MFiX - Multiphase Flow with Interphase Exchanges

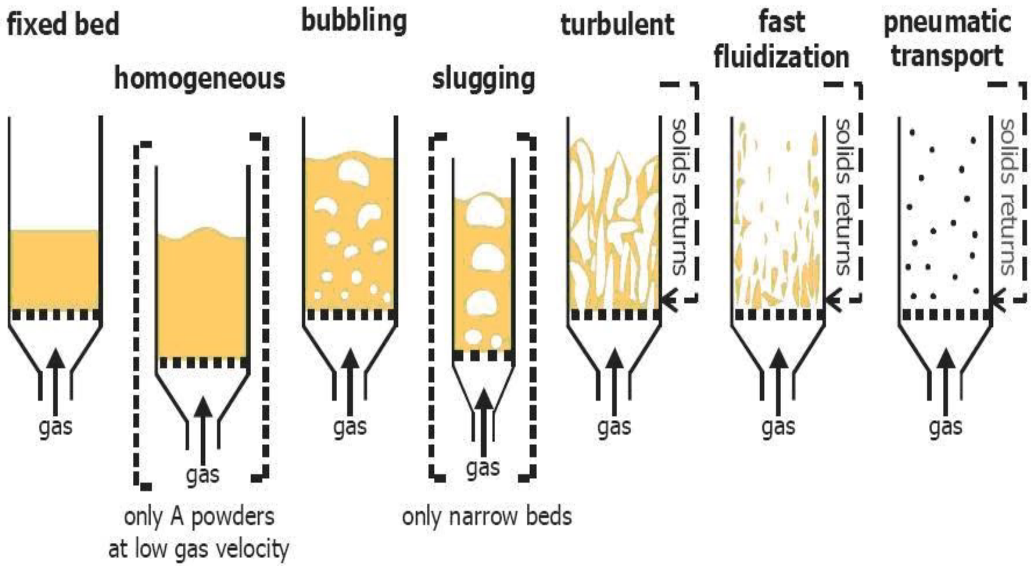
Software tools and expertise to address multiphase flow challenges in research, design, and optimization

Jeff Dietiker, Multiphase Flow Science Group, NETL/LRST

Use Simulation Tools to Predict Performance

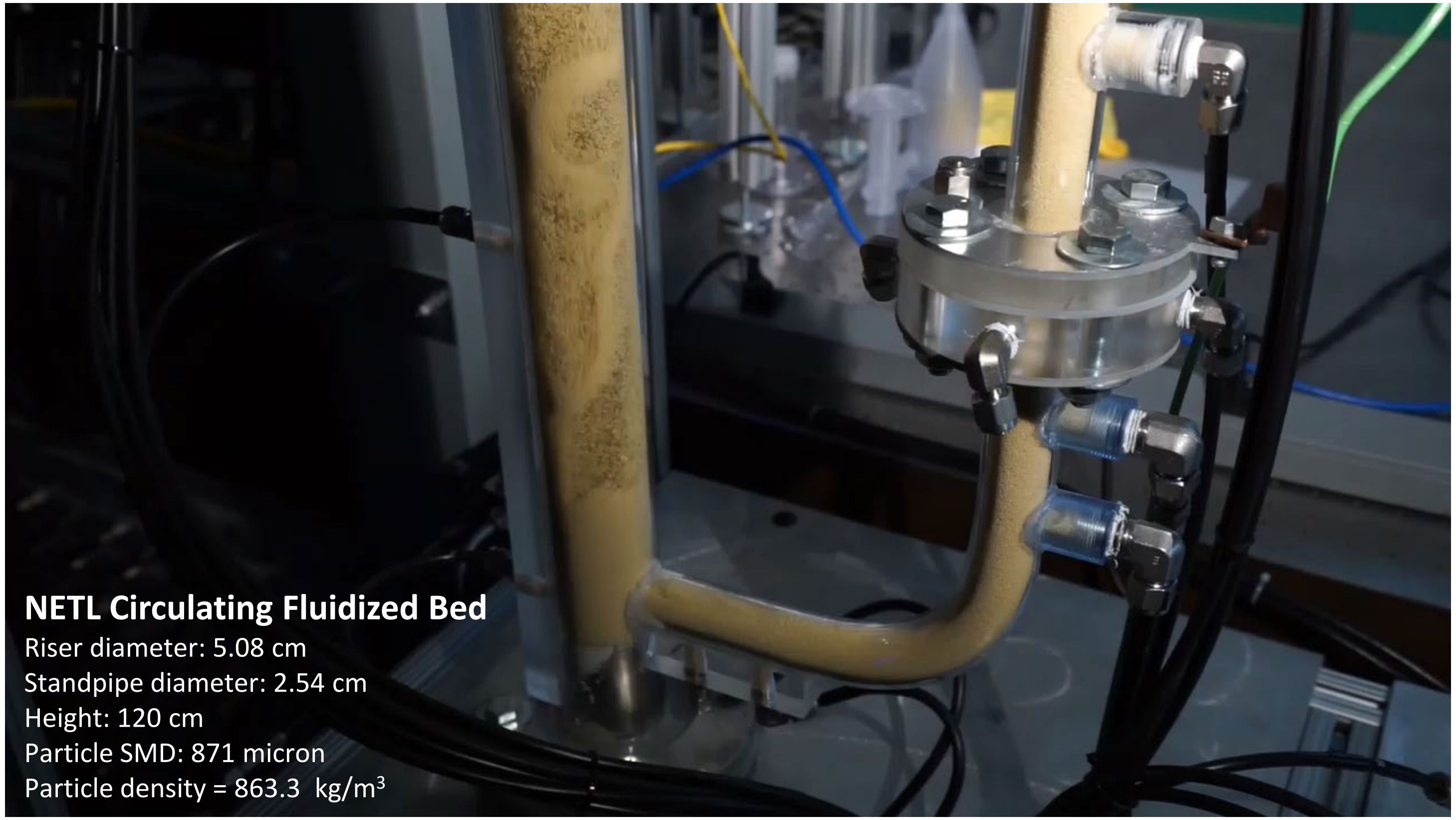
Gas-solid fluidization is very challenging to accurately model

- Fluidized bed: solid particles are suspended in a fluid-like state
- With Increasing of gas velocity, several fluidization regimes can be observed – often in the same reactor!



Increasing Gas Velocity

J. Ruud van Ommen, 2003



NETL Circulating Fluidized Bed
Riser diameter: 5.08 cm
Standpipe diameter: 2.54 cm
Height: 120 cm
Particle SMD: 871 micron
Particle density = 863.3 kg/m^3

MFiX Suite of Multiphase CFD Software

Capabilities and Benefits

NATIONAL ENERGY TECHNOLOGY LABORATORY

MFiX **is NETL flagship computational fluid dynamic (CFD) code**

- **Versatile toolset** for understanding the behavior and characterizing the performance of energy conversion processes
- **Accelerate reactor development and reduce cost** by using multiphase flow reactor modeling and simulation tools
- **Optimizes performance** for equipment and unit operations, enabling more throughput and less process downtime
- **Reduces design risks** when validated by predictive science-based calculations, lowering risk in obtaining return on investment

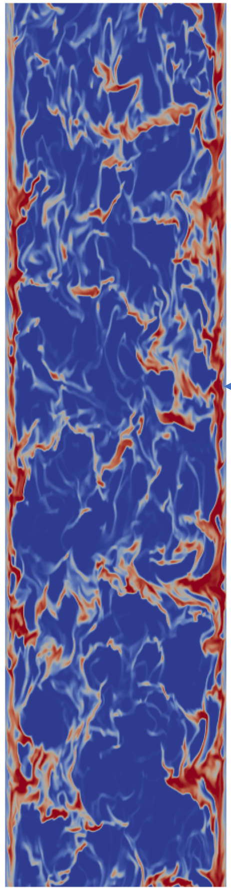
- MFiX-TFM (Two-Fluid Model)
- MFiX-DEM (Discrete Element Model)
- MFiX-PIC (Multiphase Particle-In-Cell)
- MFiX-CGDEM (Coarse Grain DEM)
- MFiX Exa (Exascale) – under development
- C3M multiphase chemistry management software
- Nodeworks: Optimization and UQ Toolsets

MFS Software Portfolio

MFiX Suite of Multiphase CFD Software

NATIONAL ENERGY TECHNOLOGY LABORATORY

Managing the tradeoff between accuracy and time to solution



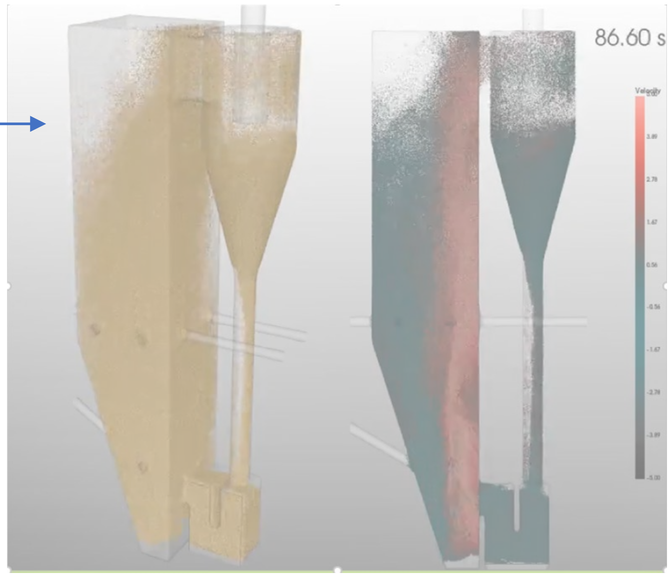
Time to Solution

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*



MFiX Exa — *Exascale: New code for new generation of computers*

ROM
Reduced Order Models: Simplified models with limited application

Model Uncertainty

MFiX-TFM : Model Overview

Continuous and disperse phases (e.g., gas and solids) are treated as coexisting continua.

