APPLICATION OF A FILTERED EULER-LAGRANGE FORMALISM TO LARGE-SCALE SIMULATIONS OF DILUTE AND DENSE FLUID-PARTICLE FLOWS

NETL 2013 MULTIPHASE FLOW WORKSHOP
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JESSE CAPECELATRO, OLIVIER DESJARDINS
SIBLEY SCHOOL OF MECHANICAL AND AEROSPACE ENGINEERING
CORNELL UNIVERSITY

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NATIONAL RENEWABLE ENERGY LABORATORY
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Multiphase flows in energy applications

• Multi-physics and multi-scale problem
  – Highly turbulent
  – Triple-phase
  – Complex geometries
  – Chemically reacting (including heat transfer + phase change)

• Computational Thermo-Fluids Laboratory led by Dr. Olivier Desjardins
  – http://ctflab.mae.cornell.edu
  – Multi-scale and multi-physics problems
  – Massively parallel computing
  – Phase interface tracking
  – Immersed boundaries for modeling complex geometries

Chemically reacting flows (Dr. Pepiot)
Multi-scale issue in turbulent particle-laden flows

Macroscale
- Large number of particles: \( \mathcal{O}(10) \)
- Length scales: m

Mesoscale
- Clustering
- Bubbling
- Particle size segregation
- Turbulence modulation

Microscale
- Wakes
- Particle collisions
- Phase change

Burlington, Vermont

Xu & Zhu, 2011

NASA
Outline

• Filtered Euler-Lagrange framework
  – Mathematical formulation
  – Numerical implementation

• Application to dense particle-laden flows
  – Gas-solid fluidized beds
  – Liquid-solid slurries

• Application to dilute particle-laden flows
  – Turbulent channel
  – Moderately-dilute riser

• Summary & conclusions
Ingredients for developing predictive multiphase tools\textsuperscript{1}

- Based on mathematical formulation derived from first-principles
- Numerically stable and convergent implementation
- Accurate and consistent models for unclosed terms
- Highly scalable

\textsuperscript{1} S. Subramaniam, Lagrangian-Eulerian methods for multiphase flows, \textit{IJMF}, (2013)
Mathematical formulation

First-principle equations

- **Gas phase**: Variable-density low-Mach Navier-Stokes equations
  \[
  \frac{\partial \rho_f}{\partial t} + \nabla \cdot (\rho_f \mathbf{u}_f) = 0
  \]
  \[
  \frac{\partial \rho_f \mathbf{u}_f}{\partial t} + \nabla \cdot (\rho_f \mathbf{u}_f \otimes \mathbf{u}_f) = \nabla \cdot \mathbf{\tau} + \rho_f \mathbf{g}
  \]
  \[
  \mathbf{\tau} = -p \mathbf{I} + \mu \left[ \nabla \mathbf{u}_f + \nabla \mathbf{u}_f^T - \frac{2}{3} (\nabla \cdot \mathbf{u}_f) \mathbf{I} \right]
  \]

- **Particles**: Newton’s second law of motion
  \[
  m_p \frac{d \mathbf{u}_p}{dt} = \int_{S_p} \mathbf{\tau} \cdot \mathbf{n} \ dS + \mathbf{F}_{p}^{\text{col}} + m_p \mathbf{g}
  \]
  \[
  \frac{d \mathbf{x}_p}{dt} = \mathbf{u}_p
  \]
  \[
  I_p \frac{d \mathbf{\omega}_p}{dt} = \int_{S_p} \frac{d_p}{2} \mathbf{n} \times (\mathbf{\tau} \cdot \mathbf{n}) \ dS + \sum_j \frac{d_p}{2} \mathbf{n} \times \mathbf{f}_{t,j \rightarrow p}^{\text{col}}
  \]

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

Volume-filtered description\(^2\)

- **Objective**: formulate equations for particle-laden flows that allow \(\Delta x \gg d_p\)
- **Introduce local volume filter** based on convolution product with kernel \(g(r)\)
  - \(\delta_f \gg d_p\): enabling the use of microscale models
  - \(\delta_f \ll L_{meso}\): mesoscale structures are fully resolved

- **Local volume fraction** 
  \[
  \varepsilon_f(x, t) = \int_{V_f} g(|x - y|) dy
  \]

- **Allows to define filtered variable** \(\bar{a}\) from point variable \(a\)
  \[
  \varepsilon_f \bar{a}(x, t) = \int_{V_f} a(y, t) g(|x - y|) dy \quad a = \bar{a} + a'
  \]
Mathematical formulation

Volume-filtering the Navier-Stokes equations

- **Continuity**
  \[
  \frac{\partial}{\partial t} (\varepsilon_f \rho_f) + \nabla \cdot (\varepsilon_f \rho_f \mathbf{u}_f) = 0
  \]

