A Massively Parallel Euler-Lagrange Strategy for Simulating Fluidized Bed Reactors

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Jesse Capecelatro, Olivier Desjardins
Sibley School of Mechanical and Aerospace Engineering
Cornell University

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Cornell University
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Motivation

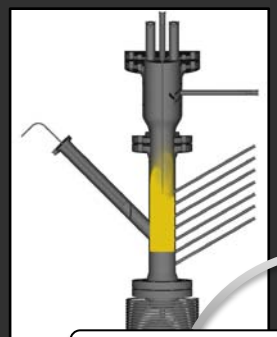
- Particle-laden flows are an important type of multiphase flow
- Common in many natural and industrial processes
- Fluidized bed reactors are ideal for gasification /pyrolysis
  - Easily scalable
  - Efficient mixing
  - Uniform temperature distribution
- Range of phenomenon exist in particle flows
  - Bubbling
  - Clustering

Spiegel (2009)

Horio & Kuroki (1994)

Objective

- Develop simulation strategy investigate complex multiphase flow dynamics
- Use first-principle based methods to optimize reactors
- Provide closures for larger scale modeling approaches
- Useful to have successful representation at each scale to elucidate the physics

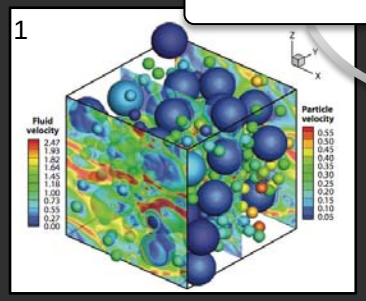


Lab scale

- Model drag, collisions, etc.
- Couple phases
- $d_p \approx 0.1dx$-$1dx$

Microscale

- Resolve flow around each particle
- $d_p \approx 10dx$-$50dx$



Industrial scale

- DSMC
- Euler-Euler
- Relies heavily on modeling

1. Tenneti & Subramaniam (2010)

Mathematical Formulation

Pointwise Description

- *Gas phase:* Variable-density / low-Mach Navier-Stokes equations

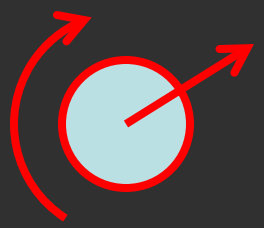
$$\frac{\partial \rho_f}{\partial t} + \nabla \cdot (\rho_f \boldsymbol{u}_f) = 0$$

$$\frac{\partial}{\partial t}(\rho_f \boldsymbol{u}_f) + \nabla \cdot (\rho_f \boldsymbol{u}_f \otimes \boldsymbol{u}_f) = \nabla \cdot \boldsymbol{\tau} + \rho_f \boldsymbol{g}$$

$$\boldsymbol{\tau} = -p\boldsymbol{\mathcal{I}} + \mu \left[(\nabla \boldsymbol{u}_f + \nabla \boldsymbol{u}_f^{\mathsf{T}}) - \frac{2}{3} \ (\nabla \cdot \boldsymbol{u}_f)\boldsymbol{\mathcal{I}} \right]$$

- *Particles:* Newton's second law of motion

$$\frac{d\boldsymbol{x}_p}{dt} = \boldsymbol{u}_p$$



$$m_p \frac{d\boldsymbol{u}_p}{dt} = \int_{S_p} \boldsymbol{\tau} \cdot \boldsymbol{n} \ d\boldsymbol{y} + F^{\mathrm{col}} + m\boldsymbol{g}$$

$$I_p \frac{d\boldsymbol{\omega}_p}{dt} = \int_{S_p} \frac{d_p}{2} \boldsymbol{n} \times (\boldsymbol{\tau} \cdot \boldsymbol{n}) \ d\boldsymbol{y} + \sum_{j=1}^{n_p} \boldsymbol{f}_{t,j \to p}^{\mathrm{col}}$$

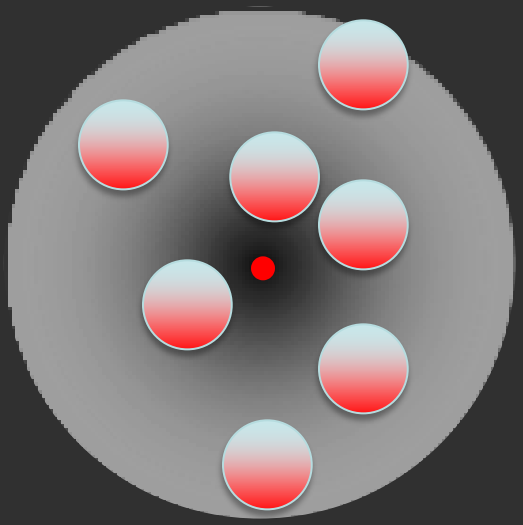
- *Boundary conditions:* no-slip and no-penetration at surface of particle
- *Collision force:* contact mechanics

Mathematical Formulation

Volume-Filtered Description

- Following the work of Anderson & Jackson (1967)
- Objective: formulate equations for particle-laden flows that allow $\Delta x \gg d_p$
- Introduce local volume filter based on convolution product with kernel $g(r)$
  - Characteristic width of kernel needs to be $\gg d_p$
  - Flow features on the scale of the particles are filtered out, enabling $\Delta x \gg d_p$
    - Leads to local mean voidage:

$$\varepsilon_f(\boldsymbol{x}, t) = \int_{V_{f\infty}(t)} g(|\boldsymbol{x} - \boldsymbol{y}|) d\boldsymbol{y}$$



  - Allows to define filtered variable $\overline{a}$ from point variable a :

$$\varepsilon_f \overline{a}(\boldsymbol{x}, t) = \int_{V_{f\infty}(t)} a(\boldsymbol{y}, t)\, g(|\boldsymbol{x} - \boldsymbol{y}|) d\boldsymbol{y}$$

  - No commutation between filtering and differentiation due to particle surface contributions

Mathematical Formulation

Volume-Filtered Description

- For variable density flows $\widetilde{a} = \dfrac{\varepsilon_f \overline{\rho_f a}}{\varepsilon_f \overline{\rho_f}}$
- In general, decompose point variable a as $a = \overline{a} + a'$ or $a = \widetilde{a} + a''$

$$\frac{\partial \varepsilon_f \overline{\rho_f}}{\partial t} + \nabla \cdot (\varepsilon_f \overline{\rho_f} \widetilde{\boldsymbol{u}_f}) = \boldsymbol{S}_\rho$$

$$\frac{\partial}{\partial t}(\varepsilon_f \overline{\rho_f} \widetilde{\boldsymbol{u}_f}) + \nabla \cdot (\varepsilon_f \overline{\rho_f} \widetilde{\boldsymbol{u}_f} \otimes \widetilde{\boldsymbol{u}_f}) = \nabla \cdot \overline{\boldsymbol{\tau}} - \nabla \cdot \boldsymbol{R}_u + \varepsilon_f \overline{\rho_f} \boldsymbol{g} + \boldsymbol{S}_{\rho u} - \boldsymbol{F}^{\text{inter}}$$

$$\boldsymbol{S}_\rho = \sum_{i=1}^{n_p} \int_{S_p} \rho_f \boldsymbol{n} \cdot \frac{d\boldsymbol{r}_i}{dt} g(|\boldsymbol{x} - \boldsymbol{y}|) \; d\boldsymbol{y}$$

$$\boldsymbol{S}_{\rho u} = \sum_{i=1}^{n_p} \int_{S_p} \rho_f \boldsymbol{n} \cdot \frac{d\boldsymbol{r}_i}{dt} \otimes \boldsymbol{u}_f g(|\boldsymbol{x} - \boldsymbol{y}|) \; d\boldsymbol{y}$$

