NATIONAL ENERGY TECHNOLOGY LABORATORY

Coupled MFIX-DEM: Verification and Validation

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U.S. DEPARTMENT OF ENERGY

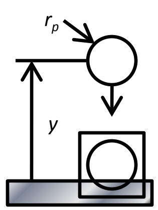
Goals: Verification and Validation

To gain confidence & increase adoption

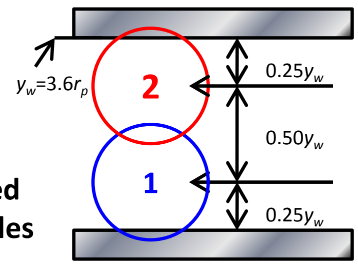
Verification

- DEM

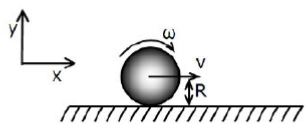
free falling particle



two stacked particles

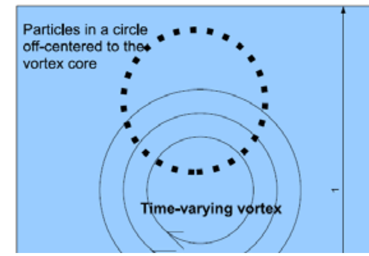


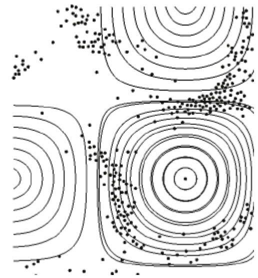
balling slipping on rough surface



- Continuum Discrete Method (CDM)

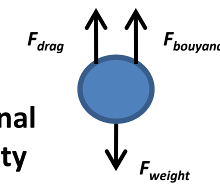
circle advection in an oscillating vortex field





particle motion in a Taylor-Green vortex

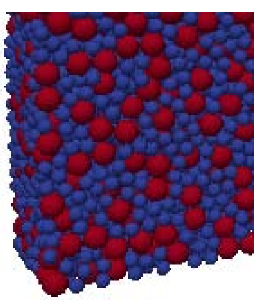
terminal velocity

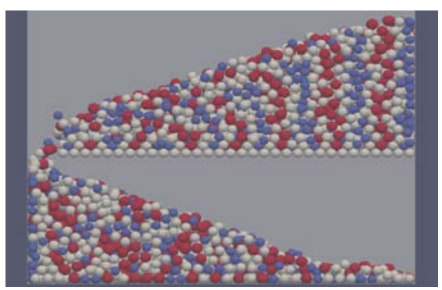


Validation (in progress)

- DEM

random packing



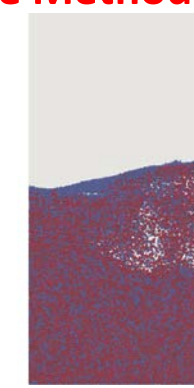


repose angle

- Continuum Discrete Method (CDM)

3D spout bed

Link et al., 2008, Fig. 9



bubbling fluidized beds

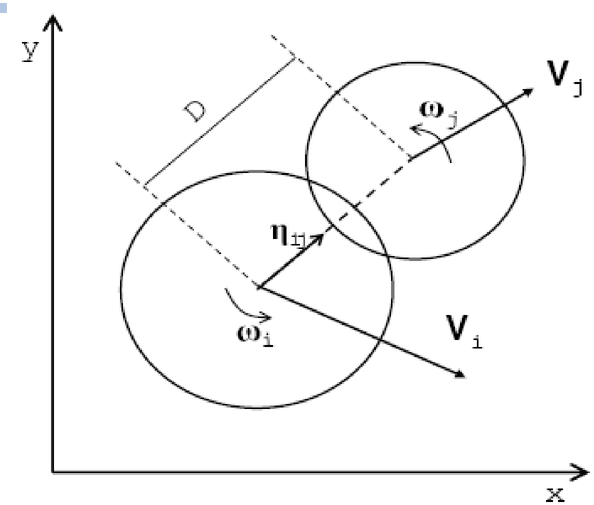
DEM Theory

Newton's Laws

$$\frac{d\mathbf{X}^{(i)}(t)}{dt} = \mathbf{V}^{(i)}(t),$$

$$m^{(i)}\frac{d\mathbf{V}^{(i)}(t)}{dt} = m^{(i)}\mathbf{g} + \mathbf{F}_{\mathrm{d}}^{(i\in k,m)}(t) + \mathbf{F}_{\mathrm{c}}^{(i)}(t),$$

$$I^{(i)}\frac{d\omega^{(i)}(t)}{dt} = \frac{1}{2}D^{(i)}\boldsymbol{\eta}\times\mathbf{F}_{\mathrm{c}}^{(i)}(t),$$

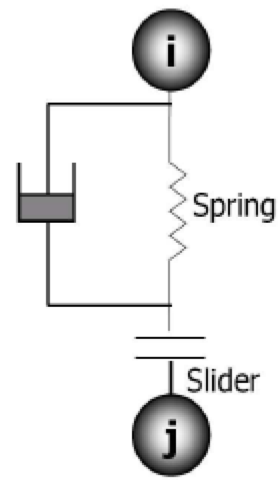


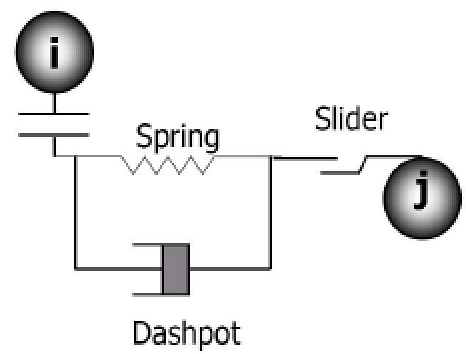
Soft-sphere model

$$\mathbf{F}_{\mathrm{c}}^{(i)}(t) = \sum_{\substack{j=1\\ j\neq i}}^{N}\left(\mathbf{F}_{ij}^{\mathrm{S}}(t) + \mathbf{F}_{ij}^{\mathrm{D}}(t)\right),$$

$$\mathbf{F}_{\mathrm{n}ij}(t) = \mathbf{F}_{\mathrm{n}ij}^{\mathrm{S}}(t) + \mathbf{F}_{\mathrm{n}ij}^{\mathrm{D}}(t),$$

$$\mathbf{F}_{\mathrm{t}ij}(t) = \mathbf{F}_{\mathrm{t}ij}^{\mathrm{S}}(t) + \mathbf{F}_{\mathrm{t}ij}^{\mathrm{D}}(t).$$





Linear-sprint dashpot (default model)

$$\eta_{\mathrm{n}m\ell} = \frac{2\sqrt{m_{\mathrm{eff}}k_{\mathrm{n}m\ell}}\,|\ln e_{\mathrm{n}m\ell}|}{\sqrt{\pi^2+\ln^2 e_{\mathrm{n}m\ell}}}$$

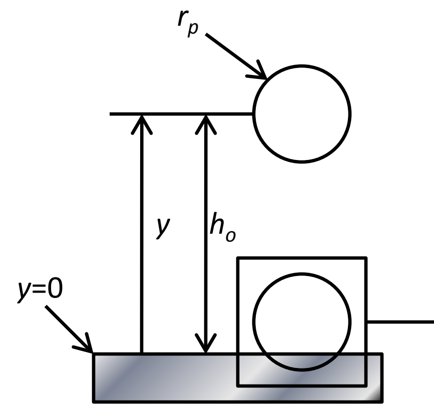
normal dashpot

NETL

Case 1: Freely Falling Particle

r_p =10cm,
ρ_p =2.6g/cm^3
g =980cm/s^2
h_o =50cm

- A smooth particle freely falling under gravity from its initial position bounces upon collision with a fixed wall
- Motion described in three stages: free fall, contact, rebound



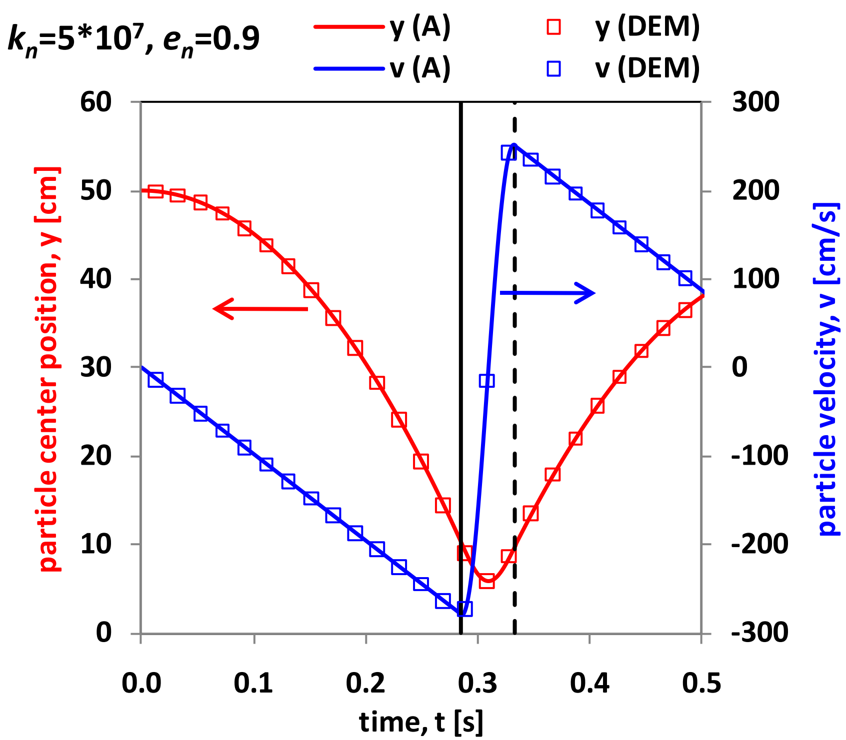
Contact Stage:

