NATIONAL ENERGY TECHNOLOGY LABORATORY

MPPIC model implementation in MFIX: frictional solid-stress model

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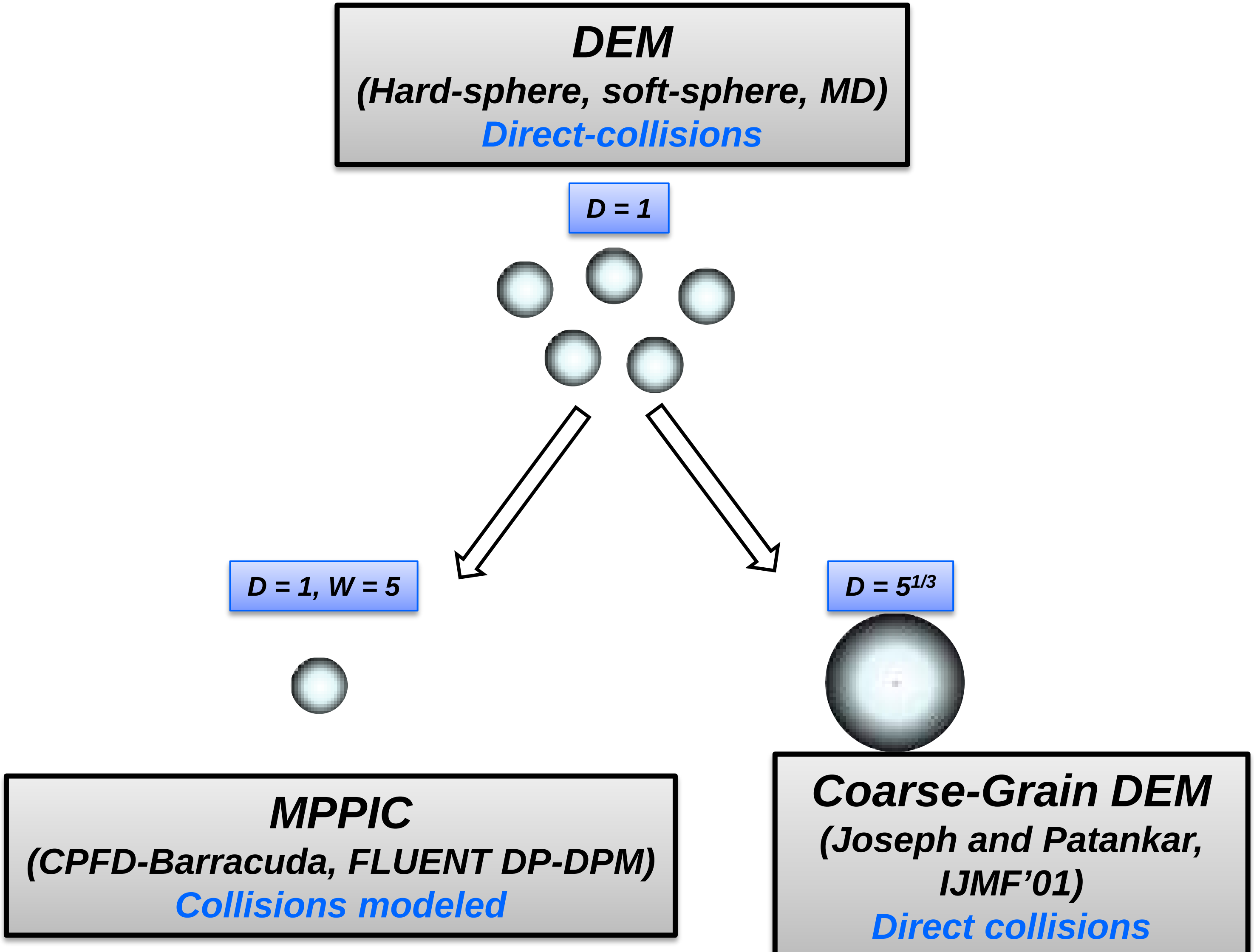
U.S. DEPARTMENT OF ENERGY

Comparison b/w different discrete methods



MPPIC: current state-of-the-art

- ✓ *“IT WORKS!!!” “IT’S FAST”*
- ✓ **Demonstrated to be a useful tool for quick turnaround simulations at pilot/device scales**
- ✓ **Several commercial implementations (Barracuda by CPFD, Dense-phase-DPM by ANSYS)**
- ✓ **Hard to ascertain and further develop sub-models (such as collision, friction, etc.)**
  - ✓ Confusion among users regarding the exact form of models
- ➢ ***Objective of this study:*** **understand, implement, and document MPPIC model in open-source MFIX code to probe its accuracy and speed**

MPPIC model details

Carrier Phase: averaged Navier-Stokes equation

$$\frac{\partial(\varepsilon_{\mathrm{g}}\rho_{\mathrm{g}})}{\partial t} + \nabla \cdot (\varepsilon_{\mathrm{g}}\rho_{\mathrm{g}}\mathbf{v}_{\mathrm{g}}) = 0$$

$$\frac{D}{Dt}(\varepsilon_{\mathrm{g}}\rho_{\mathrm{g}}\mathbf{v}_{\mathrm{g}}) = \nabla \cdot \overline{\overline{S}}_{\mathrm{g}} + \varepsilon_{\mathrm{g}}\rho_{\mathrm{g}}\mathbf{g} - \mathbf{F}_{\mathrm{drag}}$$

A_{coll} is the collision operator used to model collisions in the ***kinetic*** and ***frictional*** regimes.

Robust implementation of ***frictional regime*** A_{coll} is critical to stability of MPPIC model

Dispersed Phase

$$\frac{d\mathbf{X}_{\mathrm{p}}}{dt} = \mathbf{V}_{\mathrm{p}}$$

$$m\frac{d\mathbf{V}_{\mathrm{p}}}{dt} = m\mathbf{g} + \mathbf{F}_{\mathrm{p,drag}} + m\mathbf{A}_{\mathrm{coll}}$$

Particle trajectory evolution

$$\boxed{m\frac{d\mathbf{V}_\mathrm{p}}{dt} = m\mathbf{g} + \mathbf{F}_{\mathrm{p,drag}} + m\mathbf{A}_{\mathrm{coll}}}$$

$$\mathbf{X}_\mathrm{p}^{n+1} = \mathbf{X}_\mathrm{p}^{n} + \Delta t \mathbf{V}_\mathrm{p}^{n+1}$$

$$\mathbf{V}_\mathrm{p}^{n+1} = \widetilde{\mathbf{V}}_\mathrm{p} + \mathbf{V}_{\mathrm{p}\tau}$$

$$\widetilde{\mathbf{V}}_\mathrm{p} = \mathbf{V}_\mathrm{p}^{n} + \left(\mathbf{g} + \frac{\mathbf{F}_{\mathrm{p,drag}}}{m}\right)\Delta t$$

Drag+body force

$$\widetilde{\mathbf{V}}_\mathrm{p} \xrightarrow{A_{\mathrm{coll}}} \mathbf{V}_{\mathrm{p}\tau}$$

Impulse velocity

How is A_{coll} applied ?