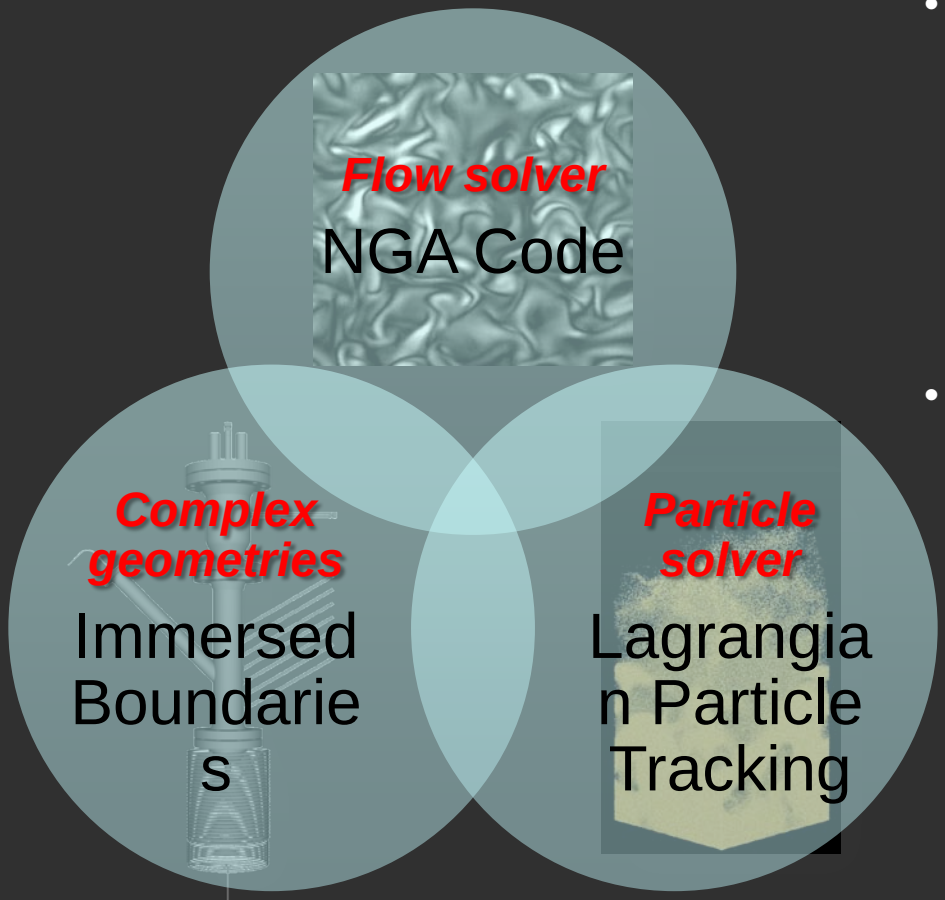
$$\overline{\boldsymbol{\tau}} = -p\boldsymbol{\mathcal{I}} + \mu \left[(\nabla \overline{\boldsymbol{u}_f} + \nabla \overline{\boldsymbol{u}_f}^{\mathsf{T}}) - \frac{2}{3} \; (\nabla \cdot \overline{\boldsymbol{u}_f}) \boldsymbol{\mathcal{I}} \right] + \boldsymbol{R}_\mu$$

$$\boldsymbol{F}^{\text{inter}} = \sum_{i=1}^{n_p} g(|\boldsymbol{x} - \boldsymbol{x}_p|) \int_{S_p} \boldsymbol{\tau} \cdot \boldsymbol{n} \; d\boldsymbol{y}$$

$$\int_{S_p} \boldsymbol{\tau} \cdot \boldsymbol{n} \; d\boldsymbol{y} \approx V_p \nabla \cdot \overline{\boldsymbol{\tau}} + \boldsymbol{f}_p^{\text{drag}}$$

$$\boldsymbol{R}_u = \varepsilon_f \overline{\rho_f} \widetilde{\boldsymbol{u}_f'' \otimes \boldsymbol{u}_f''}$$

Computational Approach



- NGA[2]
  - Arbitrarily high-order DNS/LES code
  - Massively parallel
  - Conservation of mass, momentum, and kinetic energy
- Immersed Boundary[3]
  - Based on cut-cell approach
  - Discrete conservation of mass and momentum
  - Fully implicit implementation to handle small cut-cells

2. O. Desjardins, G. Blanquart, G. Balarac, H. Pitsch, High order conservative finite difference scheme for variable density low Mach number turbulent flows, Journal of Computational Physics 227 (2008) 7125– 7159.
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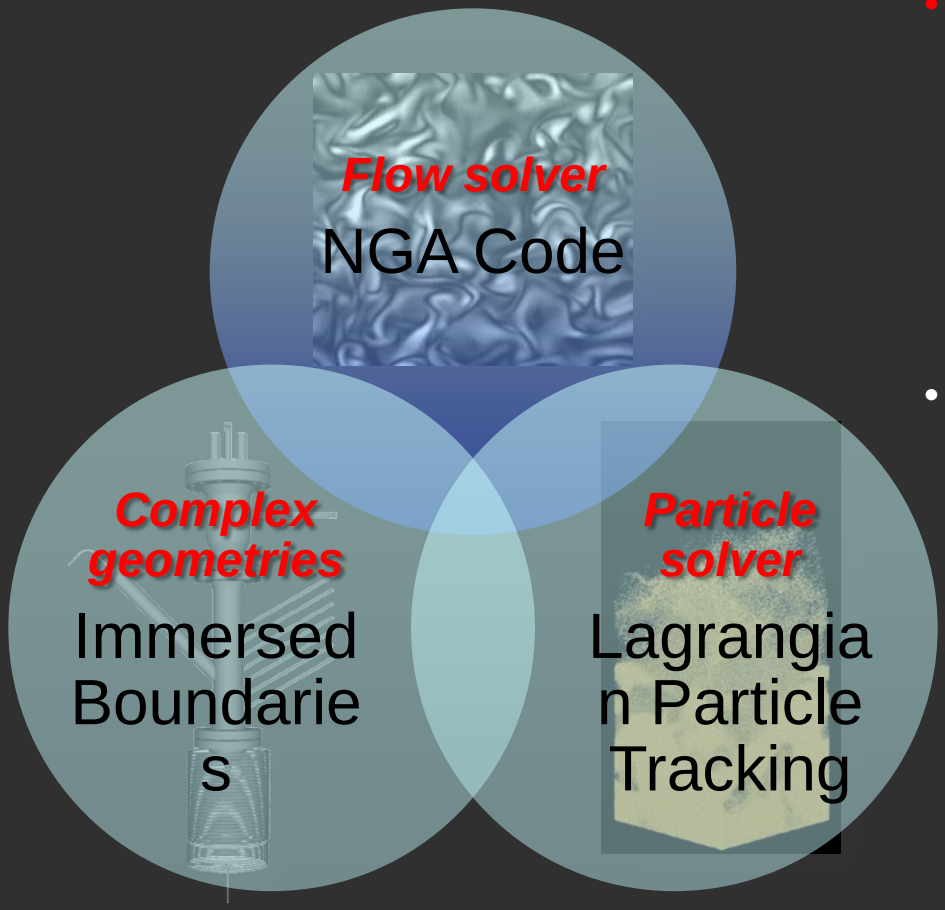

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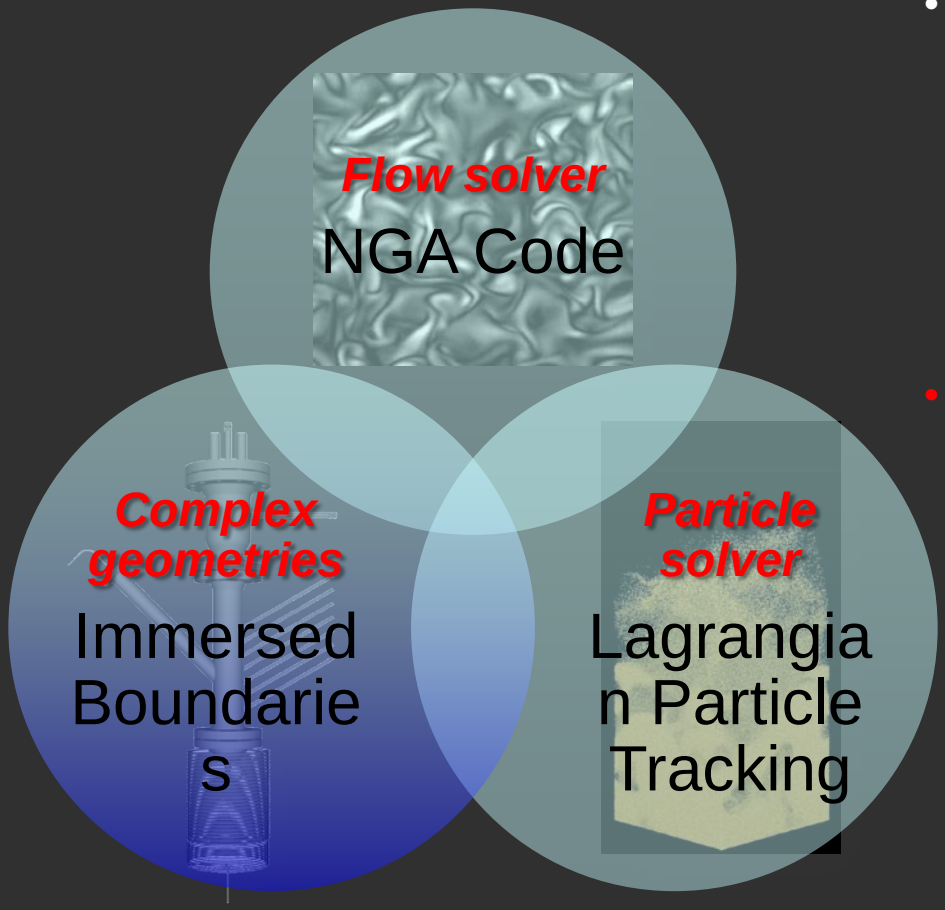

