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

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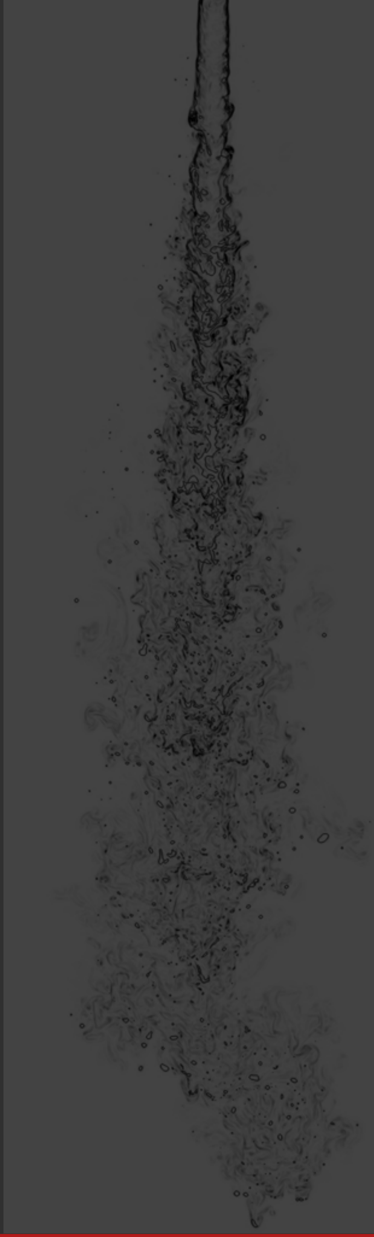
# Motivation

- 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

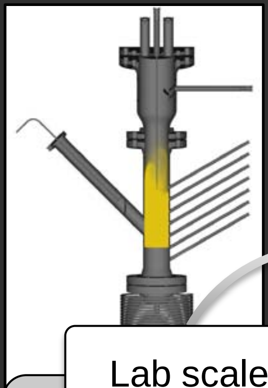

Spiegel (2009)


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

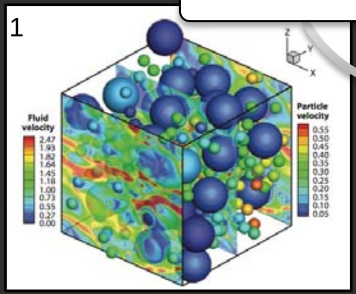


**Lab scale**

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

**Microscale**

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




**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

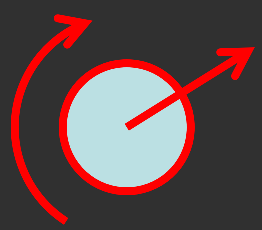
$$\frac{\partial \rho_f}{\partial t} + \nabla \cdot (\rho_f \boldsymbol{u}_f) = 0$$

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

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

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

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



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

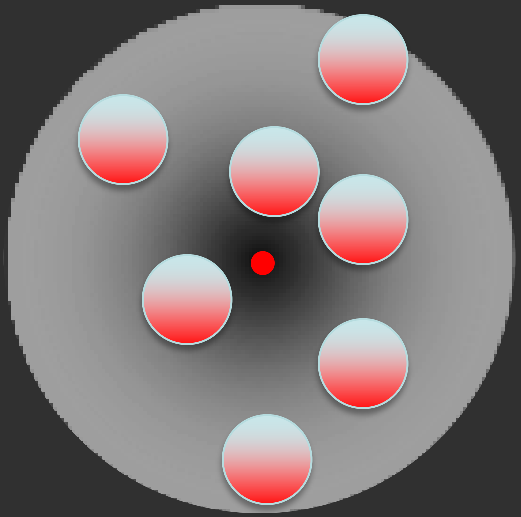
$$I_p \frac{d\boldsymbol{\omega}_p}{dt} = \int_{S_p} \frac{d_p}{2} \boldsymbol{n} \times (\boldsymbol{\tau} \cdot \boldsymbol{n}) \; d\boldsymbol{y} + \sum_{j=1}^{n_p} \boldsymbol{f}^{\mathrm{col}}_{t,j \to p}$$

- *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 $\Delta x \gg d_p$



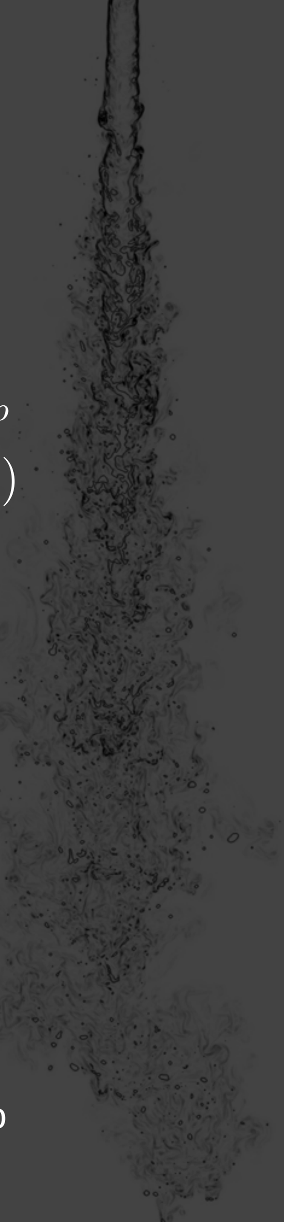
  - Leads to local mean voidage:

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

  - 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



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# 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 $a = \widetilde{a} + a''$

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

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

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

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

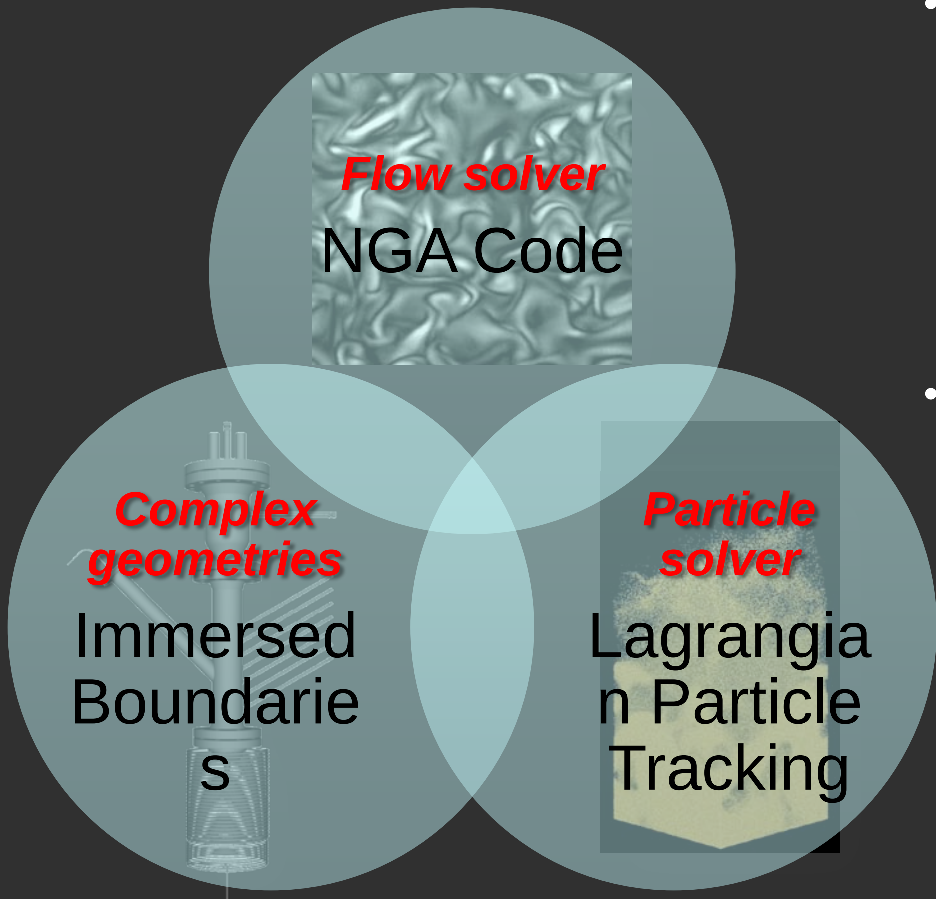
$$\boldsymbol{S}_{\rho u} = \sum_{i=1}^{n_p} \int_{S_p} \rho_f \boldsymbol{n} \cdot \frac{d\boldsymbol{r}_i}{dt} \otimes \boldsymbol{u}_f g(|\boldsymbol{x} - \boldsymbol{y}|) \; d\boldsymbol{y}$$