$$\left(\mathbf{X}_\mathrm{p}^{n+1}, \mathbf{V}_\mathrm{p}^{n+1}\right) \xrightarrow[\text{Specular}]{\text{Wall B.C.}} \left(\mathbf{X}^{*}{}_\mathrm{p}^{n+1}, \mathbf{V}^{*}{}_\mathrm{p}^{n+1}\right)$$

A_{coll} implementation (frictional regime)

$$m\frac{d\mathbf{V}_\mathrm{p}}{dt} = m\mathbf{g} + \mathbf{F}_{\mathrm{p,drag}} + m\mathbf{A}_{\mathrm{coll}}$$

$$\mathbf{X}_\mathrm{p}^{n+1} = \mathbf{X}_\mathrm{p}^{n} + \Delta t \mathbf{V}_\mathrm{p}^{n+1}$$

$$\mathbf{V}_\mathrm{p}^{n+1} = \widetilde{\mathbf{V}}_\mathrm{p} + \mathbf{V}_{\mathrm{p}\tau}$$

$$\widetilde{\mathbf{V}}_\mathrm{p} = \mathbf{V}_\mathrm{p}^{n} + \left(\mathrm{g} + \frac{\mathbf{F}_{\mathrm{p,drag}}}{m}\right)\Delta t$$

$$\widetilde{\mathbf{V}}_\mathrm{p} \xrightarrow{A_{\mathrm{coll}}} \mathbf{V}_{\mathrm{p}\tau}$$

$$\left(\mathbf{X}_\mathrm{p}^{n+1}, \mathbf{V}_\mathrm{p}^{n+1}\right) \xrightarrow[\text{Specular}]{\text{Wall B.C.}} \left(\mathbf{X}_\mathrm{p}^{*n+1}, \mathbf{V}_\mathrm{p}^{*n+1}\right)$$

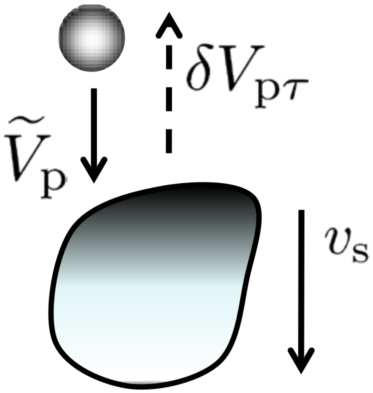
$$\chi = \varepsilon_\mathrm{s} \qquad \varepsilon_\mathrm{s} \geq \varepsilon_{\mathrm{s}_\mathrm{cp}}$$
$$= 0 \qquad \text{otherwise}$$

$$\delta \mathbf{V}_{\mathrm{p}\tau} = -\nabla \chi$$

χ is like a coloring function used to indicate the close-packed regions. $\delta \mathbf{u}_{\mathrm{p}\tau}$ is non-zero inside *and* at the interfaces of close-packed regions. It only indicates the direction of the correction due to close-packing.

A_{coll} implementation

Case 1



if $\left|\widetilde{V}_p\right| > |v_s|$

REBOUND

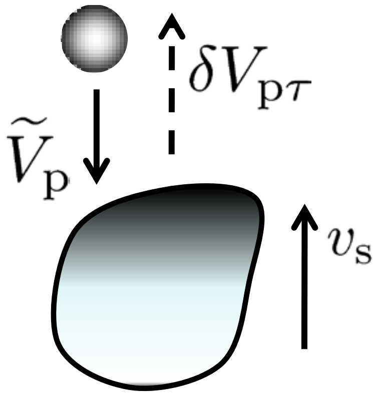
$$V_p^{n+1} = v_s - e_1^{fric}(\widetilde{V}_p - v_s) \uparrow\downarrow$$

else

SLOW DOWN

$$V_p^{n+1} = e_2^{fric}\widetilde{V}_p \downarrow$$

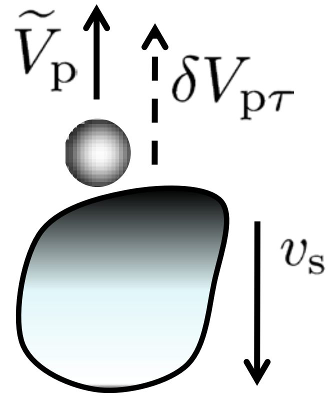
Case 2



REBOUND

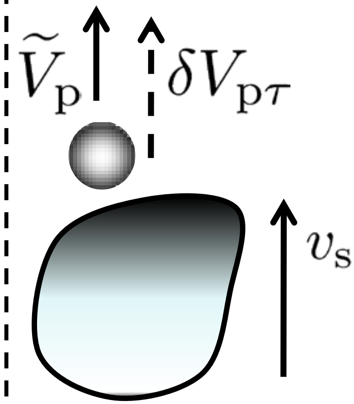
$$V_p^{n+1} = v_s - e_1^{fric}(\widetilde{V}_p - v_s) \uparrow$$

Case 3



DO NOTHING

Case 4



if $\widetilde{V}_p < v_s$

BUMP

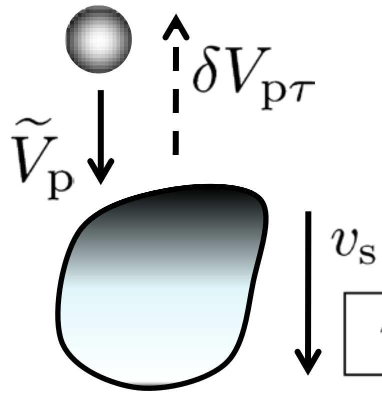
$$V_p^{n+1} = v_s - e_1^{fric}(\widetilde{V}_p - v_s) \uparrow$$

else

DO NOTHING

A_{coll} implementation (Summary)

Case 1

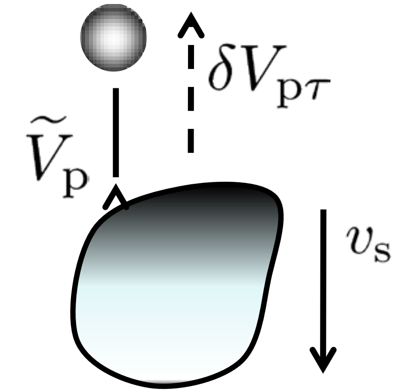


v_s: average solids velocity

$$\mathbf{V}_{rel} = \widetilde{\mathbf{V}}_{\mathbf{p}} - \mathbf{v}_{\mathbf{s}}$$