Highlights

- Long track record of successfully supporting DOE-FE priorities
- Computationally efficient
- Historical workhorse for large-scale FE applications

Technical limitations

- Unable to efficiently model phenomena like particle size distributions
- Relies on complex constitutive relations to approximate solid stresses
- Ad hoc extension to multiple solids phases

Fluid continuity equation:

$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g) + \nabla \cdot (\varepsilon_g \rho_g \boldsymbol{u}_g) = \mathcal{S}_g$$

Fluid momentum equation:

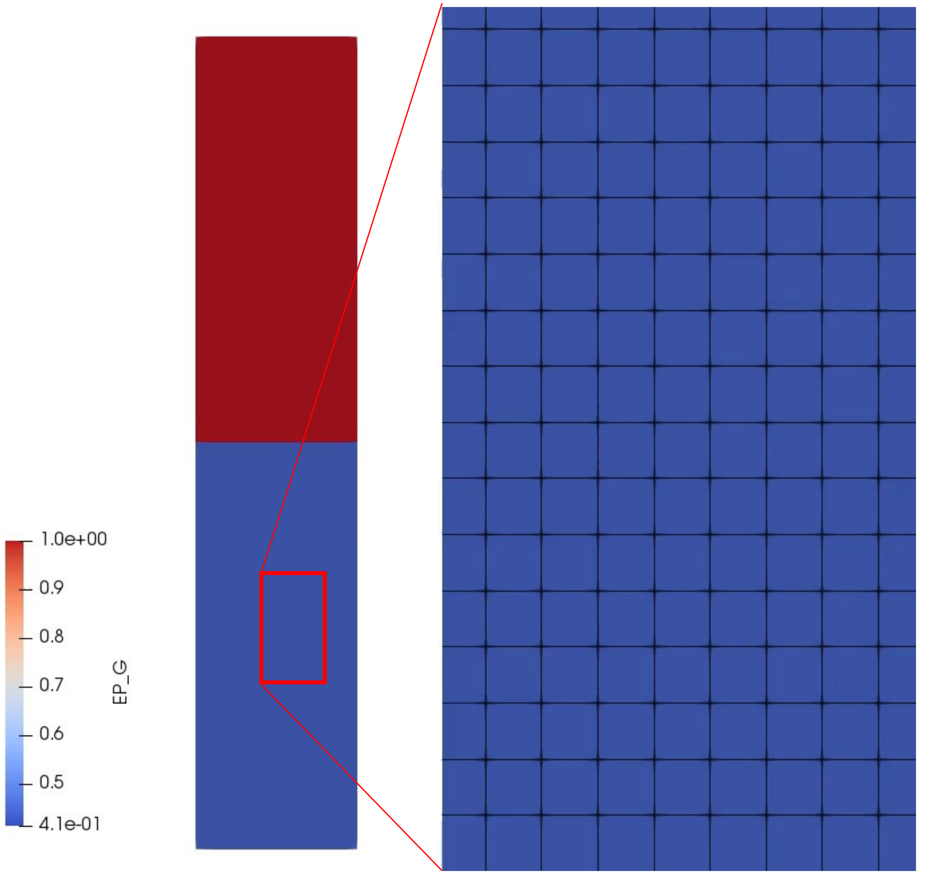
$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g \boldsymbol{u}_g) + \nabla \cdot (\varepsilon_g \rho_g \boldsymbol{u}_g \boldsymbol{u}_g)$$
$$= -\varepsilon_g \nabla p_g + \nabla \cdot \boldsymbol{\tau}_g + \varepsilon_g \rho_g \boldsymbol{g} + \sum_m \boldsymbol{\mathcal{I}}_{g,m}$$

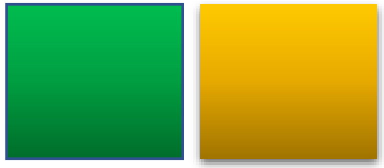
Solids continuity equation:

$$\frac{\partial}{\partial t}(\varepsilon_m \rho_m) + \nabla \cdot (\varepsilon_m \rho_m \boldsymbol{u}_m) = \mathcal{S}_m$$

Solids momentum equation:

$$\frac{\partial}{\partial t}(\varepsilon_m \rho_m \boldsymbol{u}_m) + \nabla \cdot (\varepsilon_m \rho_m \boldsymbol{u}_m \boldsymbol{u}_m)$$
$$= -\nabla p_m + \nabla \cdot \boldsymbol{\tau}_m + \varepsilon_m \rho_m \boldsymbol{g} - \boldsymbol{\mathcal{I}}_{g,m}$$





Solver time: Fluid Solid
(one solids phase)

MFiX-DEM : Discrete Element Model

Fluid is a continuum and particles are individually tracked, resolving particle-particle-wall collisions

Advantages

- Uses first principles to account for particle interactions, reducing model complexity.
- Fewer complex closures results in less overall model uncertainty.
- Only open-source, fully coupled CFD-DEM code designed for reacting flows.

Technical limitations

- Computationally expensive, limiting the size of systems that can be modeled.
- Fluid-particle interaction is closed using drag models.

Fluid continuity equation:

$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g) + \nabla \cdot (\varepsilon_g \rho_g \boldsymbol{u}_g) = \mathcal{S}_g$$

Fluid momentum equation:

$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g \boldsymbol{u}_g) + \nabla \cdot (\varepsilon_g \rho_g \boldsymbol{u}_g \boldsymbol{u}_g)$$

$$= -\varepsilon_g \nabla p_g + \nabla \cdot \boldsymbol{\tau}_g + \varepsilon_g \rho_g \boldsymbol{g} + \sum_p \boldsymbol{\mathcal{I}}_{g,p}$$

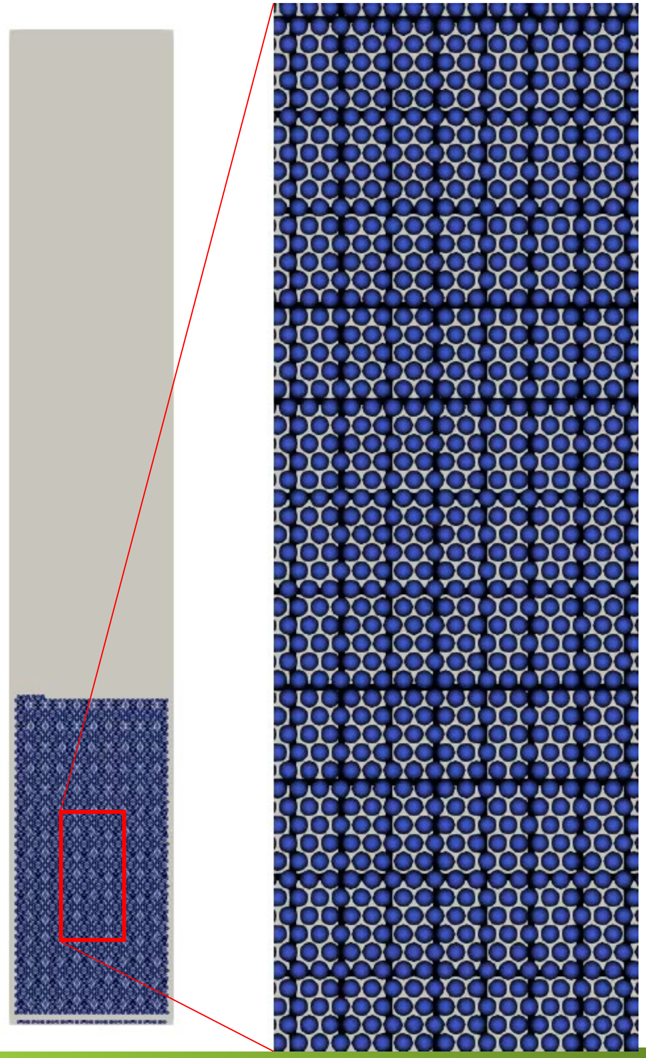
Particle continuity equation:

$$\frac{\partial}{\partial t}(m_p) = \mathcal{S}_p$$

Particle momentum equations:

$$m_p \frac{\partial \boldsymbol{u}_p}{\partial t} = m\boldsymbol{g} + \boldsymbol{F}_{coll} - \boldsymbol{\mathcal{I}}_{g,p}$$

$$I_p \frac{\partial \boldsymbol{\omega}_p}{\partial t} = \boldsymbol{\mathcal{T}}$$



MFiX-DEM : Discrete Element Model

Fluid is a continuum and particles are individually tracked, resolving particle-particle-wall collisions

Advantages

- Uses first principles to account for particle interactions, reducing model complexity.
- Fewer complex closures results in less overall model uncertainty.
- Only open-source, fully coupled CFD-DEM code designed for reacting flows.

Technical limitations

- Computationally expensive, limiting the size of systems that can be modeled.
- Fluid-particle interaction is closed using drag models.

