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MFIX Phi

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

M. Adepu, S. Chen
A. Gel, Y. Jiao, H. Emady, C. Tong, J. Hu and N. Ellingwood

2016 Crosscutting Research And Rare Earth Elements Portfolios Review, Pittsburgh, PA
04/21/2016

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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: Manogna Adepu
- PhD candidate, SEMTE

- GRA: Shaohua Chen
- PhD candidate, SEMTE

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MFIX-DEM Phi Team Member at Lawrence Livermore National Laboratory (LLNL)

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

MFIX-DEM Phi Team Members at Sandia National Laboratory (SNL)

- 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 & and Computational Sciences, University of Iowa (2014)
- Expertise: Data parallel algorithms for GPU, FEM, CFD, HPC, Digital Lung Project

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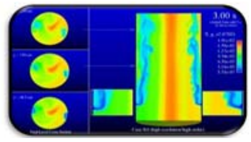
MFIX Open Source Suite
(https://mfix.netl.doe.gov)

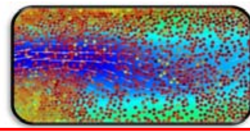
(1) MFIX-TFM (Eulerian-Eulerian)

	Serial	†DMP	‡SMP
Momentum Equations	•	•	•
Energy Equations	•	•	•
Species Equations	•	•	•
Chemical Reactions	•	•	
Cartesian cut-cell	•	•	□



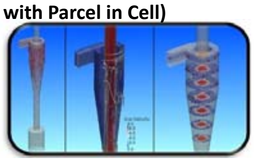
(2) MFIX-DEM (Eulerian-Lagrangian with CFD+DEM or DEM only)

	Serial	†DMP	‡SMP
Momentum Equations	•	•	•
Energy Equations	•		
Species Equations	•		
Chemical Reactions	•		
Cartesian cut-cell	○	○	



(3) MFIX-PIC (Eulerian-Lagrangian with Parcel in Cell)

	Serial	†DMP	‡SMP
Momentum Equations	•		○
Energy Equations			
Species Equations			
Chemical Reactions			
Cartesian cut-cell	○		□



• – implemented and fully tested
○ – implemented with limited testing
□ – not tested or status unknown

(4) MFIX-Hybrid (Eulerian-Lagrangian-Eulerian blend of TFM + DEM)

Source: MFIX 2015-1 user guide.

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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)

$$\frac{\partial}{\partial t}(\varepsilon_m \rho_m) + \nabla \cdot (\varepsilon_m \rho_m \vec{v}_m) = \sum_{l=1}^{N_m} R_{ml}$$

Momentum conservation

$$\frac{\partial}{\partial t}(\varepsilon_m \rho_m \vec{v}_m) + \nabla \cdot (\varepsilon_m \rho_m \vec{v}_m \vec{v}_m) = \nabla \cdot \overline{\overline{S}}_m + \varepsilon_m \rho_m \vec{g} + \sum_n \vec{I}_{mn}$$

Granular energy conservation (m ≠ g)

$$\frac{3}{2}\varepsilon_m \rho_m \left(\frac{\partial \Theta_m}{\partial t} + \vec{v}_m \cdot \nabla \Theta_m\right) = \nabla \cdot \vec{q}_{\Theta_m} + \overline{\overline{S}}_m : \nabla \vec{v}_m - \varepsilon_m \rho_m J_m + \Pi_{\Theta_m}$$

Energy conservation

$$\varepsilon_m \rho_m C_{pm}\left(\frac{\partial T_m}{\partial t} + \vec{v}_m \cdot \nabla T_m\right) = -\nabla \cdot \vec{q}_m + \sum_n \gamma_{mn}(T_n - T_m) - \Delta H_{rm}$$

Species mass conservation

$$\frac{\partial}{\partial t}(\varepsilon_m \rho_m X_{ml}) + \nabla \cdot (\varepsilon_m \rho_m X_{ml} \vec{v}_m) = R_{ml}$$

* MFIX: **M**ultiphase **F**low with **I**nterphase e**X**changes

MFIX
https://mfix.netl.doe.gov

R&D100 Award 2007

FLC Mid-Atlantic Region Tech-Transfer Award 2006

Sources:
- Syamlal et al. "MFIX Documentation, Theory Guide," DOE/METC-94/1004, NTIS/DE94000087 (1993)
- Benyahia et al. "Summary of MFIX Equations 2005-4", From URL http://www.mfix.org/documentation/MfixEquations2005-4-3.pdf, July 2007.