V_{rel}: parcel's relative velocity wrt close-pack

$$\mathbf{V}_p^{\mathbf{n+1}} = \mathbf{v}_\mathbf{s} - \mathbf{e}_\mathbf{1}^{\text{fric}} \mathbf{V}_{\text{rel}}; \quad \text{if} \quad \mathbf{V}_{\text{rel}}.(\delta \mathbf{V}_{p\tau}) < \mathbf{0}$$



$$\text{if } \left|\widetilde{V}_p\right| > |v_s|$$

REBOUND

$$V_p^{n+1} = v_s - e_1^{\text{fric}}(\widetilde{V}_p - v_s)$$

else

SLOW DOWN

$$V_p^{n+1} = e_2^{\text{fric}} \widetilde{V}_p$$

Case 1b

Comparison with existing literature

$$m\frac{d\mathbf{V}_{\mathsf{p}}}{dt} = m\mathbf{g} + \mathbf{F}_{\mathsf{p,drag}} + m\mathbf{A}_{\mathsf{coll}}$$

$$\mathbf{V}_{\mathsf{p}}^{n+1} = \widetilde{\mathbf{V}}_{\mathsf{p}} + \mathbf{V}_{\mathsf{p}\tau}$$

$$\widetilde{\mathbf{V}}_{\mathsf{p}} = \mathbf{V}_{\mathsf{p}}^{n} + \left(\mathbf{g} + \frac{\mathbf{F}_{\mathsf{p,drag}}}{m}\right)\Delta t$$

No inter-particle collision term so far

Snider, D. M., An incompressible 3-D MP-PIC model for dense particle flows, JCP (2001)

Comparison with existing literature

$$m\frac{d\mathbf{V}_\mathsf{p}}{dt} = m\mathbf{g} + \mathbf{F}_{\mathsf{p,drag}} + m\mathbf{A}_{\mathsf{coll}}$$

$$\mathbf{V}_\mathsf{p}^{n+1} = \widetilde{\mathbf{V}}_\mathsf{p} + \mathbf{V}_{\mathsf{p}\tau}$$

$$\tau = \frac{P_\mathsf{s}\varepsilon_\mathsf{s}^\beta}{\max\left[\varepsilon_{\mathsf{scp}} - \varepsilon_\mathsf{s}, \epsilon\left(1-\varepsilon_\mathsf{s}\right)\right]}$$

Isotropic inter-particle stress (Harris and Crighton)

$$\delta\mathbf{V}_{\mathsf{p}\tau} = -\frac{\Delta t \boldsymbol{\nabla}\tau}{\rho_\mathsf{s}\varepsilon_\mathsf{s}}$$

Decides the direction of solid-stress correction velocity

$$(\boldsymbol{\nabla}\tau).\mathbf{e}_k \leq 0$$

$${V'}_{p\tau_k} = \min\left(\mathbf{e}_k \cdot \delta\mathbf{V}_{\mathsf{p}\tau}, (1+\gamma)(\mathbf{v}_s - \widetilde{\mathbf{V}}_\mathsf{p}) \cdot \mathbf{e}_k\right)$$

$$V_{p\tau_k} = \max\left({V'}_{p\tau_k}, 0\right)$$

Matters mostly near close-packing, otherwise statistical noise!

Comparison with existing literature

$$m\frac{d\mathbf{V}_\mathrm{p}}{dt} = m\mathbf{g} + \mathbf{F}_{\mathrm{p,drag}} + m\mathbf{A}_{\mathrm{coll}}$$

$$\mathbf{V}_\mathrm{p}^{n+1} = \widetilde{\mathbf{V}}_\mathrm{p} + \mathbf{V}_{\mathrm{p}\tau}$$

$$\tau = \frac{P_\mathrm{s}\varepsilon_\mathrm{s}^{\beta}}{\max\left[\varepsilon_{\mathrm{scp}} - \varepsilon_\mathrm{s}, \epsilon\left(1-\varepsilon_\mathrm{s}\right)\right]}$$

$$\delta\mathbf{V}_{\mathrm{p}\tau} = -\frac{\Delta t \boldsymbol{\nabla}\tau}{\rho_\mathrm{s}\varepsilon_\mathrm{s}}$$

$$(\boldsymbol{\nabla}\tau).\mathbf{e}_k \leq 0$$

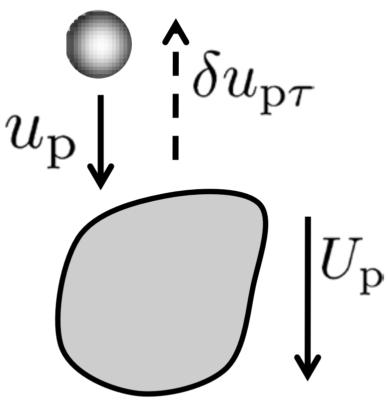
$$V'_{p\tau_k} = \min\left(\mathbf{e}_k \cdot \delta\mathbf{V}_{\mathrm{p}\tau}, (1+\gamma)(\mathbf{v}_s - \widetilde{\mathbf{V}}_\mathrm{p}) \cdot \mathbf{e}_k\right)$$

$$V_{p\tau_k} = \max\left(V'_{p\tau_k}, 0\right)$$

WHAT DO THESE LIMITERS IMPLY ?

Explanation of limiters

Case 1



if $|u_p| > |U_p|$

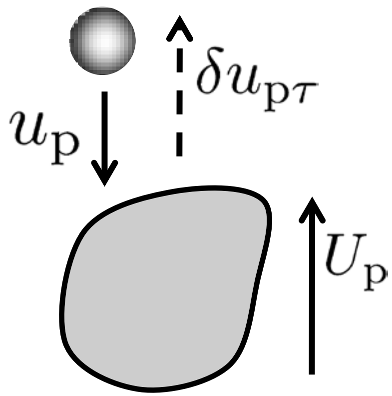
REBOUND

$$u_{p\tau} = (1+\gamma)(U_p - u_p)$$

else

DO NOTHING

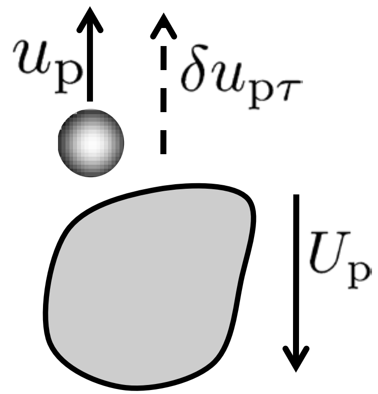
Case 2



REBOUND

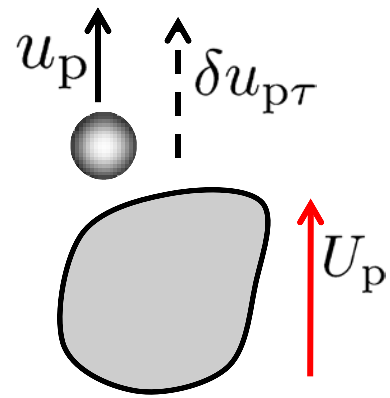
$$u_{p\tau} = (1+\gamma)(U_p - u_p)$$

Case 3



DO NOTHING

Case 4



if $u_p < U_p$

BUMP

$$u_{p\tau} = (1+\gamma)(U_p - u_p)$$

else

DO NOTHING

$$\mathbf{u}_p^{n+1} = \tilde{\mathbf{u}}_p + \mathbf{u}_{p\tau}$$

$$\delta \mathbf{u}_{p\tau} = -\frac{\Delta t \nabla \tau}{\rho_s \varepsilon_s}$$

$$(\nabla \tau).\mathbf{e}_k \leq 0$$

$$u'_{p\tau_k} = \min\left(\mathbf{e}_k \cdot \delta \mathbf{u}_{p\tau}, (1+\gamma)(\mathbf{U}_p - \mathbf{u}_p) \cdot \mathbf{e}_k\right)$$