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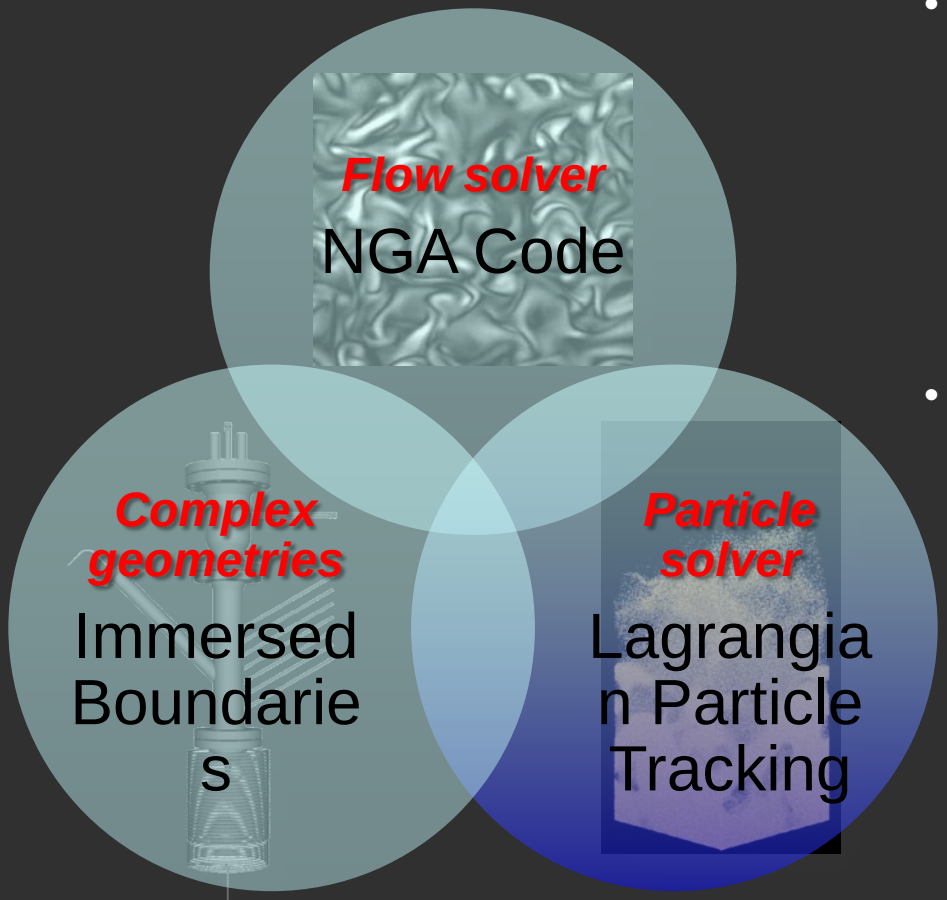

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NGA Computational Platform

- NGA solves the volume-filtered equations with the following assumptions & models

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Drag model of Tenneti & Subramaniam (2011

$$\boldsymbol{f}_i^{\text{drag}} = \frac{1}{\tau_p}\left(\widetilde{\boldsymbol{u}_f} - \boldsymbol{u}_p\right) F\left(\varepsilon_f, \mathsf{Re}_p\right)$$

$$\tau_p = \frac{\rho_p d_p^2}{18 \mu \varepsilon_f} \quad \mathsf{Re_p} = \frac{\varepsilon_\mathsf{f} \rho_\mathsf{f} \left|\widetilde{\mathsf{u}_\mathsf{f}} - \mathsf{u_p}\right| \mathsf{d_p}}{\mu}$$

$$F(\varepsilon_f, \mathrm{Re}_p) = \frac{1 + 0.15 \mathrm{Re}_p^{0.687}}{\varepsilon_f^2} + \frac{5.81\left(1-\varepsilon_f\right)}{\varepsilon_f^2} + \frac{0.48\left(1-\varepsilon_f\right)^{1/3}}{\varepsilon_f^3} + \varepsilon_f\left(1-\varepsilon_f\right)^3 \mathrm{Re}_p \left(0.95 + \frac{0.61\left(1-\varepsilon_f\right)^3}{\varepsilon_f^2}\right)$$

4. S. Tenneti, R. Garg, S. Subramaniam, Drag law for monodisperse gas- solid systems using particle-resolved direct numerical simulation of flow past fixed assemblies of spheres, International journal of multiphase flow 37 (2011) 1072–1092.

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$$\overline{\boldsymbol{\tau}} = -p\boldsymbol{\mathcal{I}} + \mu^* \left[(\nabla \overline{\boldsymbol{u}_f} + \nabla \overline{\boldsymbol{u}_f}^{\mathsf{T}}) - \frac{2}{3} (\nabla \cdot \overline{\boldsymbol{u}_f}) \boldsymbol{\mathcal{I}} \right] + \cancel{\boldsymbol{R}_u}$$

Drag model of Tenneti & Subramaniam (2011

Effective viscosity model of Gibilaro et al. (2007)[5]

$$\mu^* = \mu \varepsilon_f^{-2.8}$$

$$\boldsymbol{f}_i^{\text{drag}} = \frac{1}{\tau_p} (\widetilde{\boldsymbol{u}_f} - \boldsymbol{u}_p) F(\varepsilon_f, \mathsf{Re}_p)$$

$$\tau_p = \frac{\rho_p d_p^2}{18 \mu \varepsilon_f} \quad \mathsf{Re_p} = \frac{\varepsilon_f \rho_f |\widetilde{\mathsf{u}_f} - \mathsf{u_p}| \, \mathsf{d_p}}{\mu}$$

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5. L. Gibilaro, K. Gallucci, R. Di Felice, P. Pagliai, On the apparent viscosity of a fluidized bed, Chemical engineering science 62 (2007) 294–300.

Lagrangian Particle Tracking

- A set of 9 coupled ODEs are solved for each individual particle
- Time advancement based on
  - 2nd order Runge-Kutta for particle ODEs
  - 2nd order coupling between gas and particles phase

$$\frac{d\boldsymbol{x}_p}{dt} = \boldsymbol{u}_p$$

$$m_p \frac{d\boldsymbol{u}_p}{dt} = \int_{S_p} \boldsymbol{\tau} \cdot \boldsymbol{n} \; d\boldsymbol{y} + F^{\mathrm{col}} + m\boldsymbol{g}$$

$$I_p \frac{d\boldsymbol{\omega}_p}{dt} = \int_{S_p} \frac{d_p}{2} \boldsymbol{n} \times (\boldsymbol{\tau} \cdot \boldsymbol{n}) \; d\boldsymbol{y} + \sum_{j=1}^{n_p} \boldsymbol{f}^{\mathrm{col}}_{t,j\to p}$$

- Collisions based on soft sphere approach[6] modified for parallel efficiency
- Exchange between phases
  - Gas phase data is interpolated to the particle location using trilinear interpolation
  - Particle data is filtered onto the Eulerian mesh with an implicit/conservative smoothing operation

6. P. Cundall, O. Strack, A discrete numerical model for granular assemblies, 1979.

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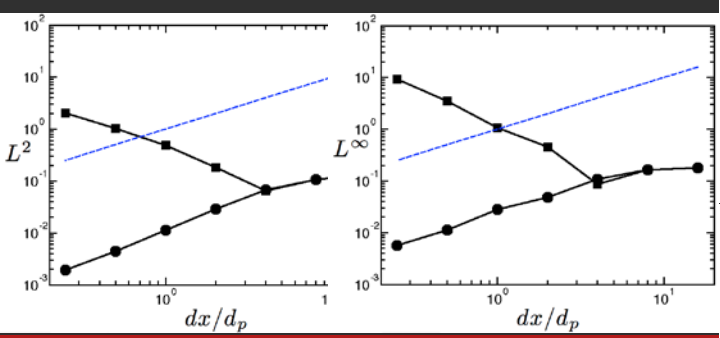
Particle Data to Eulerian Mesh