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MFIX* Open Source Multiphase Flow Flow Solver Suite:

MFIX Discrete Element Method (DEM) Equations:

MFiX
https://mfix.netl.doe.gov

Newtonian Equations for Particles

$$\frac{d\mathbf{X}^{(i)}(t)}{dt} = \mathbf{V}^{(i)}(t),$$

$$m^{(i)}\frac{d\mathbf{V}^{(i)}(t)}{dt} = \mathbf{F}_{\mathrm{T}}^{(i)} = m^{(i)}\mathbf{g} + \mathbf{F}_{\mathrm{d}}^{(i\in k,m)}(t) + \mathbf{F}_{\mathrm{c}}^{(i)}(t),$$

$$I^{(i)}\frac{d\omega^{(i)}(t)}{dt} = \mathbf{T}^{(i)}$$

Particle Contact Force Models

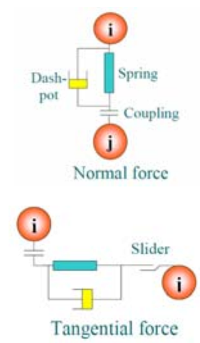
$$\mathbf{F}_{\mathrm{n}ij}(t) = \mathbf{F}_{\mathrm{n}ij}^{\mathrm{S}}(t) + \mathbf{F}_{\mathrm{n}ij}^{\mathrm{D}}(t) \qquad \mathbf{F}_{\mathrm{t}ij}(t) = \mathbf{F}_{\mathrm{t}ij}^{\mathrm{S}}(t) + \mathbf{F}_{\mathrm{t}ij}^{\mathrm{D}}(t)$$

Drag Forces on Particles

$$\mathbf{F}_{\mathrm{d}}^{(i\in k,m)} = -\nabla P_{\mathrm{g}}(\mathbf{x}_k)\mathcal{V}_{\mathrm{m}} + \frac{\beta_{\mathrm{m}}^{(k)}\mathcal{V}_{\mathrm{m}}}{\varepsilon_{sm}}\left(\mathbf{v}_{\mathrm{g}}(\mathbf{x}_k) - \mathbf{v}_{sm}(\mathbf{x}_k)\right)$$

Solid-Fluid Momentum Transfer

$$\mathbf{I}_{gm}^{k} = -\varepsilon_{sm}\nabla P_{\mathrm{g}}(\mathbf{x}_k) + \beta_{\mathrm{m}}^{(k)}\left(\mathbf{v}_{\mathrm{g}}(\mathbf{x}_k) - \mathbf{v}_{sm}(\mathbf{x}_k)\right)$$



Sources:
- R Garg, J Galvin, T Li, S Pannala, "Documentation of open-source MFIX–DEM software for gas-solids flows" (2010)

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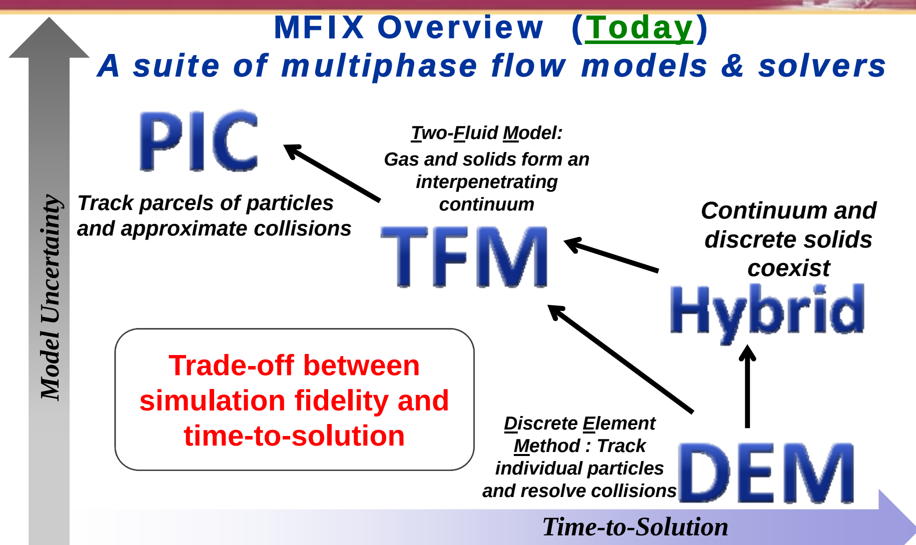
MFIX Overview (Today)

A suite of multiphase flow models & solvers



Source: Musser et al. "MFIX Update", 2014 NETL Workshop on Multiphase Flow Science (2014)

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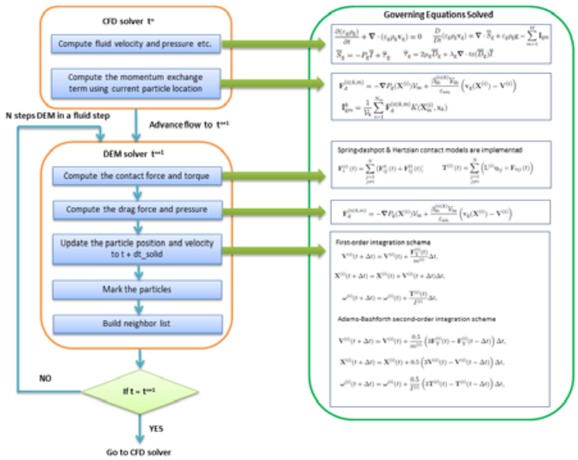
MFIX: A Unified Framework and Code Base for Eulerian-Lagrangian and Lagrangian Treatment of Multiphase Flows