$$u_{p\tau_k} = \max\left(u'_{p\tau_k}, 0\right)$$

Snider's model vs. the new model

$$\mathbf{V}_{\mathrm{p}}^{n+1} = \widetilde{\mathbf{V}}_{\mathrm{p}} + \mathbf{V}_{\mathrm{p}\tau}$$

$$\tau = \frac{P_{\mathrm{s}}\varepsilon_{\mathrm{s}}^{\beta}}{\max\left[\varepsilon_{\mathrm{scp}} - \varepsilon_{\mathrm{s}}, \epsilon\left(1-\varepsilon_{\mathrm{s}}\right)\right]}$$

$$\delta\mathbf{V}_{\mathrm{p}\tau} = -\frac{\Delta t \boldsymbol{\nabla}\tau}{\rho_{\mathrm{s}}\varepsilon_{\mathrm{s}}}$$

$$(\boldsymbol{\nabla}\tau).\mathbf{e}_k \leq 0$$

$$V'_{p\tau_k} = \min\left(\mathbf{e}_k \cdot \delta\mathbf{V}_{\mathrm{p}\tau}, (1+\gamma)(\mathbf{v}_s - \widetilde{\mathbf{V}}_{\mathrm{p}}) \cdot \mathbf{e}_k\right)$$

$$V_{p\tau_k} = \max\left(V'_{p\tau_k}, 0\right)$$

$$\mathbf{V}_{\mathrm{rel}} = \widetilde{\mathbf{V}}_{\mathbf{p}} - \mathbf{v}_{\mathbf{s}}$$

V_{rel}: parcel's relative velocity wrt close-pack

$$\mathbf{V}_{\mathrm{p}}^{\mathbf{n+1}} = \mathbf{v}_{\mathbf{s}} - \gamma \mathbf{V}_{\mathrm{rel}}; \quad \text{if} \quad \mathbf{V}_{\mathrm{rel}}.(\delta\mathbf{V}_{\mathrm{p}\tau}) < \mathbf{0}$$

Two parameter model: P_s and γ

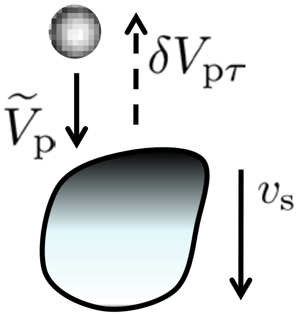
Case 1b

$$\chi = \varepsilon_{\mathrm{s}} \quad \varepsilon_{\mathrm{s}} \geq \varepsilon_{\mathrm{scp}}$$
$$= 0 \quad \text{otherwise}$$

$$\delta\mathbf{V}_{\mathrm{p}\tau} = -\boldsymbol{\nabla}\chi$$

$$\mathbf{V}_{\mathrm{rel}} = \widetilde{\mathbf{V}}_{\mathbf{p}} - \mathbf{v}_{\mathbf{s}}$$

+



$$\mathbf{V}_{\mathrm{p}}^{\mathbf{n+1}} = \mathbf{v}_{\mathbf{s}} - \mathbf{e}_{\mathbf{1}}^{\mathrm{fric}} \mathbf{V}_{\mathrm{rel}};$$
$$\text{if} \quad \mathbf{V}_{\mathrm{rel}}.(\delta\mathbf{V}_{\mathrm{p}\tau}) < \mathbf{0}$$

$$\text{if} \left|\widetilde{V}_{\mathrm{p}}\right| < |v_{\mathrm{s}}|$$

SLOW DOWN

$$V_{\mathrm{p}}^{n+1} = e_2^{\mathrm{fric}} \widetilde{V}_{\mathrm{p}}$$

Two parameter model: e_1^{fric} and e_2^{fric}

STILL DOESN'T WORK!

A simple case of particles sedimenting in a vertical channel blows up due to the inability of the frictional model to sustain specified close-packing

Fix?

Cases 1-4

$$\chi = \varepsilon_s \quad \varepsilon_s \geq \varepsilon_{scp}$$
$$= 0 \quad \text{otherwise}$$

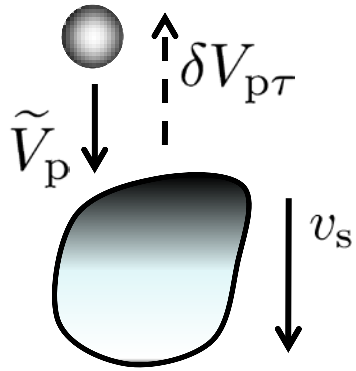
$$\delta \mathbf{V}_{p\tau} = -\nabla \chi$$

$$\mathbf{V}_{rel} = \widetilde{\mathbf{V}}_{\mathbf{p}} - \mathbf{v}_{\mathbf{s}}$$

$$\mathbf{V}_{p}^{\mathbf{n+1}} = \mathbf{v}_{\mathbf{s}} - \mathbf{e}_{\mathbf{1}}^{\text{fric}} \mathbf{V}_{rel};$$
$$\text{if} \quad \mathbf{V}_{rel}.(\delta \mathbf{V}_{p\tau}) < \mathbf{0}$$

\+

Case 1b



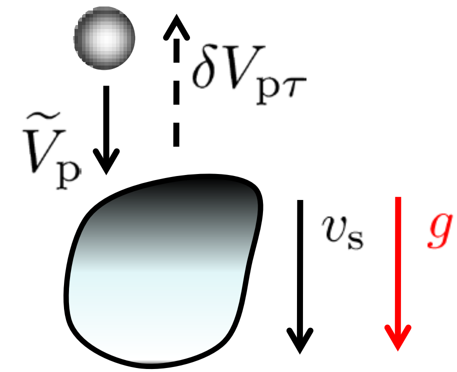
$$\text{if } \left|\widetilde{V}_p\right| < |v_s|$$

SLOW DOWN

$$V_p^{n+1} = e_2^{\text{fric}} \widetilde{V}_p$$

\+

Case 1a



$$\left|\widetilde{V}_p\right| <> |v_s|$$

ALWAYS REBOUND

$$V_p^{n+1} = -e_1^{\text{fric}} \widetilde{V}_p$$

Results in unconditionally stable solver (does not guarantee any results)
Still a 2-parameter model

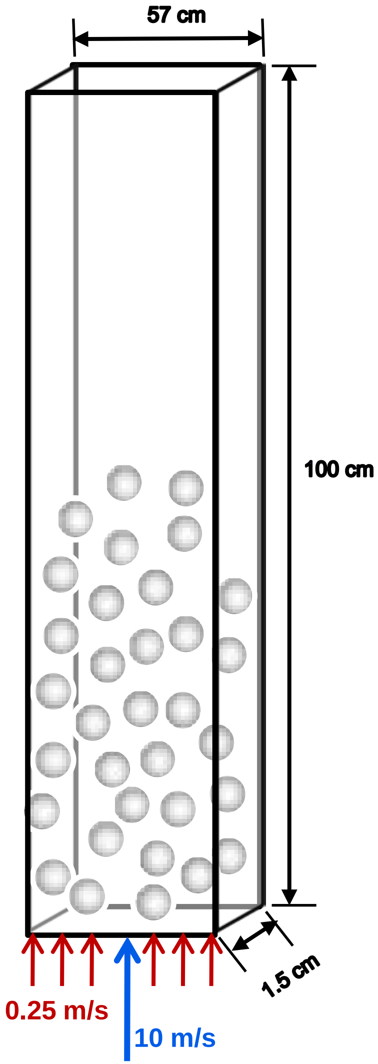
Other features/limitations/future development

