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

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

1. Tenneti & Subramaniam (2010)
Mathematical Formulation

Pointwise Description

- Gas phase: Variable-density / low-Mach Navier-Stokes equations
  \[
  \frac{\partial \rho_f}{\partial t} + \nabla \cdot (\rho_f \mathbf{u}_f) = 0
  \]
  \[
  \frac{\partial}{\partial t} (\rho_f \mathbf{u}_f) + \nabla \cdot (\rho_f \mathbf{u}_f \otimes \mathbf{u}_f) = \nabla \cdot \mathbf{\tau} + \rho_f \mathbf{g}
  \]
  \[
  \mathbf{\tau} = -p\mathbf{I} + \mu \left[ (\nabla \mathbf{u}_f + \nabla \mathbf{u}_f^T) - \frac{2}{3} (\nabla \cdot \mathbf{u}_f) \mathbf{I} \right]
  \]
- Particles: Newton’s second law of motion
  \[
  \frac{d\mathbf{x}_p}{dt} = \mathbf{u}_p
  \]
  \[
  m_p \frac{d\mathbf{u}_p}{dt} = \int_{S_p} \mathbf{\tau} \cdot \mathbf{n} \, d\mathbf{y} + F_{col}^{col} + mg
  \]
  \[
  I_p \frac{d\mathbf{\omega}_p}{dt} = \int_{S_p} \frac{d\mathbf{p}}{2} \mathbf{n} \times (\mathbf{\tau} \cdot \mathbf{n}) \, d\mathbf{y} + \sum_{j=1}^{n_p} f_{t,j\rightarrow p}^{col}
  \]
- 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**:
    \[
    \varepsilon_f (\mathbf{x}, t) = \int_{V_f(\infty)(t)} g(|\mathbf{x} - \mathbf{y}|) d\mathbf{y}
    \]
  - Allows to define **filtered variable** $\overline{a}$ from point variable $a$:
    \[
    \varepsilon_f \overline{a} (\mathbf{x}, t) = \int_{V_f(\infty)(t)} a (\mathbf{y}, t) g(|\mathbf{x} - \mathbf{y}|) d\mathbf{y}
    \]
  - No commutation between filtering and differentiation due to particle surface contributions
Mathematical Formulation

**VOLUME-FILTERED DESCRIPTION**

• For variable density flows

\[
\bar{a} = \frac{\varepsilon_f \rho_f \bar{a}}{\varepsilon_f \rho_f}
\]

• In general, decompose point variable \( a \) as \( a = \bar{a} + a' \) \( \Rightarrow u = \bar{a} + a'' \)

\[
\frac{\partial \varepsilon_f \rho_f}{\partial t} + \nabla \cdot (\varepsilon_f \rho_f \bar{u}_f) = S_\rho
\]

\[
\frac{\partial}{\partial t} (\varepsilon_f \rho_f \bar{u}_f) + \nabla \cdot (\varepsilon_f \rho_f \bar{u}_f \otimes \bar{u}_f) = \nabla \cdot \bar{\tau} - \nabla \cdot R_u + \varepsilon_f \rho_f g + S_{\rho u} - F_{\text{inter}}
\]

\[
S_\rho = \sum_{i=1}^{n_p} \int_{S_p} \rho_f n \cdot \frac{d r_i}{d t} g(|x - y|) \ dy
\]

\[
S_{\rho u} = \sum_{i=1}^{n_p} \int_{S_p} \rho_f n \cdot \frac{d r_i}{d t} \otimes u_f g(|x - y|) \ dy
\]

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

\[
F_{\text{inter}} = \sum_{i=1}^{n_p} g(|x - x_p|) \int_{S_p} \bar{\tau} \cdot n \ dy
\]

\[
\int_{S_p} \bar{\tau} \cdot n \ dy \approx V_p \nabla \cdot \bar{\tau} + f_p^{\text{drag}}
\]

\[
R_u = \varepsilon_f \rho_f \bar{u}_f'' \otimes \bar{u}_f''
\]
Computational Approach

- **NGA²**
  - Arbitrarily high-order DNS/LES code
  - Massively parallel
  - Conservation of mass, momentum, and kinetic energy

- **Immersed Boundary³**
  - Based on cut-cell approach
  - Discrete conservation of mass and momentum
  - Fully implicit implementation to handle small cut-cells

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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.
Computational Approach

- **NGA\textsuperscript{2}**
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Computational Approach