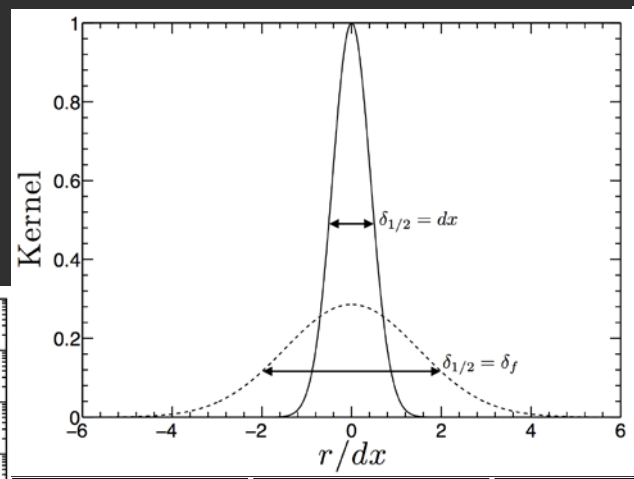
- Need to transfer ε_f and $\boldsymbol{F}^{\text{inter}}$ to underlying mesh consistent with mathematical formulation
- Filtering needs to be based on particle size not mesh
- Filter based on the convolution of mollification and Laplacian smoothing
  - Mollification: extrapolate particle data to neighboring cells
  - Diffusion: smooth data with specified width
- Filter width δ_f is independent of the mesh size

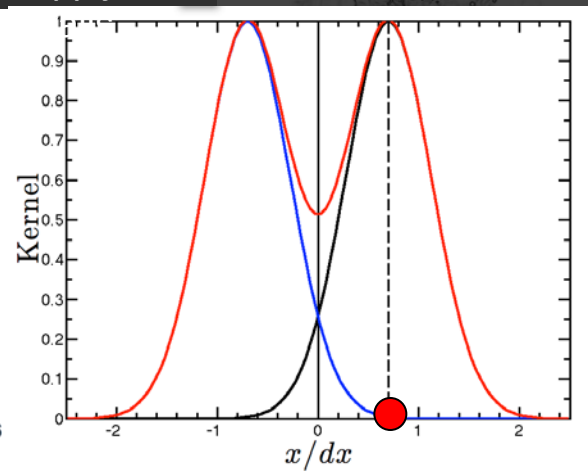
Gaussian diffusion

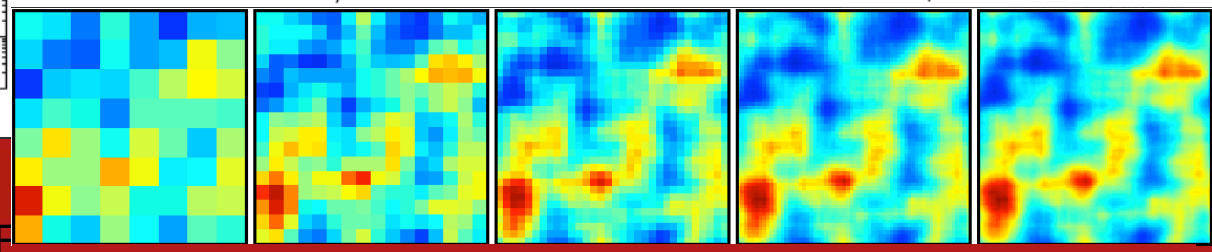
Introduce image particle to apply Neumann condition near

L-norm error





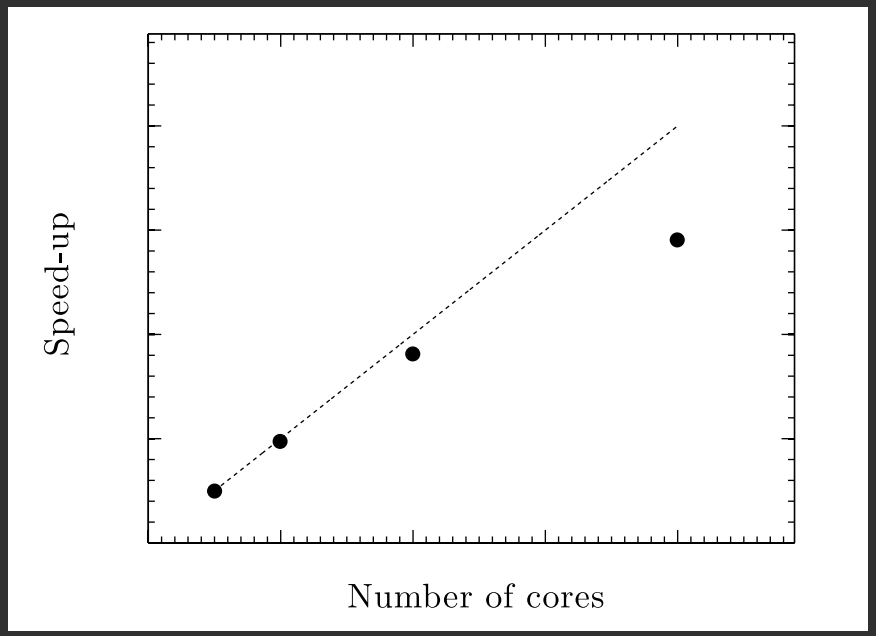


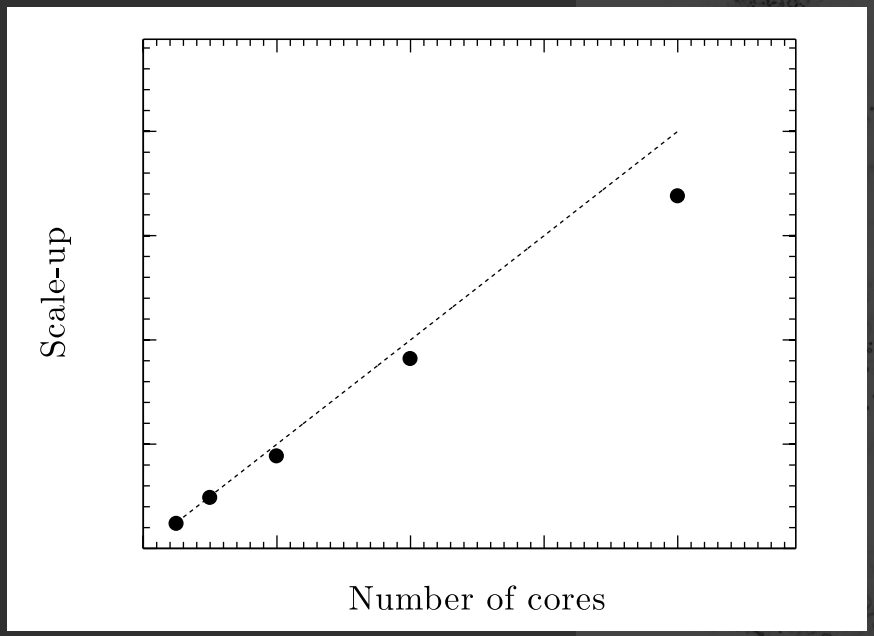


$dx = 4d_p$ $dx = 2d_p$ $dx = d_p$ $dx = d_p/2$ $dx = d_p/4$

Parallel Performance

- Parallelization: MPI (domain decomposition)
- Scaling performed on Red Mesa (Sandia National Labs)
- 134 million cells, 383 million particles