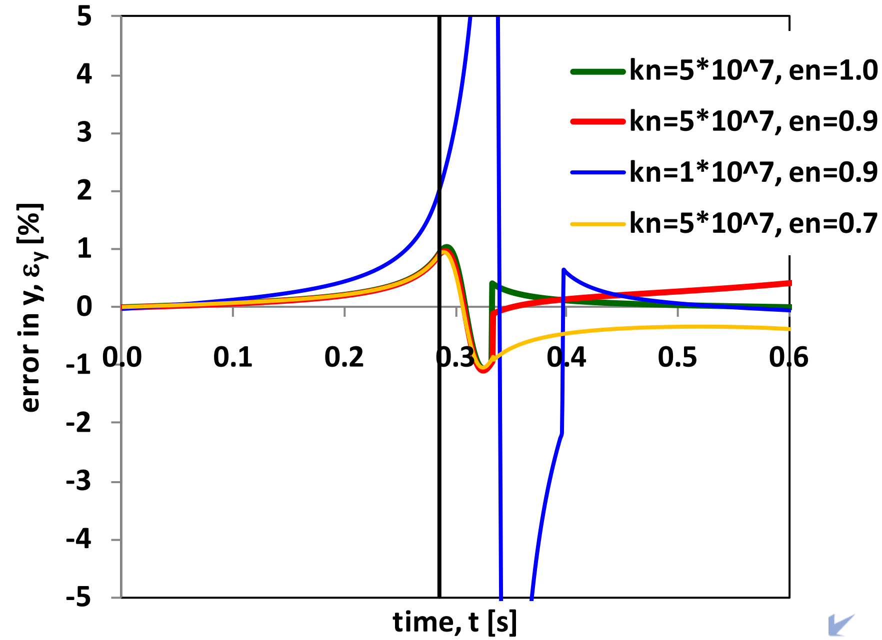
$$\ddot{y} = F_b + F_k + F_d$$

$$F_b = -g$$

$$F_k = -\frac{k}{m_p}\left(y - r_p\right)$$

$$F_d = -\frac{\eta_n}{m_p}\dot{y}$$

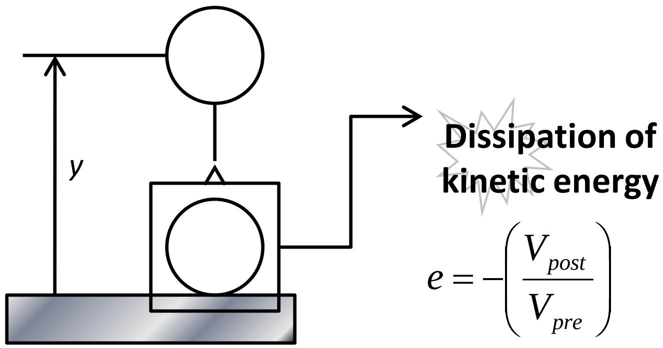




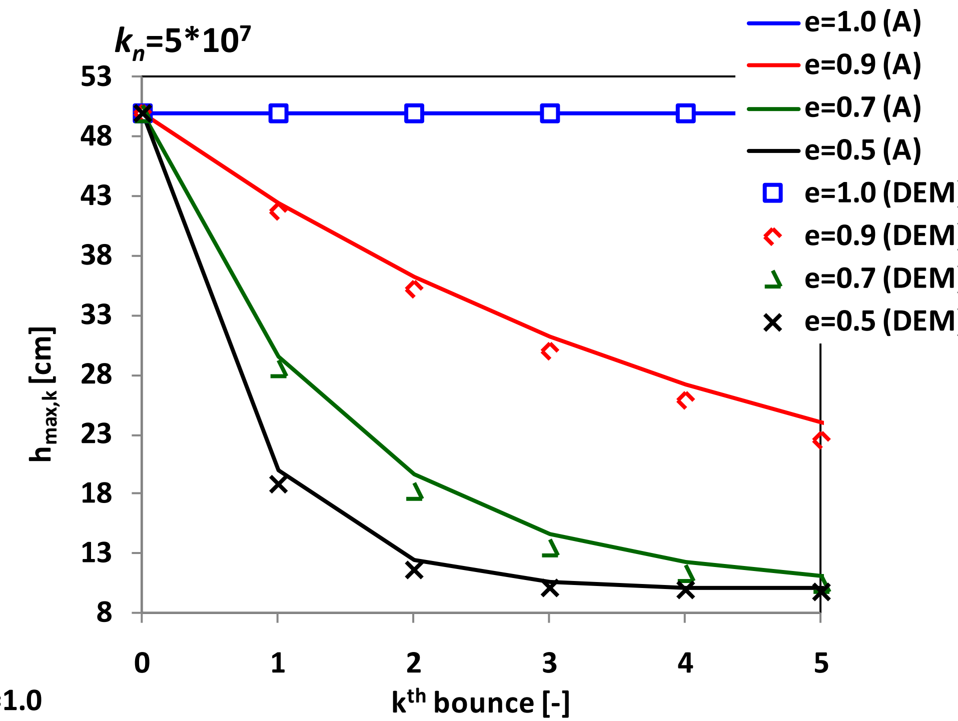
Following the work of Chen et al., Int. J. of Geomech., 2007

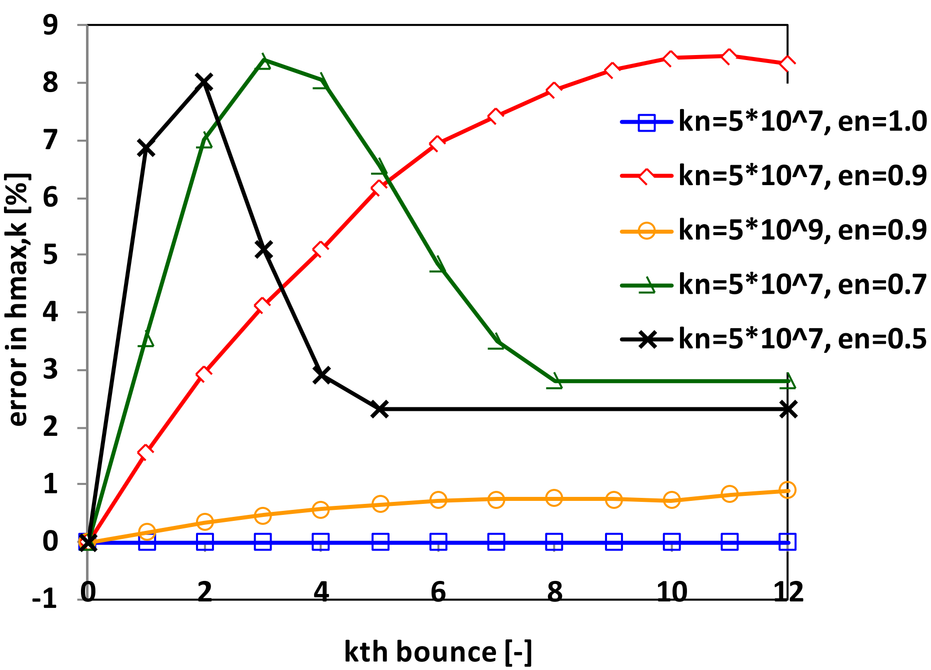
Case 1: Comparison with Hard-Sphere Model

- No contact stage : instantaneous collision



$$e = -\left(\frac{V_{post}}{V_{pre}}\right)$$



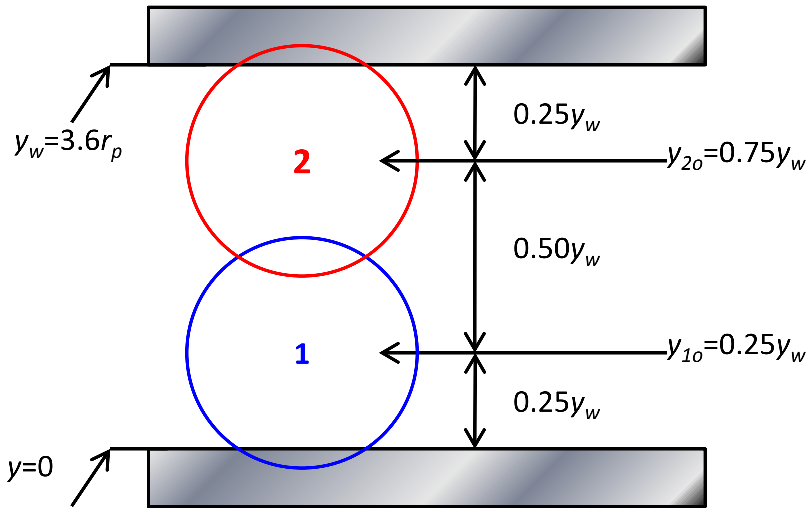


Error essentially reflects difference in hard-sphere vs. soft-sphere treatment

Case 2: Two Stacked Particles

r_p =0.05cm,
ρ_{p1} =20g/cm^3
ρ_{p2} =10g/cm^3
k_n =10^{6}dyne/cm
g =980cm/s^2

- A system of two stacked particles compressed between two fixed walls under gravity
- Equal size particles
- Top particle is twice as dense as upper particle