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

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

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

# 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.**

**3. P. Pepiot, O. Desjardins, Direct numerical simulation of dense particle-laden flows using a conservative immersed-boundary technique, Center of Turbulence Research, Summer program 2010.**

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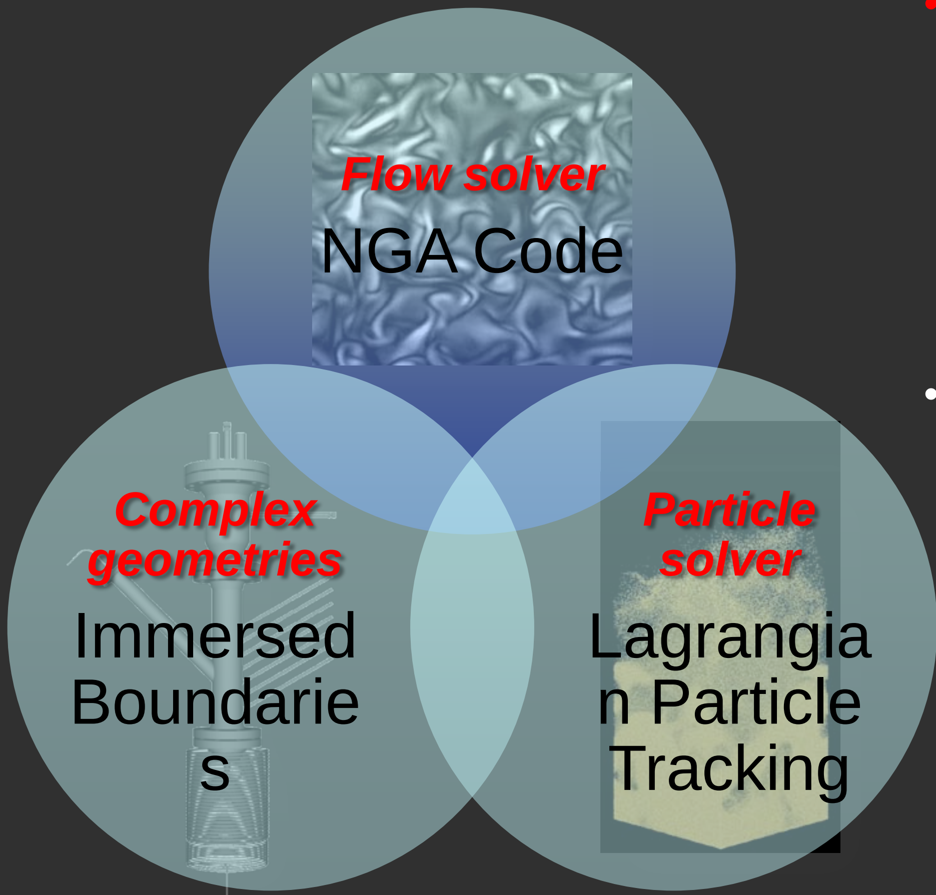


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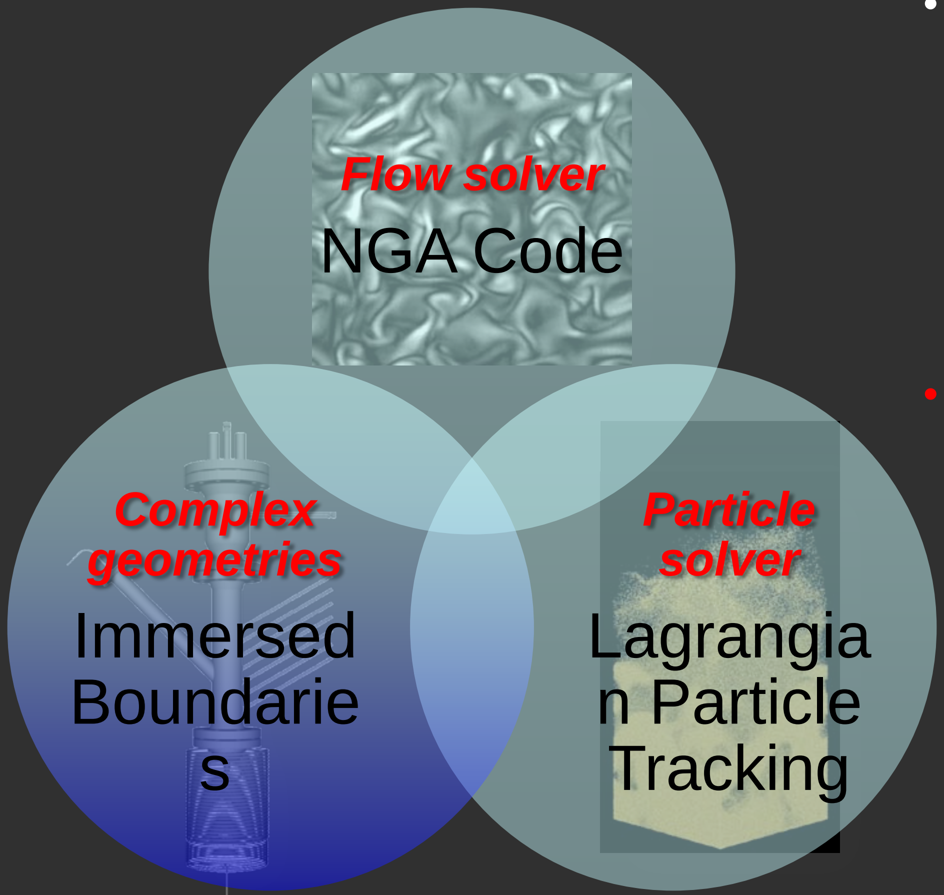


