Sensitivity Analysis of Particle-In-Cell Modeling Parameters in MFiX-PIC

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MFiX Suite Overview (No math!)

- **DNS** (Direct Numerical Simulation): fine scale, accurate simulations for limited size domain
- **MFiX DEM** (Discrete Element Method): track individual particles and resolve collisions
- **MFiX TFM** (Two-Fluid Model): gas and solids form an interpenetrating continuum
- **MFiX PIC** (Particle-In-Cell): track parcels of particles and approximate collisions

- **ROM** (Reduced Order Models): simplified models with limited application

- **Model Uncertainty**

- **Time to Solution**

**MFiX fluid solver**

- Lagrangian
  - DEM
  - PIC

- Eulerian
  - TFM

**Scale Levels**

- **Micro-scale**
  - DNS
- **Meso-scale**
  - CFD-DEM
  - TFM
- **Macro-scale**
  - MP-PIC
  - Filtered-TFM
MFiX Suite Overview (Math!)

**Fluid solver**
\[
\frac{\partial}{\partial t}(\varepsilon_g \rho_g) + \frac{\partial}{\partial x_j}(\varepsilon_g \rho_g U_{gj}) = \sum_{n=1}^{N_g} R_{gn}
\]
\[
\frac{\partial}{\partial t}(\varepsilon_g \rho_g U_{gi}) + \frac{\partial}{\partial x_j}(\varepsilon_g \rho_g U_{gj} U_{gi}) = -\varepsilon_g \frac{\partial P_g}{\partial x_i} + \varepsilon_g \rho_g g_i + S_{gi}
\]

**MFiX-TFM**
\[
\frac{\partial}{\partial t}(\varepsilon_m \rho_m) + \frac{\partial}{\partial x_j}(\varepsilon_m \rho_m U_{mj}) = \sum_{n=1}^{N_m} R_{mn}
\]
\[
\frac{\partial}{\partial t}(\varepsilon_m \rho_m U_{mi}) + \frac{\partial}{\partial x_j}(\varepsilon_m \rho_m U_{mj} U_{mi}) = -\varepsilon_m \frac{\partial P_m}{\partial x_i} + \frac{\partial \tau_{mi} j}{\partial x_j} + \varepsilon_m \rho_m g_i + S_{mi}
\]

**MFiX-DEM**
\[
\frac{d m_p}{d t} = \sum_{n=1}^{N} R_n
\]
\[
\frac{d \mathbf{V}_p}{d t} = \beta (\mathbf{U}_g - \mathbf{V}_p) - \frac{1}{\rho_p} \nabla p + \mathbf{F}_c + \mathbf{g}
\]
\[
\mathbf{F}_c = \sum_j (\mathbf{F}_{n j} + \mathbf{F}_{t j})
\]

**MFiX-PIC**
\[
\frac{d m_p}{d t} = \sum_{n=1}^{N} R_n
\]
\[
\frac{d \mathbf{V}_p}{d t} = \beta (\mathbf{U}_g - \mathbf{V}_p) - \frac{1}{\rho_p} \nabla p - \frac{1}{\epsilon_p \rho_p} \nabla \tau_p + \mathbf{g}
\]
\[
\tau_p = \frac{P_p \epsilon_p}{\max(\epsilon_{cp} - \epsilon_p, \delta(1 - \epsilon_p))}
\]
Why PIC?

• Gas-solid flows common in industrial applications

• Limitation of Eulerian-Eulerian approach:
  • Framework to include additional phases needs several constitutive relations which increase uncertainty
  • Limitation to resolve sharp interfaces (Continuum models tend to follow gradients)

• Limitation of Eulerian-Lagrangian approach:
  • Particle count in industrial-scale systems of the order of billions, not tractable with a naïve approach such as Discrete Element Modeling

• Need for speed !!
• Framework for graphical programming using nodes and connections

• Underlying library for optimization/UQ work.

• Integrates with MFiX GUI

• For more information: https://mfix.netl.doe.gov/nodeworks/

Courtesy: Justin Weber, NETL
Surrogate modeling and analysis toolset

Design of Experiments

Model evaluation (MFiX, etc.)

Response Surface Construction

Optimization, Sensitivity, Uncertainty

Courtesy: Justin Weber, NETL
NETL VV&UQ Roadmap

**Features**

Survey of subject matter experts

Systematic design of experiments and simulation campaign

Tollgates for reviews, analysis and discussions with stakeholders

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**Validation and Uncertainty Quantification**

- Define research objectives & general problem classification
- Identify and define application specific constraints
- Identify Quantities of Interest (QoI)
- Query subject matter experts (SMEs)
- Assess feedback
- Yes: Tollgate review prior to testing
- No: Revision

- Computational model setup
- Simulation Campaign design & prior tollgate review
- Campaign execution
- QA & preliminary analysis
- Analysis & Stakeholder Tollgate
- Model Bias Analysis
- Simulation Campaign
- Experimental Campaign
- Quantitative Analysis
- Next research objective

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Plan overview

- **Cases selected to cover a broad range of flow conditions**
  - Particle Settling: $U/U_{mf} < 1.0$ ($P_0 \sim 1$) (Simulation campaign)
  - Bubbling Fluidized bed: $U/U_{mf} \sim 1$ ($P_0 \sim 10$)
  - Circulating Fluidized bed: $U/U_{mf} >> 1.0$ ($P_0 \sim 100$)