Fluid continuity equation:

$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g) + \nabla \cdot (\varepsilon_g \rho_g \boldsymbol{u}_g) = \mathcal{S}_g$$

Fluid momentum equation:

$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g \boldsymbol{u}_g) + \nabla \cdot (\varepsilon_g \rho_g \boldsymbol{u}_g \boldsymbol{u}_g)$$

$$= -\varepsilon_g \nabla p_g + \nabla \cdot \boldsymbol{\tau}_g + \varepsilon_g \rho_g \boldsymbol{g} + \sum_p \boldsymbol{\mathcal{I}}_{g,p}$$

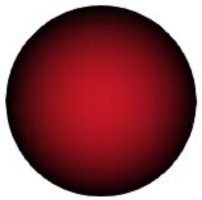
Particle continuity equation:

$$\frac{\partial}{\partial t}(m_p) = \mathcal{S}_p$$

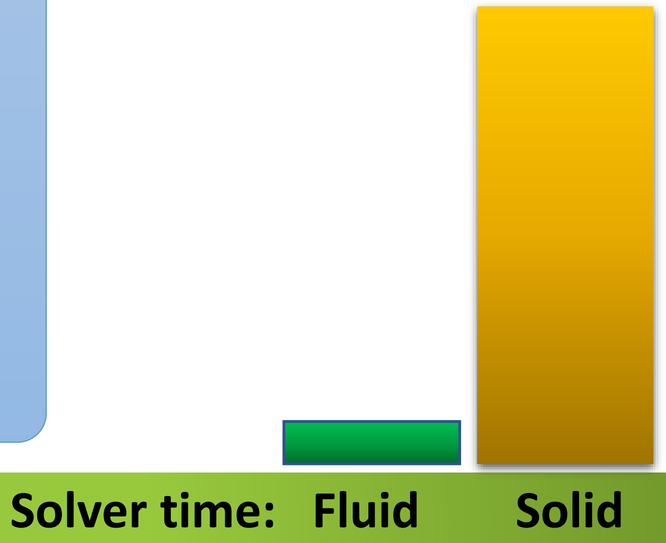
Particle momentum equations:

$$m_p \frac{\partial \boldsymbol{u}_p}{\partial t} = m\boldsymbol{g} + \boldsymbol{F}_{coll} - \boldsymbol{\mathcal{I}}_{g,p}$$

$$I_p \frac{\partial \boldsymbol{\omega}_p}{\partial t} = \boldsymbol{\mathcal{T}}$$



P-P and P-W collisions are resolved (soft sphere)



MFiX-PIC : (Multiphase) Particle-in-Cell

Fluid is a continuum and particles are tracked as parcels, solid-stress model approximates collisions

Advantages

- Computationally efficient
- Able to track particle-scale phenomena like time-histories and size distributions
- Only open-source, PIC model

Technical limitations

- Relies on a continuum stress model to approximate particle-particle interactions
- Strong dependence on implementation

Formally released: April, 2019

Fluid continuity equation:

$$\frac{\partial}{\partial t}\left(\varepsilon_g \rho_g\right) + \nabla \cdot \left(\varepsilon_g \rho_g \boldsymbol{u}_g\right) = \mathcal{S}_g$$

Fluid momentum equation:

$$\frac{\partial}{\partial t}\left(\varepsilon_g \rho_g \boldsymbol{u}_g\right) + \nabla \cdot \left(\varepsilon_g \rho_g \boldsymbol{u}_g \boldsymbol{u}_g\right)$$

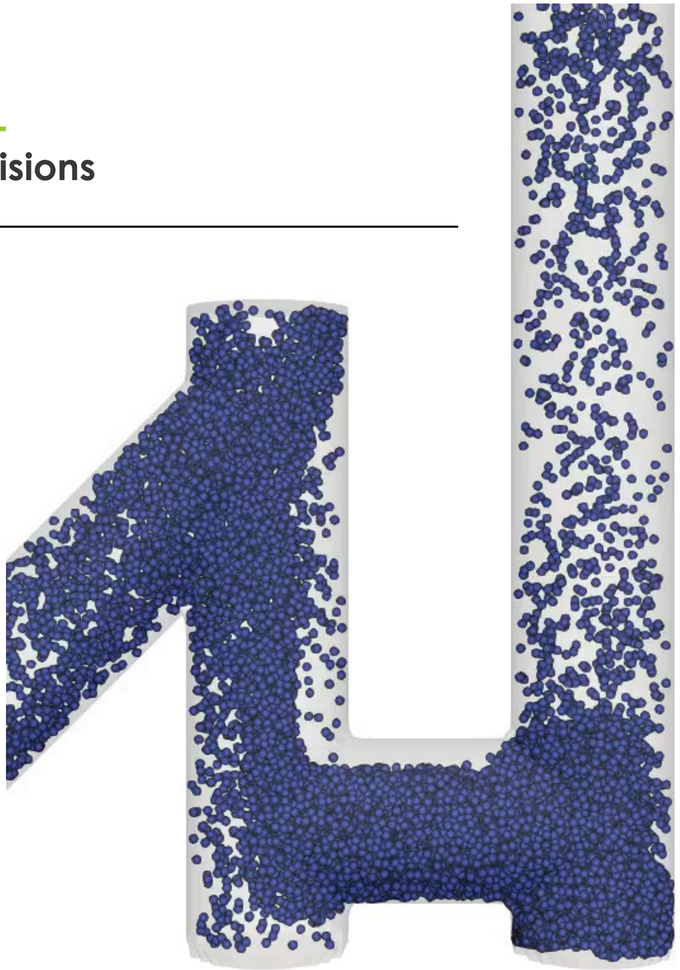
$$= -\varepsilon_g \nabla p_g + \nabla \cdot \boldsymbol{\tau}_g + \varepsilon_g \rho_g \boldsymbol{g} + \sum_p \boldsymbol{\mathcal{I}}_{g,p}$$

Parcel continuity equation:

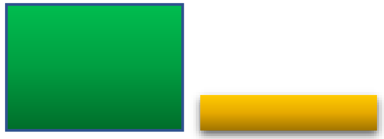
$$\frac{\partial}{\partial t}\left(m_p\right) = \mathcal{S}_p$$

Parcel momentum equation:

$$m_p \frac{\partial \boldsymbol{u}_p}{\partial t} = m\boldsymbol{g} + \nabla \tau_p - \boldsymbol{\mathcal{I}}_{g,p}$$

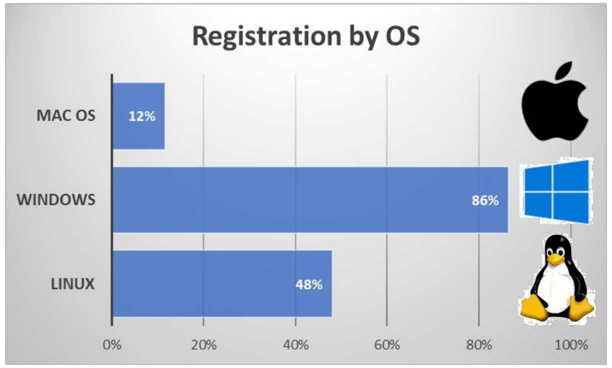


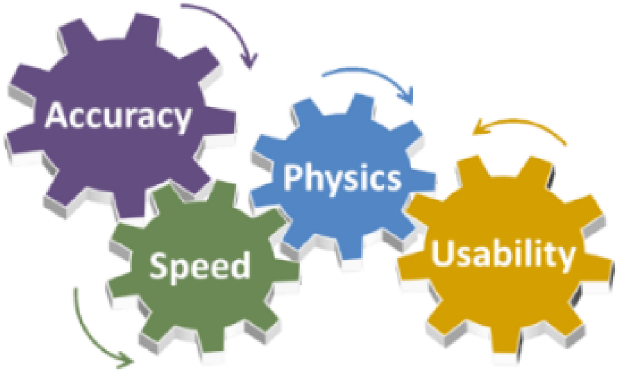
Parcel collisions are not resolved



Graphical User Interface (GUI)

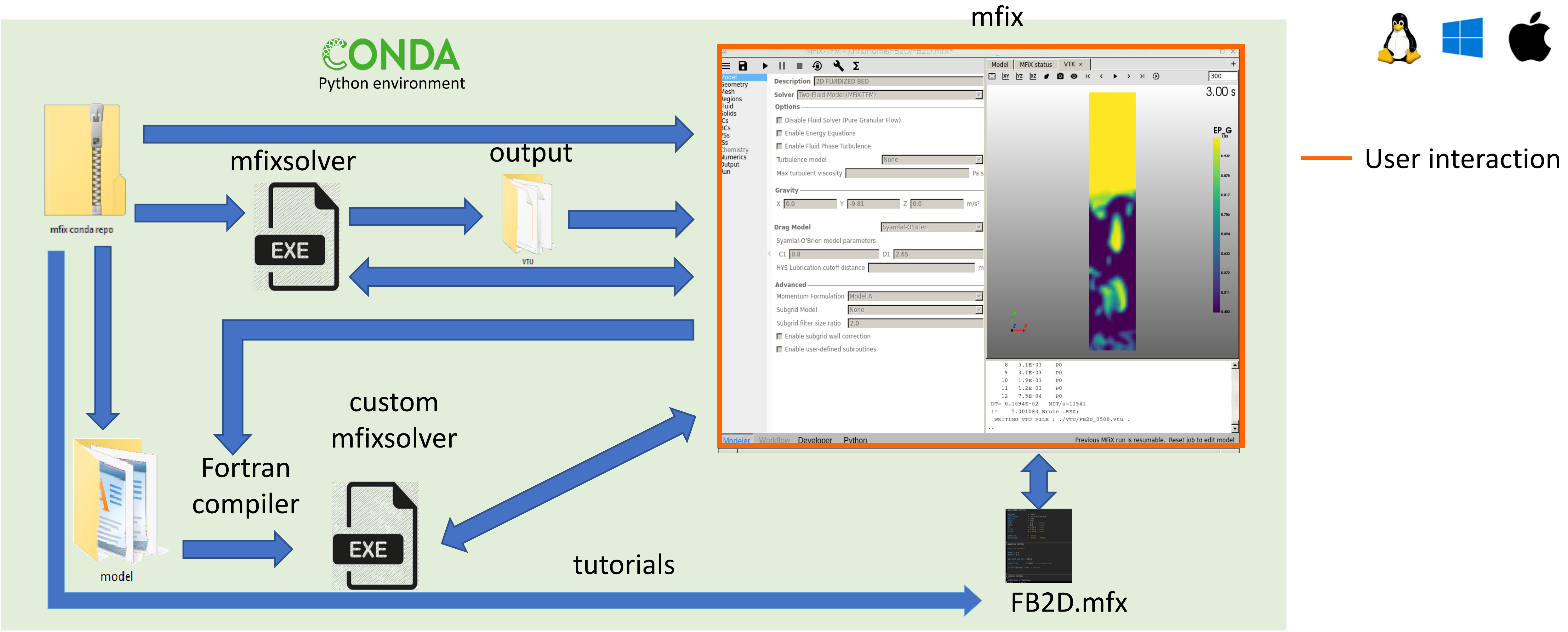
- **Open-source (https://mfix.netl.doe.gov)**
- **Motivation: Better serve MFiX community**
  – Improve usability of MFiX
  – Support Linux, macOS and Windows OS
  – Decrease time to setup, reduce error
- **Solution: Graphical User Interface**
  - Released in 2017
  - Between 1 and 4 releases per year