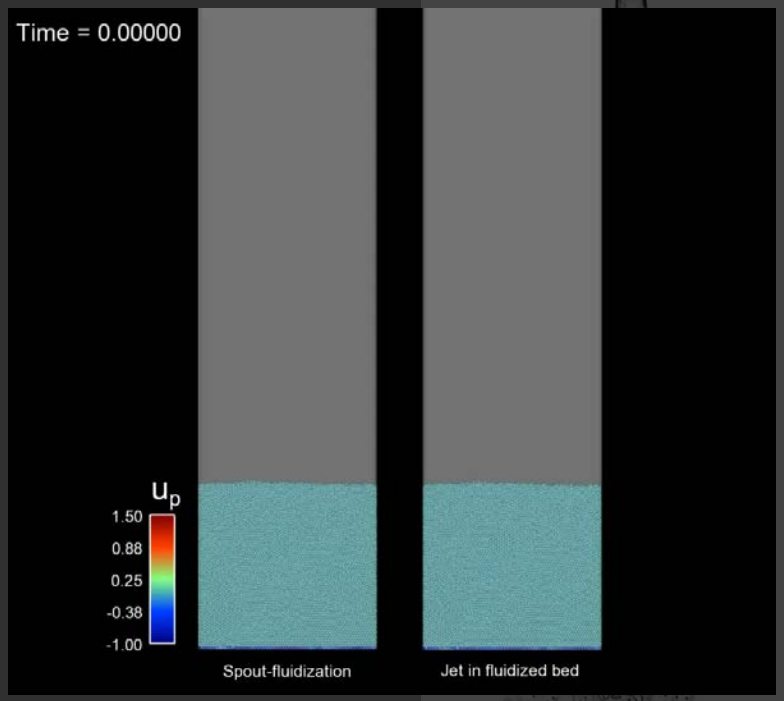


Initial validation

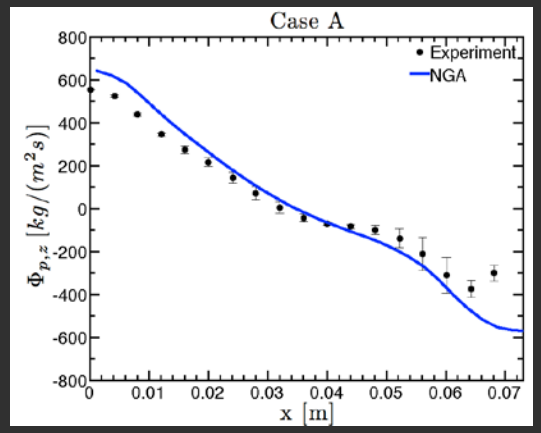
Spout fluidization (*Link et al., 2005*)

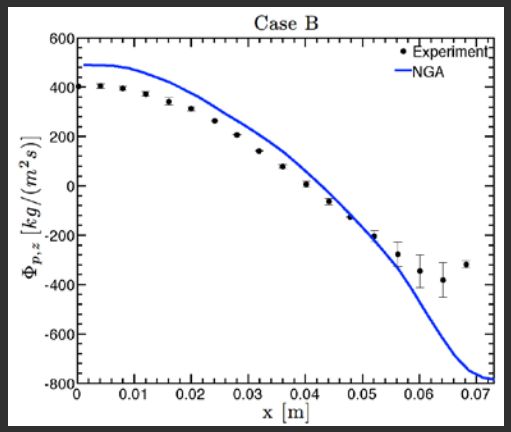
- Case A: u_{bg}= 1.5 m/s, u_{sp}=30 m/s
- Case B: u_{bg}= 3.0 m/s, u_{sp}=20 m/s

Bed dimensions [m]	0.75 x 0.15 x 0.015
Spout width [m]	0.01
Particle diameter [m]	0.0025
Particle density [kg/m^3]	2526
Number of particles [-]	245,000
Grid [-]	300 x 60 x 6

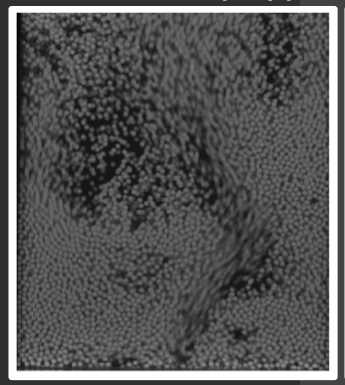


Particle mass flux





Case B (exp)

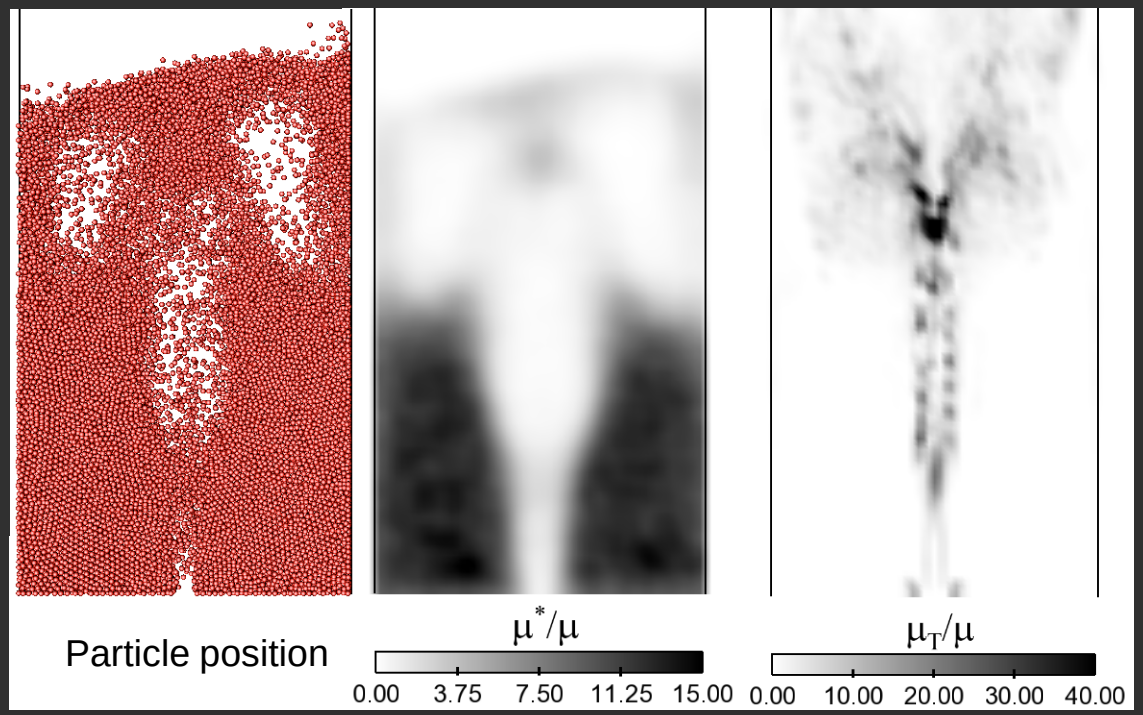


Case B (sim)

Initial validation

Spout fluidization, case A

- Dynamic Smagorinsky eddy viscosity model[8] to close $\boldsymbol{R}_u$
- Based on Lagrangian averaging[9]
- SGS model does not account for turbulence modulation by particles
- Spatial segregation between models



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Computational Thermo-Fluids Laboratory

8. M. Germano, U. Piomelli, P. Moin, W.H. Cabot, A dynamic subgrid-scale eddy viscosity model, Phys. Fluids A 3 (1991) 1760–1765.
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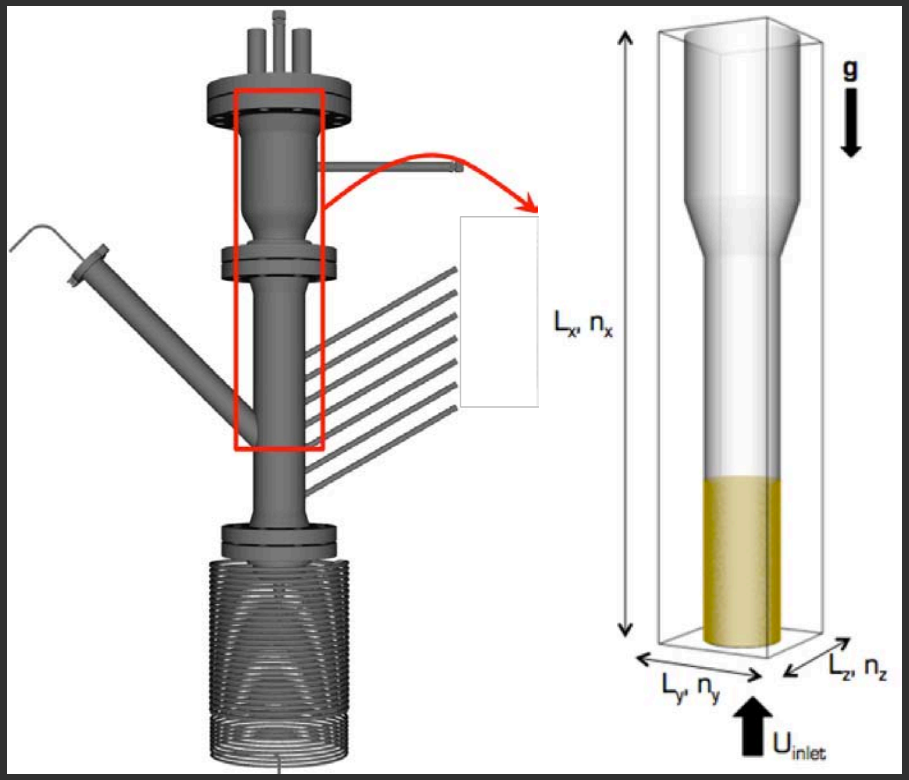
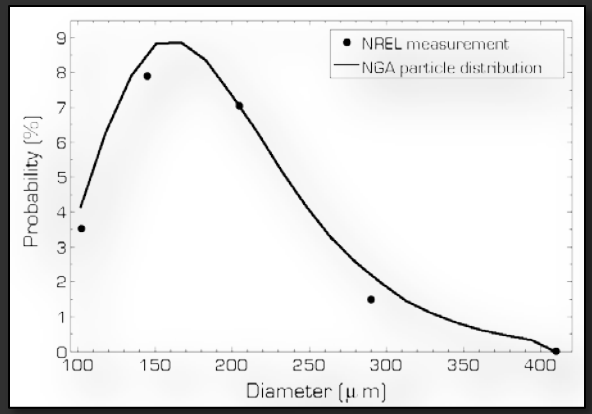
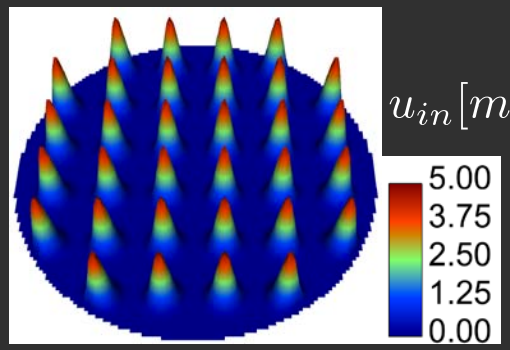
Half-scale simulation of NREL's 4-in fluidized bed reactor