Particle 1 force balance:

$$\ddot{y}_1 = F_{1b} + F_{1kw} + F_{12k} + F_{1dw} + F_{12d}$$

$$F_{1b} = -g \qquad F_{1kw} = -\frac{k_{nw}}{m_1}\left(y_1 - r_p\right)$$

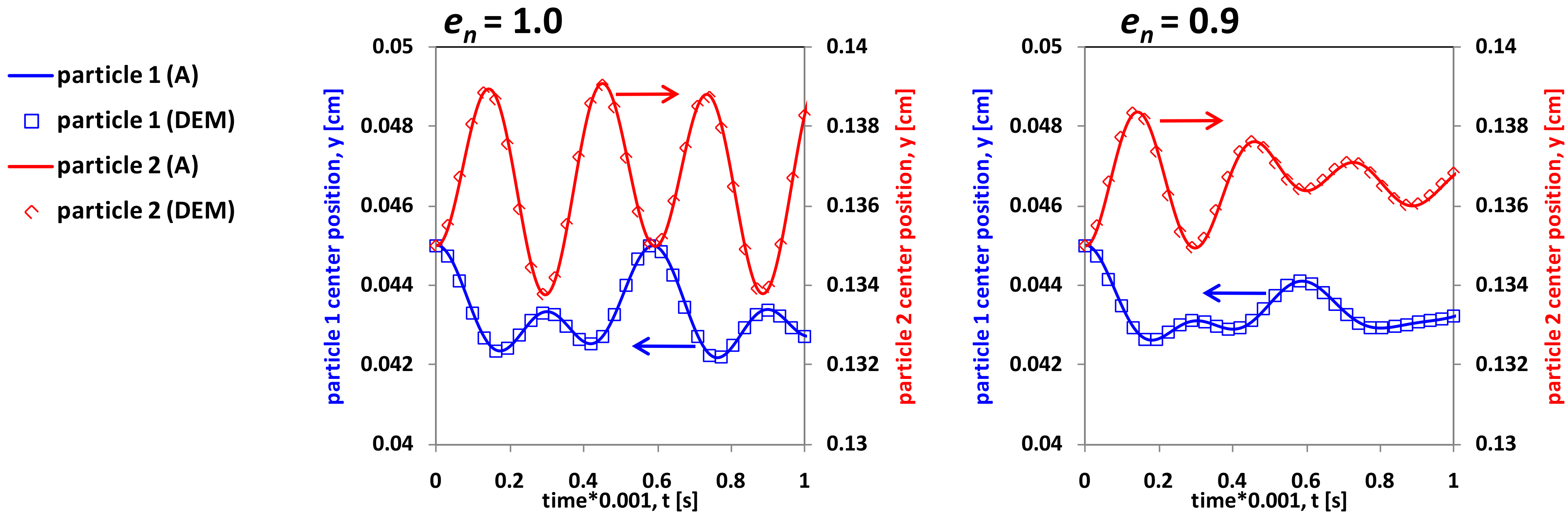
$$F_{12k} = -\frac{k_n}{m_1}\left(2r_p - \left(y_2 - y_1\right)\right)$$

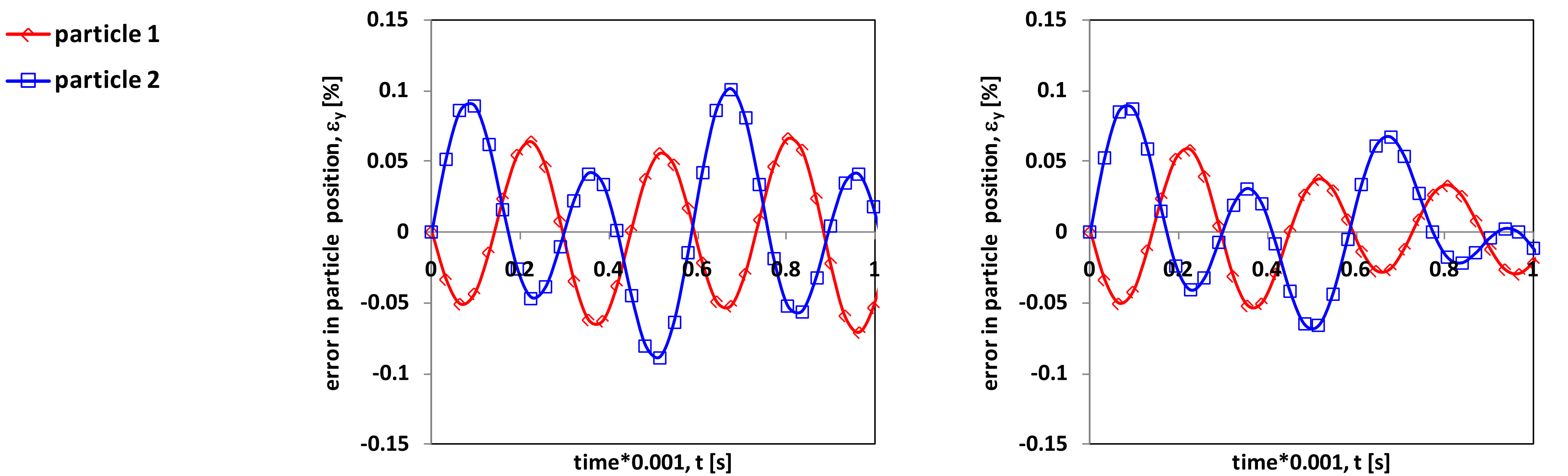
$$F_{1dw} = -\frac{\eta_{n1w}}{m_1}\dot{y}_1$$

$$F_{12d} = -\frac{\eta_{n12}}{m_1}\left(\dot{y}_1 - \dot{y}_2\right)$$

Following the work of Chen et al., Int. J. of Geomech., 2007

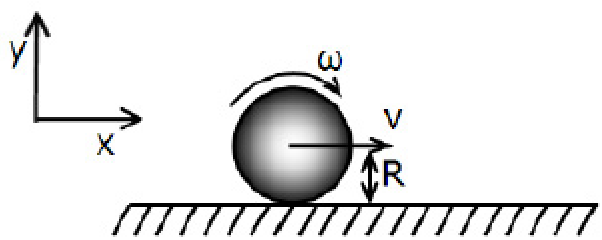
Case 2: Results





Case 3: Ball Slipping on a Rough Surface

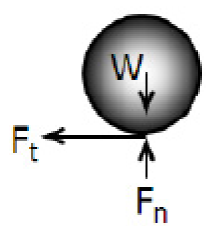
- A ball is released on a rough surface with finite translational velocity (v_o) but zero angular velocity
- Sliding friction will create an angular velocity and reduce v_o until there is zero slip at point of contact ($v_x = \omega R$ at $t = t_s$)

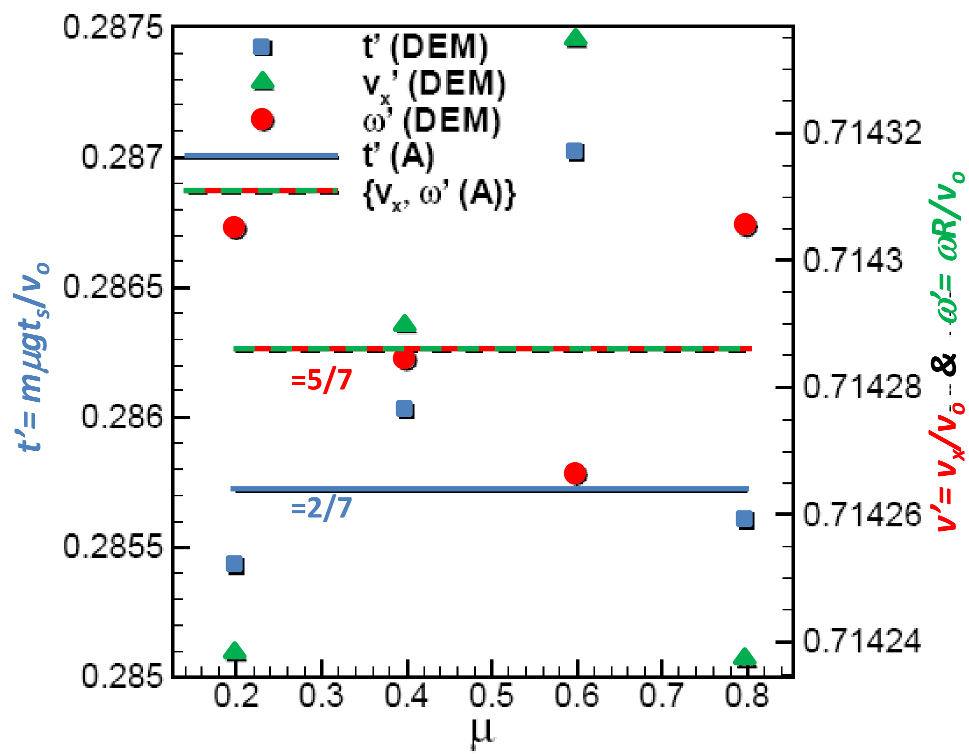


Particle motion:

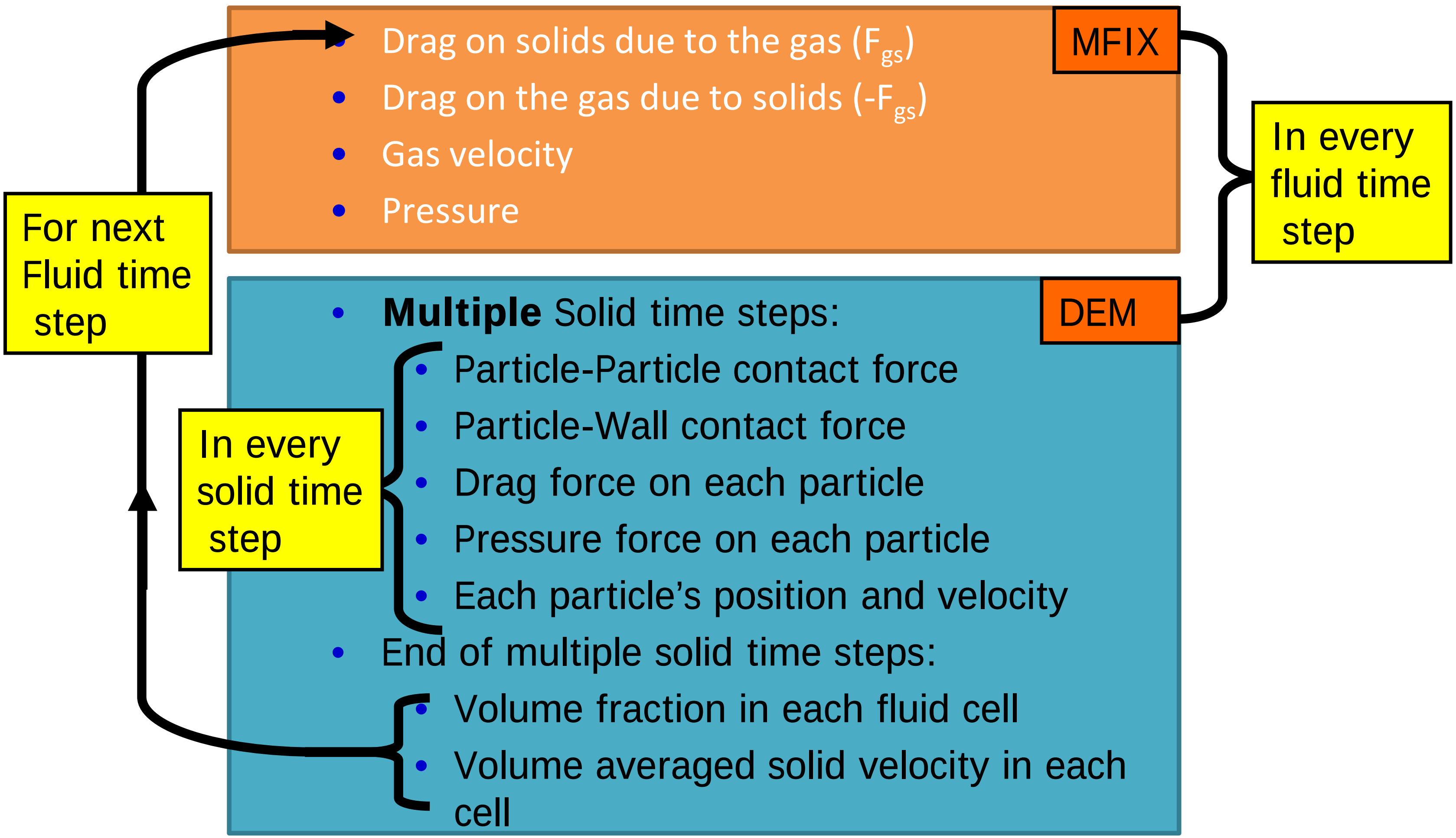
$$\frac{dv_x}{dt} = \frac{-F_t}{m} - \mu g$$

$$\frac{d\omega}{dt} = \frac{\mu m g R}{I}$$





CDM: MFIX-DEM Coupling

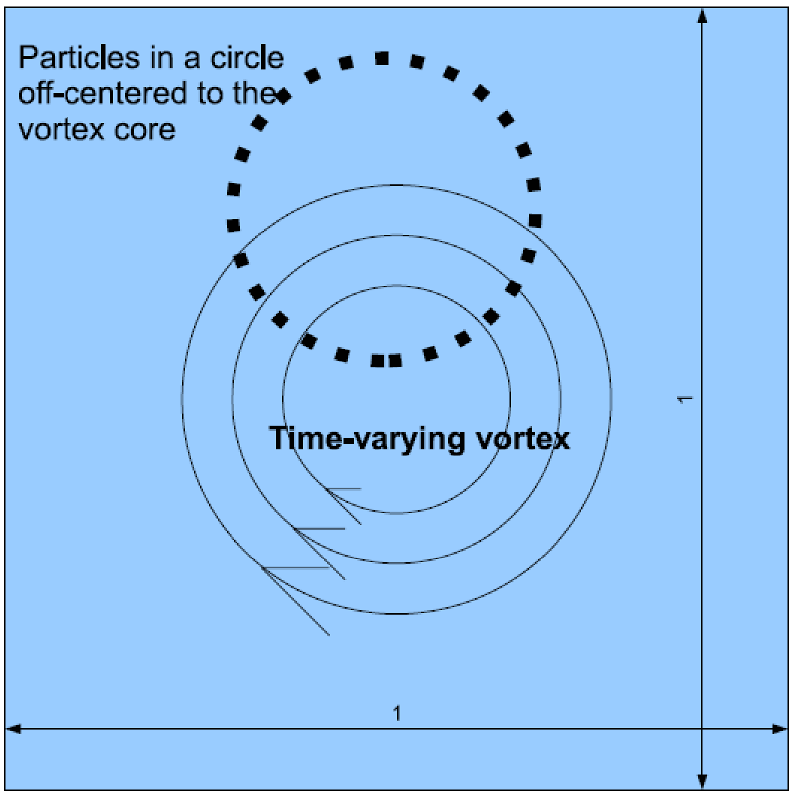


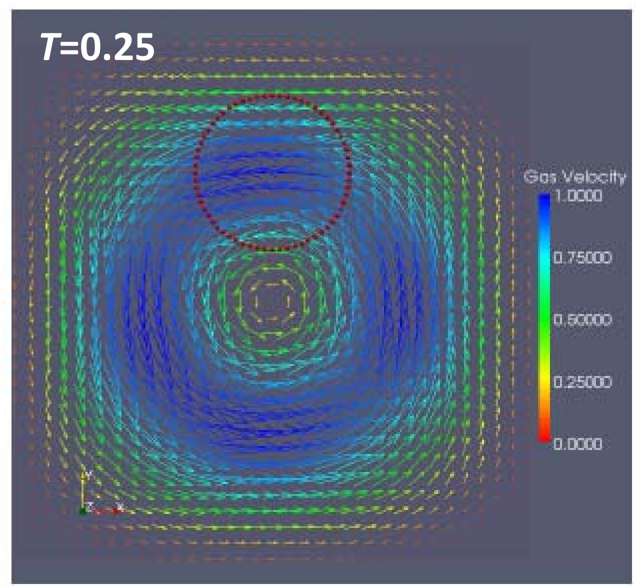
Case 4: Advection of a Circle in an Oscillating Vortex Field

- Particles of zero mass are arranged in a circle (2D) or sphere (3D) and subject to an off-centered oscillating vortex field

$$u = 2\sin^2(\pi x)\sin(2\pi y)\cos(\pi t/T),$$

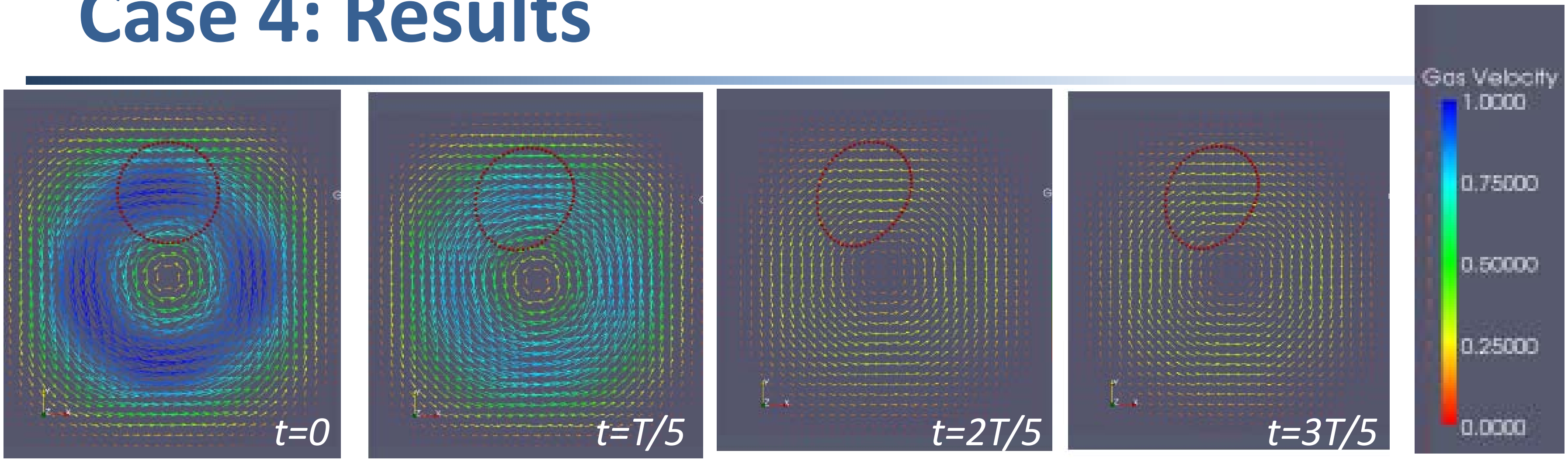
$$v = -\sin(2\pi x)\sin^2(\pi y)\cos(\pi t/T).$$