- **Momentum**
  \[
  \frac{\partial}{\partial t} (\varepsilon_f \rho_f \mathbf{u}_f) + \nabla \cdot (\varepsilon_f \rho_f \mathbf{u}_f \otimes \mathbf{u}_f) = \nabla \cdot (\mathbf{\tau} - \mathbf{R}_u) + \varepsilon_f \rho_f \mathbf{g} - \mathbf{F}_{\text{inter}}
  \]
  \[
  \mathbf{\tau} = -\mathbf{p} \mathbf{I} + \mu \left[ \nabla \mathbf{u}_f + \mathbf{u}_f \nabla - \frac{2}{3} (\nabla \cdot \mathbf{u}_f) \mathbf{I} \right] + \mathbf{R}_\mu
  \]

- **Interphase exchange**
  \[
  \mathbf{F}_{\text{inter}} = \sum_{p=1}^{n_p} g(|\mathbf{x} - \mathbf{x}_p|) \mathbf{f}_{\text{inter}}^p
  \]
  \[
  \mathbf{f}_{\text{inter}}^p \approx \mathbf{V}_p \nabla \cdot \mathbf{\tau} + \mathbf{f}_{\text{drag}}^p
  \]
Ingredients for developing predictive multiphase tools

- Numerically stable and convergent implementation
- Accurate and consistent models for unclosed terms
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- Highly scalable

Consistent framework from point-particle to full DNS

• Accurate solution of the equations requires $\Delta x \ll \delta_f$
• Model closures depend on $\delta_f$
• What is the appropriate choice for $\delta_f$?

$$\int_{V_f} \nabla \cdot \tau g(|x - y|) \, dy = \nabla \cdot (\varepsilon_f \overline{\tau}) - \sum_{p=1}^{n_p} \int_{S_p} n \cdot \tau g(|x - y|) \, dy$$

- Microscale models might break down
- Cannot resolve boundary layers

Ray & Collins, 2011
Consistent framework from point-particle to full DNS

- Accurate solution of the equations requires $\Delta x \ll \delta_f$
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\[
\int_{V_f} \nabla \cdot \tau_g(|x - y|) \, dy = \nabla \cdot (\varepsilon_f \bar{T}) - \sum_{p=1}^{n_p} \int_{S_p} \nabla \cdot \tau_g(|x - y|) \, dy
\]

- Drag model of Tenneti et al. (2011)
- Soft-sphere collision model (Cundall & Strack 1979)
- Lagrangian Dynamic Smagorinsky SGS model of Meneveau et al. (2000)
- Effective viscosity (Gibilaro 2007)

- Microscale models might break down
- Cannot resolve boundary layers
- Better capture turbulence and mesoscale dynamics
- Can handle large number of particles

Ray & Collins, 2011
Numerical implementation

Filter discretization

• Direct implementation becomes too expensive
• Filter based on the convolution of mollification and Laplacian smoothing\(^2\)
  1. Mollification: transfer particle data to neighboring cells
  2. Diffusion: smooth data with specified width
• Fully conservative, implicit treatment
• Special care is needed at the walls

Particle influence on mesh

Two-step filter

Near-wall treatment

Filter discretization

- Direct implementation becomes too expensive
- Filter based on the convolution of mollification and Laplacian smoothing

1. Mollification: transfer particle data to neighboring cells
2. Diffusion: smooth data with specified width

- Fully conservative, implicit treatment
- Special care is needed at the walls

Numerical implementation


Filter width $\delta_f$ is independent of the mesh size

$\Delta x = 4d_p$  $\Delta x = 2d_p$  $\Delta x = d_p$  $\Delta x = d_p/2$  $\Delta x = d_p/4$

Error

$1^\text{st}$-order (—)
Single-step (■)
Two-step (●)

1st-order (—)
Single-step (■)
Two-step (●)
Ingredients for developing predictive multiphase tools

Ingredients for developing predictive multiphase tools

- Numerically stable and convergent implementation ✓
- Accurate and consistent models for unclosed terms ?
- Based on mathematical formulation derived from first-principles ✓
- Highly scalable

Numerical implementation

Computational platform

NGA\(^4\)

- Arbitrarily high-order multi-physics DNS/LES code
- Conservation of mass, momentum, and kinetic energy
- Highly scalable

4. O. Desjardins, G. Blanquart, G. Balarac, H. Pitsch, High order conservative finite difference scheme for variable density low Mach number turbulent flows, JCP (2008)
Ingredients for developing predictive multiphase tools

Predictive multiphase tool

- Numerically stable and convergent implementation
- Based on mathematical formulation derived from first-principles
- Accurate and consistent models for unclosed terms
- Highly scalable

Application to dense gas-solid flows

Bubble statistics

Particle flux

Segregation rate
Application to liquid-solid slurries

- Compared with experiments by Roco & Balakrishnam (1985)
- Two cases simulated
  - Re=85,000 (above critical deposition velocity)
  - Re=42,660 (below critical deposition velocity)
- Force liquid mass flow rate in a periodic pipe
- 768 x 156 x 156 mesh
- 19 M polydisperse particles

Application to liquid-solid slurries

Computational Thermo-Fluids Lab

Time = 0.0000

Velocity [m/s]
- 19,000,000 particles
- Re=42,660
- Density ratio=2.5

Volume fraction
- 1.50
- 1.12
- 0.75
- 0.38
- 0.00
- 0.70
- 0.52
- 0.35
- 0.17
- 0.00
Application to liquid-solid slurries

Excellent agreement with experiments

(a) Experimental data (Roco and Balakrishnam, 1985).

