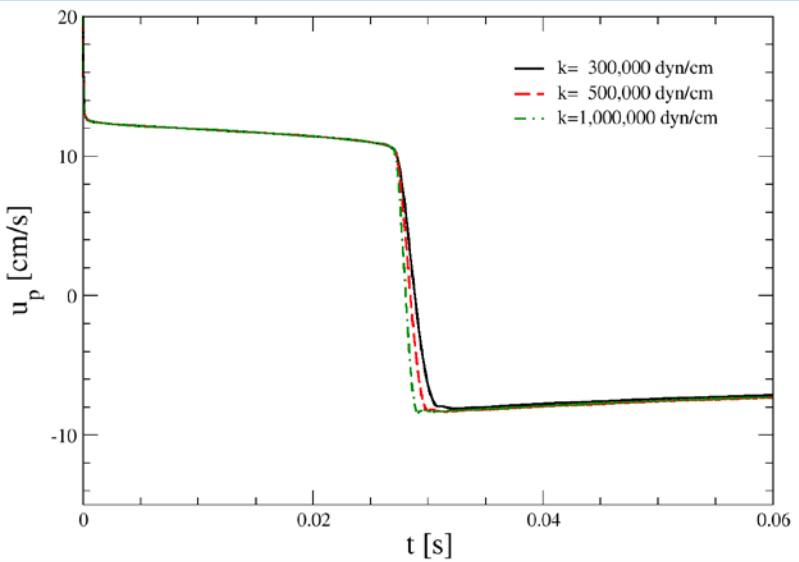
Image courtesy : Joesph et al. *

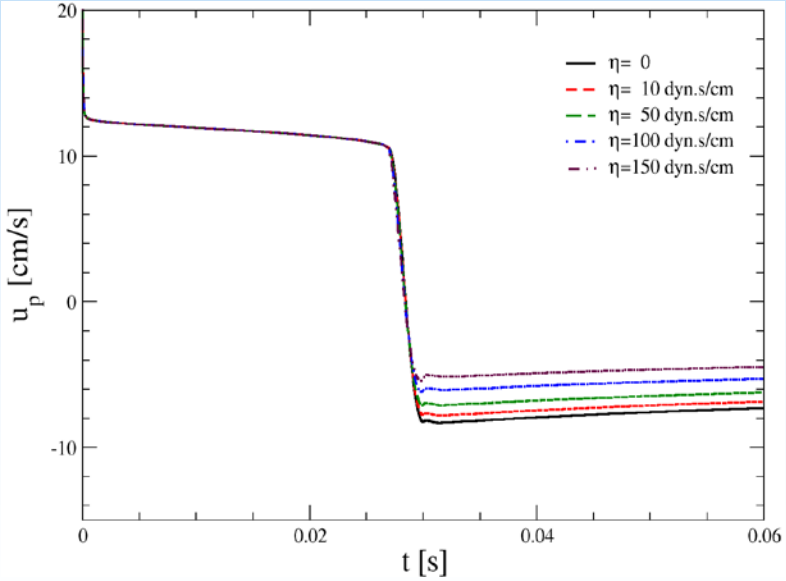
- DNS + Collision Model
  - fluid field is directly solved by DNS
  - collision is handled by the soft-sphere model
    - select model parameters to match experimental data

* 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)

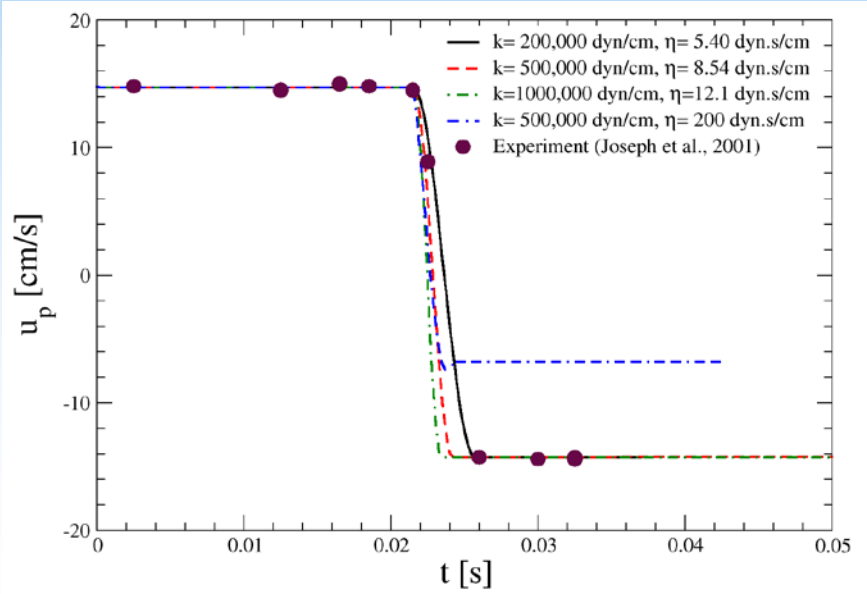
- Simulations are done using DNS combined with the soft-sphere collision model
- Study the effect of model parameters to the dynamics of particle in collision
  - Spring stiffness affects the duration time of collision
  - Damping coefficient affects the rebounding velocity