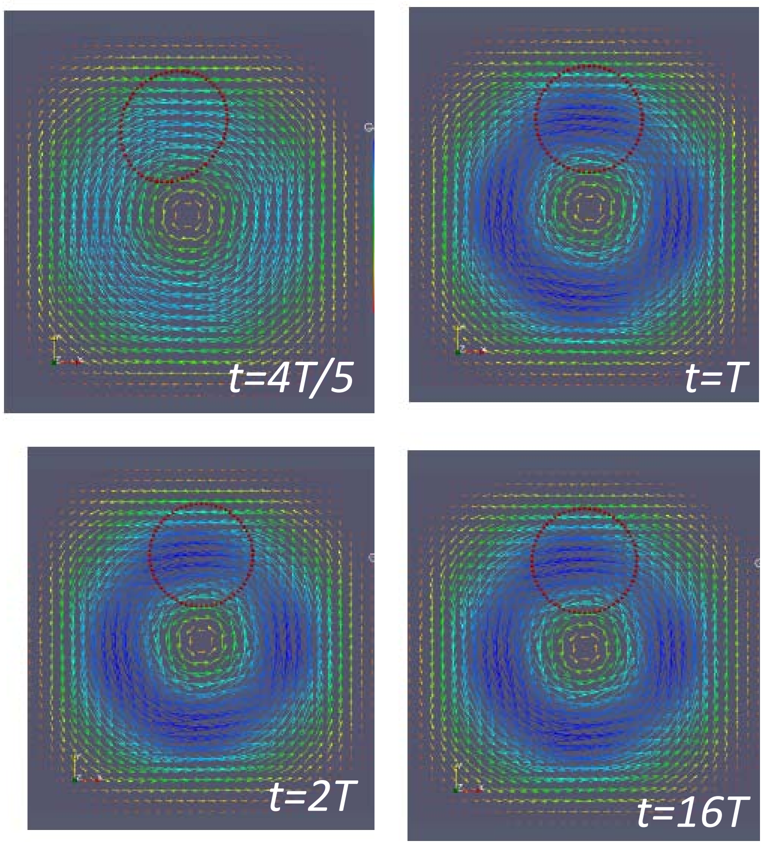


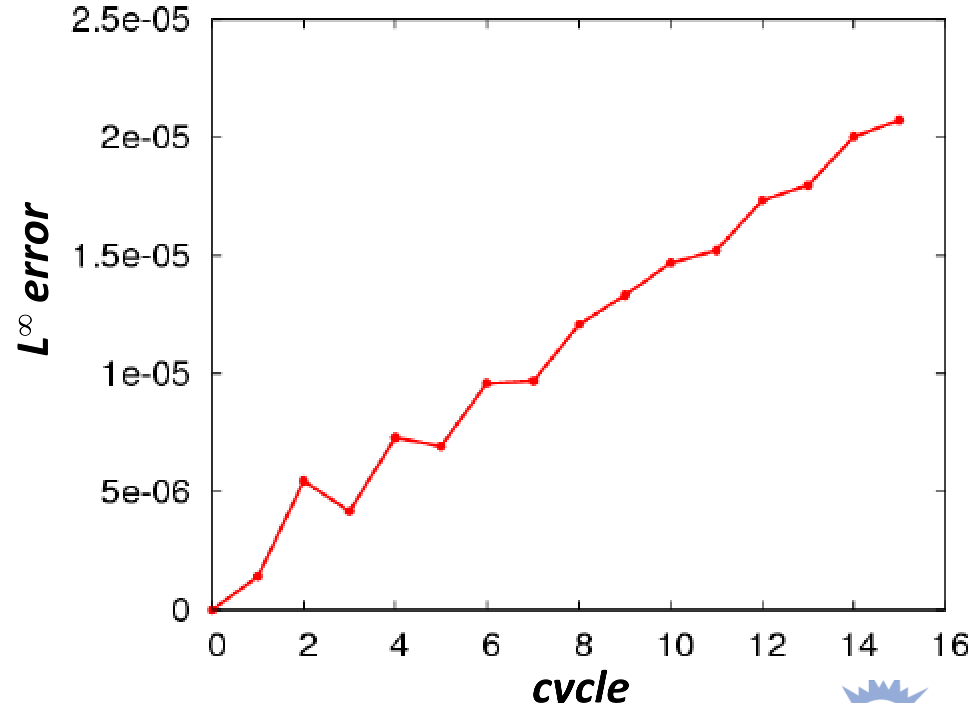


Setup has been by others used to test advection algorithms (Rider & Kothe, 1998; Liovic et al., 2006; Leveque, 1996)

Case 4: Results







Case 5: Particle Motion in Vortex

r_p =0.01cm,
ρ_p =1.8g/cm^3
v =0.05
μ_g =varied

- Particles with finite mass are subject to a 2D vortex gas field

$$u_g = -\cos(k_x x)\sin(k_y y),$$

$$v_g = \sin(k_x x)\cos(k_y y),$$

- The extent of gas-solids interaction is quantified by the particle Stokes number

$$St = \frac{\tau_p}{\tau_g}$$

$$\tau_p = \frac{\rho_p {d_p}^2}{18\mu_g}$$ particle response/ relaxation time

$$\tau_g = \frac{L}{U}$$ fluid time-scale

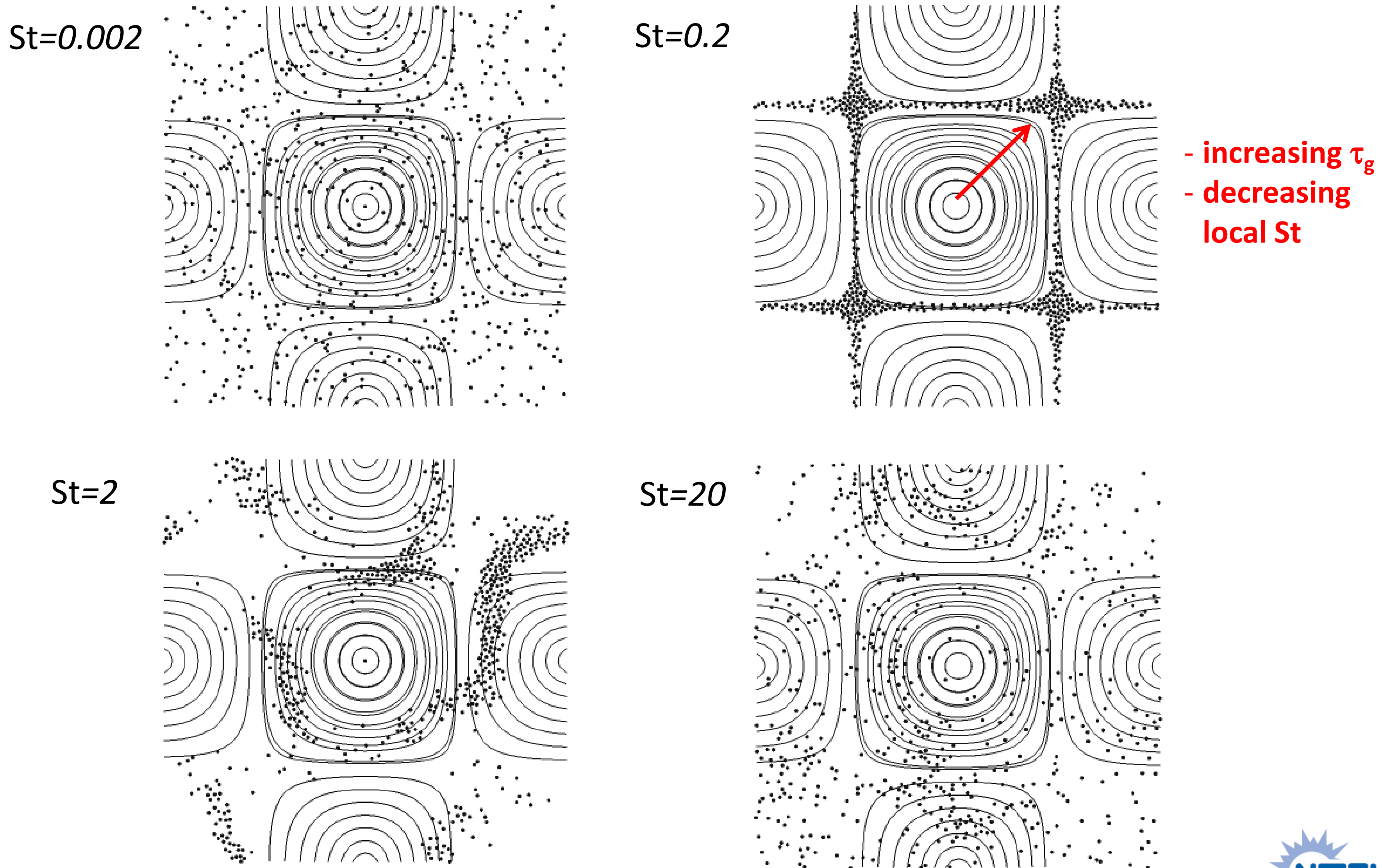
St << 1 ~ particles become flow tracers (drag dominates)

St ~ O(1) ~ particles follow local pathlines that circulate around large scale vortices

St >> 1 ~ particles move with their initial trajectories (inertia dominates)

Results

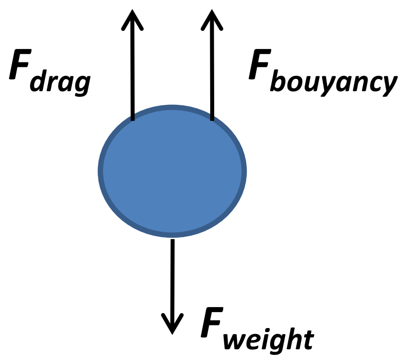
$$St = \frac{\tau_p}{\tau_g}$$



Case 6: Particle Terminal Velocity

r_p =0.01cm,
ρ_p =2.0g/cm^3
ρ_g =1.2x10^{-3}g/cm^3
μ_g =1.8x10^{-5} Pa.s
v_g =40cm/s

- Terminal velocity of a single small particle freely falling under gravity through a gas phase

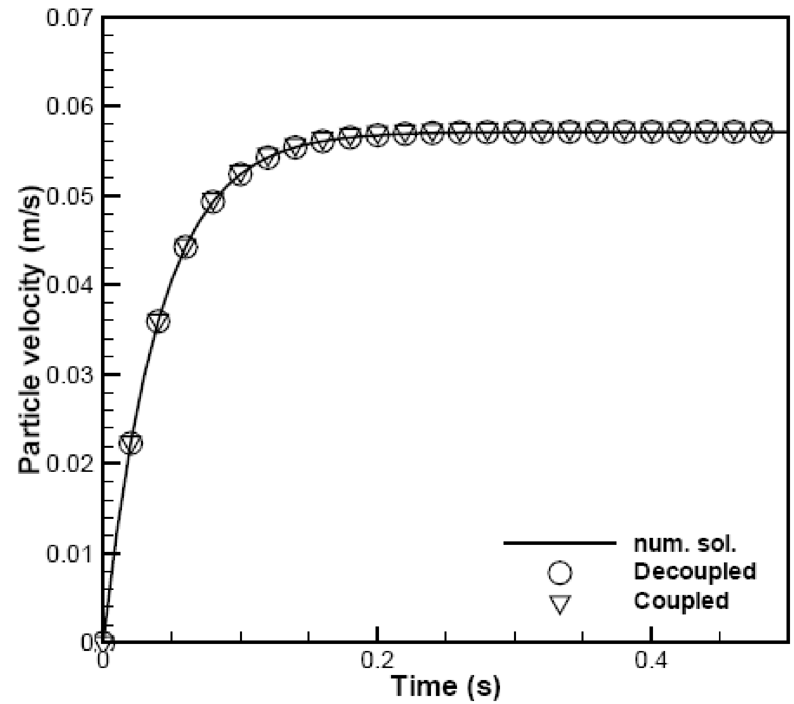


Particle motion:

$$\frac{d\mathbf{v}_p}{dt} = \frac{\mathrm{g}(\rho_p - \rho_g)}{\rho_p} - \frac{3}{4}\frac{\rho_g\,|\mathbf{v}_p - \mathbf{v}_g|^2}{d_p\rho_p}C_d,$$

$$C_d = \frac{24}{\mathrm{Re}}(1 + 0.15\mathrm{Re}^{0.687})$$

Schiller & Naumann (1933)