- ❑ Specular reflections at wall
- ❑ No friction at the walls
- ❑ No collisions in the viscous regime
- ❑ Robust extension to cut-cell

Model development thought process

- ✓ **Three problems were chosen: sedimentation, spouted bed, and uniformly fluidized bed**
- ✓ **Any frictional model or a wild guess was tested by running all three problems**
  - ➢ Lot of times very encouraging results for one problem led to blow up of simulations for other problems
  - ➢ A stable model did not always imply a physically plausible model. The first model I tried was the most stable one but nothing really moved in that model either!
- ✓ **The final model is a trade off between numerical stability and physics. There are many other variants of this model possible…..**

Sample Problem 1: Kuiper's jet

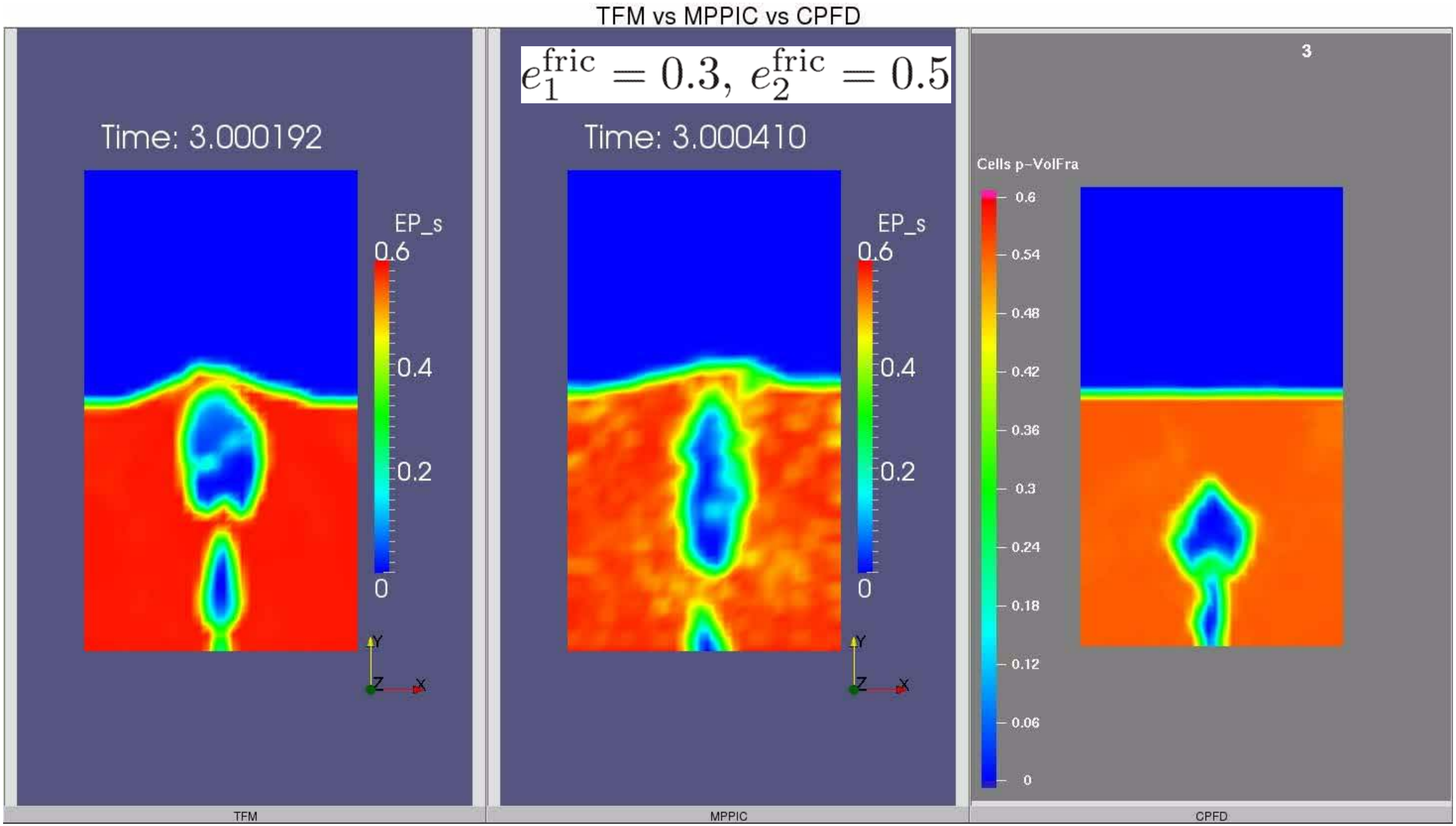


Properties
Solids: $D_p = 0.05$ cm, $\rho_p = 2.6$ g/cm^3 Total number of particles (DEM) = 36 million Total number of parcels (MPPIC) = 4,560 ~ **8000** particles per parcel
Gas: Air at standard conditions
Bed Dimension= (57x100x1.5) cm^3 ≡ (31x60x1) cells
No slip wall BC's for gas and free slip for solids phase mean velocity
Drag model: Wen & Yu / Ergun Pressure of bed weight = 7.1 kPa