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

External Coupling

LIGGGHTS®

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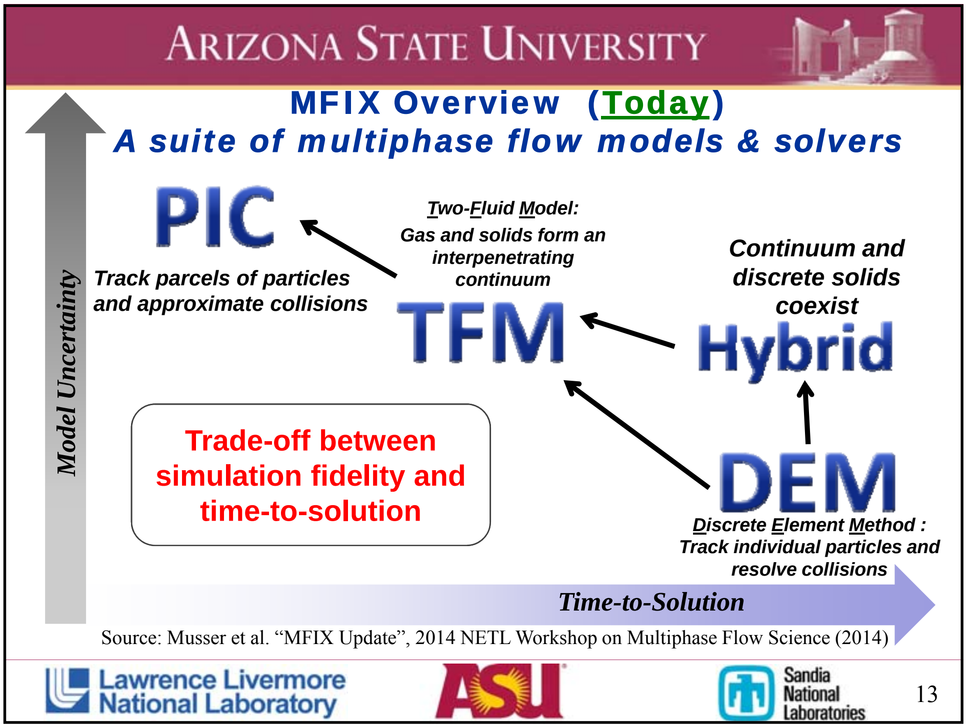
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MFIX Overview (Today)
A suite of multiphase flow models & solvers
PIC
Track parcels of particles and approximate collisions
Two-Fluid Model:
Gas and solids form an interpenetrating continuum
TFM
Continuum and discrete solids coexist
Hybrid
Trade-off between simulation fidelity and time-to-solution
DEM
Discrete Element Method :
Track individual particles and resolve collisions
Model Uncertainty
Time-to-Solution
Source: Musser et al. "MFIX Update", 2014 NETL Workshop on Multiphase Flow Science (2014)
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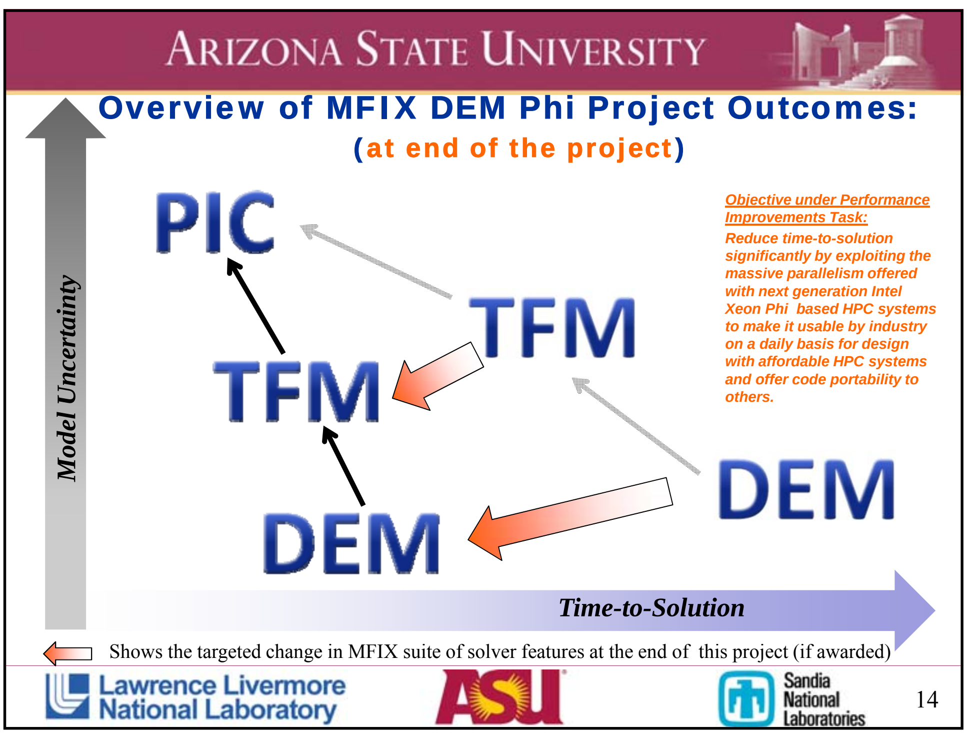
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Overview of MFIX DEM Phi Project Outcomes:
(at end of the project)
PIC
TFM
TFM
DEM
DEM
Objective under Performance Improvements Task:
Reduce time-to-solution significantly by exploiting the massive parallelism offered with next generation Intel Xeon 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.
Model Uncertainty
Time-to-Solution
Shows the targeted change in MFIX suite of solver features at the end of this project (if awarded)
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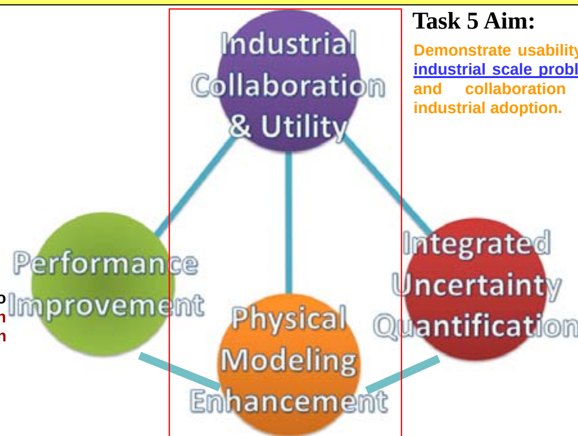
MFIX-DEM Phi: Performance and Capability Improvements Towards Industrial Grade Open-source DEM Framework with Integrated Uncertainty Quantification