Summary of Verification Study

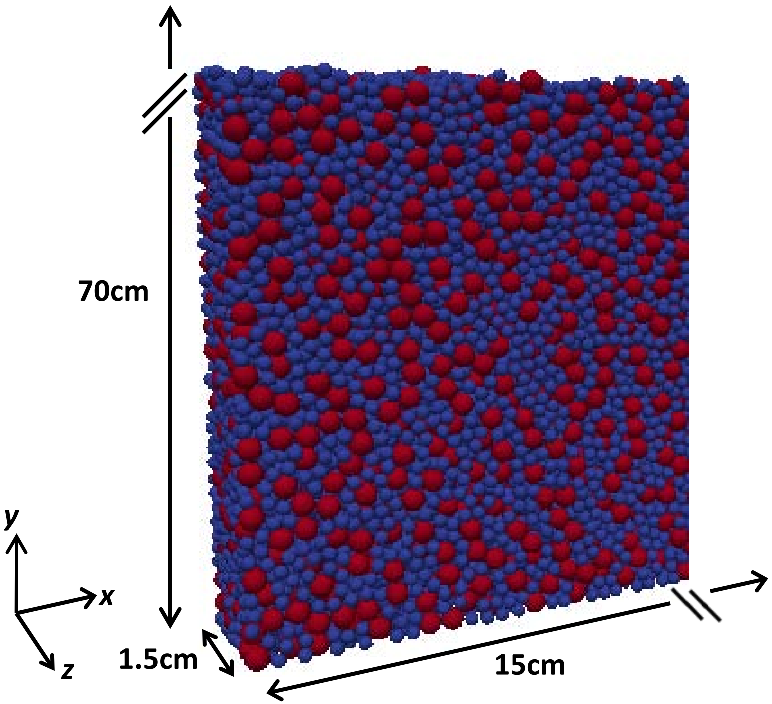
- Cases 1 and 2 involving a freely falling particle and two stacked particles targeted the implementation of the normal collision model and the time stepping algorithm
- Case 3 (ball slipping) targeted implementation of the tangential force model
- Cases 4 and 5 (advection & vortex flow) targeted the interpolation routines
- Case 6 (terminal velocity) served as a relatively simple test of the drag force
- All of these cases demonstrate fairly good agreement with the corresponding analytical solution (when available) or yielded the anticipated behavior

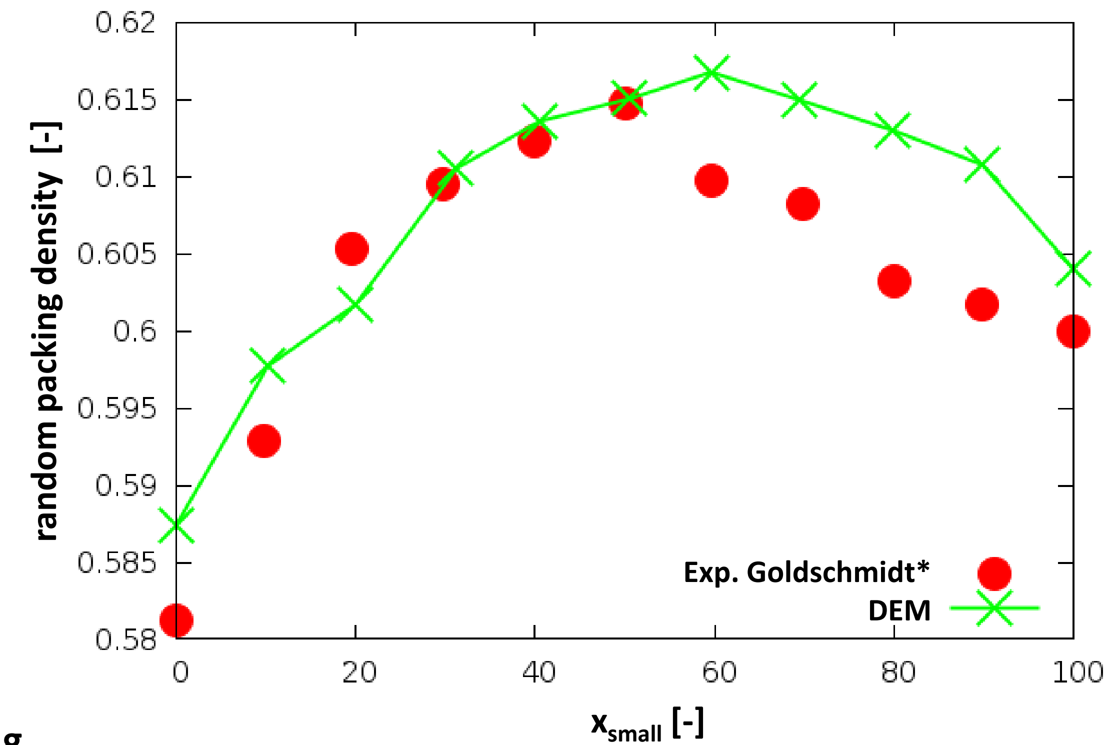
Garg, Galvin, Li and Pannala, Submitted to Powder Technology, 2010

Case 1: Random Packing of Binary Mixture

d_{p1} =0.152cm,
d_{p2} =0.249cm,
ρ_p =2.52g/cm^3
M_t =200g

- **Simulation setup: particles are randomly seeded, spaced far apart, in a pseudo 2D column and allowed to settle under gravity**





Additional comparisons for random packing of binary mixtures possible:

- **various correlations (e.g. Yu & Standish, 1987; Fedors & Landel, 1979)**
- **systematic experiments (e.g. McGreary, 1961; Jeschar, et al., 1975)**

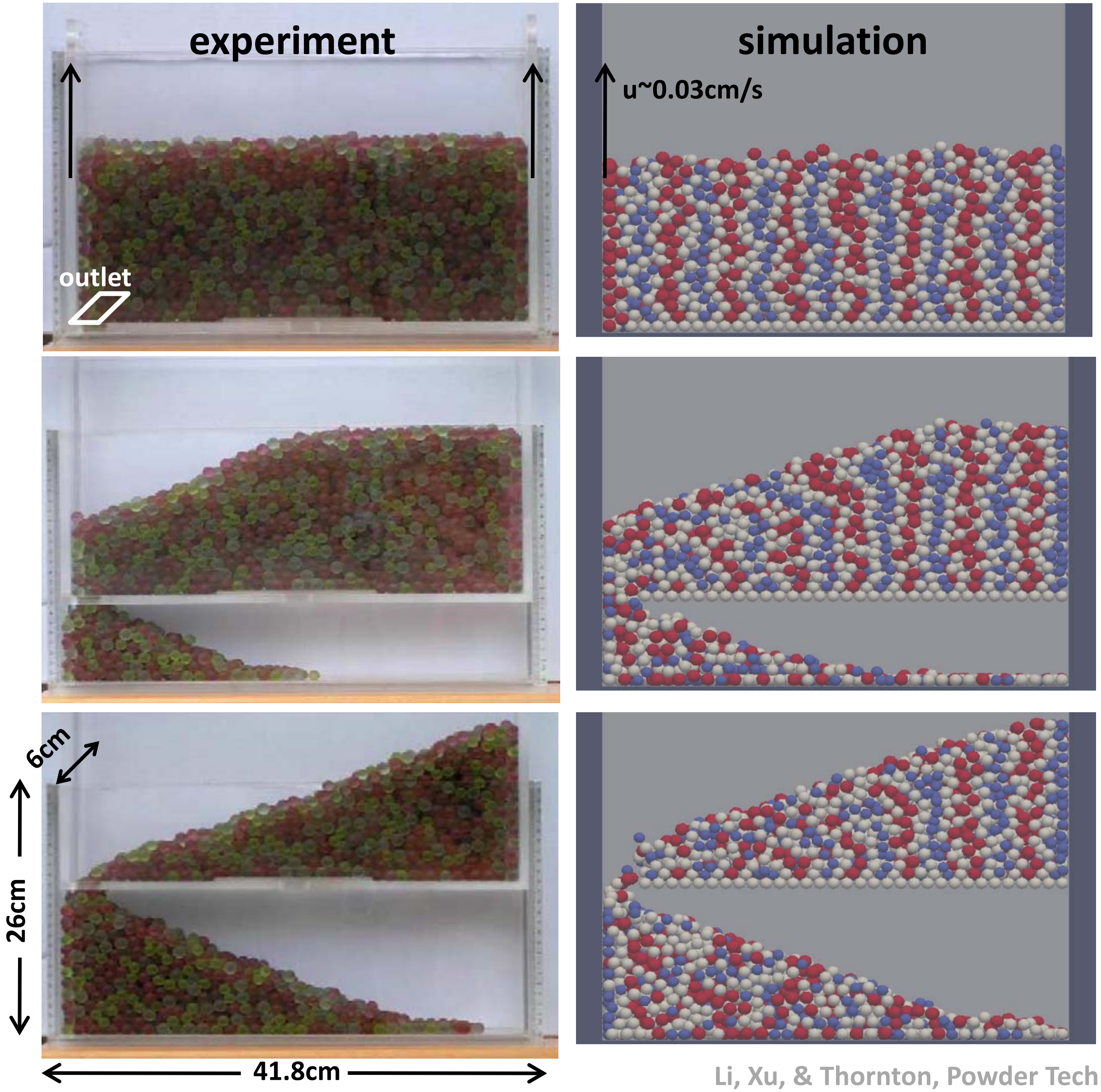
Similar trends are predicted with relative error less than 2%

