MFiX-DEM Phi: Performance and Capability Improvements Towards Industrial Grade Open-source DEM Framework with Integrated Uncertainty Quantification

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04/21/2016

Presentation Outline

- The Project Team
- Technical Background/Motivation for The Project
- Potential Significance of The Results of The Work
- Physical Modeling Enhancement
- Industrial Collaboration and Utility
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MFIX-DEM Phi team: ASU campus

- PI: Aytekin Gel
  - PhD, West Virginia U. 1999
  - MBA, ASU, 2007
  - Professor of Practice, School of Computing, Informatics, Decision Systems Engineering (SCIDSE), ASU
  - Expertise: HPC, CFD, UQ, multiphase reactive flow, Six Sigma for Quality
  - 16 years of startup company exp.
  - Involved with MFIX since 1999
  - Award: Team Member of R&D 100, 2007

- Co-PI: Heather Emady
  - PhD, Purdue U. 2012
  - Assistant Professor, School of Engineering, Materials, Transport and Energy (SEMTE)
  - Expertise: particulate processes and product design
  - Award: Bisgrove Scholar, 2015

- Co-PI: Yang Jiao
  - PhD, Princeton U. 2010
  - Assistant Professor, School of Engineering, Materials, Transport and Energy (SEMTE)
  - Expertise: computational materials
  - Award: DARPA Young Faculty, 2014

- GRA: Shaohua Chen
  - PhD candidate, SEMTE

- GRA: Manogna Adepu
  - PhD candidate, SEMTE
The Project Team

- Co-PI: Charles Tong
- Research Scientist
- Expertise: uncertainty quantification
- Developer of open-source UQ toolbox PSUADE and CCSI Toolkit UQ framework FOQUS

- Co-PI: Jonathan Hu
- Principal Member of the Technical Staff at Sandia National Laboratories
- Expertise: highly scalable linear equation solver, developer of Trilinos Project (ML, nextgen ML: MueLu)
- Award: R&D 100 (Trilinos)

- Nathan Ellingwood
- Research Staff at Sandia National Laboratories
- Ph.D. in Applied Math & Computational Sciences, University of Iowa (2014)
- Expertise: Data parallel algorithms for GPU, FEM, CFD, HPC, Digital Lung Project

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MFIX* Open Source Multiphase Flow Solver Suite:

MFIX Two-Fluid Model (TFM) Equations Solved:

Mass conservation for phase m (m=g for gas and s for solids)
\[
\frac{\partial}{\partial t} (\rho_m \phi_m) + \nabla \cdot (\rho_m \phi_m \mathbf{v}_m) = \sum R_{ai}
\]

Momentum conservation
\[
\frac{\partial}{\partial t} (\rho_m \phi_m \mathbf{v}_m) + \nabla \cdot (\rho_m \phi_m \mathbf{v}_m \mathbf{v}_m) = \nabla \cdot \mathbf{S}_m + \rho_m \mathbf{g} + \sum \mathbf{T}_{ai}
\]

Granular energy conservation (m \neq g)
\[
\frac{3}{2} \rho_m (\frac{\partial \Theta_m}{\partial t} + \mathbf{v}_m \cdot \nabla \Theta_m) = \nabla \cdot \mathbf{q}_m + \nabla \cdot \mathbf{S}_m + \nabla \cdot \mathbf{v}_m - \rho_m \mathbf{P}_m + \Pi_m
\]

Energy conservation
\[
\rho_m C_p \left( \frac{\partial T_m}{\partial t} + \mathbf{v}_m \cdot \nabla T_m \right) = -\nabla \cdot \mathbf{q}_m + \sum \gamma_{ai} (T_m - T_{ai}) - \Delta H_{m}
\]

Species mass conservation
\[
\frac{\partial}{\partial t} (\rho_m X_{ai}) + \nabla \cdot (\rho_m X_{ai} \mathbf{v}_m) = R_{ai}
\]

Sources:

* MFIX: Multiphase Flow with Interphase Exchanges
Newtonian Equations for Particles

\[
\frac{dX_i(t)}{dt} = \dot{V}_i(t),
\]

\[
m_i \frac{d\dot{V}_i(t)}{dt} = F_i(t) = m_i \ddot{X}_i(t) + F_d^{(2)}(t) + F_c(t),
\]

\[
f(t) \frac{d\dot{V}_i(t)}{dt} = T_i(t).
\]