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

Task 2 Aim:
Increase the speed to reduce time-to-solution by optimizing modern computing platforms

Task 4 Aims:
Ensure the results of the code are accurate.
Increase usability by reducing complexity

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

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- ➢ Physical Modeling Enhancement- Enhance the Capability for Handling
  - ➢ Particle Size Distributions
  - ❑ Heat Transfer
- ❑ Industrial Collaboration and Utility

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Physical Modeling Enhancement

Enhance the Capability for Handling Particle Size Distributions

- 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.

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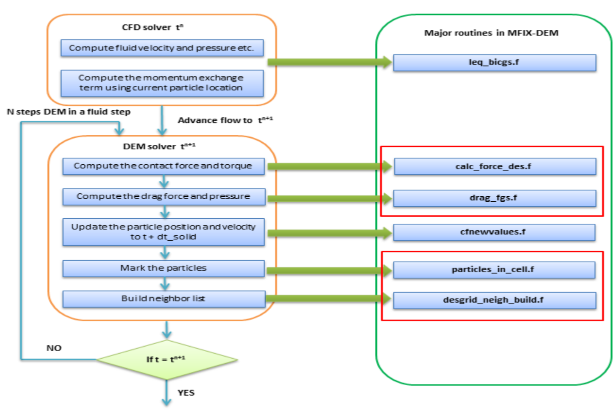
Physical Modeling Enhancement

Enhance the Capability for Handling Particle Size Distributions

Summary of subroutine modification



Implemented distribution types:
Uniform, Normal(Gaussian), LogNormal

Added commands for ICs:
IC_PSD_TYPE(ICV, Phase)
IC_PSD_MEAN_DP(ICV, Phase)
IC_PSD_STDEV(ICV, Phase)
IC_PSD_MAX_DP(ICV, Phase)
IC_PSD_MIN_DP(ICV, Phase)

Added commands for BCs:
BC_PSD_TYPE(BCV, Phase)
BC_PSD_MEAN_DP(BCV, Phase)
BC_PSD_STDEV(BCV, Phase)
BC_PSD_MAX_DP(BCV, Phase)
BC_PSD_MIN_DP(BCV, Phase)

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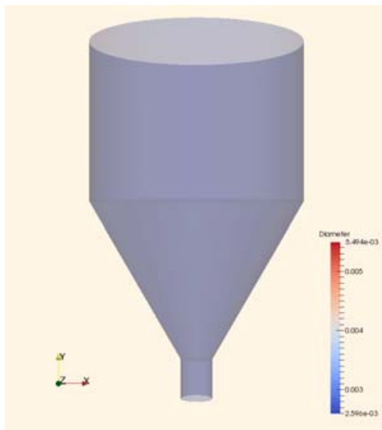
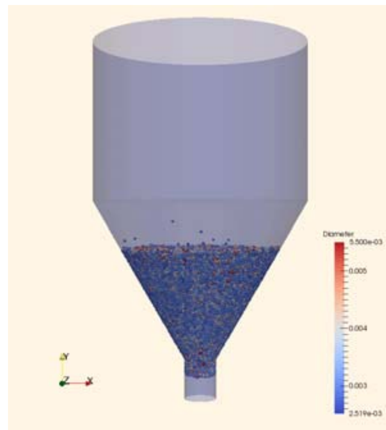
Enhance the Capability for Handling Particle Size Distributions – Preliminary Results for Bin Flow Case