(b) Simulation results.

(a) Experimental data (Roco and Balakrishnam, 1985).

(b) Simulation results.
Application to liquid-solid slurries

Capable of predicting onset of bed formation

(a) Solid concentration profile.

(b) Solid velocity profile.
Application to dilute channel flows

Simulation configuration

Domain

Mesh: 1000 x 272 x 320

\[ \Delta x^+ = 8 \quad \Delta y^+ = 4.8 \quad \Delta z^+ = 8 \]

Experimental parameters

- \[ \delta = 2 \text{ cm} \]
- \[ \text{Re}_{25} = 13,850 \]
- Bulk velocity = 9.2 m/s
- Centerline velocity, \( U_{cl} = 10.5 \)
- Particle diameter = 150 \( \mu \text{m} \)
- Particle density = 2,500 kg/m\(^3\)
- St = 50

<table>
<thead>
<tr>
<th>Wall boundary condition</th>
<th>( \text{Re}_\tau )</th>
<th>( \phi )</th>
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<tbody>
<tr>
<td>Paris &amp; Eaton (2001)</td>
<td>644</td>
<td>0.2</td>
</tr>
<tr>
<td>Benson &amp; Eaton (2003)</td>
<td>617</td>
<td>0.15</td>
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<tr>
<td>NGA</td>
<td>630</td>
<td>0.15</td>
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</table>
Application to dilute channel flows

Single-phase channel flow

Eddy viscosity contribution
Application to dilute channel flows

Particle-laden channel
Application to dilute channel flows

Particle-laden channel

Turbulence modulation & preferential concentration due to non-uniform interphase coupling

1D kinetic energy

Particle number density

\[ \frac{N_p}{\langle N_p \rangle} \]

\[ \text{Initial} \quad tU_{cl}/\delta = 2000 \]
Application to dilute channel flows

Particle-laden channel

Turbulence modulation & preferential concentration due to non-uniform interphase coupling

Extend to moderately-dilute flows
Application to risers

• Dimensional analysis

\[ Fr = \frac{U}{\sqrt{gd_p}} \quad Ar = \frac{\rho_s \rho_f d_p^3 g}{\mu^2} \quad D/d_p \]

• Experimental observations (Noymer & Glicksman, 2000)
  – Clusters fall very close to the walls (~100 μm)
  – Clusters located within hydrodynamic boundary layer
  – Cluster fall velocity independent of inflow conditions

\[ \frac{u_{cl}}{u_{mf}} = \frac{1000}{\sqrt{Ar}} \quad u_{mf} = 0.00075 \frac{\rho_s gd_p^2}{\mu} \]

\[ u_{cl} = 0.75 \sqrt{\frac{\rho_s}{\rho_f}} gd_p \]

Simulation cases

<table>
<thead>
<tr>
<th></th>
<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
<th>Case 4</th>
<th>Case 5</th>
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<tbody>
<tr>
<td>Ar</td>
<td>50</td>
<td>100</td>
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<td>2500</td>
<td>12500</td>
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<tr>
<td>D/d_p</td>
<td>320</td>
<td>150</td>
<td>150</td>
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</tr>
<tr>
<td>\langle \varepsilon_p \rangle</td>
<td>0.15%</td>
<td>1.5%</td>
<td>1.5%</td>
<td>1.5%</td>
<td>1.5%</td>
</tr>
<tr>
<td>\rho_p/\rho_f</td>
<td>2500</td>
<td>2500</td>
<td>2500</td>
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</tr>
</tbody>
</table>

• Simulation parameters
  – 3D pipe geometry (immersed boundaries)
  – Periodic in vertical direction
  – 760,000 particles
  – Mesh: 800x83x83
Application to risers

Case 4: Ar=2500

Cluster fall velocity
- Computed from tracking of identified cluster structures
- Compared to experimental correlation of Noymer & Glicksman (2000)
Conclusions

• Volume filtered formalism provides a consistent framework from point-particle to fully resolved simulations

• Pushing the validity of classical microscale models to finer meshes yields excellent results

• The proposed framework can capture a range of phenomenon including
  – Clustering
  – Bubbling
  – Segregation in particle size
  – Preferential concentration

• Looking forward
  – Study intermediate values of particle diameter to mesh size ratio \( \frac{d_p}{\Delta x} \approx 1 \sim 10 \)
  – Implement sharper / higher accuracy filters
  – Use this framework to provide closure for RANS modeling:

R.O. Fox, J. Capecelatro, O. Desjardins
Validation of a Multiphase Turbulence Model Using Mesoscale DNS of Gravity-Driven Gas-Particle Flow. 11:50-12:10 PM