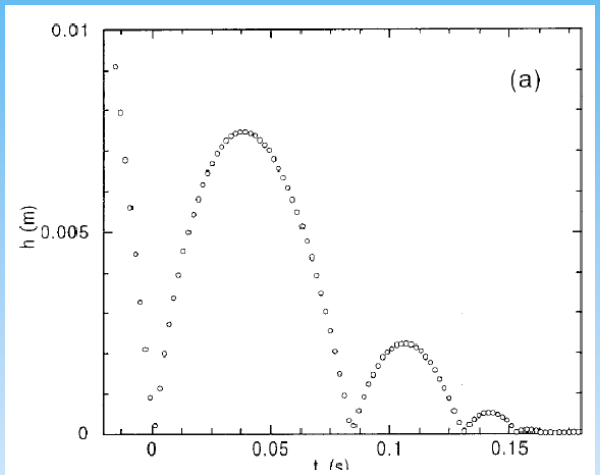
Central Particle-Wall Collision (3)

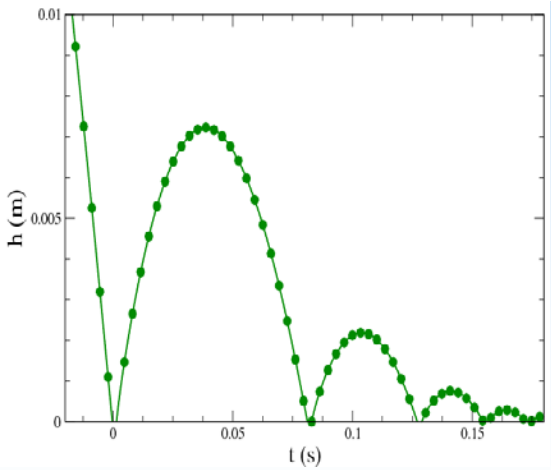
- Experimental conditions
  - Central particle-wall collision in air
  - Particle: glass sphere; d=0.635 cm, ρ_p=2.54 g/cm3;
  - Fluid: air, ρ_{air}=0.001025 g/cm^3, μ_{air}=0.018 cP, Re=62.5.
  - Wall: zerodur wall
- Best mach of model parameters
  - k=200,000dyn/cm
  - η=5.40 dyn.s/cm