Particle injection (0.4s) and settling (0.3s)



Particle discharge (4.0 s)

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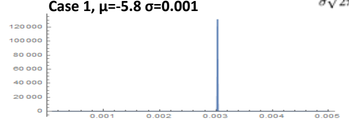
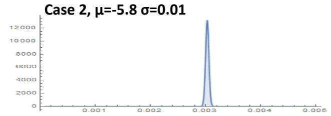
Enhance the Capability for Handling Particle Size Distributions

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

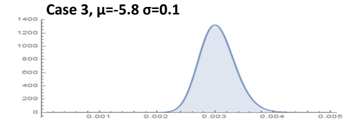
Case 1, μ=-5.8 σ=0.001



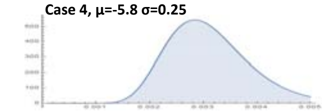
Case 2, μ=-5.8 σ=0.01



Case 3, μ=-5.8 σ=0.1



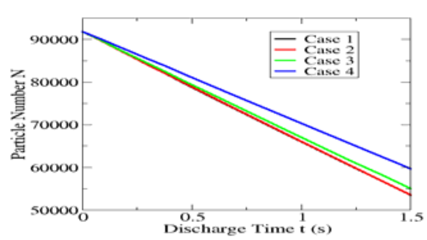
Case 4, μ=-5.8 σ=0.25



Packing Fraction

	Case 1	Case 2	Case 3	Case 4
MFIX-DEM	0.605	0.608	0.624	0.659
LAMMPS	0.609	0.604	0.633	0.662

Discharge Dynamics



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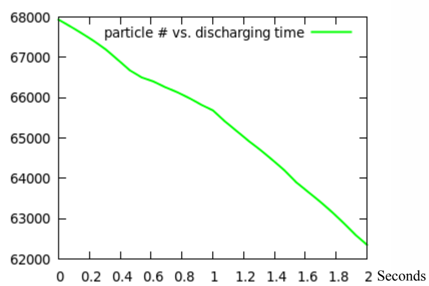
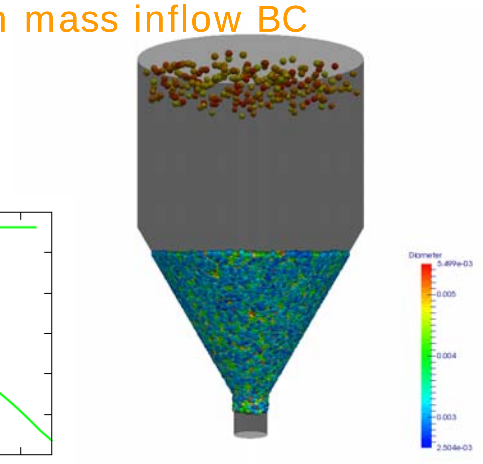
Enhance the Capability for Handling Particle Size Distributions

Hopper with mass inflow BC

Three solid phases:

phase 1, μ=-5.3 σ=0.05(MI)
phase 2, μ=-5.5 σ=0.05
phase 3, μ=-5.8 σ=0.05





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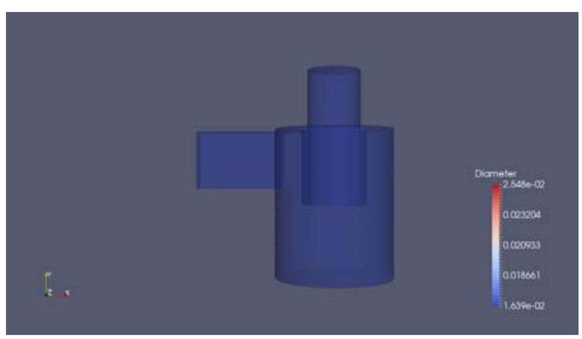
Enhance the Capability for Handling Particle Size Distributions

Cyclone

Log-Normal
μ=-3.90
σ=0.05



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  - ✓ Particle Size Distributions
  - ➢ Heat Transfer
- ❑ Industrial Collaboration and Utility

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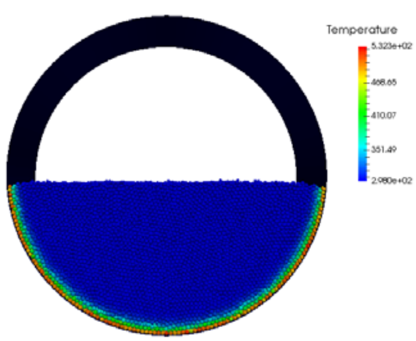
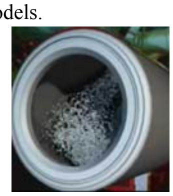
Physical Modeling Enhancement

Enhance the Capability for Handling Heat Transfer through experimental validation



Snapshot of wall HT after 2 sec of simulation.