Goldschmidt et al., Powder Technology, 2003, 138:135-159

Case 2: Angle of Repose

d_{p1} =1.113cm, d_{p2} =1.112cm, d_{p3} =1.1111cm
n_{p1} =750, n_{p2} =1500, n_{p2}=750
ρ_p =2.45g/cm^3
μ =0.1545
μ_w =0.1333

Snapshots of side discharge of glass beads



- **Setup: An inner box with an outlet at the bottom-left is moved vertically in an outer box where particles are discharged**

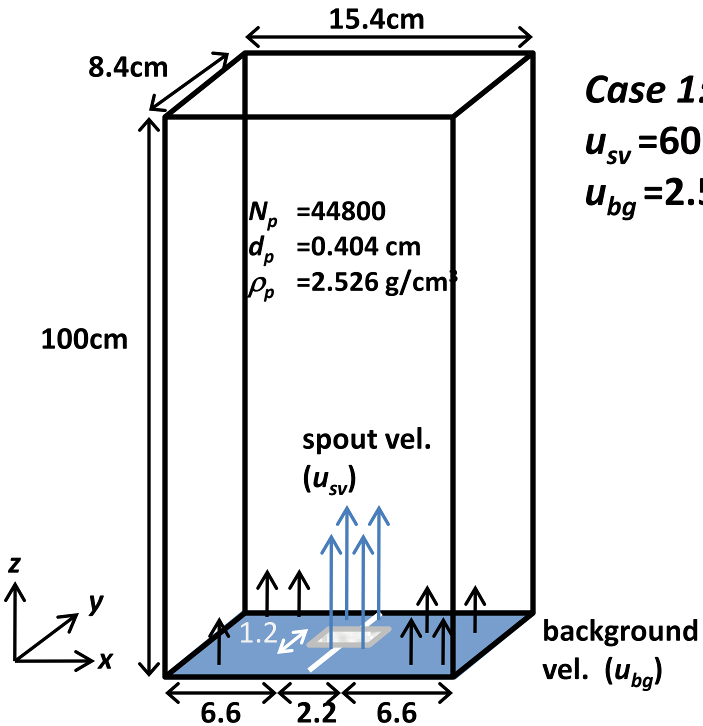
General behavior is predicted

Angle of repose is slightly under-predicted

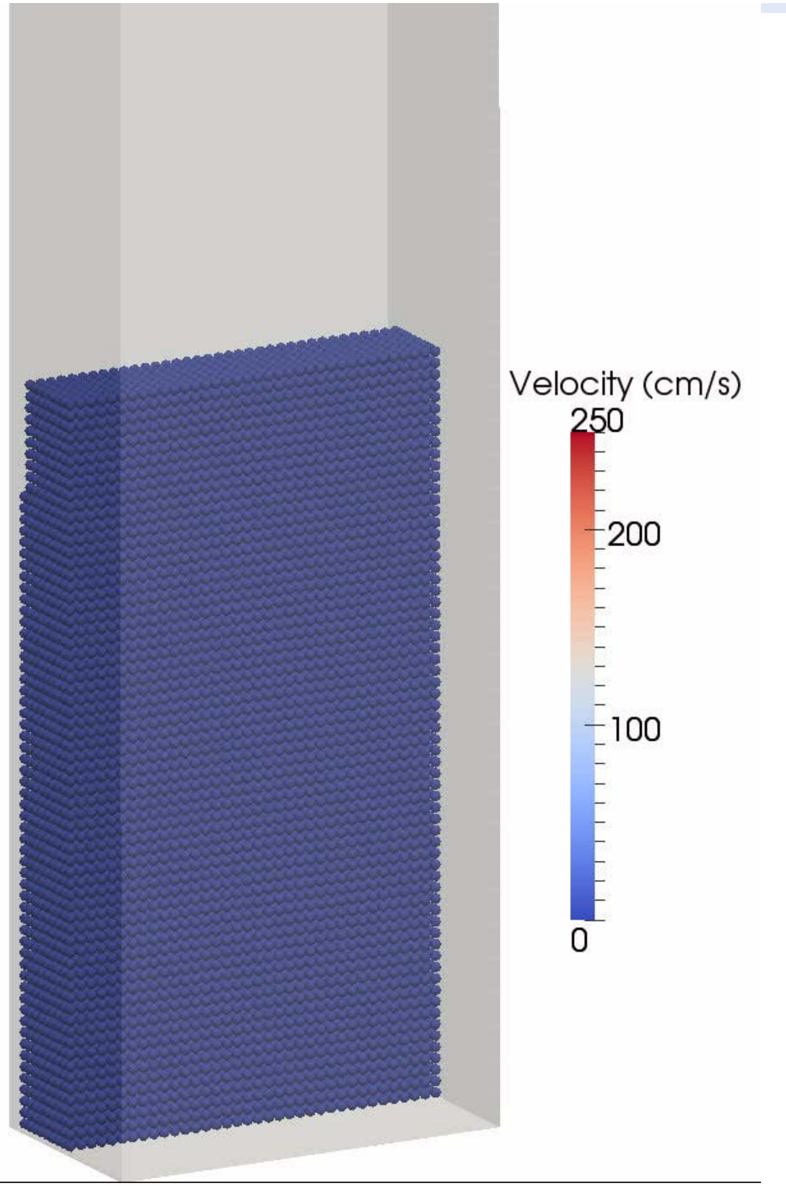
Li, Xu, & Thornton, Powder Technology, 2005, 160:219-228.

Case 3: 3D Spout Bed

- Experimental setup
  - Wide range of operating conditions (u_{bg}: 0-3.5m/s and u_{sv}:40-95m/s) wi data reported for 3 cases in 3 regim
  - Use PEPT & spectral analysis of pressure fluctuations



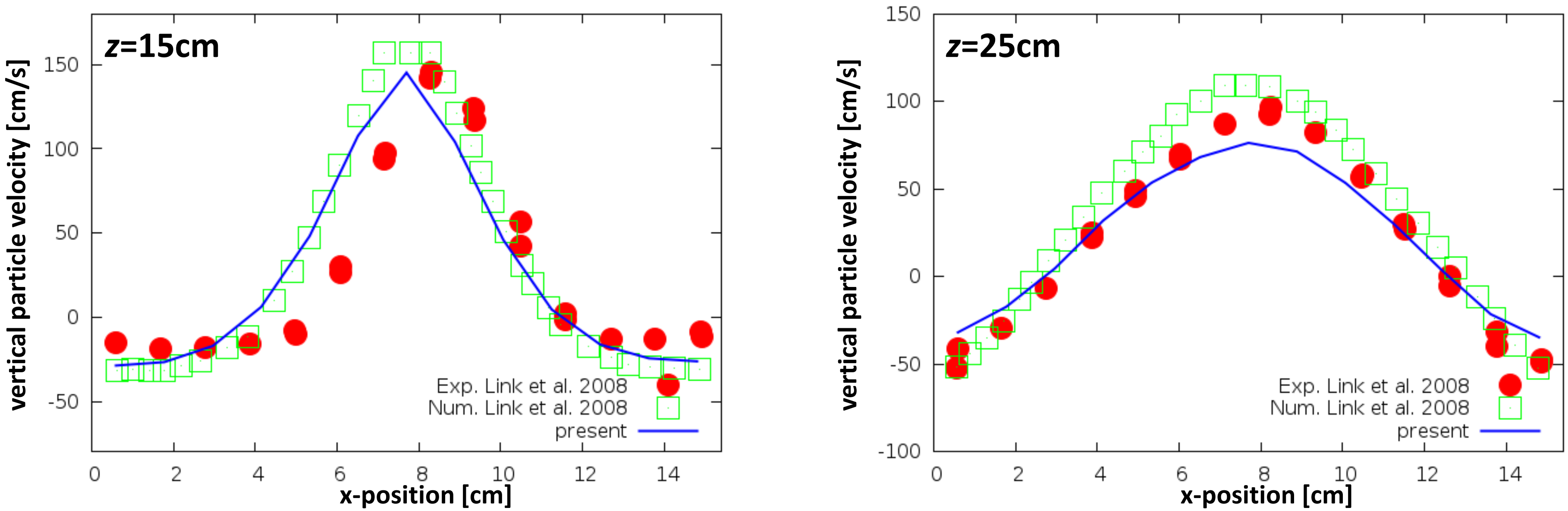
Case 1:
u_{sv} =60m/s
u_{bg} =2.5m/s



Link et al., AIChE Journal, 2008, 54:1189-1202.