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

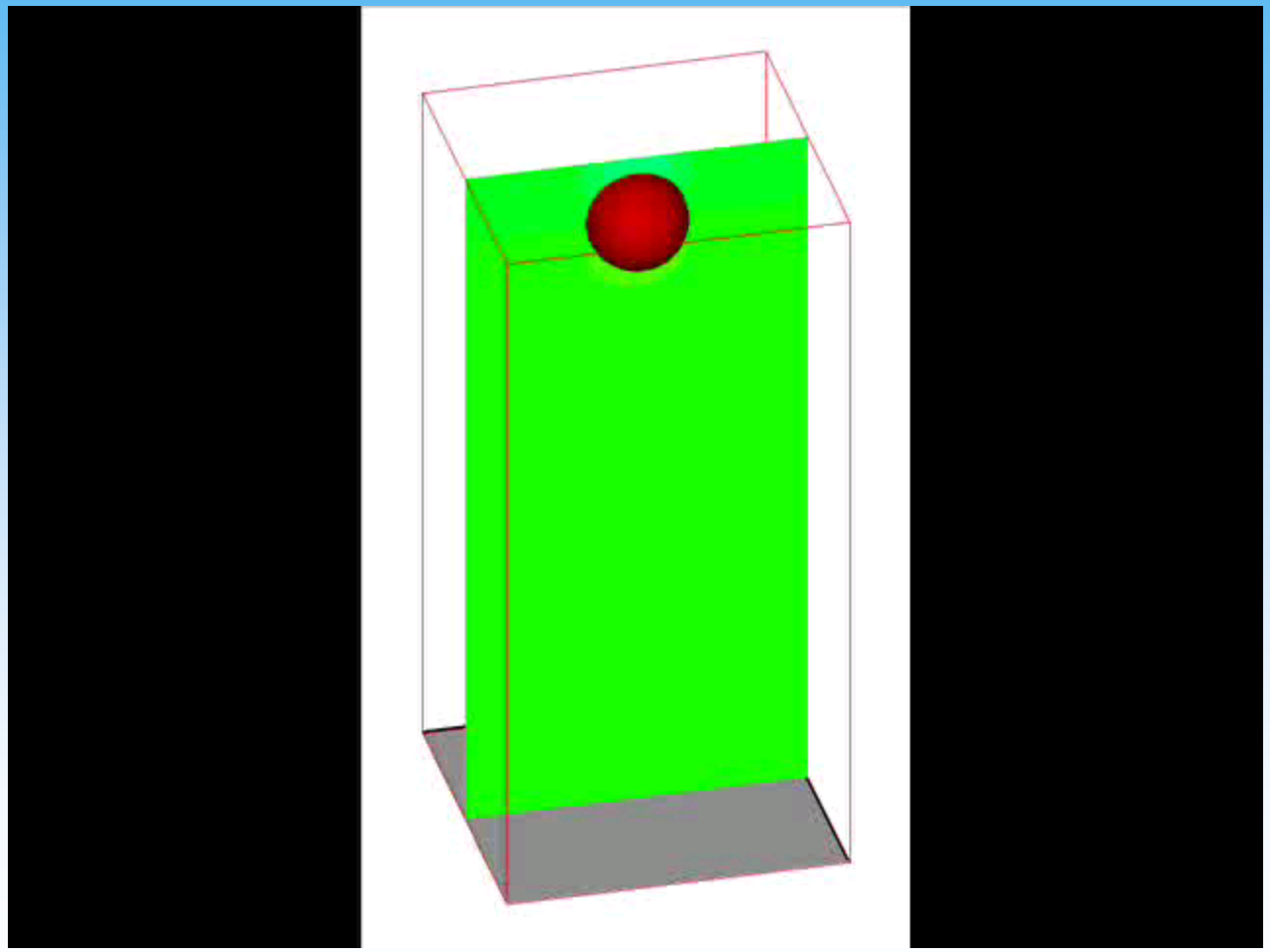
- Experimental study*
  - Sphere falling onto a plate in viscous fluid (in silicon oil RV10).
  - trajectory of a sphere (diameter is 3mm) was recorded.
- DNS numerical simulation
  - k=317,000 dyn/cm,
  - η=140 dyn.s/cm





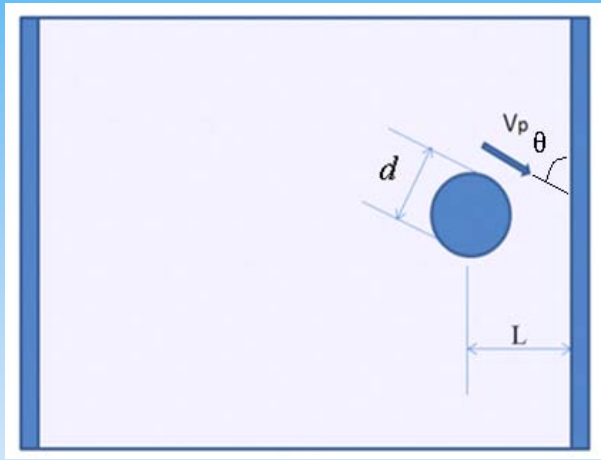
* Gondret, P.; M. Lance, & L. Petit (2002), "Bouncing motion of spherical particles in fluids," *Phys. Fluids*, **14**:643-652 .