- 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.




Source : http://www.muzzio.rutgers.edu/

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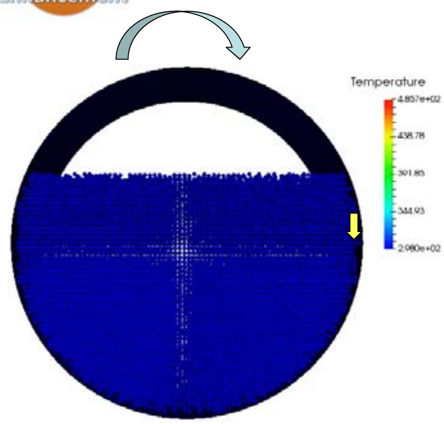
Physical Modeling Enhancement

Enhance the Capability for Handling Heat Transfer through experimental validation



Animation of wall heat transfer (2 sec)

- 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

Diameter of drum	6 inch.
Height of drum	3 inch.
Fill Volume	50 %
Number of particles	100,000
Density of particles	1500 kg/m3
Diameter of particles	0.002 m
K_s: solid conductivity	1 W/(m-K)
Cp_s: specific heat of solid	850 J/(kg-K)
K_g: air conductivity	0.0372 W(m-K)
Cp_g: specific heat of air	1020 J/(kg-K)

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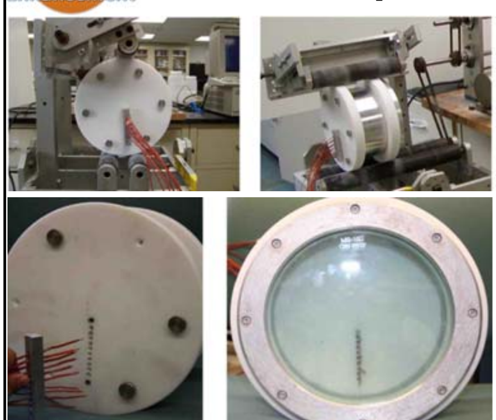
Physical Modeling Enhancement

Enhance the Capability for Handling Heat Transfer

Experimental Validation



Source: *Bodhisattwa Chaudhuri, et al. "Experimentally validated computations of heat transfer in granular materials in rotary calciners". Powder Technology 198 (2010) 6–15.*

- 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.

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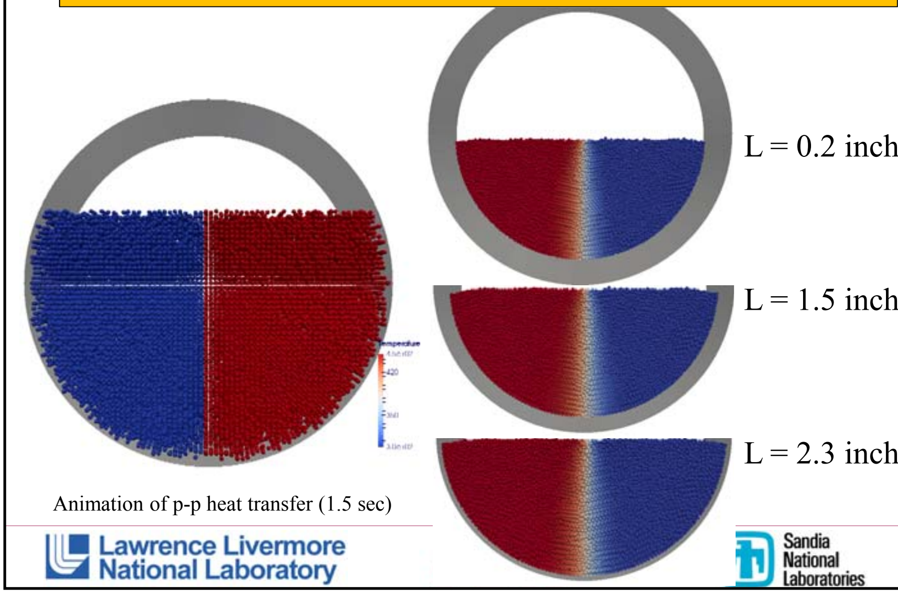
Enhance the Capability for Handling Heat Transfer: Rotary drum validation



Animation of p-p heat transfer (1.5 sec)

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Industrial Collaboration & Utility

Perform Industry Outreach and Development of Industry Cases

- 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:

P&G Procter&Gamble

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Industrial Collaboration & Utility

Perform Industry Outreach and Development of Industry Cases

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.

	Model 1
Initial # of particles	300,000
Particle diameter (m)	0.003
Particle density (kg/m³)	1000
Poisson ratio	0.25
Young's modulus (MPa)	25
Coefficient of restitution	0.5
Static friction coefficient	0.2
Rolling friction coefficient	0.0
Timestep (sec)	10[illegible]
Settling time (sec)	1.5
Flow time (sec)	3.0

Model parameters for bin flow simulations.