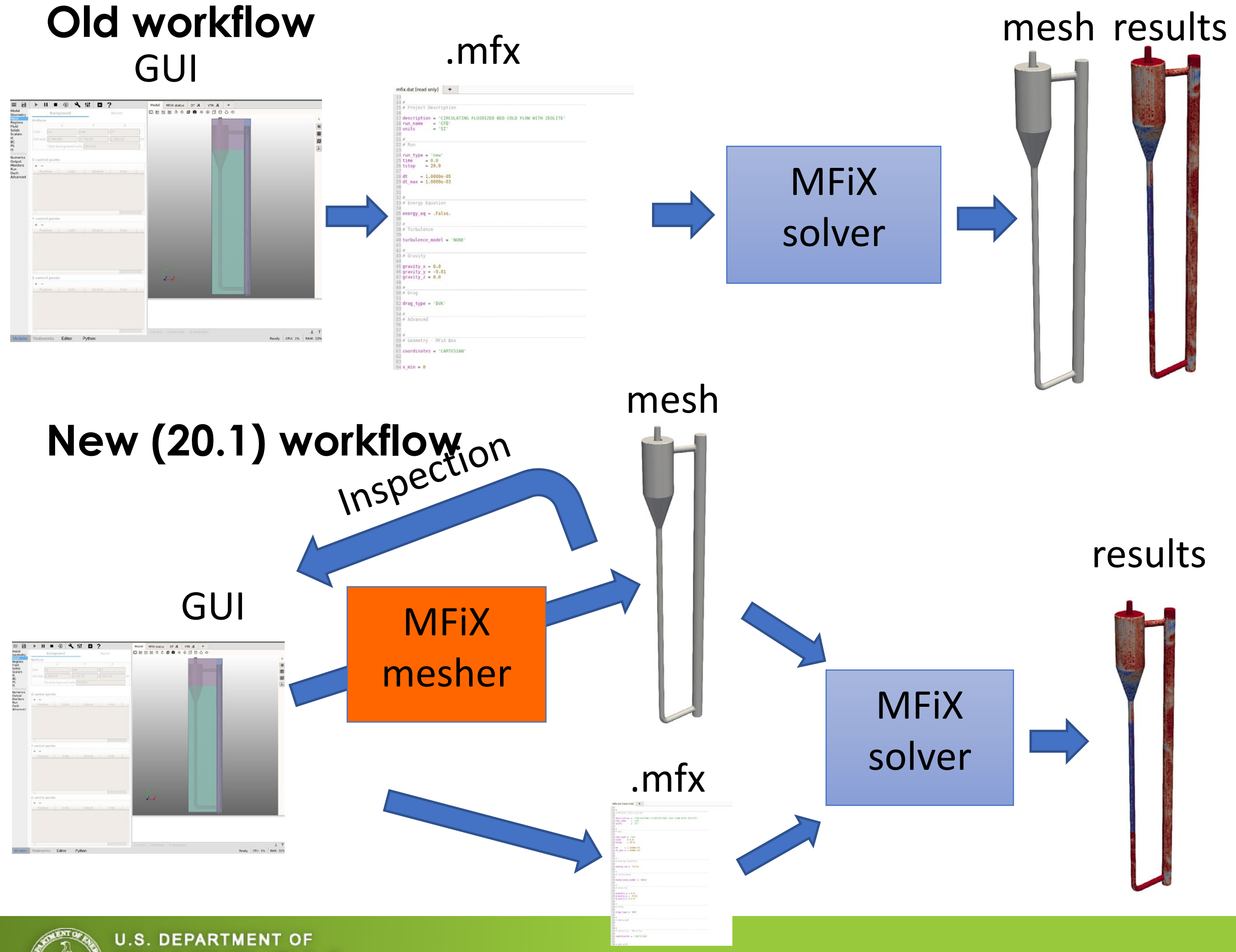


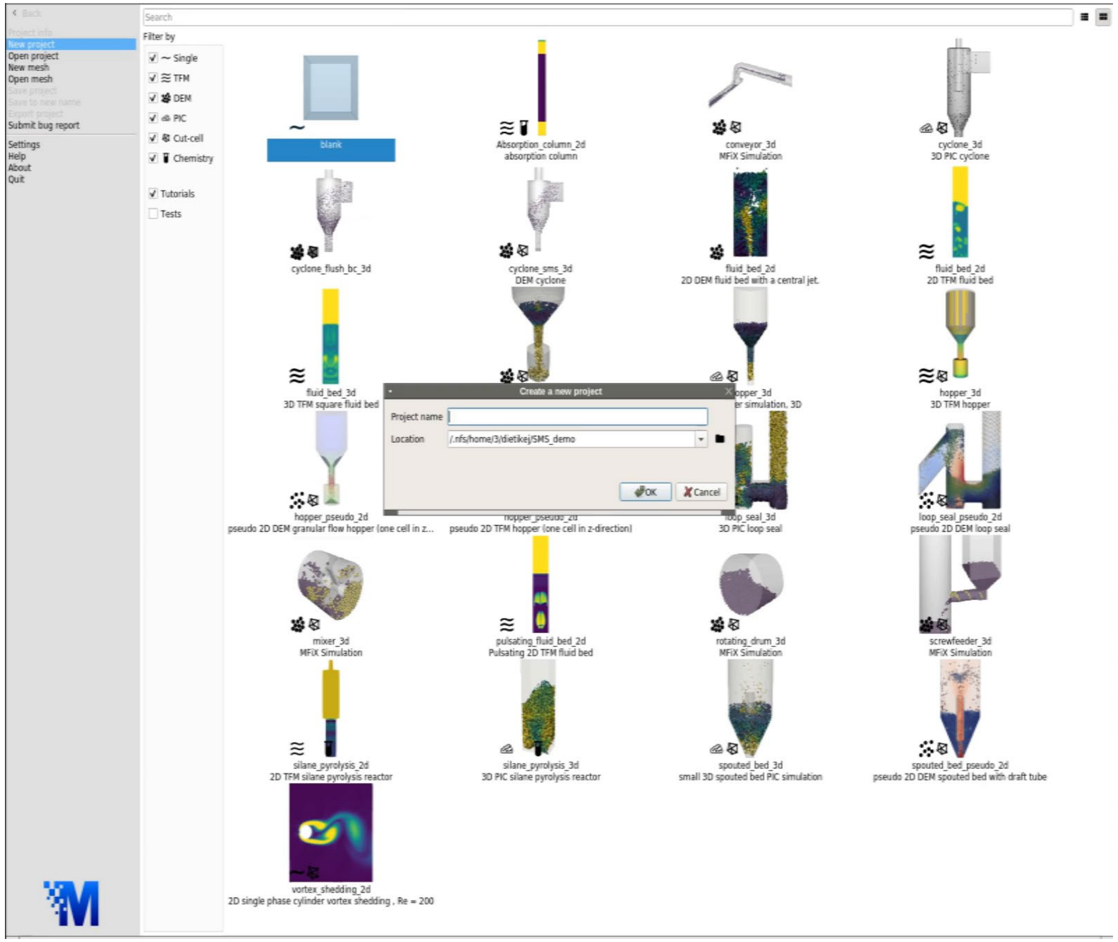
MFiX usability improvement

NETL Multiphase Flow Science
Home of the MFiX Software Suite.
https://mfix.netl.doe.gov