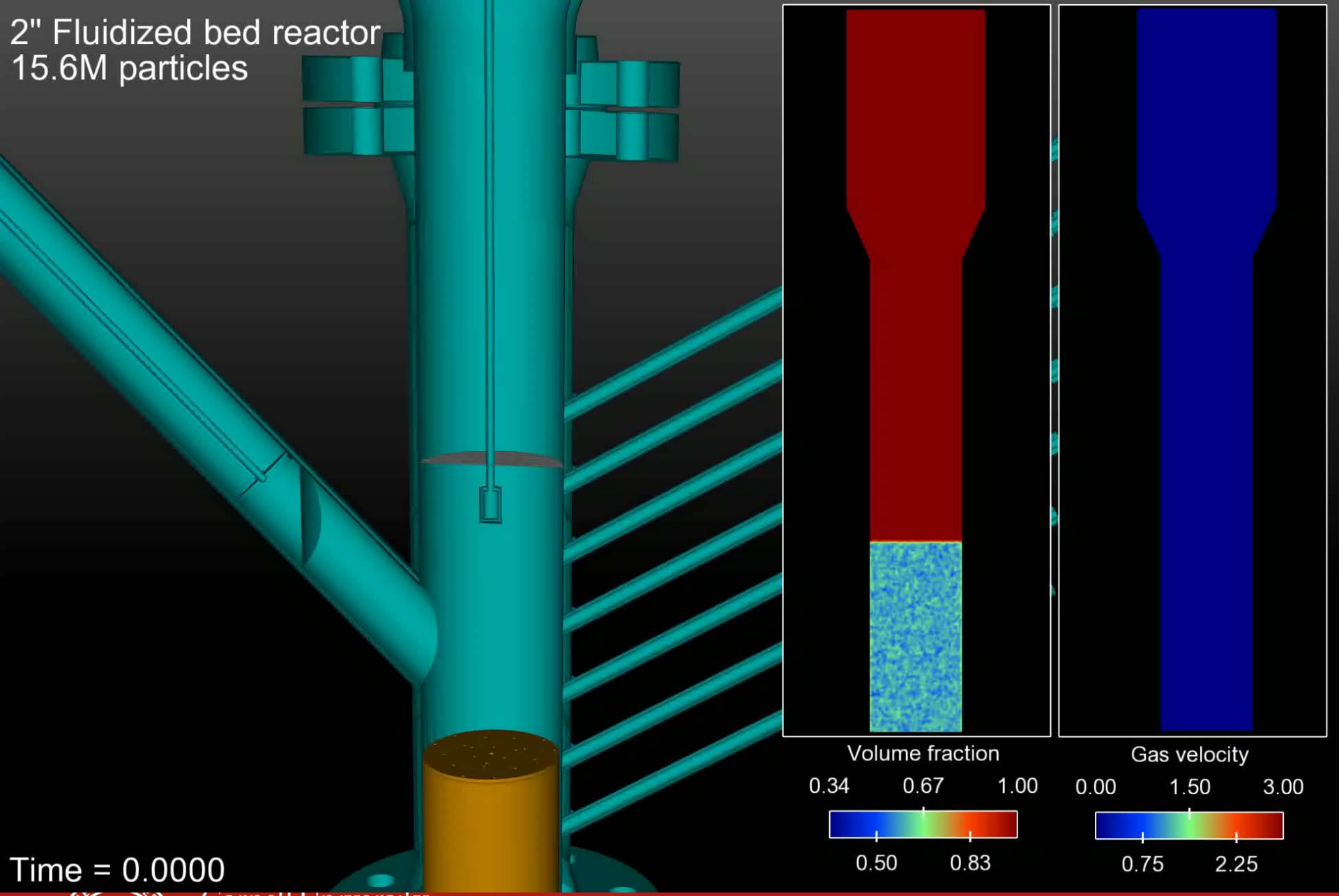
- National Renewable Energy Laboratory operates a 4-inch fluidized bed reactor for biomass gasification





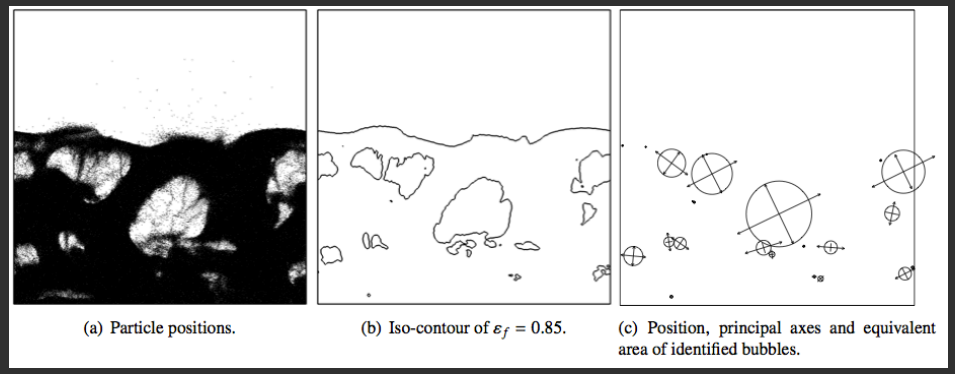


- $u_{in} = 6 \rightarrow 12U_{mf}$
- 15.6 M particles
- 20 M grid cells
- 576 cores on Marvin (Cornell cluster)

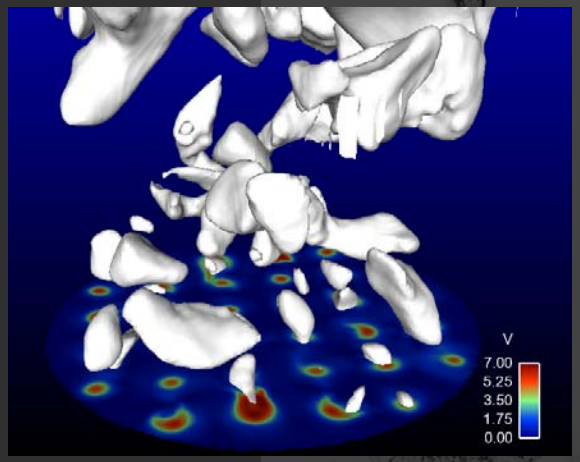

2" Fluidized bed reactor
15.6M particles
Volume fraction
0.34
0.67
1.00
0.50
0.83
Gas velocity
0.00
1.50
3.00
0.75
2.25
Time = 0.0000

Bubble characterization

- Structure identification algorithm[10]
  - Band-growth algorithm to identify bubbles