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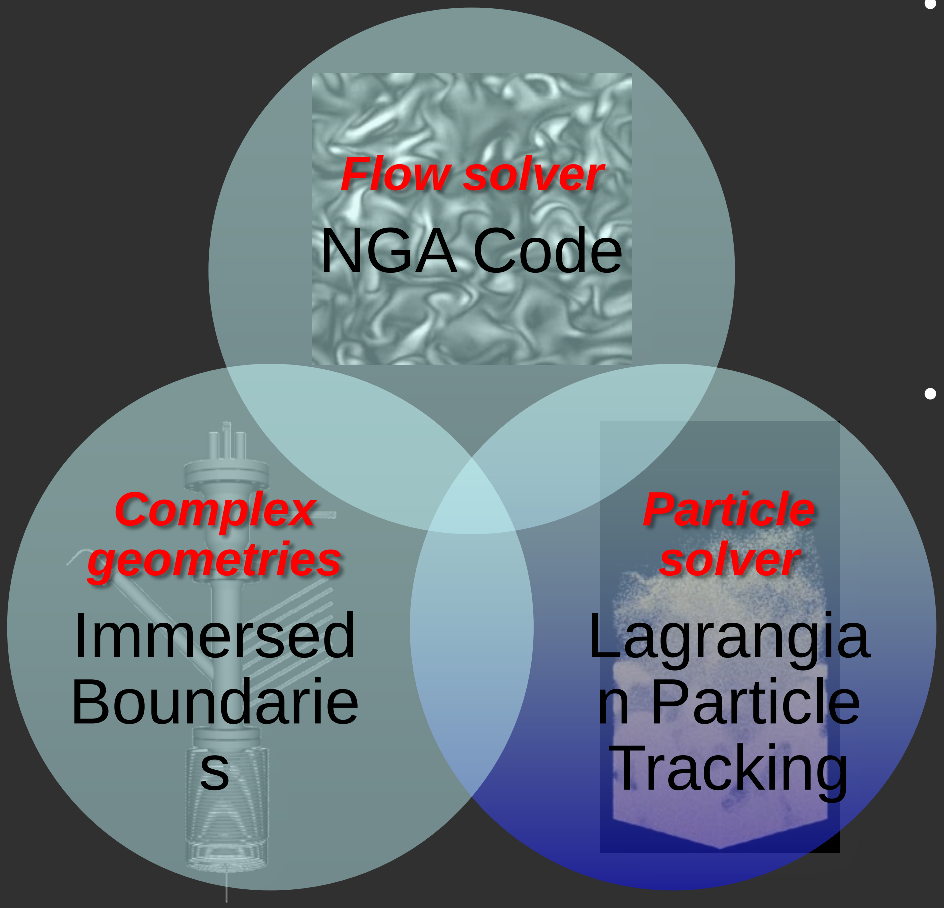


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# NGA Computational Platform

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

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

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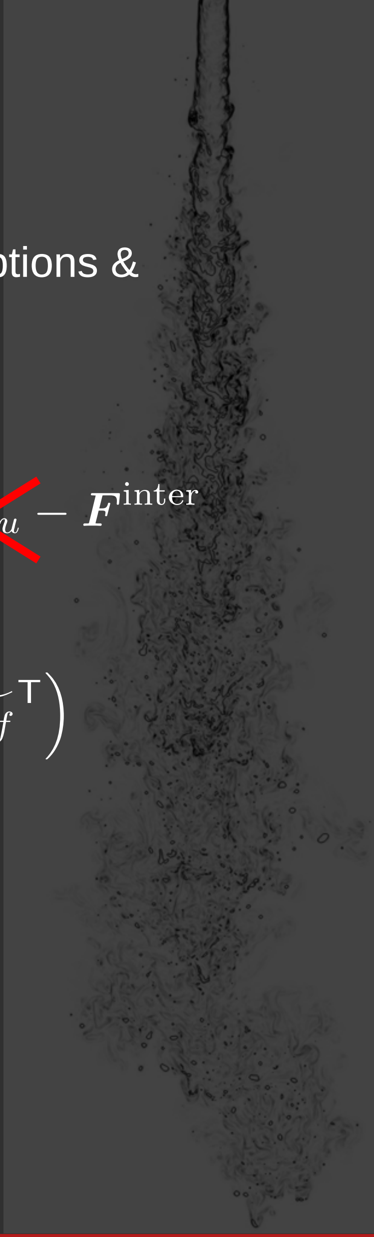

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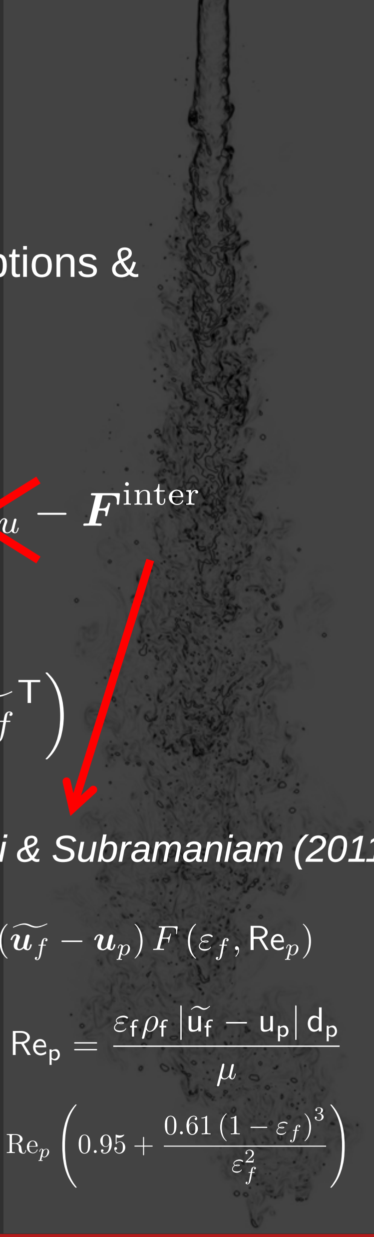

*Drag model of Tenneti & Subramaniam (2011)*

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

$$\tau_p = \frac{\rho_p d_p^2}{18 \mu \varepsilon_f} \quad \mathrm{Re}_p = \frac{\varepsilon_f \rho_f \left|\widetilde{u}_f - u_p\right| d_p}{\mu}$$

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



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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*Drag model of Tenneti & Subramaniam (2011*

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

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

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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

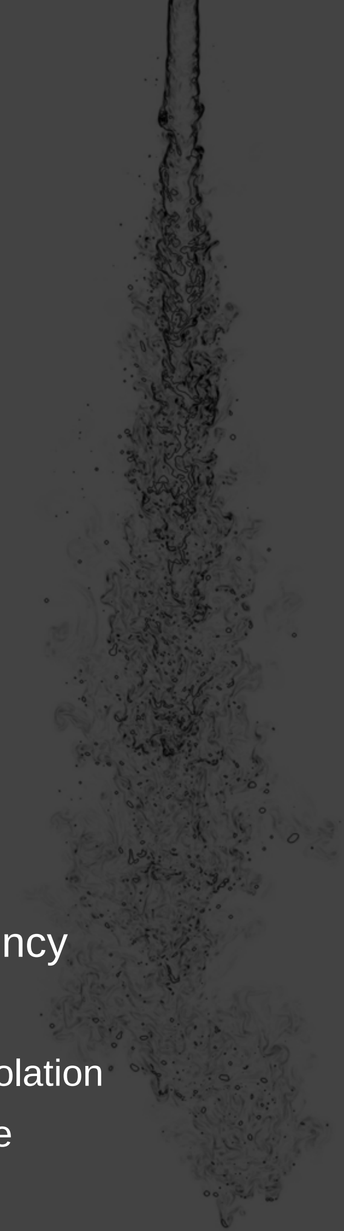
- A set of 9 coupled ODEs are solved for each individual particle
- Time advancement based on
  - 2nd order Runge-Kutta for particle ODEs
  - 2nd order coupling between gas and particles phase