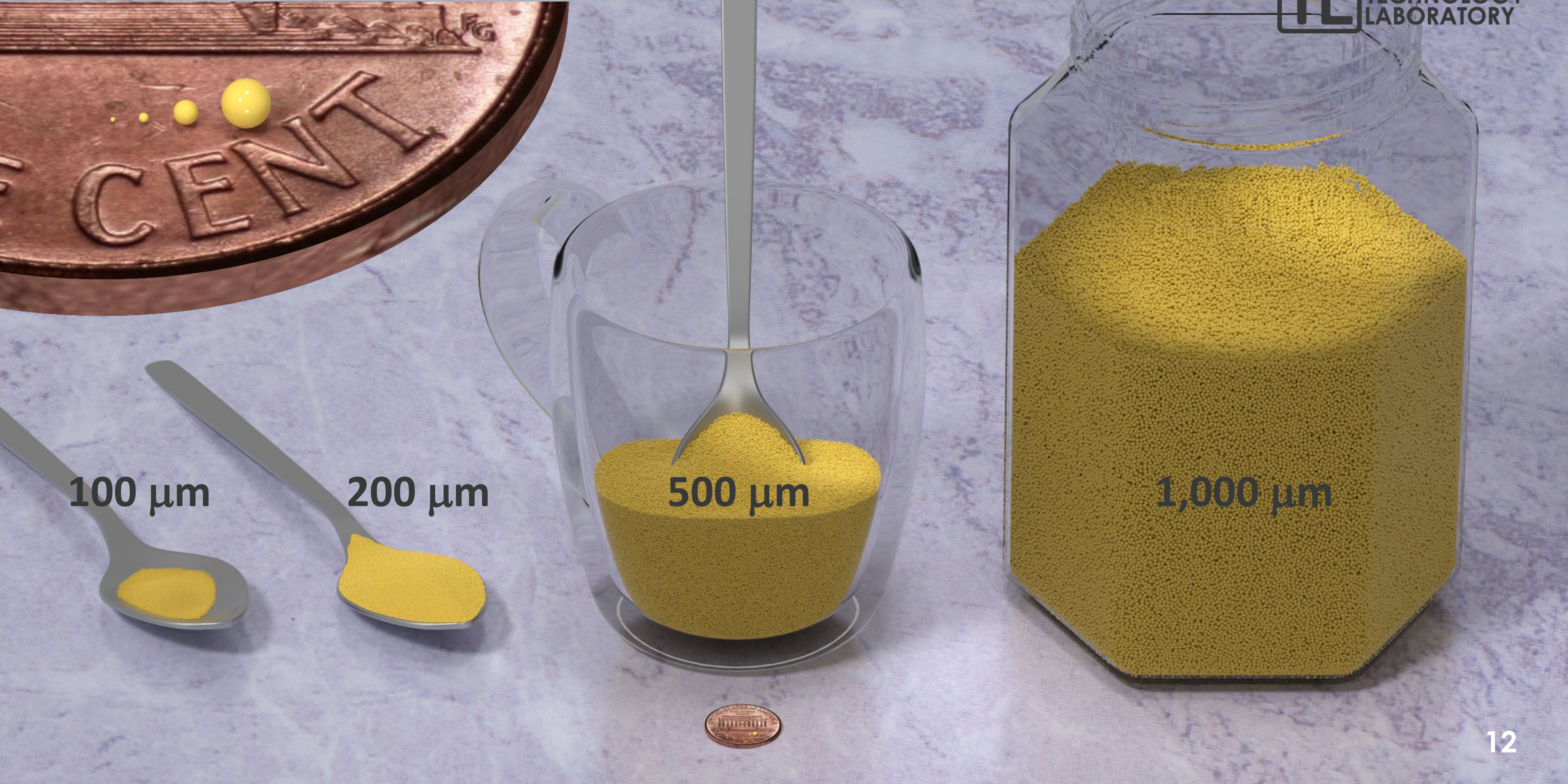
Preprocessor development





What can be modeled with 1 Million particles?

NATIONAL ENERGY TECHNOLOGY LABORATORY



Enabling large Scale simulations

DEM example

Height = 0.68 m

Particle diameter = 800 microns

Particle count = 500,000 particles

Enabling large Scale simulations

Height = 4.0 m (x6)
Particle count = 650 Millions (x1,300)
☒ **DEM**
☑ **PIC,** Parcel counts = 13 Millions

Height = 0.68 m
Particle count = 500,000
☑ **DEM**

Multiphase Particle In Cell (MP-PIC)

Use MP-PIC for computational speed and averaged accuracy

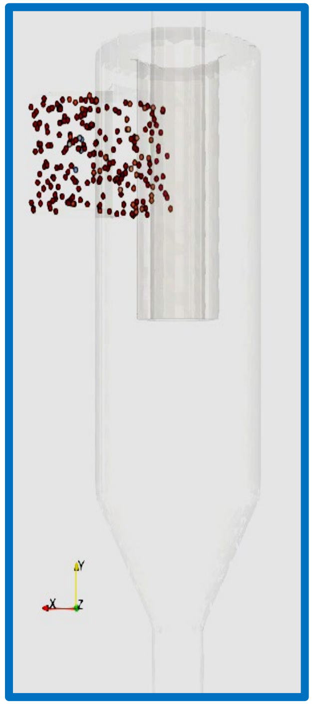
REDUCED ACCURACY ↑ — SOLIDS REPRESENTATION (vertical axis)

INCREASED COMPUTATIONAL SPEED → — GENERALIZED IDEA FOR PARTICLE INTERACTIONS (horizontal axis)

	Collision Resolved	Momentum Conservation	Solid Stress Gradient
Parcel	**CGPM** ✓ Coarse Grained Particle Method **Masaaki et al. 2000** **Sakai and Koshizuka,2009**	**CGHS** Coarse Grained Hard Sphere **Lu et al., 2017**	MFiX PIC **MP-PIC** Multi Phase Particle In Cell **Andrews and O'Rourke, 1996** ✓
Particle	MFiX DEM **CFD-DEM** Computation Fluid Dynamic-Discrete Element Method **Tsuji et al., 1993** ✓	**ED/TD HS** Event Driven/ Time Driven Hard Sphere **Hoomans et al., 1996** **Ouyang and Li, 1999**	

Particle Flow in Cyclone

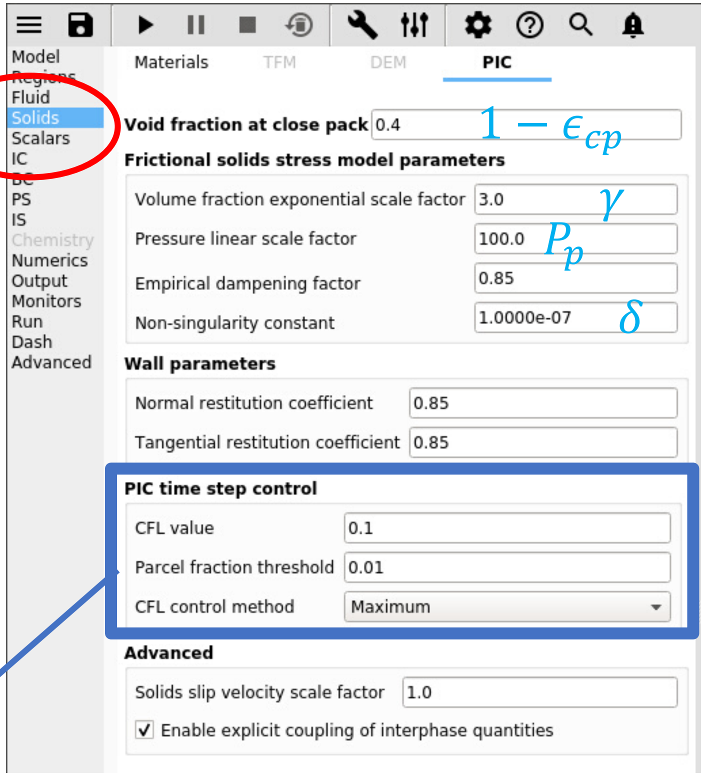
MP-PIC can significantly reduce computational effort, and in the right type of application, maintain accuracy.



Multiphase Particle In Cell (MP-PIC)

Basic Set-Up Information

The PIC model parameters are clustered under the Solids tab.



New in 20.2: PIC CFL setting

- Need for CFL identified by QA program
- Allows consistent results with large Fluid time step
- Showed speed up of 3 for a cyclone simulation

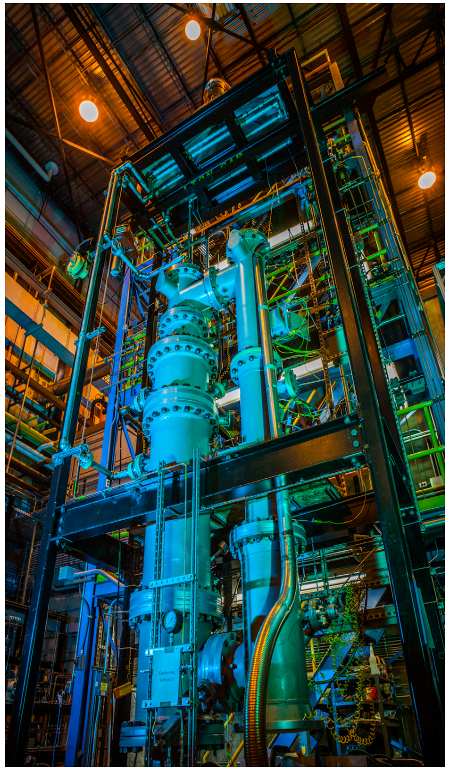
Some parameters that a user defines directly influence the momentum equation through solids stress calculation.