Particle Contact Force Models

\[
F_{ij}(t) = F_{ij}^p(t) + F_{ij}^{(2)}(t) \quad F_{ij}(t) = F_{ij}^p(t) + F_{ij}^{(2)}(t)
\]

Drag Forces on Particles

\[
p_d^{(2)} = -\nabla P_g(x_i) \nu_i + \frac{\rho_d(x_i)}{\kappa_m} (\nu_i(x_i) - \nu_m(x_i))
\]

Solid-Fluid Momentum Transfer

\[
\dot{T}_{gm} = -\kappa_m \nabla P_g(x_i) + \rho_d^{(2)} (\nu_i(x_i) - \nu_m(x_i))
\]


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**ARIZONA STATE UNIVERSITY**

**MFIX Overview (Today)**

*Trade-off between simulation fidelity and time-to-solution*

**PIC**

Track parcels of particles and approximate collisions

**TFM**

Two-Fluid Model: Gas and solids form an interpenetrating continuum

**Hybrid**

Continuum and discrete solids coexist

**DEM**

Discrete Element Method: Track individual particles and resolve collisions


Flow chart illustrating the key solution processes coupling the CFD solver and DEM solver and the associated governing equations.

No need for external coupling of multiple software as done in most of the current available options such as CFDEM® coupling by CFDEMresearch GmbH:

- OpenFOAM
- LIGGGHTS®

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**MFIX Overview (Today)**

**A suite of multiphase flow models & solvers**

- **PIC**
  - Track parcels of particles and approximate collisions

- **TFM**
  - Two-Fluid Model: Gas and solids form an interpenetrating continuum

- **DEM**
  - Discrete Element Method: Track individual particles and resolve collisions

- **Hybrid**
  - Continuum and discrete solids coexist

**Trade-off between simulation fidelity and time-to-solution**


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**Overview of MFIX DEM Phi Project Outcomes:** (at end of the project)

**Objective under Performance Improvements Task:** Reduce time-to-solution significantly by exploiting the massive parallelism offered with next generation Intel Xeon Phi based HPC systems to make it usable by industry on a daily basis for design with affordable HPC systems and offer code portability to others.

**Time-to-Solution**

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Shows the targeted change in MFIX suite of solver features at the end of this project (if awarded)
**Task 2 Aim:**
Increase the speed to reduce time-to-solution by optimizing modern computing platforms

**Task 3 Aim:**
Develop physics w.r.t. the targeted application

**Task 4 Aims:**
Ensure the results of the code are accurate, increase usability by reducing complexity

**Task 5 Aim:**
Demonstrate usability for industrial scale problems and collaboration for industrial adoption.

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- The Project Team
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  - Physical Modeling Enhancement - Enhance the Capability for Handling
    - Particle Size Distributions
    - Heat Transfer
- Industrial Collaboration and Utility
New data structures have been implemented to separate geometrical and physical parameters of each particles of a solid phase, and to allow each solid phase to possess a different size distribution.

New subroutines have been written to generate initial particle configurations with built-in distributions, including Gaussian, Log-Normal, and Uniform.

New subroutines have been written to generate initial particle configurations with arbitrary user-defined particle size distributions.

Subroutines using particle radii as parameters have been modified accordingly.

The implementations have been tested in a discharging hopper case provided by one of the collaborator.
Enhance the Capability for Handling Particle Size Distributions – Preliminary Results for Bin Flow Case

Particle discharge (4.0 s) and settling (0.3 s)

Case 1, \(\mu = -5.8\ \sigma = 0.001\)

Case 2, \(\mu = -5.8\ \sigma = 0.01\)

Case 3, \(\mu = -5.8\ \sigma = 0.1\)

Case 4, \(\mu = -5.8\ \sigma = 0.25\)

Enhance the Capability for Handling Particle Size Distributions

\[ N(x, \mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma}} \exp \left(\frac{-(x-\mu)^2}{2\sigma^2}\right) \]

<table>
<thead>
<tr>
<th>Case</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>MFIX-DEM</td>
<td>0.605</td>
<td>0.608</td>
<td>0.624</td>
<td>0.659</td>
</tr>
<tr>
<td>LAMMPS</td>
<td>0.609</td>
<td>0.604</td>
<td>0.633</td>
<td>0.662</td>
</tr>
</tbody>
</table>