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

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

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

- 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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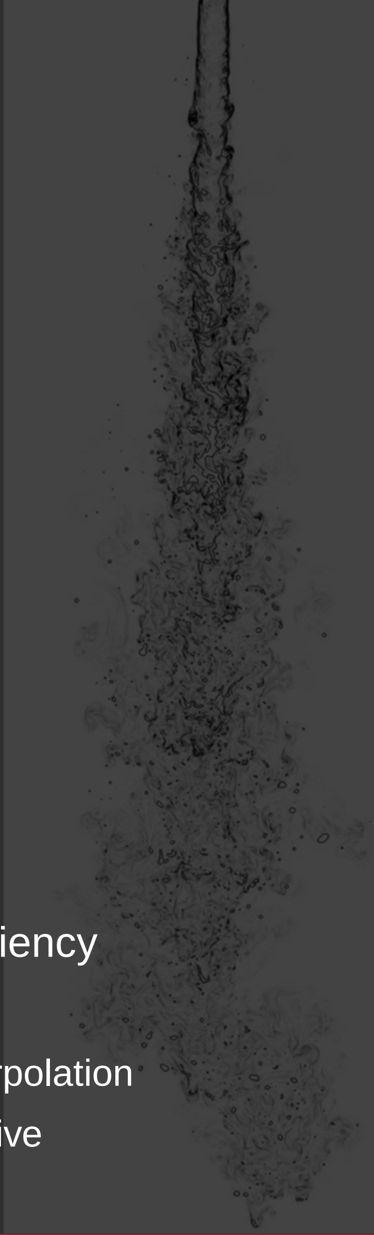



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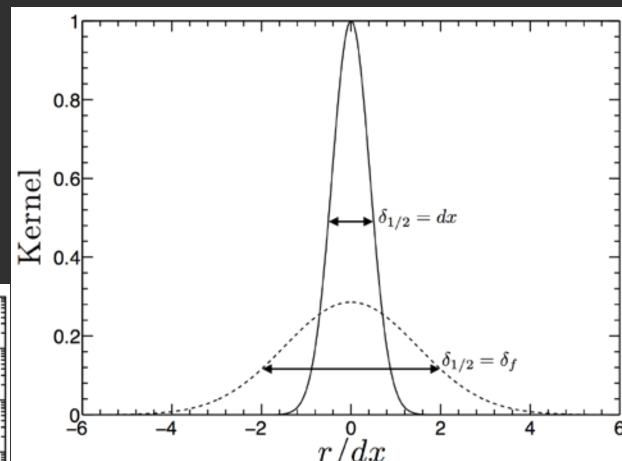
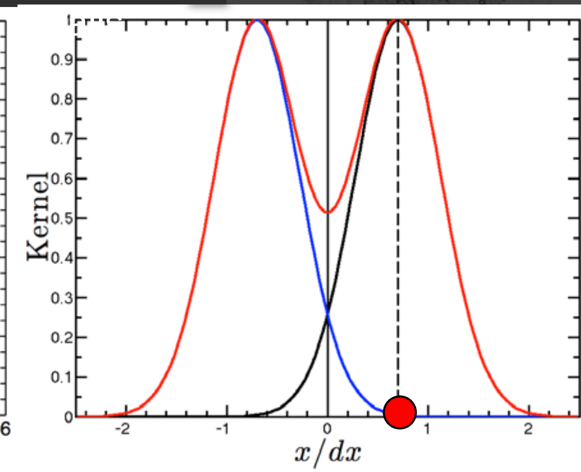
# Particle Data to Eulerian Mesh

- Need to transfer $\varepsilon_f$ 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 $\delta_f$
- Filter width $\delta_f$ is independent of the mesh size