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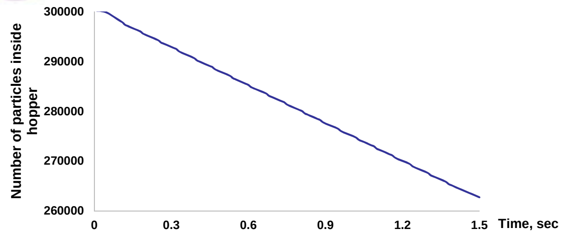
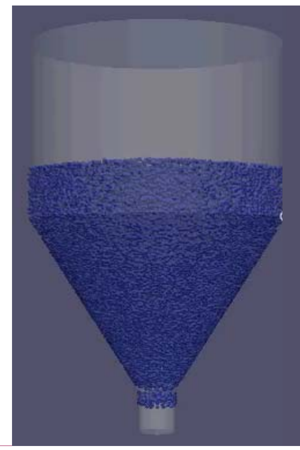
Perform Industry Outreach and Development of Industry Cases

Test Case # 1 provided by Industrial Collaborator: Preliminary Results





Results from		cores	Particles after 1.5 s	% reduction in particles
MFIX 2015-2 release version	MPI only	16	262,552	-12.50 %
LIGGGHTS (as per collaborator runs)	MPI only	20	257,997	-14.00%

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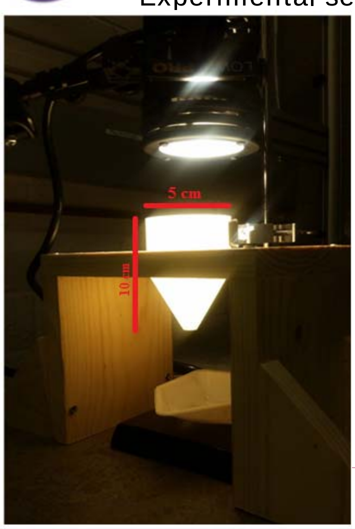
Validation of hopper discharge rate and pure granular flow

Experimental setup of the scaled down hopper



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Validation of hopper discharge rate and pure granular flow

Hopper discharge using sand

Experimental Parameters

Hopper height	10 cm
Fill height	8 cm
Total time	1.2 min
Wt. of sand	193.4 gm
Size range	[0.064 0.174] mm

- 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.

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Industrial Collaboration & Utility

The overarching goal is for MFIX-DEM to be able to solve industrial-scale problems, and to encourage its adoption by industry.

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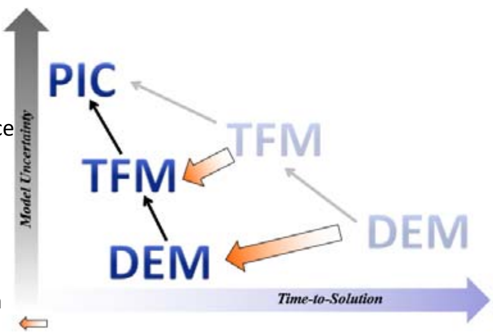
Overall goal of the project

- Lowering the barrier for industrial users and researcher in adopting MFIX in day-to-day use.
  - Physical modelling 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 system which will be available and affordable.
  - Integrated uncertainty quantification that is easy to use.



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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.
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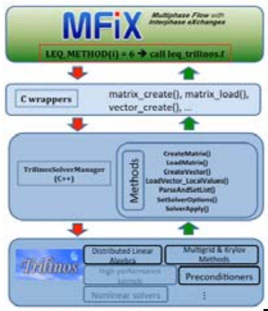
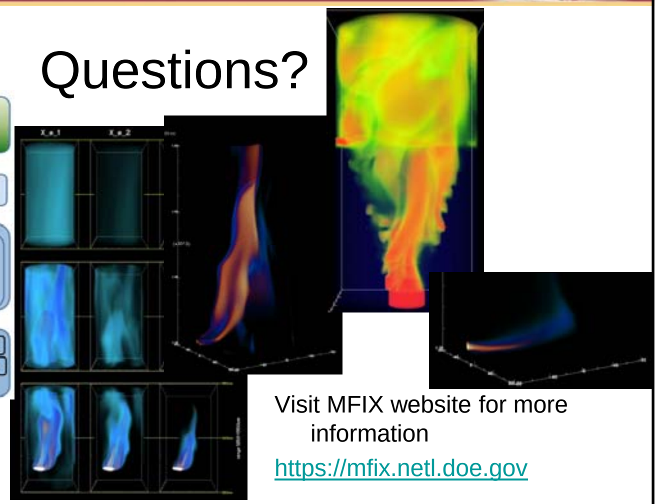
Questions?