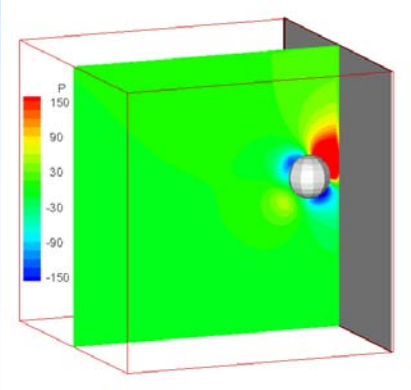
Falling of a Sphere in Oil (Animation)

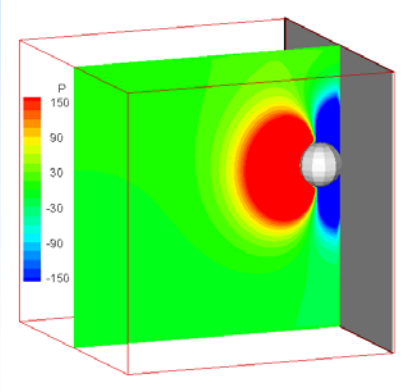


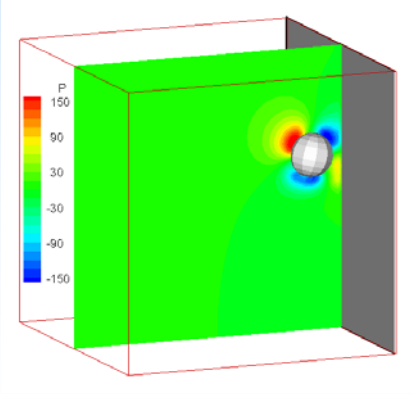
Oblique Particle-Wall Collision (1)

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



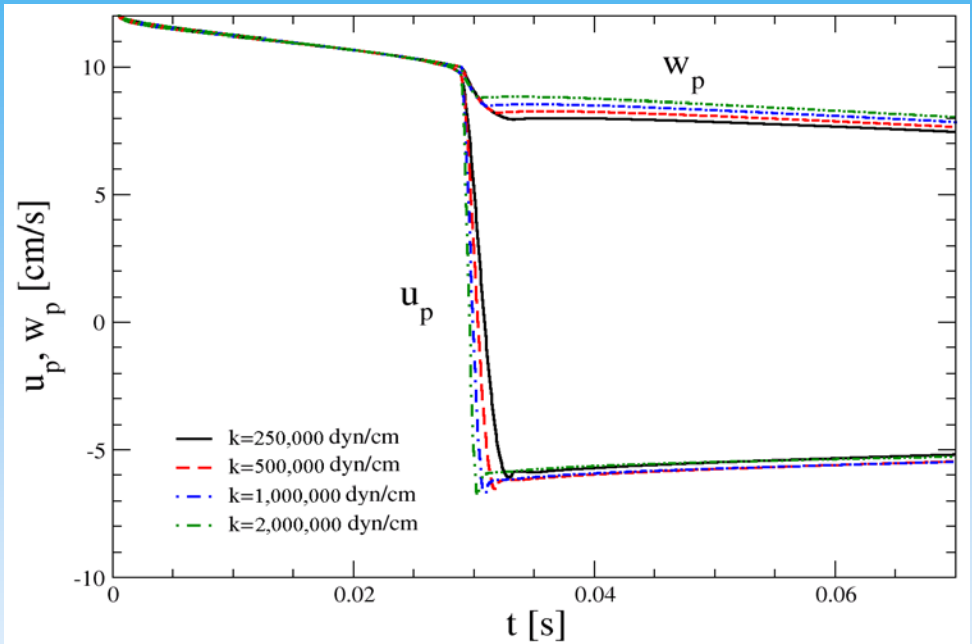






Oblique Particle-Wall Collision: Effect of Spring Stiffness

- Damping coefficient η=50 dyn.s/cm
- Spring stiffness 250,000 dyn/cm≤k≤2,000,000 dyn/cm
- Coefficient of Restitution: little change in normal direction, e≈0.65; 10% change in tangential direction e≈0.79~0.88
- Particle slips at wall
  - tangential velocity changes after collision are observed
  - experiment data supports this*