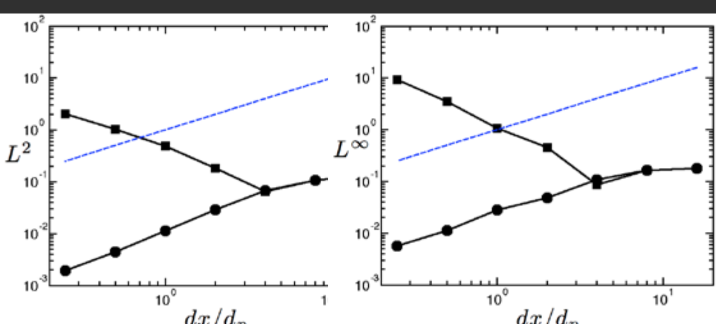
Gaussian diffusion

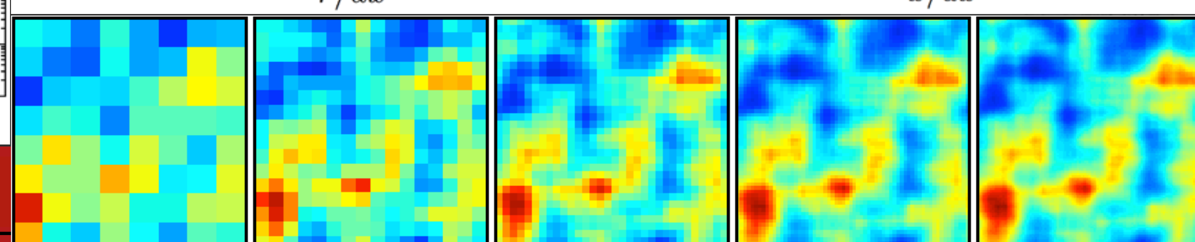



Introduce image particle to apply Neumann condition near




L-norm error

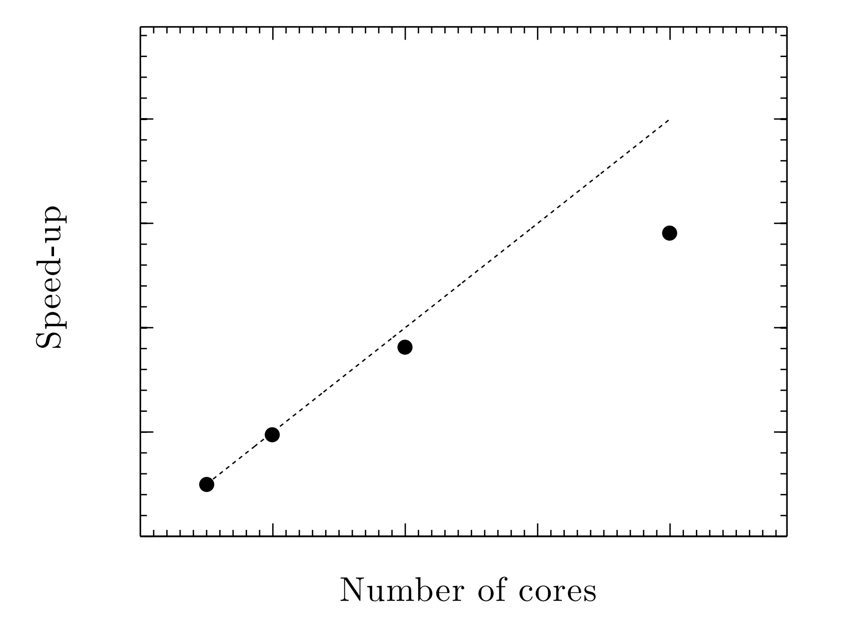


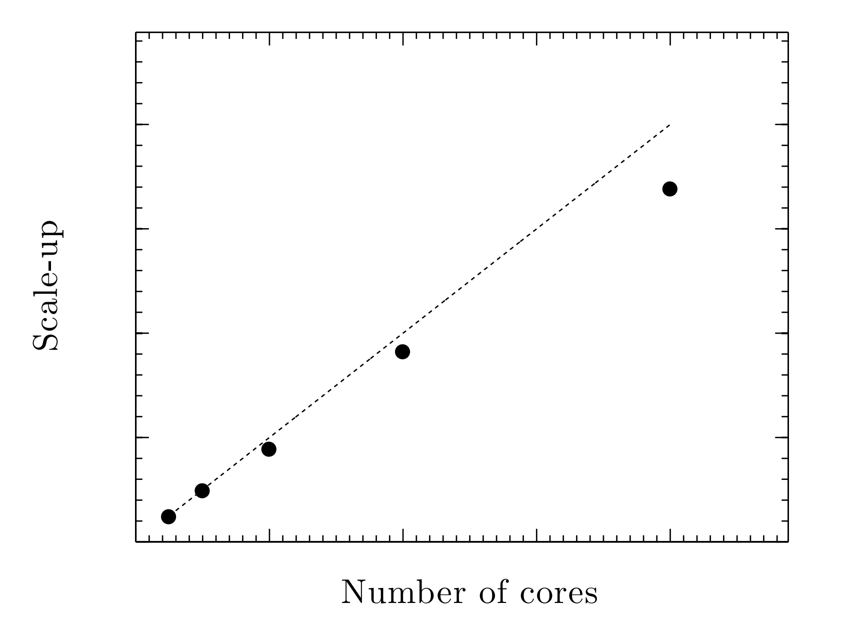



$dx = 4d_p$ $dx = 2d_p$ $dx = d_p$ $dx = d_p/2$ $dx = d_p/4$

# Parallel Performance

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



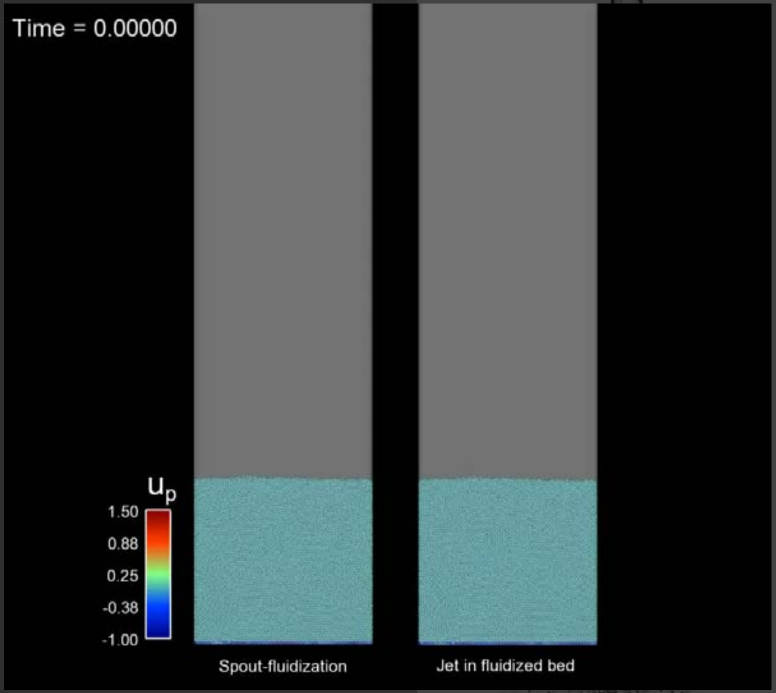



# Initial validation

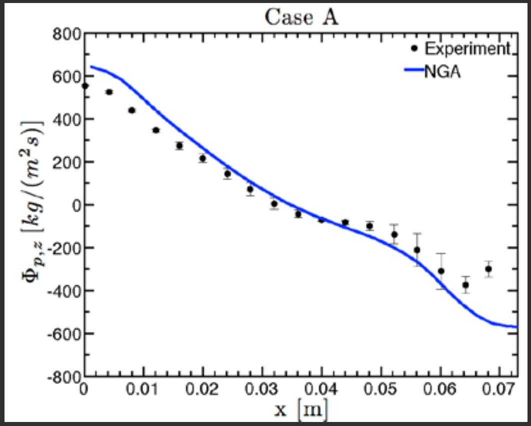
Spout fluidization (*Link et al., 2005*)

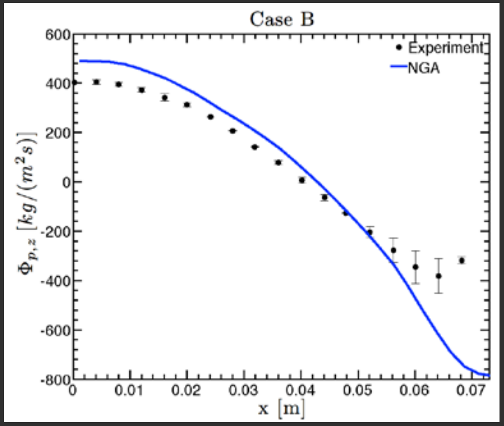
- Case A: $u_{bg}$= 1.5 m/s, $u_{sp}$=30 m/s
- Case B: $u_{bg}$= 3.0 m/s, $u_{sp}$=20 m/s

| | |
|---|---|
| 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 |

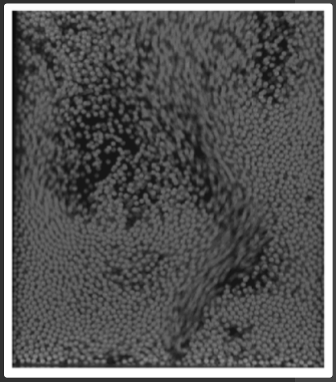



Particle mass flux




Case B (exp)

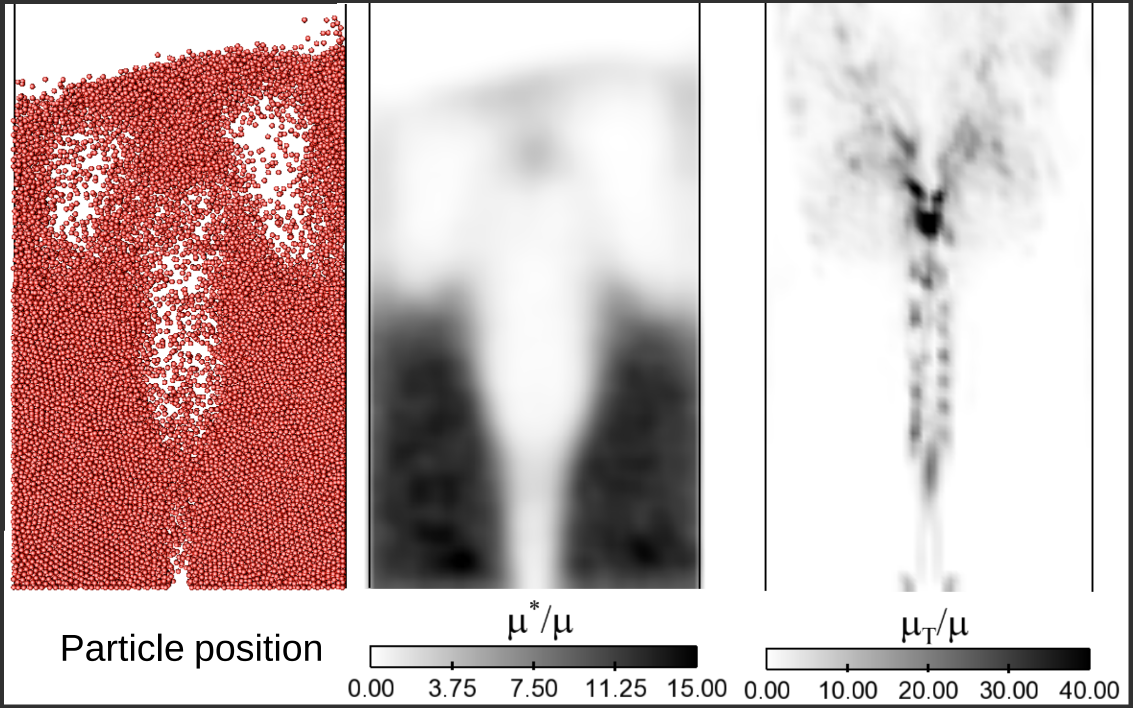


Case B (sim)