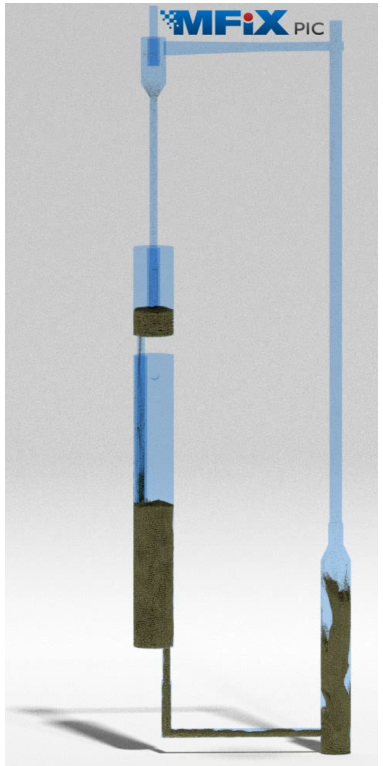
$$\tau_p = \frac{P_p \epsilon_p^{\gamma}}{\max\left(\epsilon_{cp} - \epsilon_p, \delta(1-\epsilon_p)\right)}$$

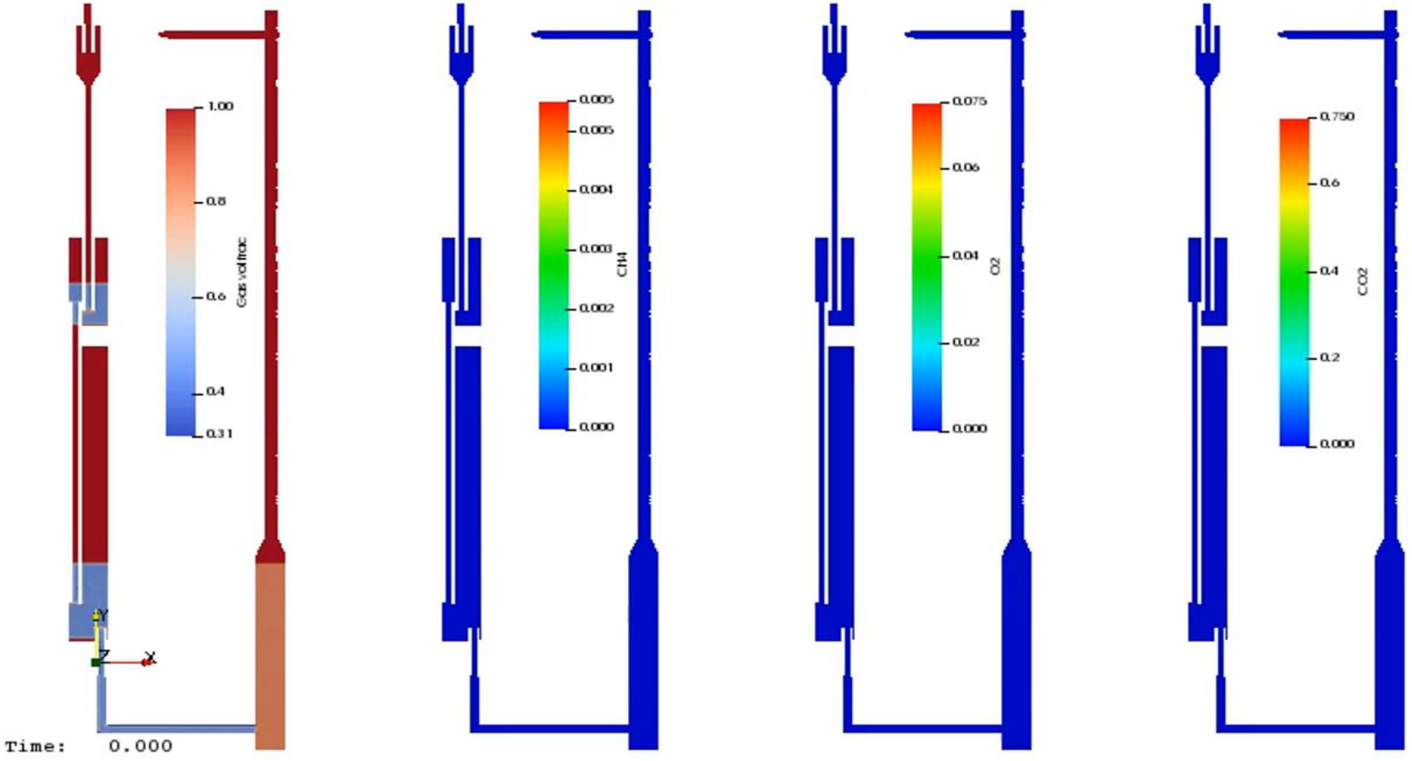
$$\frac{d\vec{V_p}}{dt} = \beta(\vec{U_g} - \vec{V_p}) - \frac{1}{\rho_p}\nabla p - \frac{1}{\epsilon_p \rho_p}\nabla \tau_p + \vec{g}$$

Other parameters act as scale factors for energy exchange between parcels and their surroundings.

Multiphase Particle In Cell (MP-PIC)







Simulation of industrial scale multi-phase flow devices is within MFiX's grasp!

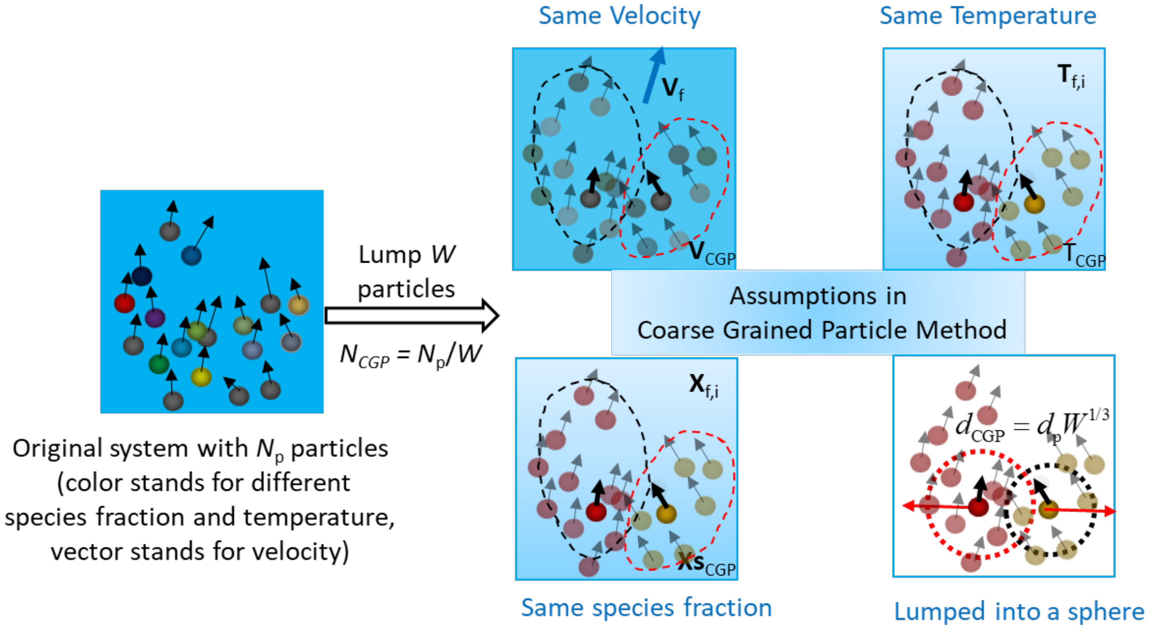
MFiX-PIC couples the MFiX Eulerian fluid solver with new Lagrangian solids stress model.

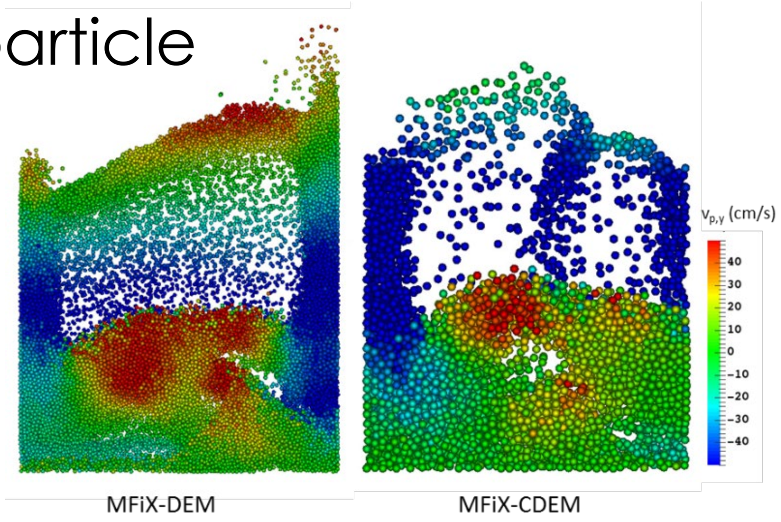
Excellent matching to pressure drop, temperature profiles and chemical species production at industrial scale.

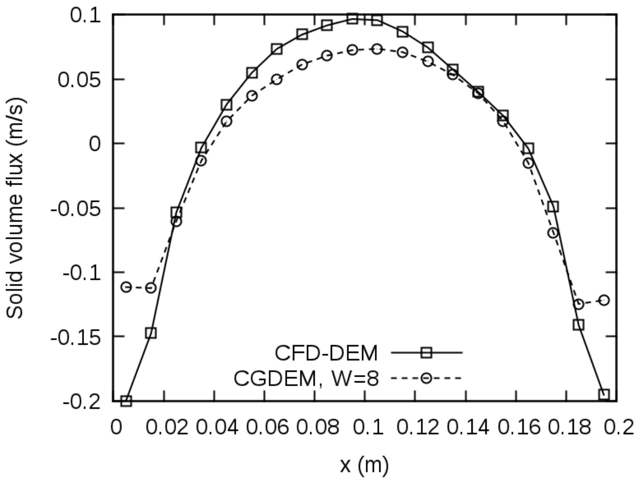
Tractable time to solution.