Flow solver
NGA Code

Complex geometries
Immersed Boundaries

Particle solver
Lagrangian Particle Tracking

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NGA Computational Platform

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

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\[
\frac{\partial \varepsilon_f \rho_f}{\partial t} + \nabla \cdot (\varepsilon_f \rho_f \vec{u}_f) = S_f
\]

\[
\frac{\partial}{\partial t} (\varepsilon_f \rho_f \vec{u}_f) + \nabla \cdot (\varepsilon_f \rho_f \vec{u}_f \otimes \vec{u}_f) = \nabla \cdot \vec{\tau} - \nabla \cdot \mathbf{R}_u + \varepsilon_f \rho_f \mathbf{g} + S_{mu} - F_{\text{inter}}
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\mathbf{R}_u = -\nu_T \left( \nabla \mathbf{u}_f + \nabla \mathbf{u}_f^T \right)
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\end{align*}
\]

\[
\mathbf{R}_u = -\nu_T \left( \nabla \bar{u}_f + \nabla \bar{u}_f^T \right)
\]

**Drag model of Tenneti & Subramaniam (2011)**

\[
f_i^{\text{drag}} = \frac{1}{\tau_p} (\bar{u}_f - \bar{u}_p) F(\varepsilon_f, \text{Re}_p)
\]

\[
\tau_p = \frac{\rho_p d_p^2}{18 \mu \varepsilon_f} \quad \text{Re}_p = \frac{\varepsilon_f \rho_f |\bar{u}_f - \bar{u}_p| d_p}{\mu}
\]

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

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\end{align*}
\]

\[
\tau = -p \mathbf{I} + \mu^* \left[ (\nabla \bar{u}_f + \nabla \bar{u}_f^T) - \frac{2}{3} (\nabla \cdot \bar{u}_f) \mathbf{I} \right] + \mathbf{R}_f
\]

Effective viscosity model of Gibilaro et al. (2007)

\[
\mu^* = \mu \varepsilon_f^{-2.8}
\]


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

\[
\frac{dx_p}{dt} = u_p
\]

\[
m_p \frac{du_p}{dt} = \int_{S_p} \tau \cdot n \, dy + F^{col} + mg
\]

\[
I_p \frac{d\omega_p}{dt} = \int_{S_p} \frac{dp}{2} n \times (\tau \cdot n) \, dy + \sum_{j=1}^{n_p} f^{col}_{t,j \rightarrow p}
\]

- 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

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Particle Data to Eulerian Mesh

- Need to transfer $\varepsilon_f$ and $\mathbf{F}_{\text{inter}}$ 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 is independent of the mesh.

Introduce image particle to apply Neumann condition near walls.

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

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bed dimensions [m]</td>
<td>0.75 x 0.15 x 0.015</td>
</tr>
<tr>
<td>Spout width [m]</td>
<td>0.01</td>
</tr>
<tr>
<td>Particle diameter [m]</td>
<td>0.0025</td>
</tr>
<tr>
<td>Particle density [kg/m³]</td>
<td>2526</td>
</tr>
<tr>
<td>Number of particles [-]</td>
<td>245,000</td>
</tr>
<tr>
<td>Grid [-]</td>
<td>300 x 60 x 6</td>
</tr>
</tbody>
</table>

Particle mass flux

Case A

Case B
Initial validation

Spout fluidization, case A

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

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

- 15.6 M particles
- 20 M grid cells
- 576 cores on Marvin (Cornell cluster)

\[ u_{in} = 6 \rightarrow 12U_{mf} \]
2" Fluidized bed reactor
15.6M particles

Time = 0.0000
Bubble characterization

- **Structure identification algorithm**\(^{10}\)
  - Band-growth algorithm to identify bubbles

- Mean bubble diameter: \(0.18 \times D_{\text{bed}}\)
- On average 8 bubbles in bed at once
- Compared results with Darton\(^{11}\) correlation
  - \(U_{\text{in}} = 6 \times U_{mf}\) (solid line)
  - \(U_{\text{in}} = 12 \times U_{mf}\) (Dashed line)

\[
D_{b} = 0.54 \left( U_{in} - U_{mf} \right)^{0.4} \left( h + 4 \sqrt{A_{0}} \right)^{0.8} g^{-0.2} 
\]

---

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\textsuperscript{12}

\textsuperscript{12} Y. He, N.G. Deen, Gas-Solid Turbulent Flow in a Circulating Fluidized Bed Riser: Experimental and Numerical Study of Monodisperse Particle Systems.
Simulation of a Turbulent Riser

- Radial Distribution Function (RDF) to characterize clustering

\[ RDF(x, r) = \frac{N_p L_z}{2dr N(N-1)} \]

- \( N \): 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

- 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…)

![Simulation Diagram](image)
Questions?