Easiest to bubble, hardest to simulate stably

Kuipers, J.A.M., A two-fluid micro balance of fluidized bed. PhD thesis, 1990

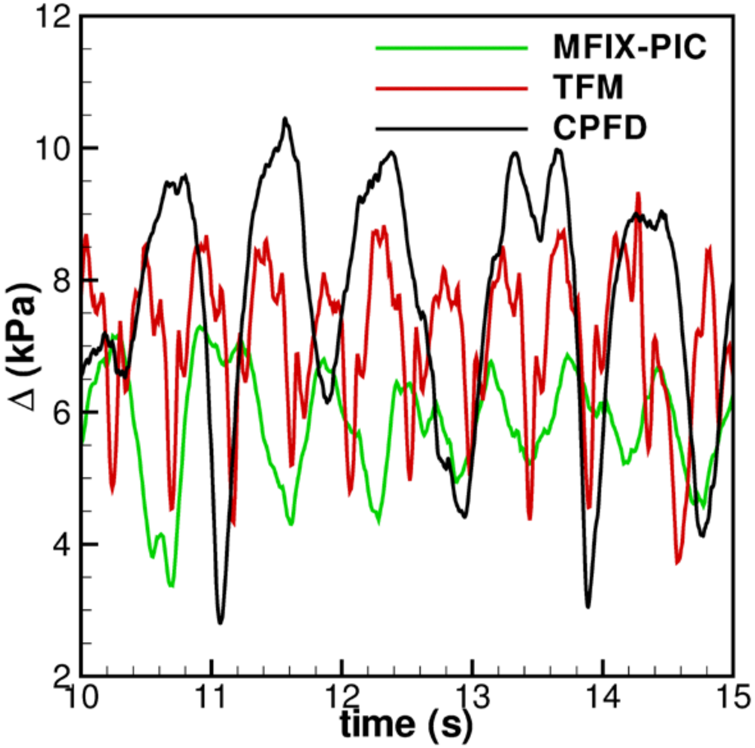
TFM vs MPPIC vs CPFD

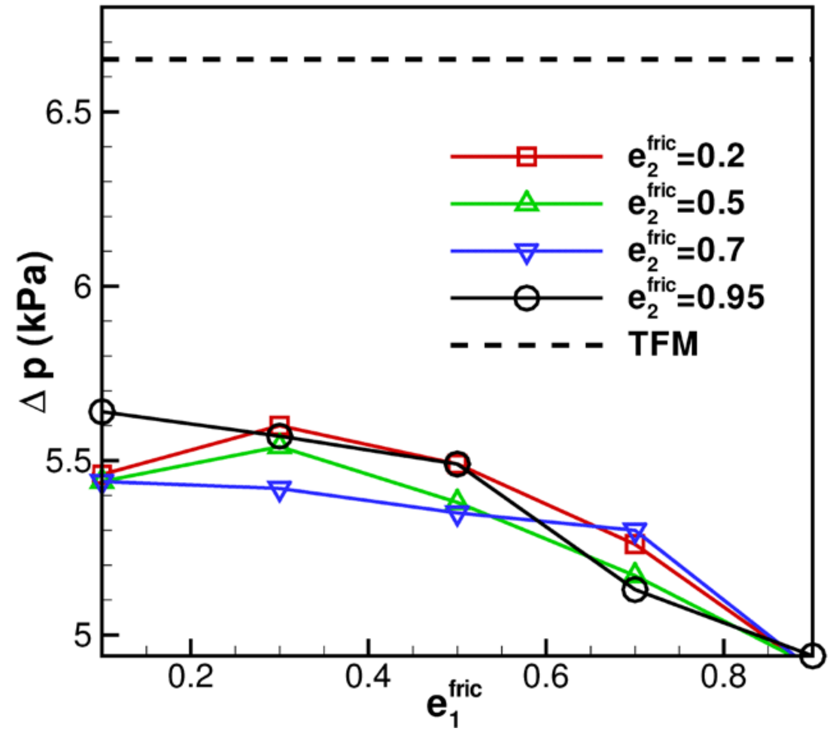


TFM **MFIX-PIC** **CPFD**

Pressure Drop

$e_1^{\mathrm{fric}} = 0.3,\ e_2^{\mathrm{fric}} = 0.5$

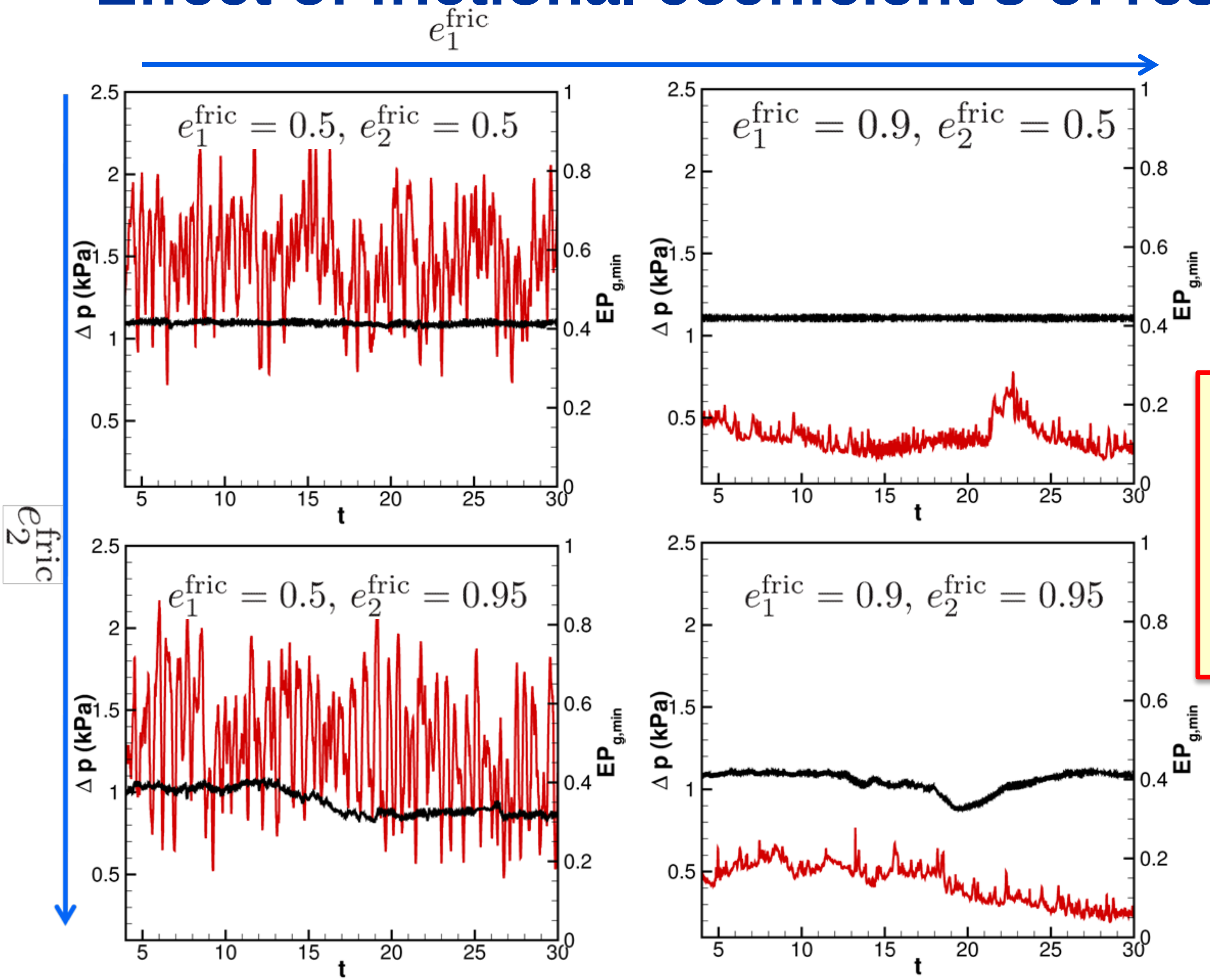




- Both MFIX-PIC and CPFD exhibit different bubble frequency with CPFD giving the lowest bubble frequency
- The amplitude of oscillations is higher in CPFD implying prediction of higher pressure fluctuations for design purposes