Coarse Grain DEM

- Particles are lumped together to create a CG particle
- CG particles collide with each other
- Heat transfer, chemical reactions
- MFiX-CGDEM formal release: 12/31/2020

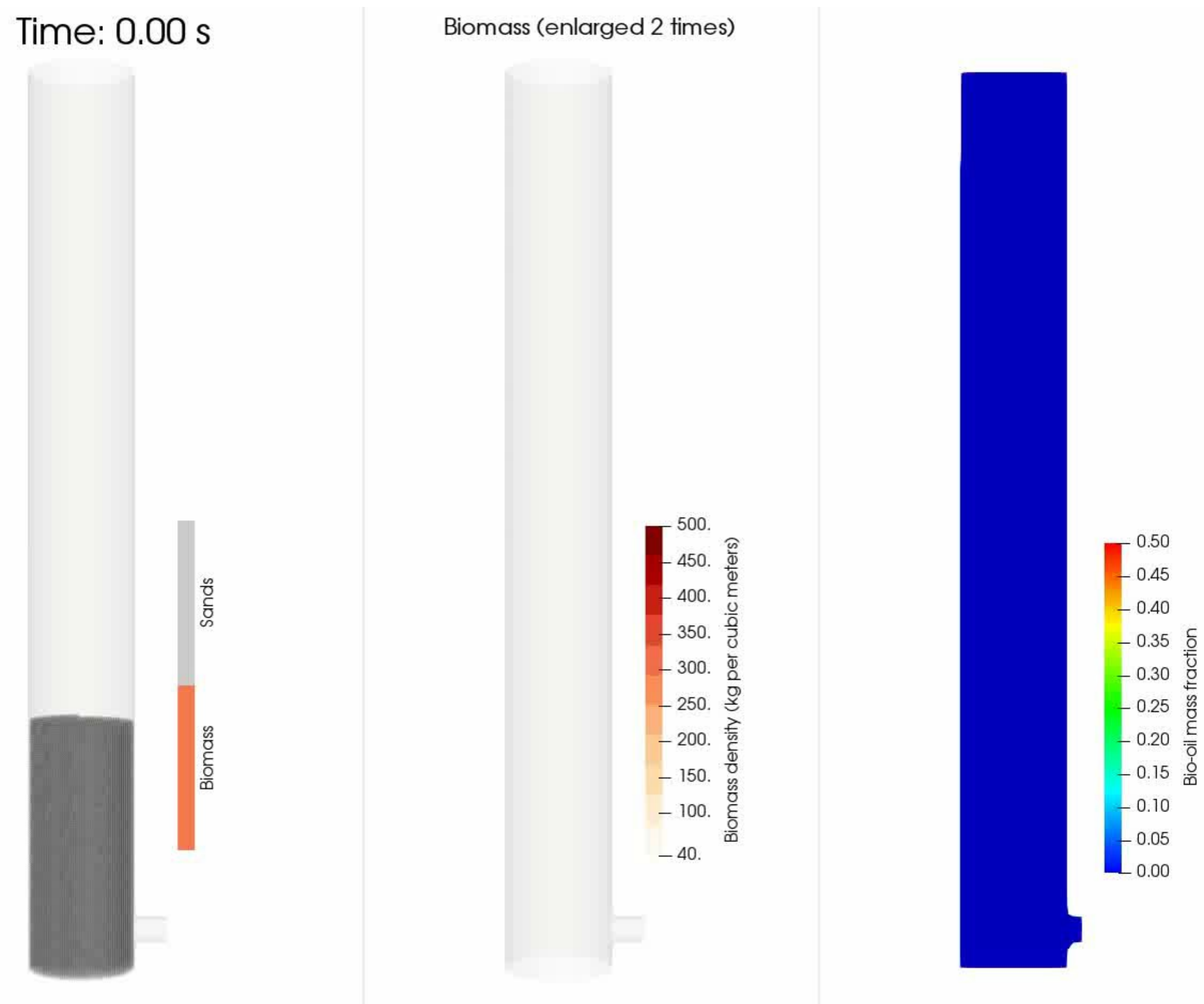




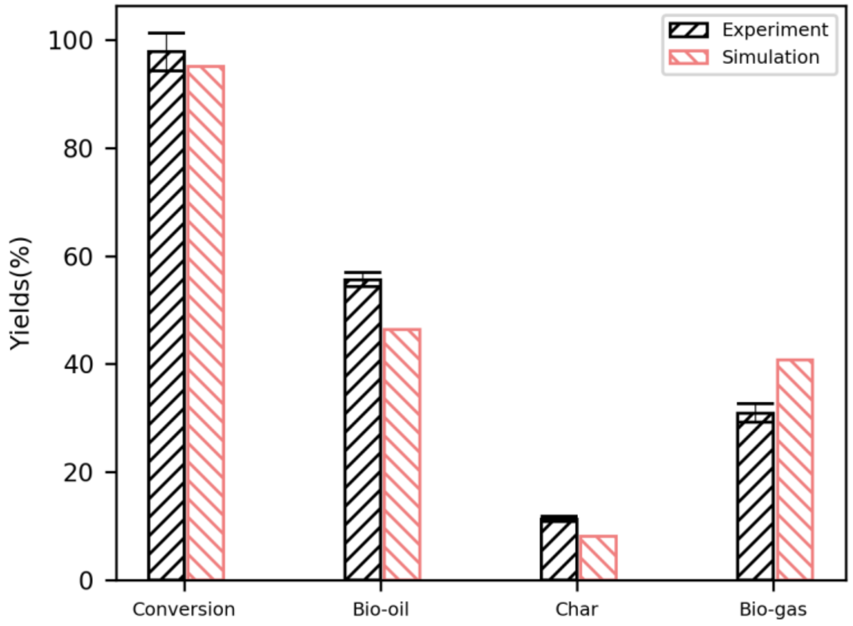


Coarse Grain DEM

CG-DEM Simulation of 2-inch Fluidized Bed Pyrolysis Reactor



1. Sands & 130 microns Biomass
2. Coarse Grained DEM Simulation
3. Hybrid drag model
4. DNS calibrated heat transfer & reaction kinetics