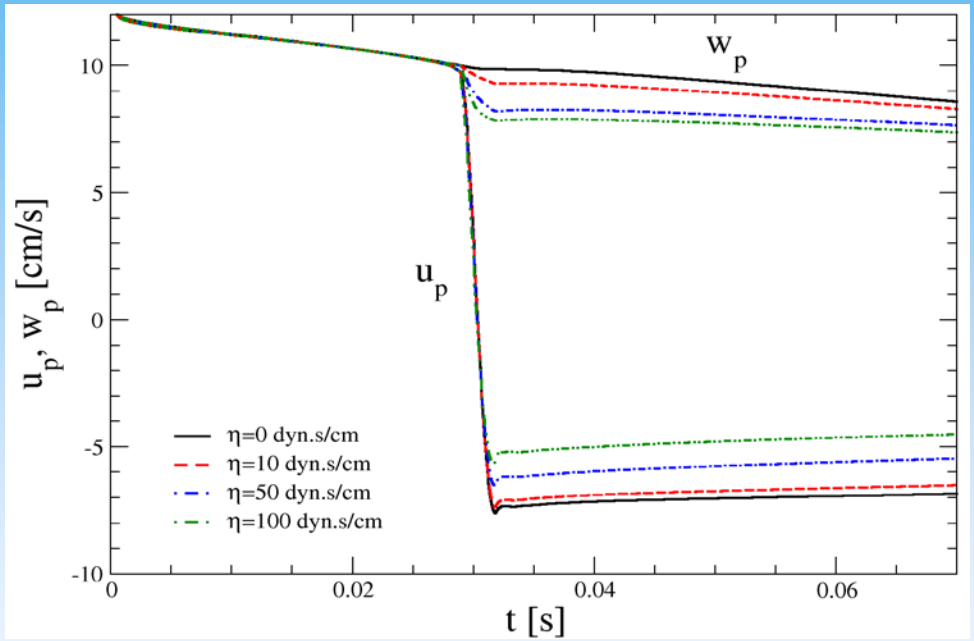


Particle normal and tangential velocity components before and after collision at damping coefficient η=50 dyn.s/cm.

*Joseph, G. G. and M. L. Hunt, "Oblique particle-wall collisions in a viscous fluid," *J. Fluid Mech.*, **510**:71-93 (2004).

Oblique Particle-Wall Collision: Effect of Damping Coefficient

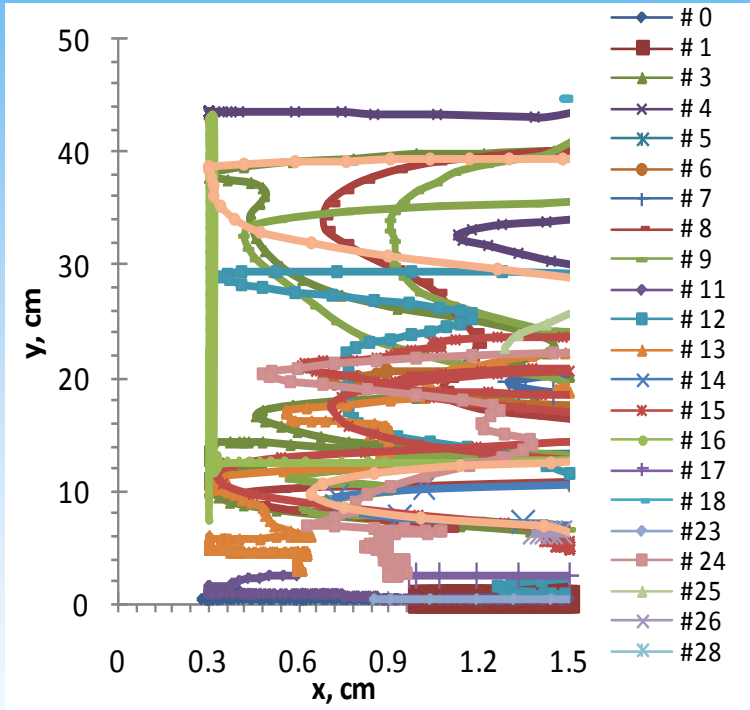
- Constant spring stiffness k=1,000,000 dyn/cm
- Damping coefficient η=0~100 dyn.s/cm
- Results of restitution coefficient, *e*
  - normal direction: e=0.76 at η=0; e=0.54 at η=100 dyn.s/cm
  - tangential direction: e=1 at η=0; e=0.78 at η=100 dyn.s/cm



Particle normal and tangential velocity components before and after collision at spring stiffness k=1,000,000 dyn/cm