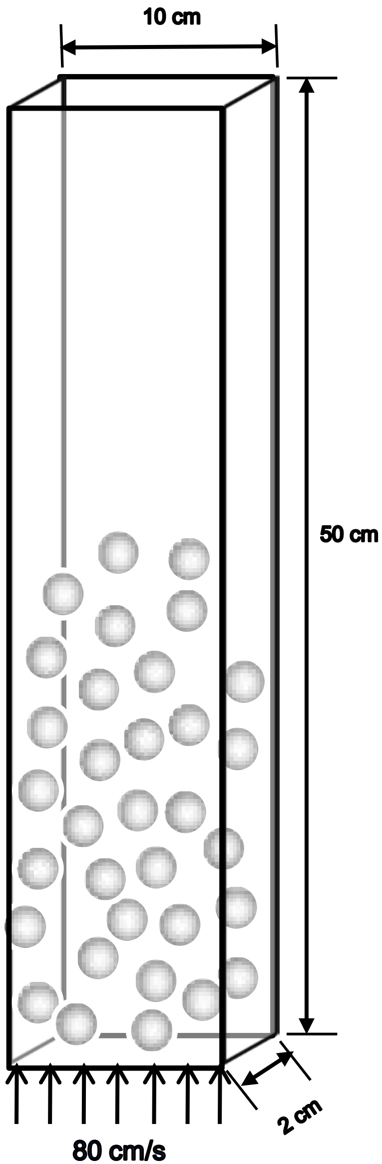
- Under-prediction of pressure drop by 15% for the best case.
- Pressure drop most sensitive to first frictional coefficient of restitution.
- Week dependence on second frictional coefficient of restitution
- Recommended values of 0.3-0.6 for both parameters
- **COMPUTATIONAL WALL TIMES:** TFM (400 mins), and MPPIC (80 mins) on a single core.

Effect of frictional coefficient's of restitution



- The model's stability does not get affected by the first coefficient of restitution.
- Recommended values of 0.3-0.6 for both parameters

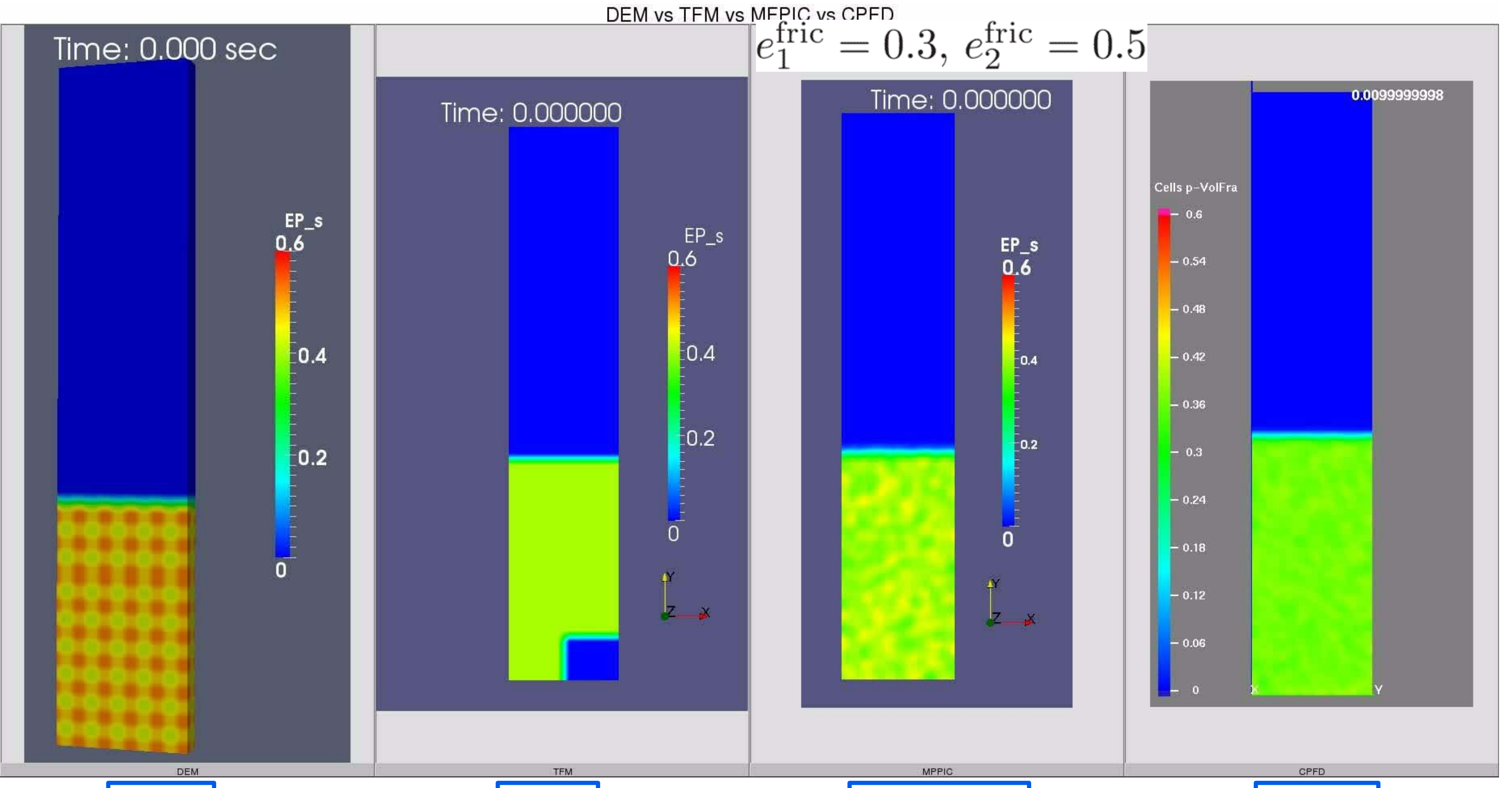
Sample Problem 2: uniformly fluidized



Properties
Solids: D_p = 0.1 cm, ρ_p = 2.5 g/cm^3 Total number of particles (DEM) = 305 K Total number of parcels (MPPIC) = 16,000 ~ **20** particles per parcel
Gas: Air at standard conditions Fluidization velocity = 80 cm/s
box dimension = (10x50x2) cm^3 ≡ (20x100x4) cells
FREE slip wall BC's for both gas and solids phase mean velocity
Drag model: Wen &Yu / Ergun Pressure of bed weight = 1.96 kPa

Easiest to simulate, hardest to bubble!