- **Summary of model parameters used:**

<table>
<thead>
<tr>
<th></th>
<th>I1 Pressure scale factor</th>
<th>I2 Volume fraction scale factor</th>
<th>I3 Statistical weight</th>
<th>I4 Volume fraction at maximum packing</th>
<th>I5 Solid slip velocity factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1: Particle Settling</td>
<td>[1,10]</td>
<td>[2.5]</td>
<td>[3.20]</td>
<td>[0.4,0.5]</td>
<td>[0.5,1.0]</td>
</tr>
<tr>
<td>C2: Fluidization</td>
<td>[1,100]</td>
<td>[2.5]</td>
<td>[10,100]</td>
<td>[0.4,0.5]</td>
<td>[0.85,0.98]</td>
</tr>
<tr>
<td>C3: Circulating Fluidized Bed</td>
<td>[1,250]</td>
<td>[2.5]</td>
<td>[4]</td>
<td>[0.4,0.5]</td>
<td>[0.85,0.98]</td>
</tr>
</tbody>
</table>

*Parameters selected based on prior sensitivity study*

\[
\frac{d\bar{V}_p}{dt} = \beta (\bar{U}_g - \bar{V}_p) - \frac{1}{\rho_p} \bar{v}_p - \frac{1}{\epsilon_p \rho_p} \bar{\tau}_p + \ddot{g}
\]

\[
\tau_p = \frac{P_0 \epsilon_p^\beta}{\max(\epsilon_{cp} - \epsilon_p, \delta(1 - \epsilon_p))}
\]
Case 1: Particle Settling

Analytical Solution:

Location of shock

\[ x(t) = -t \left( \frac{\varepsilon_S^* \varepsilon_g^* u_r^* - \varepsilon_{S0} \varepsilon_{g0} u_{r0}}{\varepsilon_S^* - \varepsilon_{S0}} \right) \]

Relative velocity (Stokes' drag)

\[ u_r = \frac{g \Delta \rho d_p^2}{18 \mu_g} \varepsilon_g^{3.65} \]
Case 1: Particle Settling

- Model parameters
  - Pressure linear scale factor (t1)
  - Exponential factor (t2)
  - Statistical weight (t3)
  - Void fraction at packing (t4)
  - Solids slip velocity factor (t5)

- Simulation campaign having 55 simulations

- Response variable: Filling shock location (m)

- Design of experiments using Latin Hypercube Sampling with genetic algorithm
Case 1: Particle Settling

- Response surface constructed using Radial basis function
- Sobol indices show the following:
  - main effects (first order)
  - interactive effects (second order)
- Code-to-Code comparison with PSUADE

Sensitivity Analysis using Sobol Indices

3D plot of the data-fitted surrogate model
*\( t_1, t_2, t_3 \) set at nominal values
Sensitivity Analysis

Case 2: Fluidization

\[ P_4, h_4 = 86.26 \text{ cm} \]

\[ h_{\text{bed}} = 15.24 \text{ cm} \]

\[ \Delta P_4 \]

\[ P_3, h_3 = 11.11 \text{ cm} \]

\[ P_2, h_2 = 6.03 \text{ cm} \]

\[ P_1, h_1 = 0.56 \text{ cm} \]

\[ h = 0 \text{ cm} \]

\[ P_0, h_0 = -14.61 \text{ cm} \]

\[ \Delta P_3 \]

\[ \Delta P_2 \]

Filter

\[ \text{ID} = 6.35 \text{ cm} \]
Case 2: Fluidization

3D plot of the data-fitted surrogate model (Radial Basis Function)

Sensitivity Analysis using Sobol Indices

- $\Delta P_2$: Pressure linear scale factor, $t_1$, set at nominal values
- $\Delta P_3$: Exponential factor, $t_2$, set at nominal values
- $\Delta P_4$: Statistical weight, $t_3$, set at nominal values
- Void fraction at packing, $t_4$
- Solids slip velocity factor, $t_5$
Sensitivity Analysis

Case 3: CFB

- Material: High density polyethylene
- Particle density: 863 kg/m³
- Mean particle diameter: 871 μm
- Particle count: 800,000

References:
- Wen & Yu (AIChE 1966)
- Gidaspow (AIChE 1990)
- BVK (CES 2007)
- HKL (JFM 2001)
Sensitivity Analysis

Case 3: CFB

3D plot of the data-fitted surrogate model (Radial Basis Function)

Interface height

**ΔP - Riser**

**ΔP - Standpipe**

*Sensitivity Analysis using Sobol Indices*

- **t1:** Pressure linear scale factor
- **t2:** Exponential factor
- **t4:** Void fraction at packing
- **t5:** Solids slip velocity factor

*ΔP, t1, t2 set at nominal values*
Summary

• **Conclusions**
  - Systematic analysis of Particle-In-Cell model parameters
  - Three different operating regimes: Settling bed, Bubbling fluidized bed and Circulating fluidized bed
  - Solids slip velocity factor and void fraction at maximum packing influence settling dynamics
  - More likely to use larger values of pressure linear scale factor at higher flow rates

• **Future work**
  - Bayesian calibration of model parameters
  - Extension to reacting multiphase flows
Thank you for your attention.

Sensitivity Analysis of Particle-In-Cell Modeling Parameters used in MFIX-PIC

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Case 1: Scatter plot matrix with response variables
Case 2: Scatter plot matrix with response variables
Case 3: Scatter plot matrix with response variables