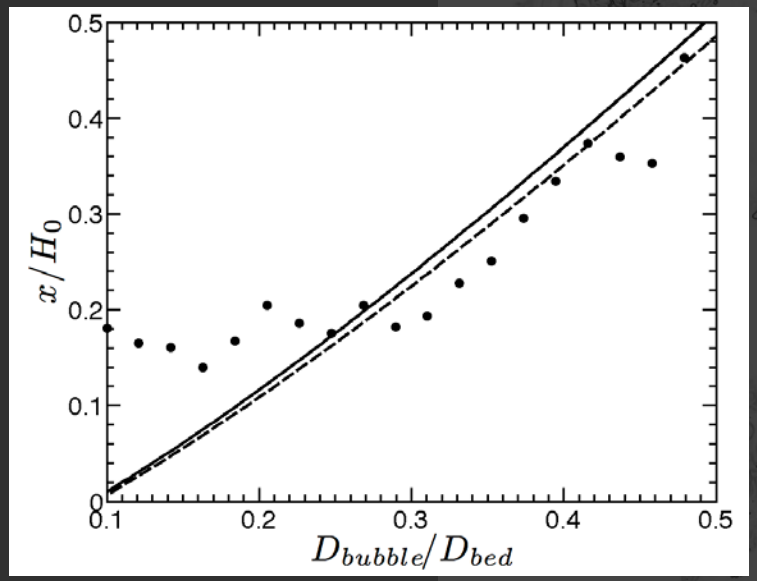


(a) Particle positions. (b) Iso-contour of $\varepsilon_f = 0.85$. (c) Position, principal axes and equivalent area of identified bubbles.



- Mean bubble diameter: 0.18*Dbed
- On average 8 bubbles in bed at once
- Compared results with Darton[11] correlation
  - Uin = 6 Umf (solid line)
  - Uin =12 Umf (Dashed line)

$$D_b = 0.54\,(U_{in} - U_{mf})^{0.4}\left(h + 4\sqrt{A_0}\right)^{0.8} g^{-0.2}$$



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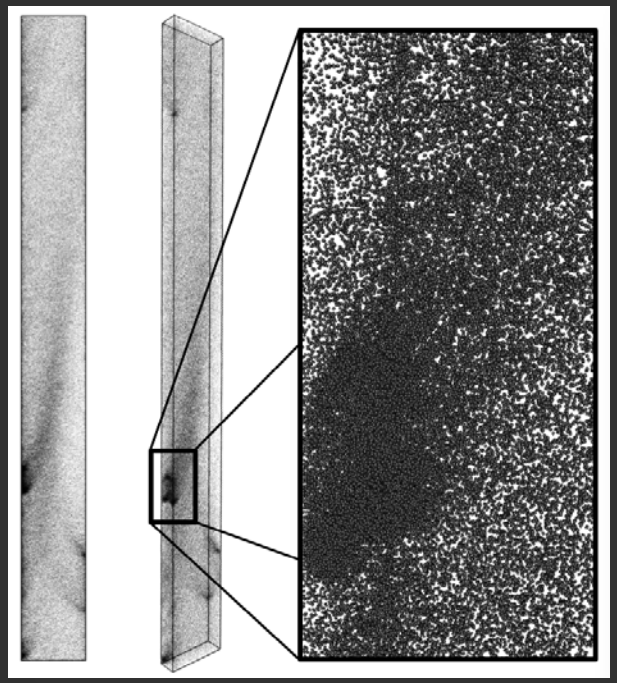
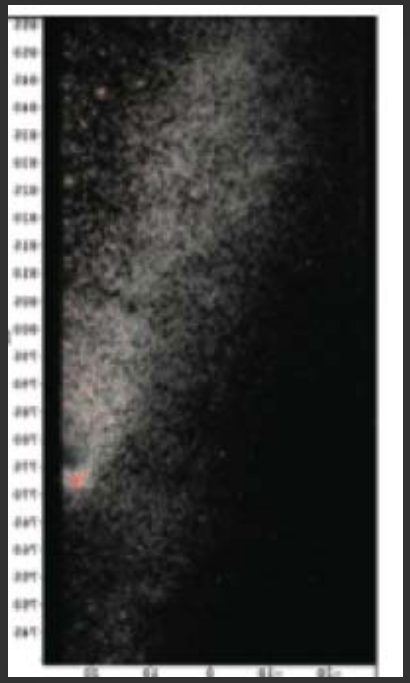
Simulation of a Turbulent Riser

- Periodic in stream-wise directions
- 266,760 particles initially uniform distribution
- 800 x 82 x 26 mesh for 0.5 m domain
- Formation of clusters along walls is observed – excellent qualitative agreement with experiments[12]





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Simulation of a Turbulent Riser

- Radial Distribution Function (RDF) to characterize clustering

$$RDF(x, \boldsymbol{r}) = \frac{N_p L_z}{2drN(N-1)}$$

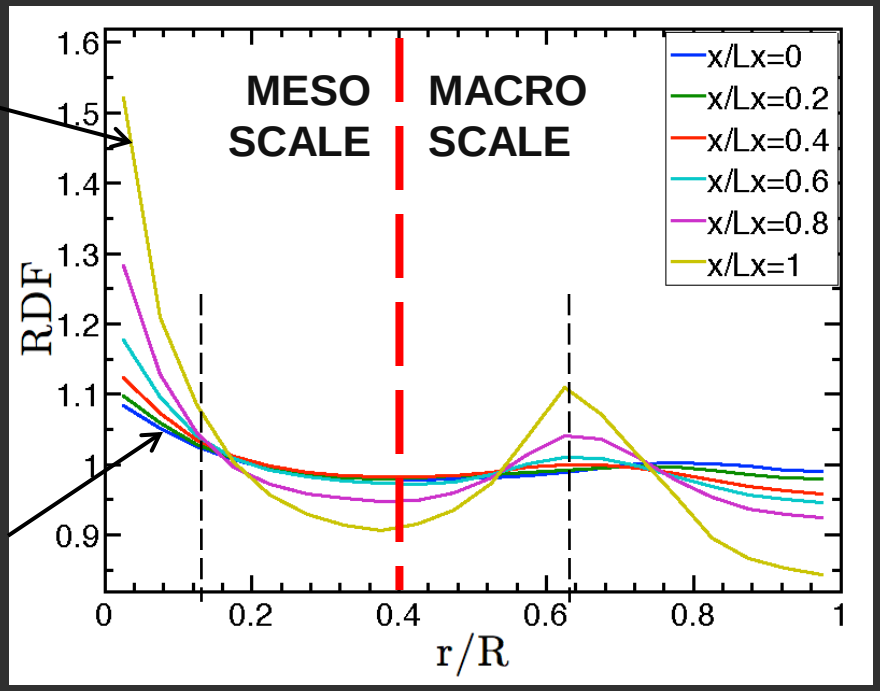
RDF=1: Uniform distribution

RDF>1: Clustering

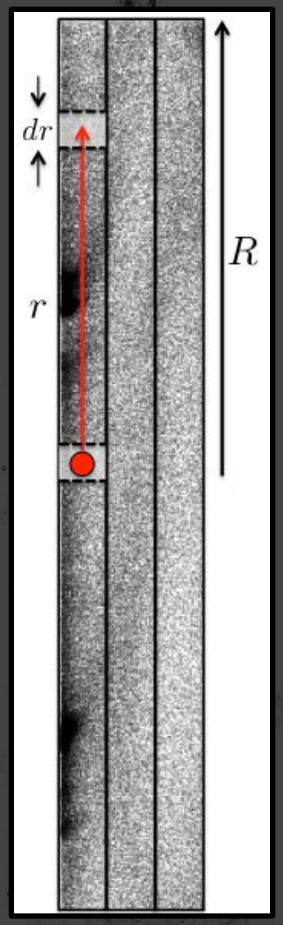
  - N: Number of particles in column
  - N_p: Number of particle pairs
  - Total possible number of pairs: N(N-1)