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#commercialscalegasifier

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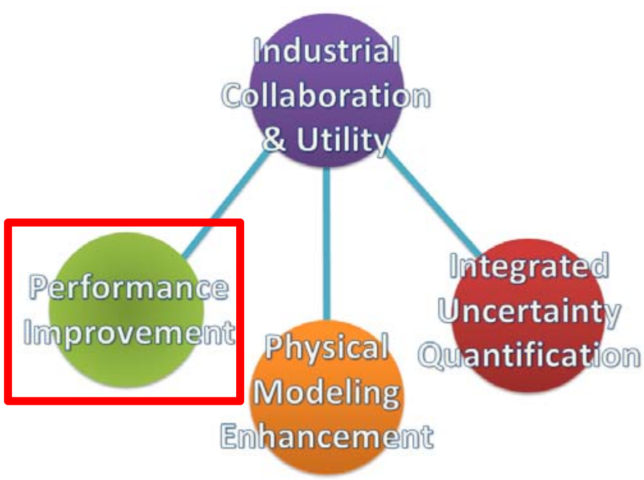
Performance and Capability Improvements



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Performance Improvement

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

TFLOP/s= Trilinos floating point operations per second

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Performance Improvement

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

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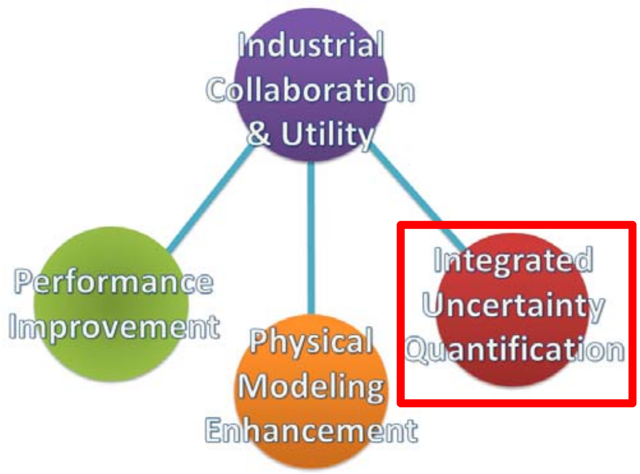
Performance and Capability Improvements



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Integrated Uncertainty Quantification

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.

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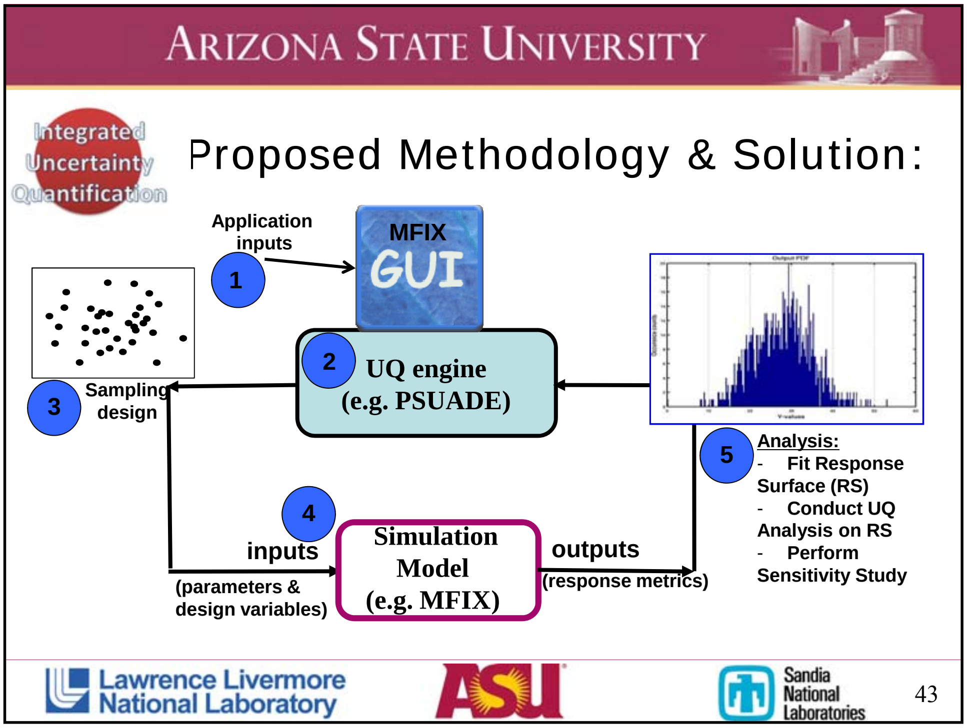
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Integrated Uncertainty Quantification
Proposed Methodology & Solution:
Application inputs
1
MFIX
GUI
2
UQ engine
(e.g. PSUADE)
3
Sampling design
4
inputs
(parameters & design variables)
Simulation Model
(e.g. MFIX)
outputs
(response metrics)
5
Analysis:
- Fit Response Surface (RS)
- Conduct UQ Analysis on RS
- Perform Sensitivity Study
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