# 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

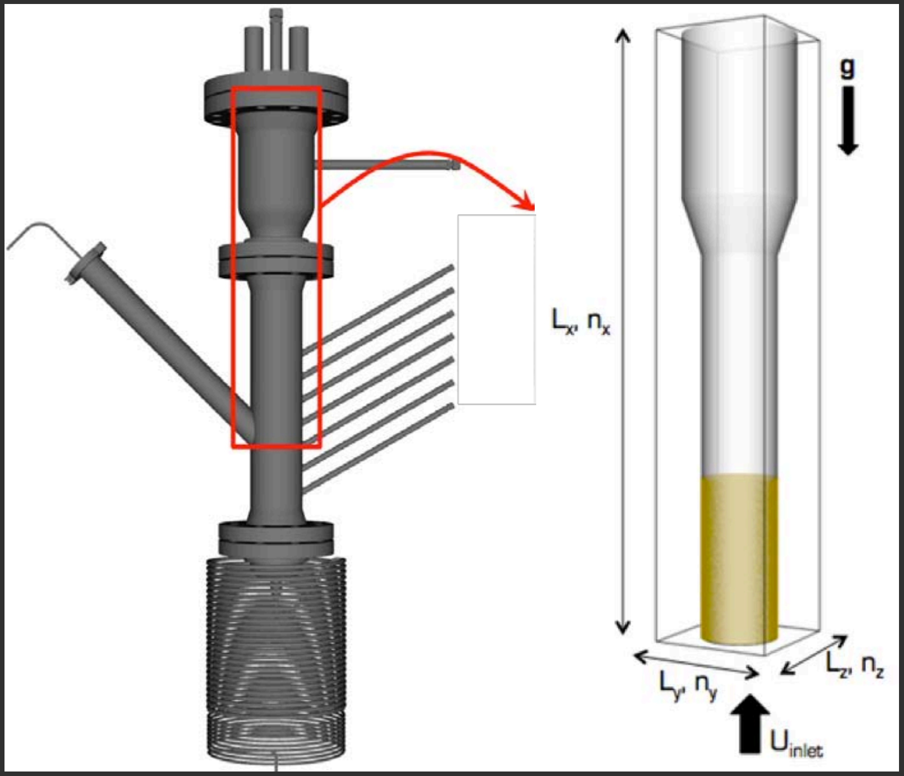


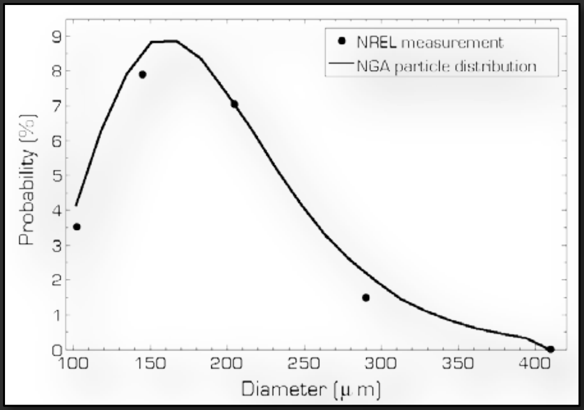


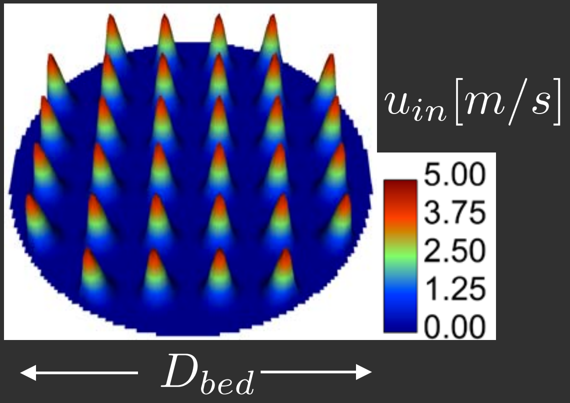

8. M. Germano, U. Piomelli, P. Moin, W.H. Cabot, A dynamic subgrid-scale eddy viscosity model, Phys. Fluids A 3 (1991) 1760–1765.
9. C. Meneveau, T.S. Lund, W.H. Cabot, A Lagrangian dynamic subgrid-scale model of turbulence, J. Fluid Mech. 319 (2000) 353–385.

# Half-scale simulation of NREL's 4-in fluidized bed reactor

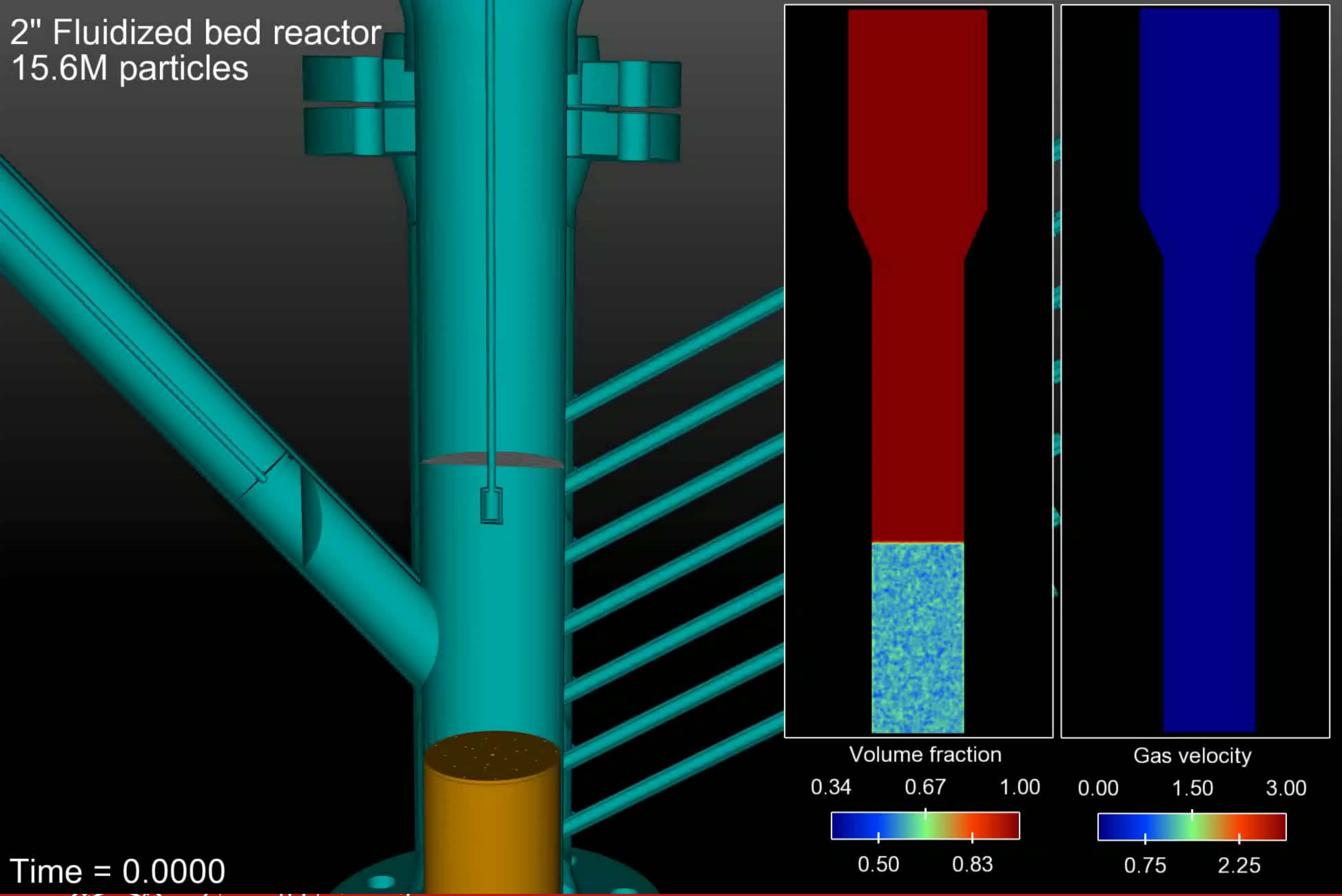
- National Renewable Energy Laboratory operates a 4-inch fluidized bed reactor for biomass gasification