Use of the DNS to Determine the Behavior of the Solid Phase Near Walls

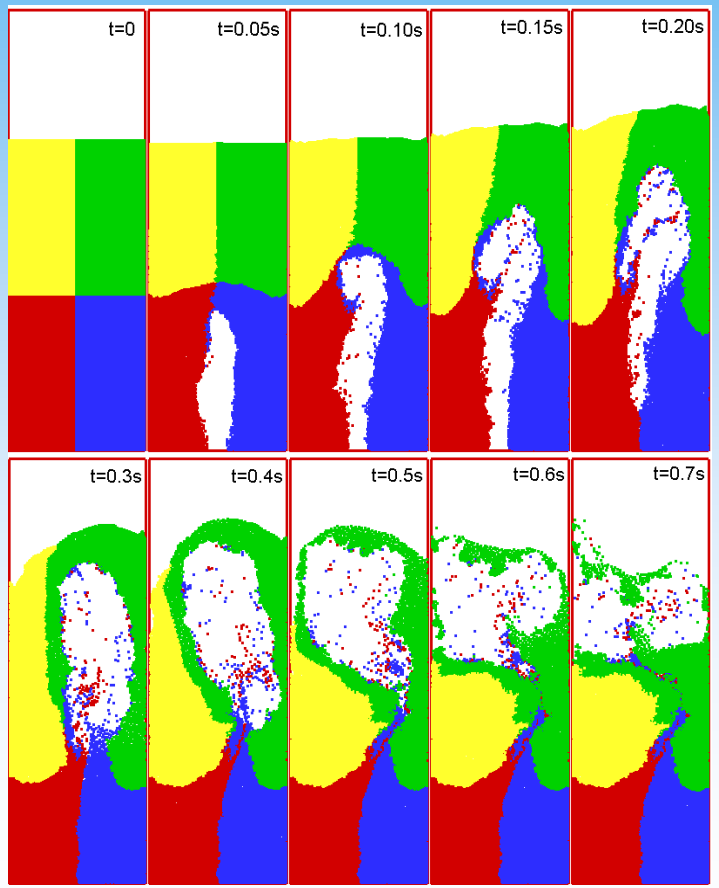
- Use the soft-sphere collision model.
- Determine collision model parameters that match experimental data
- Observe the behavior of a statistically large number of particles in the wall region.
- Determine the average particle velocity profile.
- Deduce the appropriate "boundary condition" for solid phase.

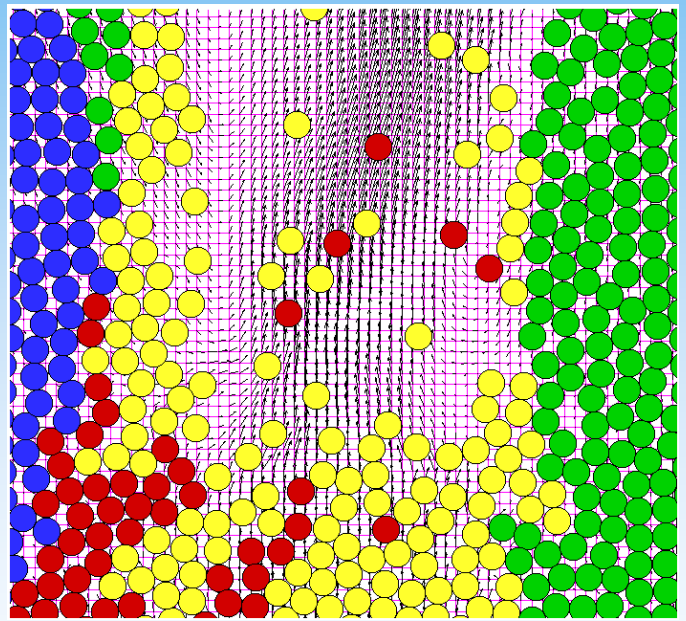


Davis, A. P., Michaelides, E. E., and Feng, Z.-G. (2010), "Particle velocity near vertical boundary - a source of uncertainty in two-fluid models," 7th International Conference on Multiphase Flow, FL. May 30-June 4, 2010.