Case 3: Time-Average Lateral Profiles in Vertical Particle Velocity

Reported in the central XZ-plane



Fair agreement with both experimental data and DEM predictions

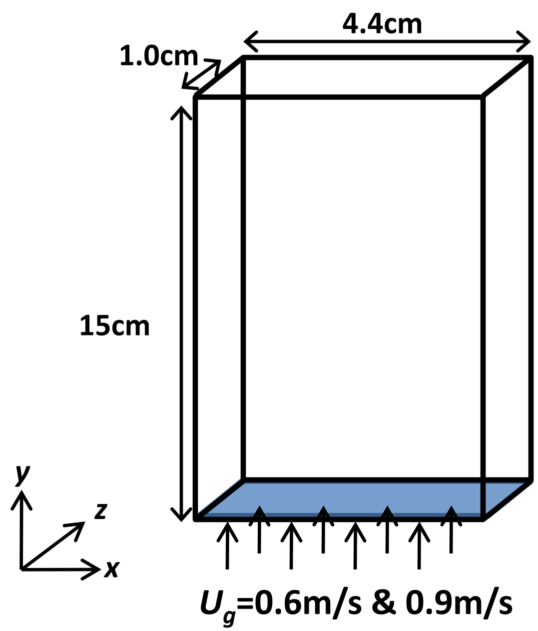
Additional comparisons possible including frequency spectra data of the pressure drop fluctuations and data for two additional cases:

- **Case 2 - Spouting-with aeration**
- **Case 3 - Jet-in-fluidized-bed**

Case 4: Bubbling Bed 1

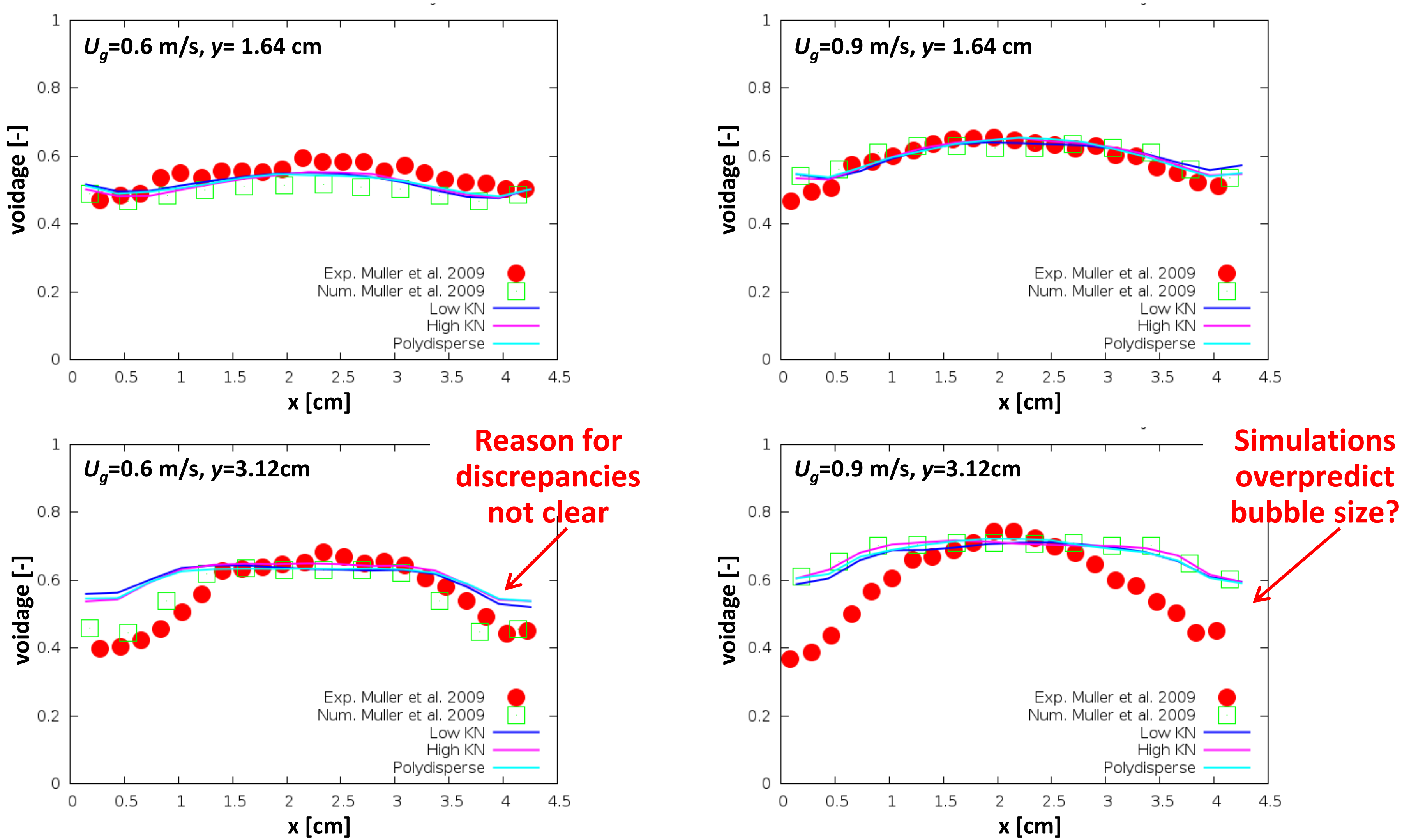
d_{p1} =0.12cm,
ρ_p =1.0g/cm^3
N_p =9240

- Experimental setup
  - Small bubbling bed of poppy seeds (**kidney shaped**) fluidized at 2 gas velocities
  - Use magnetic resonance (MR to measure time-averaged voidage map of bed
- Simulation setup
  - Same but with reduced bed height (12cm) and **spherical particles**



Muller et al., Particuology, 2009, 7:297-306

Case 4: Time-Averaged Lateral Profiles in Void Fraction

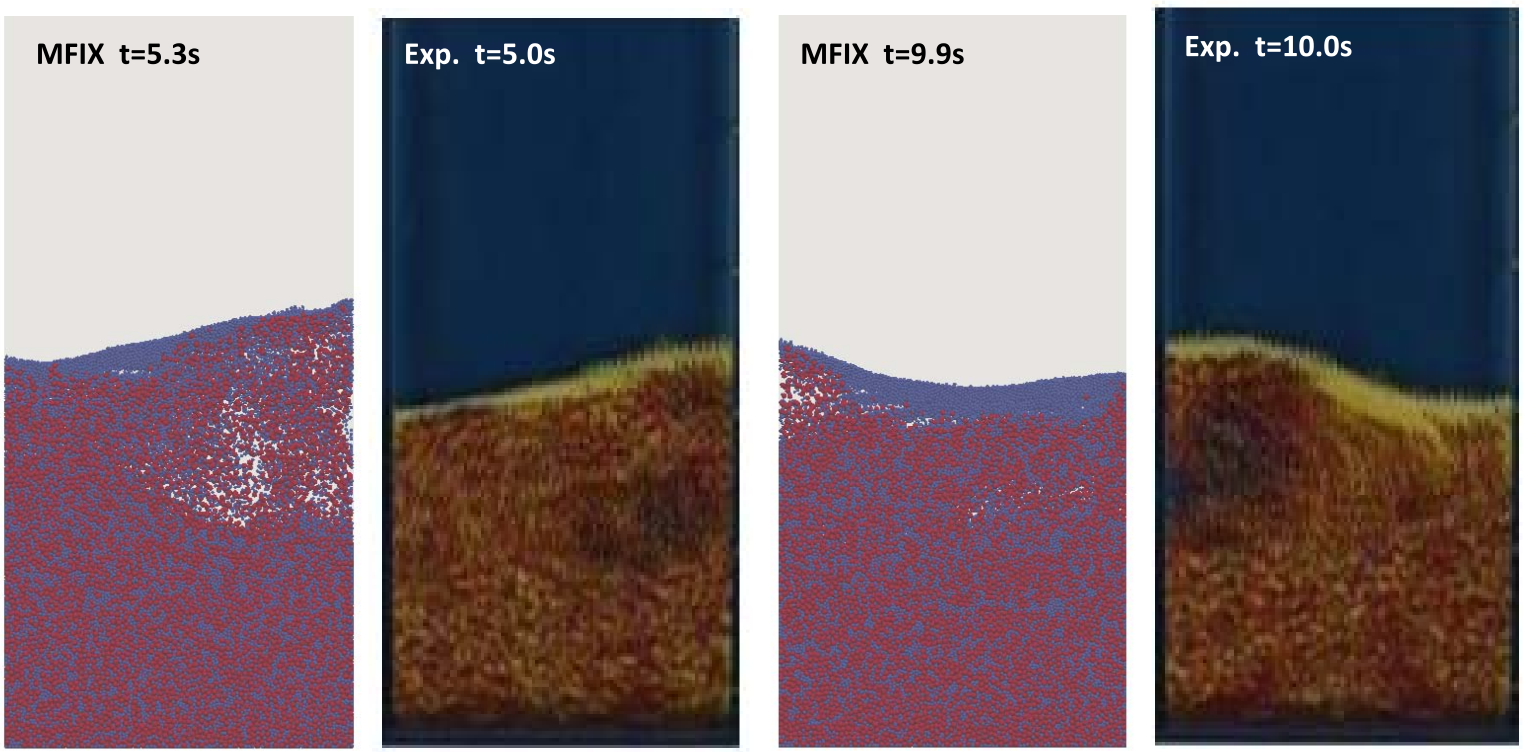


Further parametric studies needed (e.g., friction coefficient, restitution coefficient)
Additional comparisons possible with similar data on solids velocity

Case 5: Bubbling Bed 2 (Binary Segregation)

d_{p1} =0.152cm,
d_{p2} =0.249cm,
ρ_p =2.52g/cm^3
x_1 =25%
M_t =494.3g
U_g =1.2m/s

- Experimental setup
  - A psuedo 2D bubbling fluidized bed (see case 1) of a bidisperse mixture of differing sized glass particles; various compositions & operating velocities
  - Digital image analysis to measure bed expansion and segregation dynamics



Qualitative agreement

Quantitative comparison with experimental data (segregation dynamics) is underway

Goldschmidt et al., Powder Technology, 2003, 138:135-159;
van Sint Annaland et al., Chemical Engineering Science, 2009, 64: 4237-4246, Fig 6. or 7.

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Current Status and Future Plans

Validation

- Finish detailed analysis of existing cases & work on additional test cases
  - Tsuji et al., PT, 1993: 2D Fluidized Bed with a Central Jet
  - ANL Experiments (Aranson and Li, ANL): Flower bed
  - Granular plane shear flow (Saitoh and Hayakawa, PRE, 2007)

Future Work

Speed-up
- Coarse-graining (MP-PIC, CDEM etc.)
- Parallelization (SMP, DMP, GPGPUs)
- Time-stepping algorithms, MD potentials…

Utility
- Test existing constitutive models
- Interpret important experiments (e.g. clustering data from Frank)

Innovation
- Hybrid DECM algorithm
- Path to pilot and commercial-scale reactors

New Features
- Heat and Mass transfer
- Reactions
- This is one area not much is done in the literature