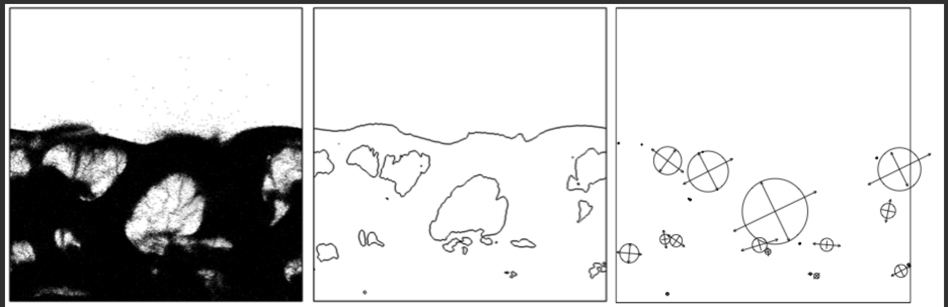




- $u_{in} = 6 \rightarrow 12U_{mf}$
- 15.6 M particles
- 20 M grid cells
- 576 cores on Marvin (Cornell cluster)

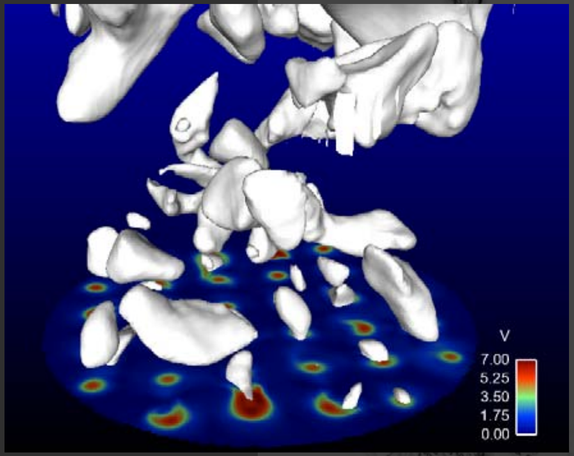

2" Fluidized bed reactor
15.6M particles
Time = 0.0000
Volume fraction
0.34 0.67 1.00
0.50 0.83
Gas velocity
0.00 1.50 3.00
0.75 2.25

# Bubble characterization

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

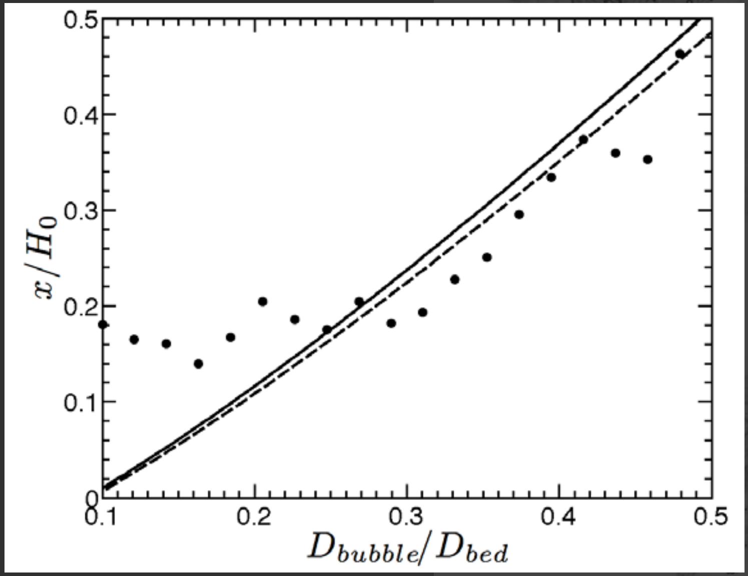


(a) Particle positions. (b) Iso-contour of $\varepsilon_f = 0.85$. (c) Position, principal axes and equivalent area of identified bubbles.




- 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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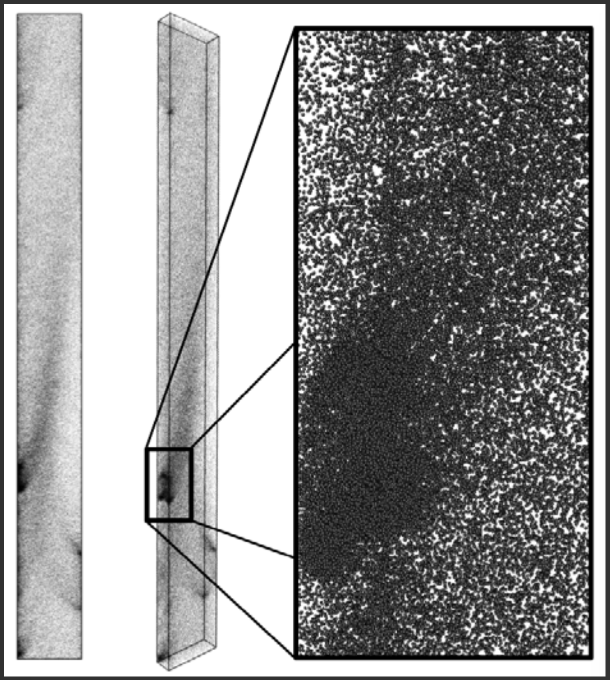
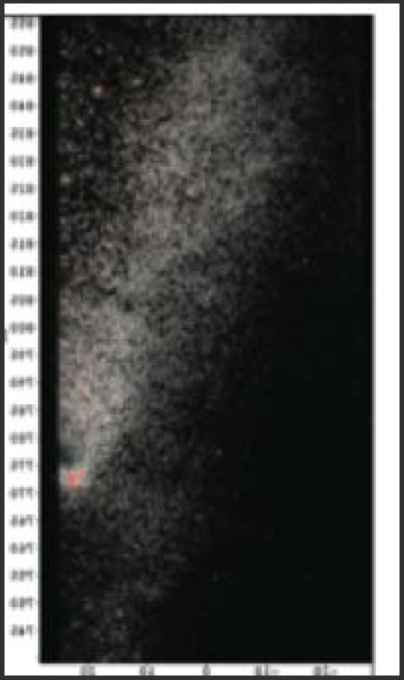
10. P. Pepiot, O. Desjardins, Numerical Analysis of Two- and Three-Dimension Fluidized Bed Reactors Using an Euler-Lagrange Approach. (2010)
11. R. Darton, R. LaNauze, J. Davidson, D. Harrison, Bubble growth due to coalescence in fluidised beds, Chemical Engineering Research and Design 55 (1977) 274–28

# 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]





**12.** Y. He, N.G. Deen, Gas-Solid Turbulent Flow in a Circulating Fluidized Bed Riser: Experimental and Numerical Study of Monodisperse Particle Systems. (2009)