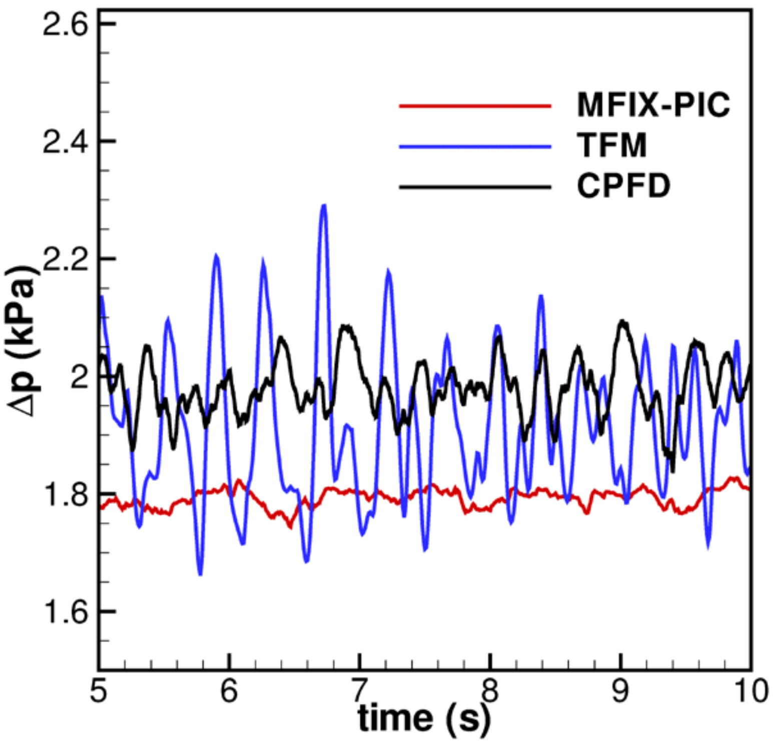
DEM vs TFM vs MPPIC vs CPFD



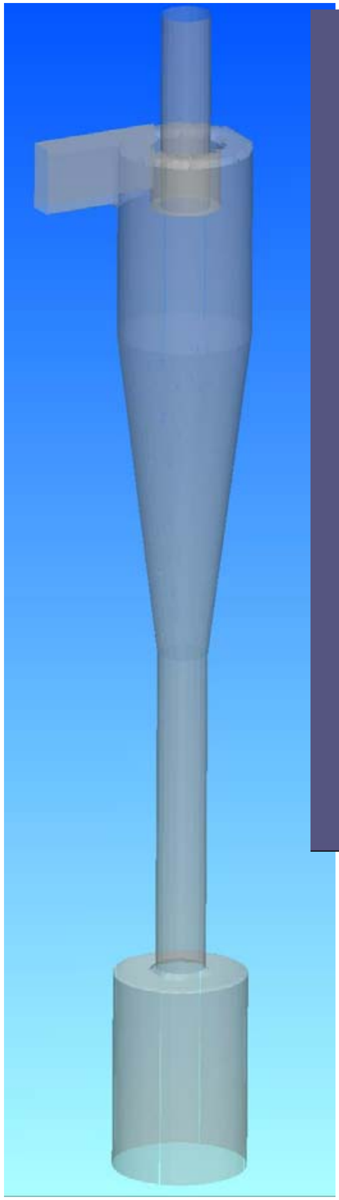
DEM **TFM** **MFIX-PIC** **CPFD**

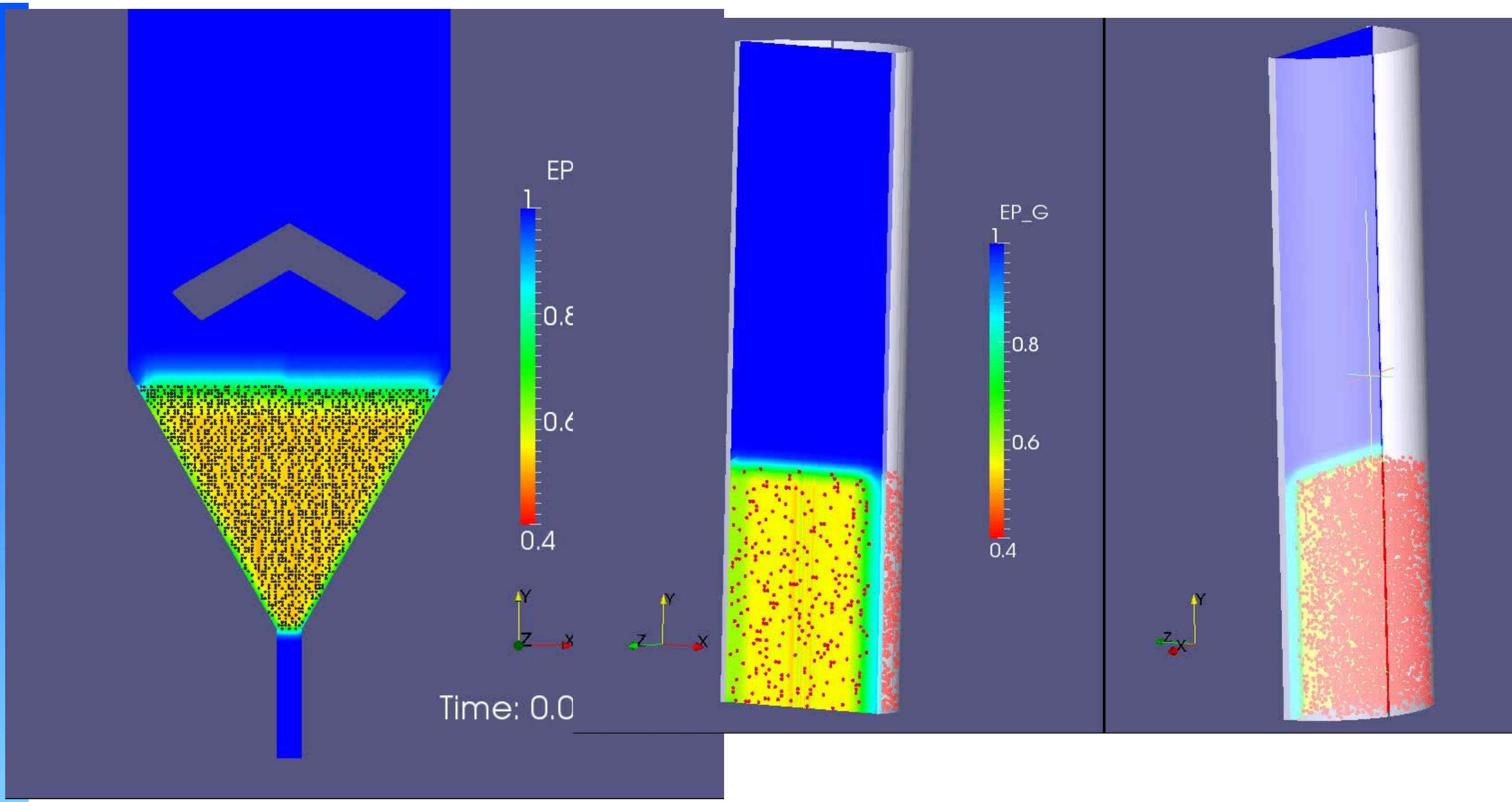
Both MFIX-PIC and CPFD do not bubble much and as a result predict low variations in pressure drop (see next slide)

Pressure drop comparison



Extension to Cartesian Grid





- **More work needed for robust extension of MPPIC model to cut-cell**
  - Forward interpolation of gas-phase velocity field
  - Calculation of solid phase frictional pressure on the Eulerian grid followed by its forward interpolation
  - Backward estimation of mean fields

Conclusions/Observations

- **MPPIC model implemented in open-source MFIX code**
  - A new limiter based on physical arguments formulated for solid-stress model
- **MPPIC model compared against other CFD models and existing commercial MPPIC model**
- **MPPIC models found to be in qualitative and limited quantitative agreements with the more accurate DEM model**
- **Need to implement additional physical models for particle-particle and particle-wall interactions**

Acknowledgments

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