Discharge Dynamics

![Diagram showing discharge dynamics](image)
Hopper with mass inflow BC

Three solid phases:
- phase 1, $\mu=-5.3$ $\sigma=0.05 (MI)$
- phase 2, $\mu=-5.5$ $\sigma=0.05$
- phase 3, $\mu=-5.8$ $\sigma=0.05$

Cyclone

Log-Normal
$\mu=-3.90$
$\sigma=0.05$
The Project Team

Technical Background/Motivation for The Project

Potential Significance of The Results of The Work

- Physical Modeling Enhancement - Enhance the Capability for Handling
  - Particle Size Distributions
  - Heat Transfer

Industrial Collaboration and Utility

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Enhance the Capability for Handling Heat Transfer through experimental validation

- Conduction, convection, and radiation occur in many multiphase processes. Particle-particle conduction is now commonly used in DEM codes, but more complex heat transfer models are necessary to more accurately simulate these processes.

- Current serial version of MFIX-DEM has codes for each of these, but they remain to be tested and validated.

- Whether drying, mixing, granulating, coating or heating, rotary drum systems are among the most common process equipment, offering efficient economical solutions. Thus, a rotary drum was selected for validating heat transfer models.

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Snapshot of wall HT after 2 sec of simulation.

Source: http://www.muzzio.rutgers.edu/
Enhance the Capability for Handling Heat Transfer through experimental validation

- The drum is held at a fixed hot temperature of 600K with particles placed in the drum with a temperature of 300K and air at 298 K. The drum is rotated at a speed of 2 RPM in clockwise direction.

- Simulating particle-wall and particle-fluid-particle heat transfer

**Simulation parameters**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diameter of drum</td>
<td>6 inch.</td>
</tr>
<tr>
<td>Height of drum</td>
<td>3 inch.</td>
</tr>
<tr>
<td>Fill Volume</td>
<td>50 %</td>
</tr>
<tr>
<td>Number of particles</td>
<td>100,000</td>
</tr>
<tr>
<td>Density of particles</td>
<td>1500 kg/m3</td>
</tr>
<tr>
<td>Diameter of particles</td>
<td>0.002 m</td>
</tr>
<tr>
<td>(K_s): solid conductivity</td>
<td>1 W/(m-K)</td>
</tr>
<tr>
<td>(C_p_s): specific heat of solid</td>
<td>850 J/(kg-K)</td>
</tr>
<tr>
<td>(K_g): air conductivity</td>
<td>0.0372 W/(m-K)</td>
</tr>
<tr>
<td>(C_p_g): specific heat of air</td>
<td>1020 J/(kg-K)</td>
</tr>
</tbody>
</table>

Animation of wall heat transfer (2 sec)

Enhance the Capability for Handling Heat Transfer

- A rolling aluminum calciner with thermocouples inserted in the radial direction.

- One side is Teflon and one side is glass for internal view.

- Particle - particle and particle - wall conduction has been validated in this paper.

- Further fluid-particle convention and radiation via particle-environment modes will be tested and validated.

Enhance the Capability for Handling Heat Transfer: Rotary drum validation

- Thermocouples and infrared camera will be used to monitor the temperature during experiments.
- Heat gun will be used to heat the walls of the drum.
- 10 thermocouples will be arranged radially and one IR camera will be arranged at a distance from the drum on the glass window side.
- To confirm heat transfer varies radially test simulation has been conducted.
- Left half of the particles are given 298 K and right half 450 K.

**Animation of p-p heat transfer (1.5 sec)**

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• FOA Objectives requires demonstration of the new capabilities with at least one industrially relevant problem.
• For a demonstration of the process to continually obtaining industry feedback was stated.
• From the beginning of this project, we teamed up with two major industrial collaborators with distinctly different application domains:

World's largest publicly traded international oil and gas company:

ExxonMobil
Research and Engineering

One of the largest global consumer goods company:

Procter & Gamble

Test Case # 1 provided by one of the Industrial Collaborator:

• Bin Flow (Hopper settling and discharge): A cylindrical hopper was initially filled with a set of spherical particles which were allowed to settle under the influence of gravity. The bottom of the hopper was then opened and the material was allowed to pour from the hopper. We track the flow rate of material from the hopper as a comparison metric case, which they use as a granular flow benchmarking test case for assessing various CFD software. Also input deck for LIGGGHTS (open-source DEM code) to facilitate comparative assessment.
Test Case # 1 provided by Industrial Collaborator: Preliminary Results

Results from cores Particles % reduction in particles

<table>
<thead>
<tr>
<th></th>
<th>cores</th>
<th>Particles after 1.5 s</th>
<th>in particles</th>
</tr>
</thead>
<tbody>
<tr>
<td>MFIX 2015-2 MPI only</td>
<td>16</td>
<td>262,552</td>
<td>-12.50 %</td>
</tr>
<tr>
<td>LIGGGHTS (as per collaborator runs) MPI only</td>
<td>20</td>
<td>257,997</td>
<td>-14.00 %</td>
</tr>
</tbody>
</table>

Experimental setup of the scaled down hopper

Validation of hopper discharge rate and pure granular flow
Validation of hopper discharge rate and pure granular flow
Hopper discharge using sand

Experimental Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hopper height</td>
<td>10 cm</td>
</tr>
<tr>
<td>Fill height</td>
<td>8 cm</td>
</tr>
<tr>
<td>Total time</td>
<td>1.2 min</td>
</tr>
<tr>
<td>Wt. of sand</td>
<td>193.4 gm</td>
</tr>
<tr>
<td>Size range</td>
<td>[0.064 0.174] mm</td>
</tr>
</tbody>
</table>

- Sand was used to demonstrate the experimental setup and working.
- Once the setup is finalized silica beads will be used for validating the granular flow.

The overarching goal is for MFIX-DEM to be able to solve industrial-scale problems, and to encourage its adoption by industry.
Lowering the barrier for industrial users and researchers in adopting MFIX in day-to-day use.

- Physical modeling enhancements to capture the physics more accurately and reduce uncertainty.
- Performance improvements to reduce time-to-solution by taking advantage of current and next generation HPC systems which will be available and affordable.
- Integrated uncertainty quantification that is easy to use.

Acknowledgments

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- Valuable feedback from MFIX Development Team at NETL is acknowledged.
- This work used the Extreme Science and Engineering Discovery Environment (XSEDE) at Texas Advanced Computing Center, which is supported by National Science Foundation grant number ACI-1053575.
- This research used resources of the National Energy Research Scientific Computing Center (NERSC), a DOE Office of Science User Facility supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.
Visit MFIX website for more information
https://mfix.netl.doe.gov

Source: Visualizations prepared by A. Gel & OLCF Visualization Support for Commercial Scale Gasifier Simulations with MFIX as part of INCITE award (2010)
https://mfix.netl.doe.gov/results.php#commercialgasifier

Performance and Capability Improvements
Background:

- Currently supercomputing capability on a desktop possible, if you can make your program to run efficiently on it!

Many in Core (MIC) from Intel,
First generation Intel Xeon Phi (named Knights Corner):
- Approximately 1 TeraFLOP/s computing capability for double precision (1st generation)

Graphical Processing Unit (GPU) from NVIDIA:
- Approximately 3 TeraFLOP/s computing capability for double precision

Proposed Methodology & Solution:

- Legacy CFD software still in demand
  - Due to extensive validation performed.
- However, require code modernization to take advantage of new HPC platforms:
  1. **Bottom-up approach**: Hot-spot guided code refactoring and optimization
  2. **Top-down approach**: Leverage external scalable solvers from Trilinos Project
Background:

- An increasing interest in the assessment of predictive credibility of simulation and computational modeling.
- Several barriers exist in the effective use of practical computational models in the engineering design process by industry:
  - Lack of user-friendly tools to perform critical analyses like uncertainty quantification
  - Lack of adequate background in statistical sciences
- Increasing computational power and parallelism offers a unique capability of performing non-intrusive UQ.
Proposed Methodology & Solution:

1. Application inputs
2. UQ engine (e.g. PSUADE)
3. Sampling design
4. Inputs (parameters & design variables)
5. Analysis:
   - Fit Response Surface (RS)
   - Conduct UQ Analysis on RS
   - Perform Sensitivity Study

Simulation Model (e.g. MFIX)