# Simulation of a Turbulent Riser

- Radial Distribution Function (RDF) to characterize clustering

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

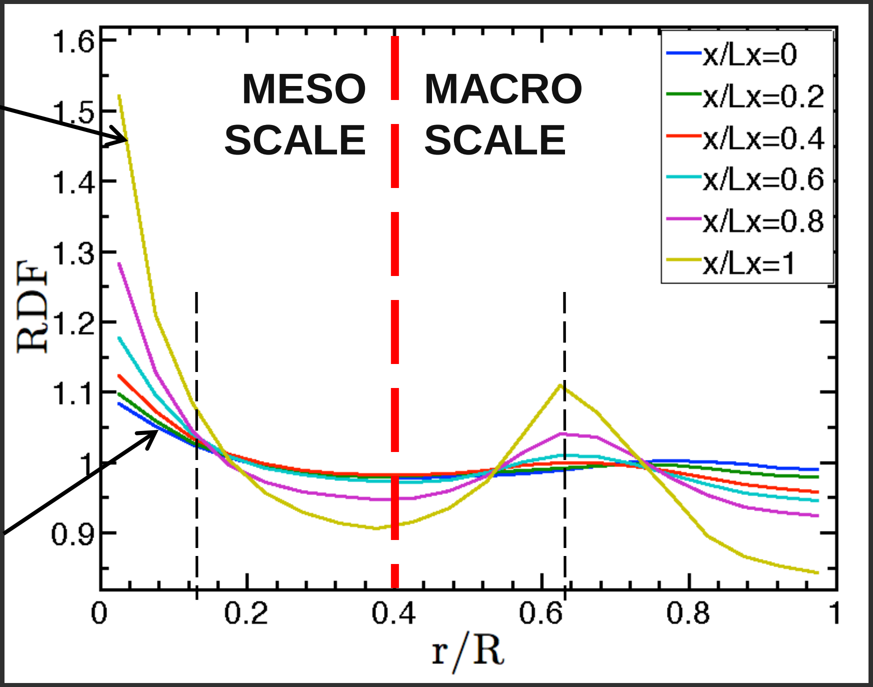
  - N: Number of particles in column
  - $N_p$: Number of particle pairs
  - Total possible number of pairs: N(N-1)

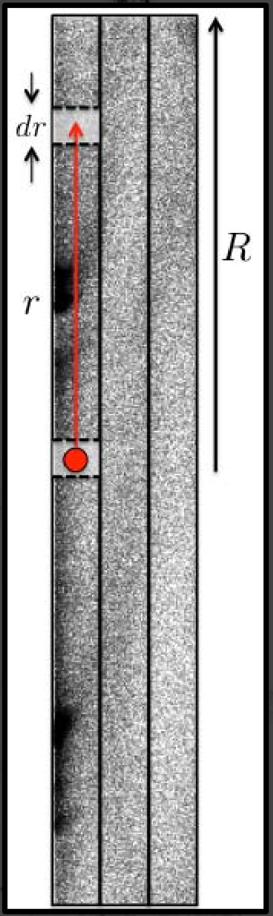
RDF=1: Uniform distribution

RDF>1: Clustering

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 $d_p$)

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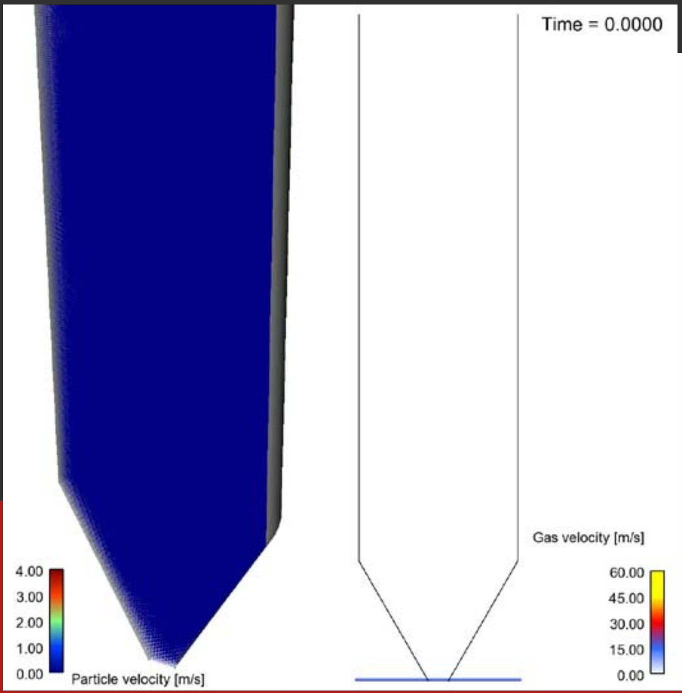
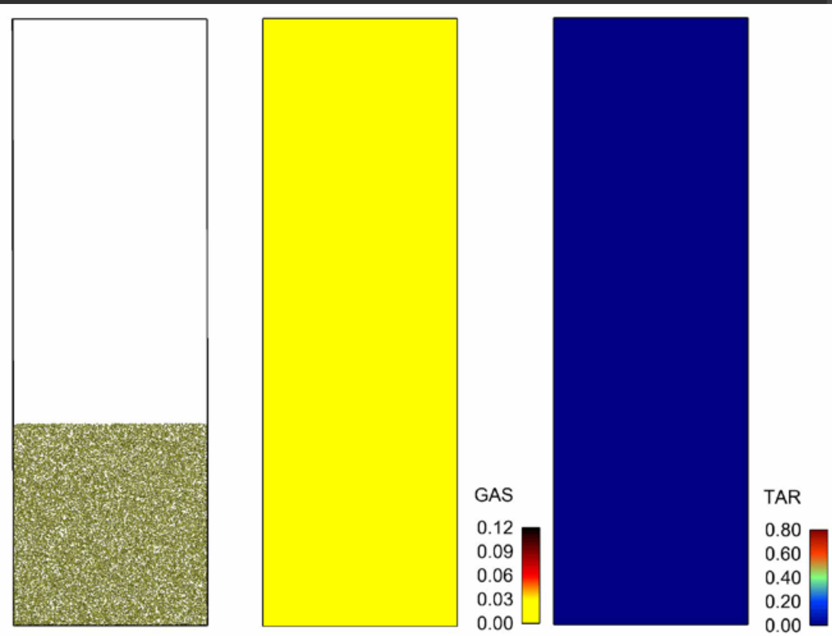
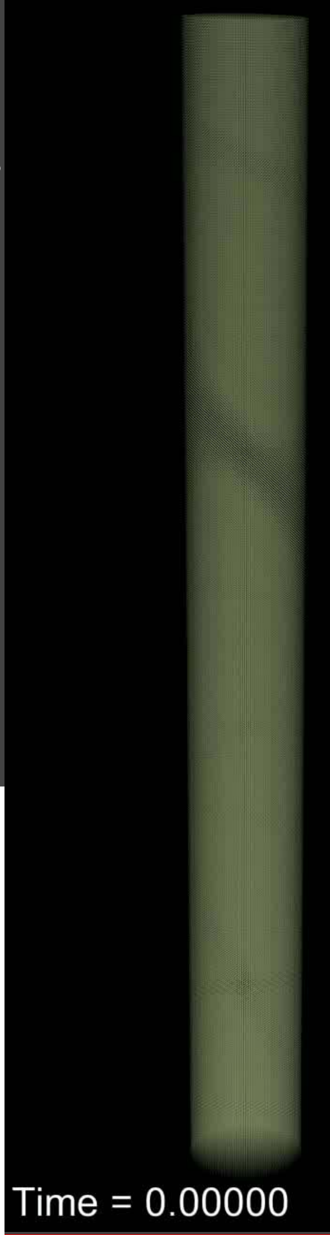
# Conclusions

- 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?