Near-wall

Duct center

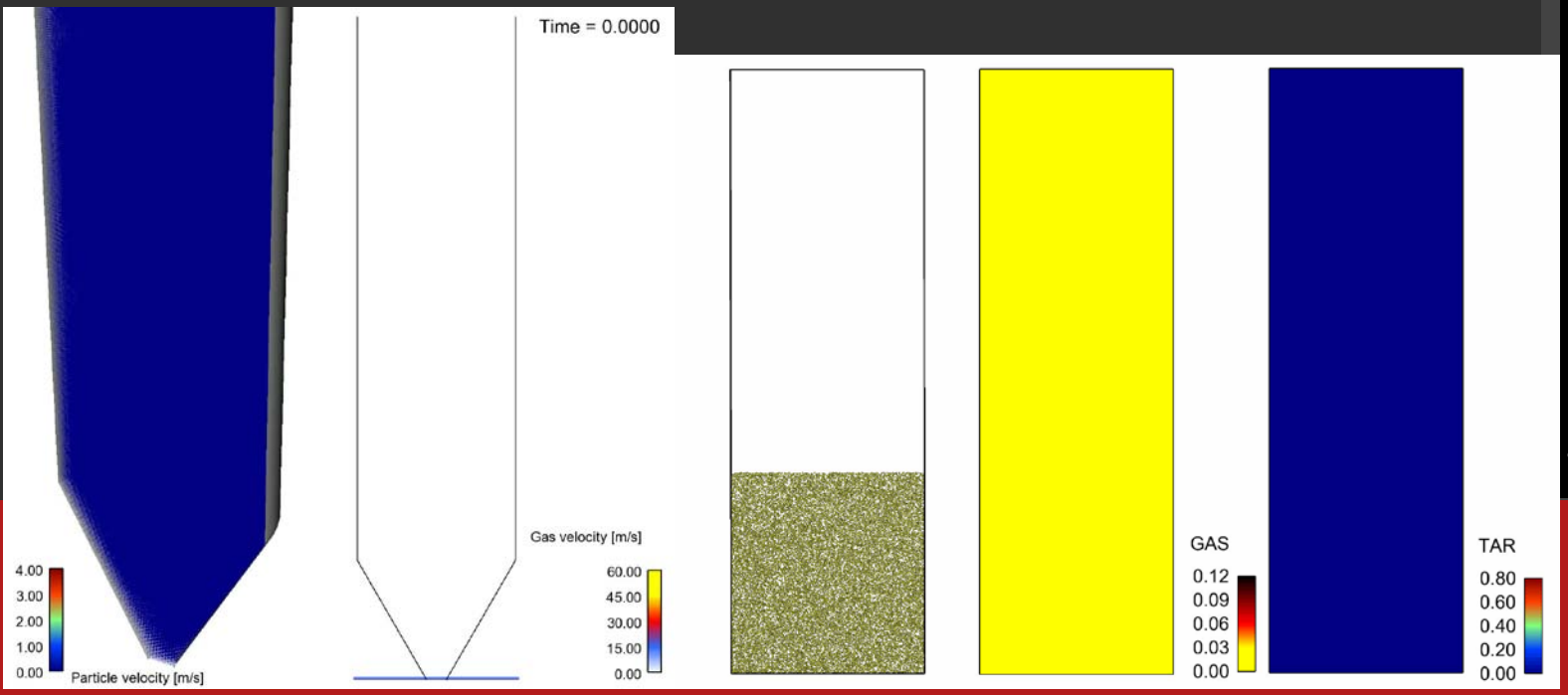


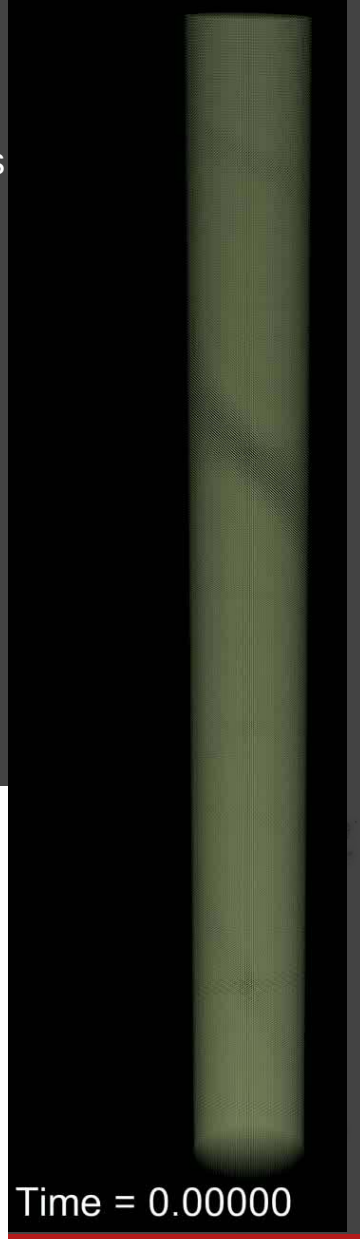
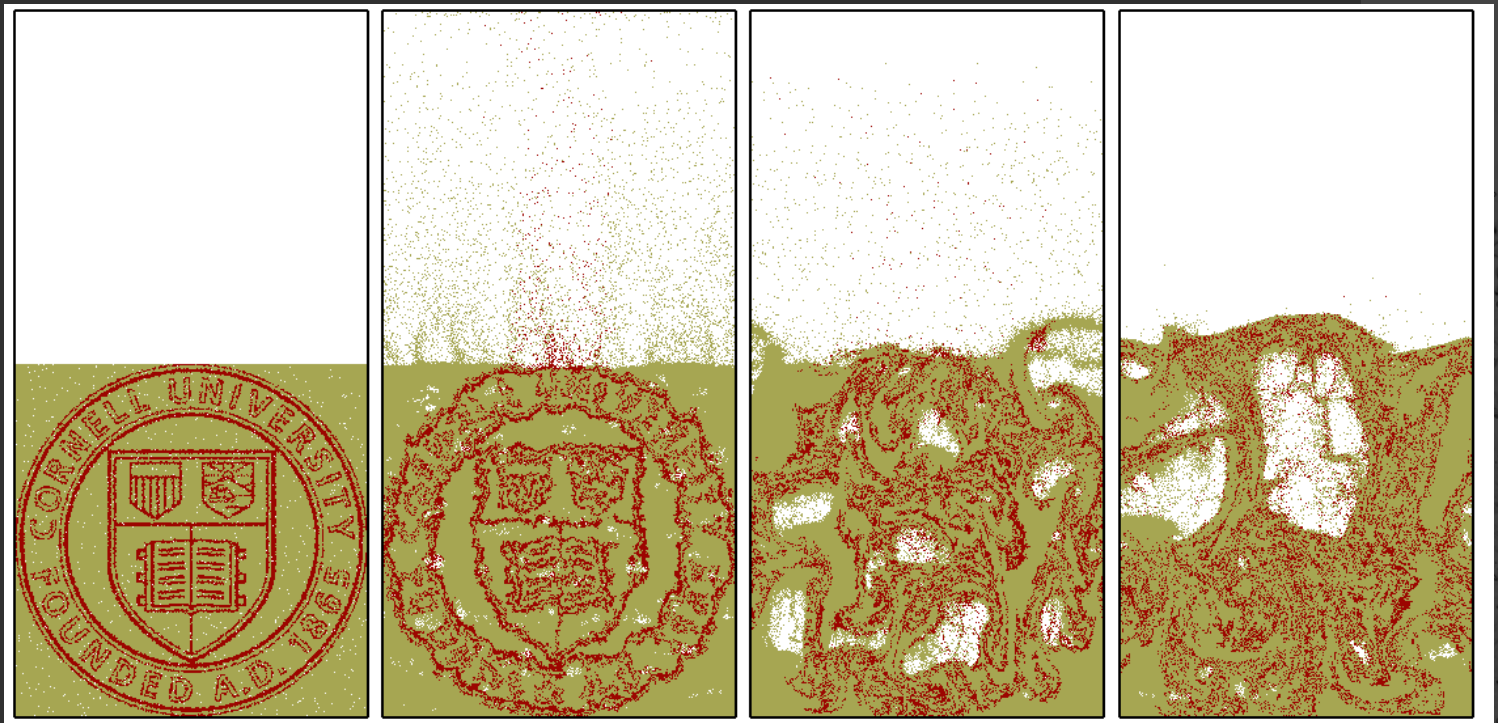
- Meso-scale
  - Maximum clustering at the walls
  - Characteristic cluster size ~ 90 d_p
- Macro-scale
  - Second peak in RDF
  - Characteristic length scale ~ L_z / 3 (or 460 d_p)



Conclusions

- Presented a simulation strategy for turbulent particle-laden flows in complex geometries
- Simulations of fluidized bed reactors show good agreement with experimental data
- Looking forward:
  - Further validation
  - Chemistry is currently being incorporated (Pepiot research group)
  - Investigate clustering in turbulent risers
  - Use resolved particle simulations for exploring the closure of the filtered equations
  - Transition to industrial scale approaches (QMOM, parcels…)





Questions?