Evolution of a “Bubble” in a Fluidized Bed

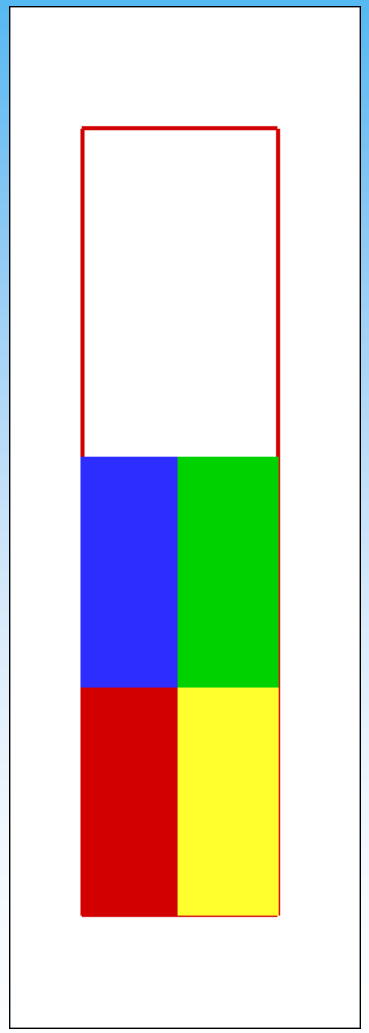
– Inject fluid for a short time to create a “bubble.” 12,000 particles are used*.





* Feng, Z-G, X. Zhang and B. 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 Engi Summer Meeting, August 1-5, 2010, Montreal, Canada.

Fluidization of 12,000 Particles



Conclusions and Future Work

- Conclusions
  - A *DNS* method has been developed for the motion and heat transfer of the particles suspended in fluid
  - *DNS* combined with the soft-sphere collision model (with proper input parameters) is able to capture the dynamics of particle-wall collisions.
  - Particle interactions close to the wall influence the particle velocities, hence, the boundary conditions of solid phase at the wall.
  - Particles "slip" near a solid wall, and slip coefficients depend on particle and fluid properties.
  - Partial slip boundary condition for solid phase should be used for TFM.
- Future work
  - Determine velocity profile of solid phase near wall to derive slip boundary condition models for solid phase
  - Incorporate the slip boundary condition models into MFIX* simulation.
  - Conduct experimental study to validate the boundary condition models.

* *MFIX* is an general-purpose computer code developed at the NETL for describing the hydrodynamics, heat transfer and chemical reaction in fluid-solids systems.

Papers Published

- **Peer Reviewed Journal Papers:**
  - 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,” *ASME J. Fluids Eng.*, accepted with revision,
  - 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.
  - Kartushinski, A., Michaelides, E. E., Rudi, U. A., Shcheglov, I. N. , and Tisler, S. V. (2010), “Numerical Simulation of Three-Dimensional Gas-Solid Particle Flow in a Horizontal Pipe,” *AIChE Journal*, 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.

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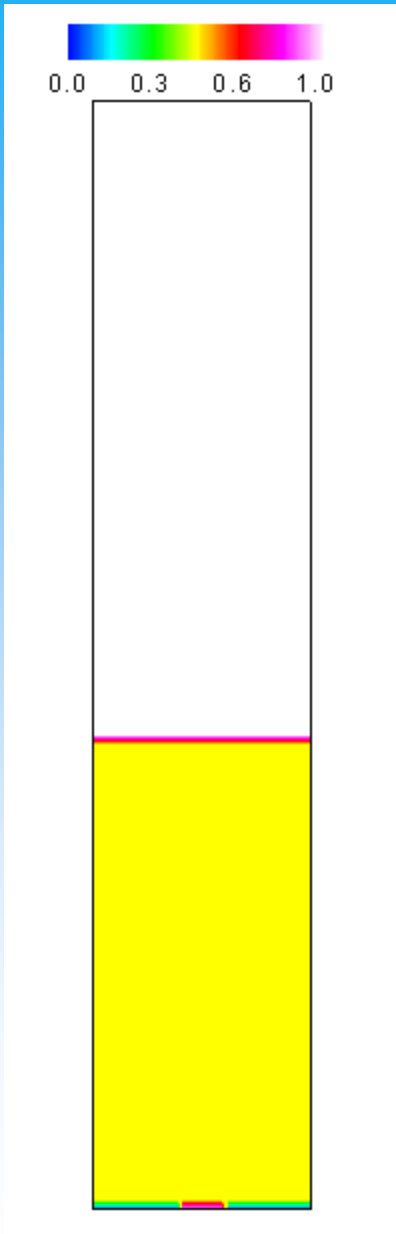
Thank you!