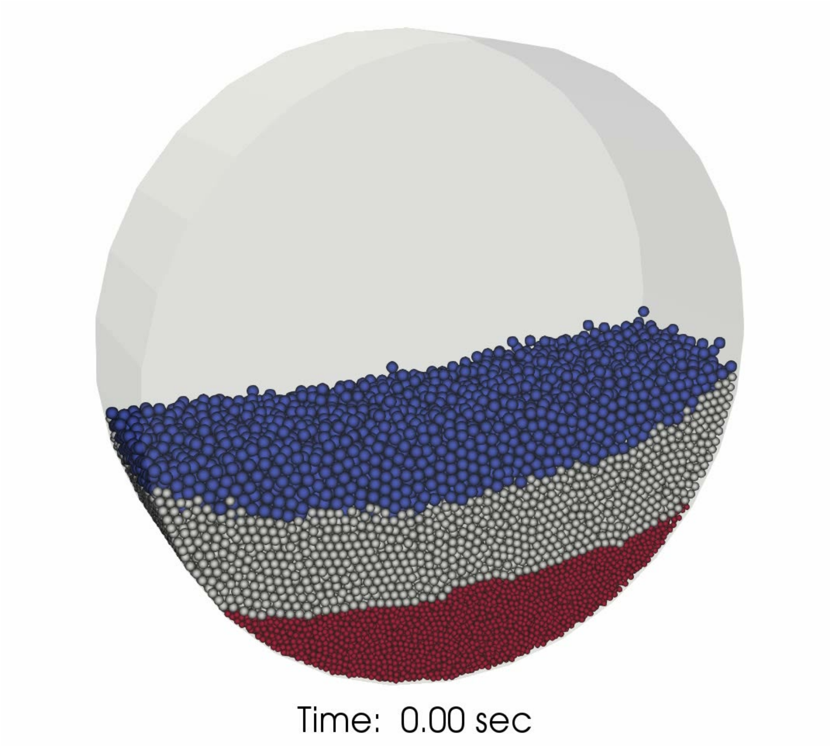


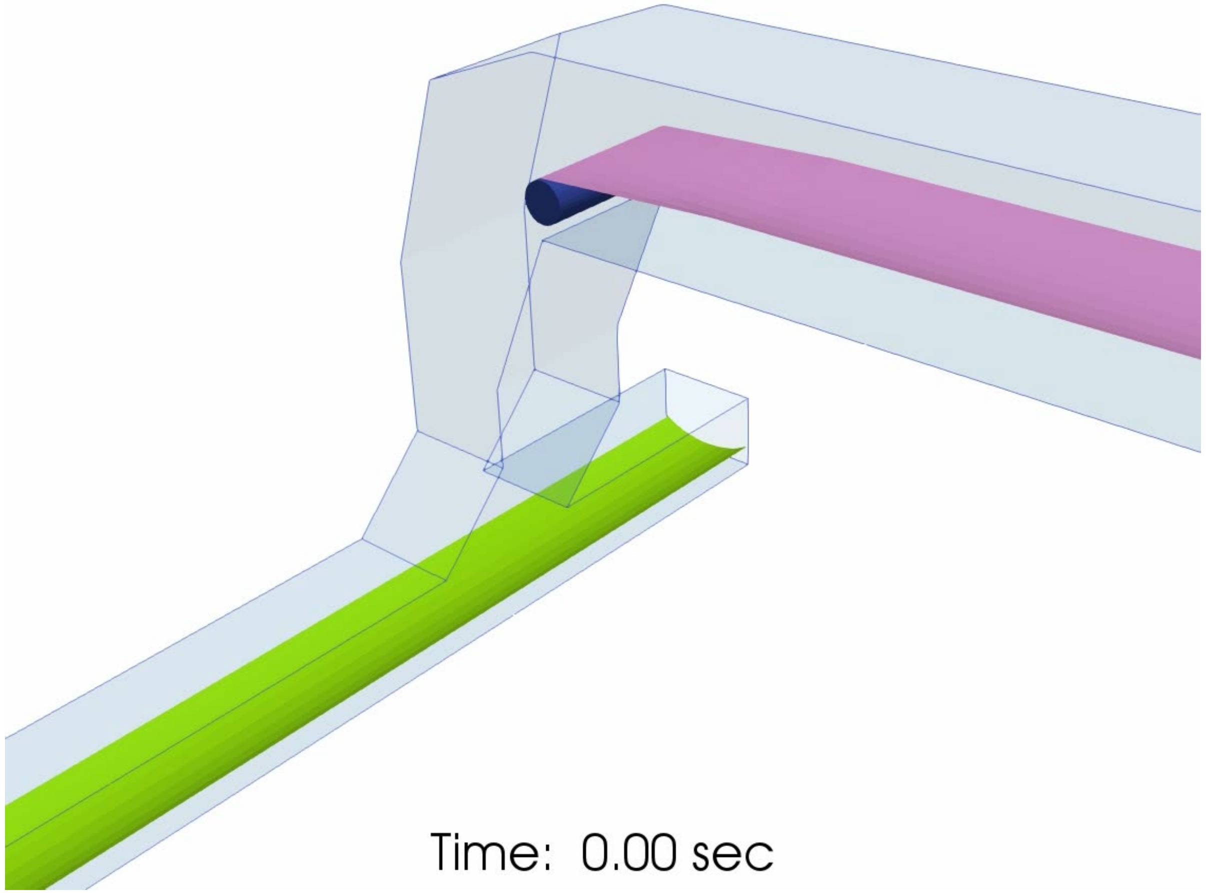
Moving geometry

Several options to represent moving geometry

Moving STL walls through tangential velocity

- Add Collection of UDFs and tutorials
- Rotating drum
- Conveyor belts

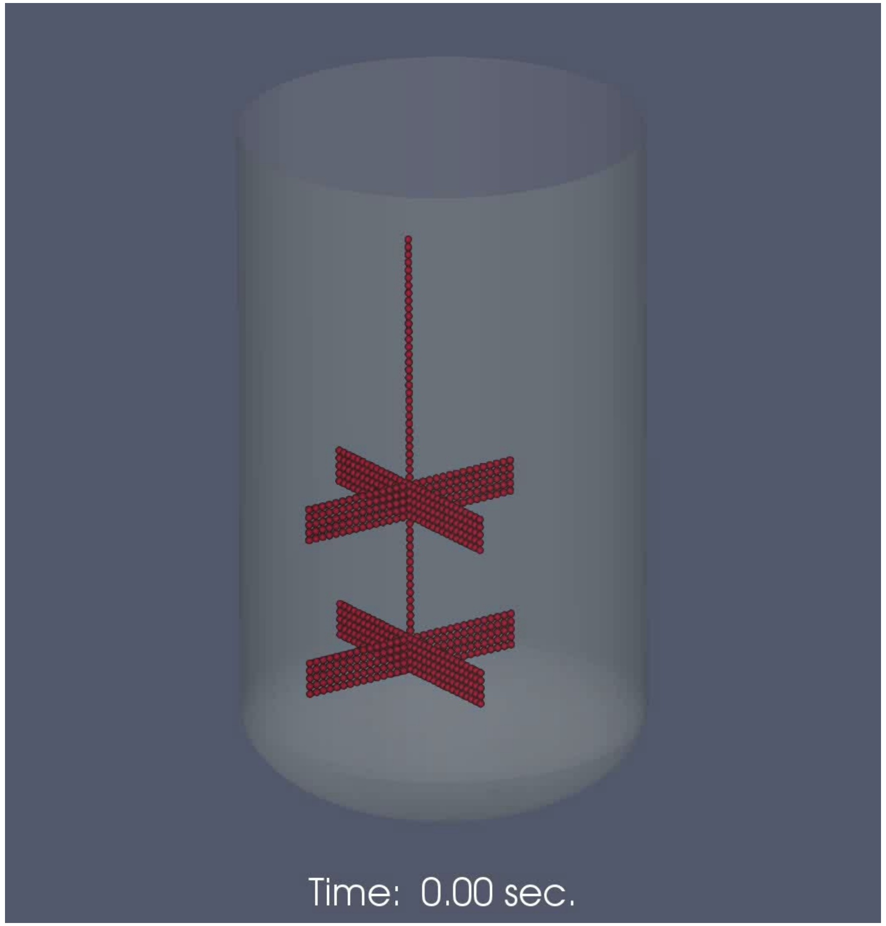




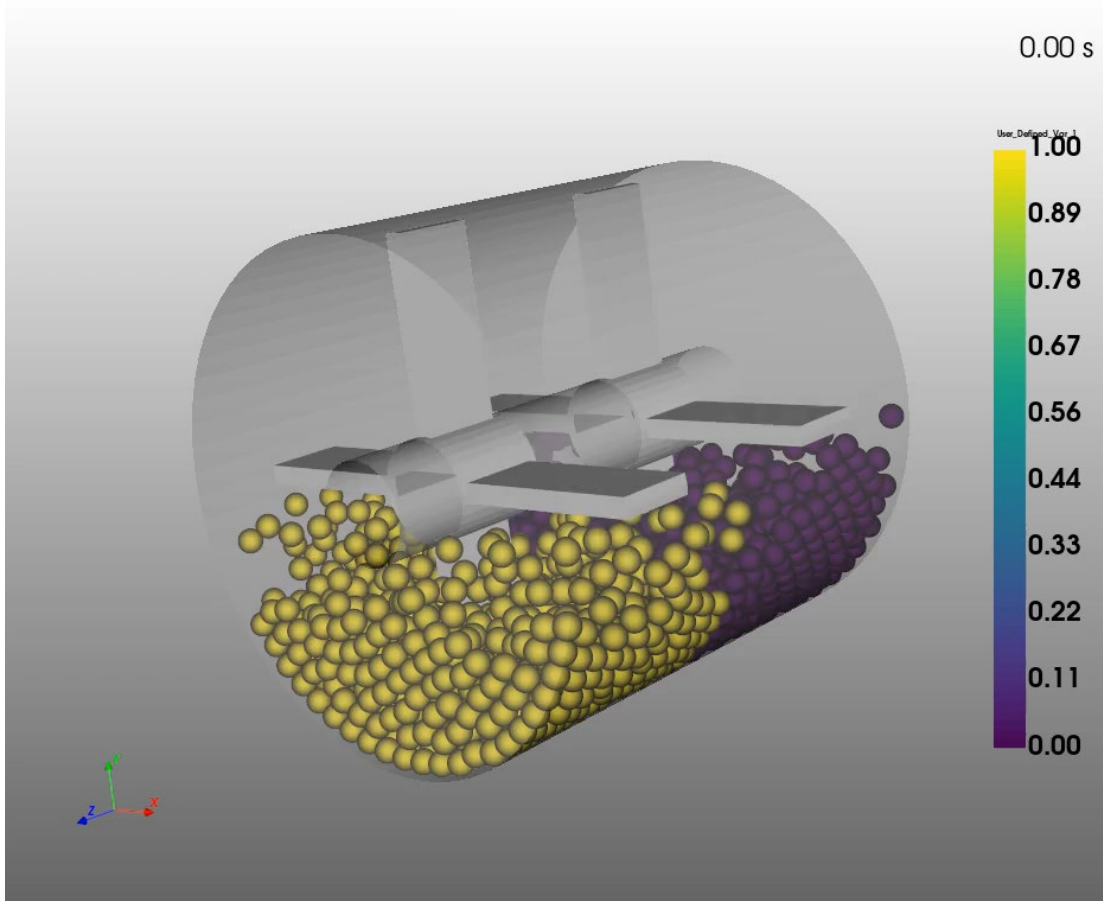
Moving geometry

Several options to represent moving geometry

Freeze or set particle velocity

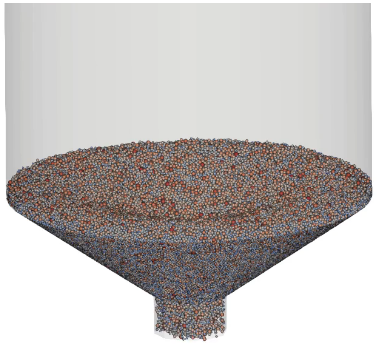


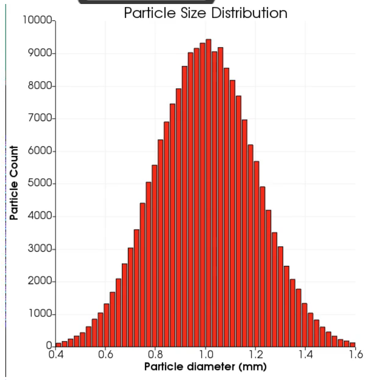
Move STL geometry (Granular DEM)

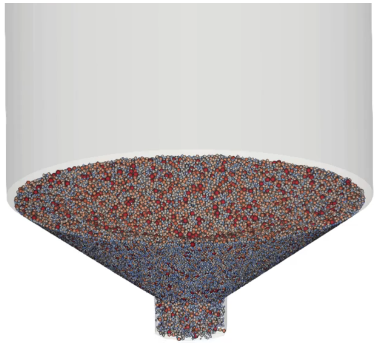


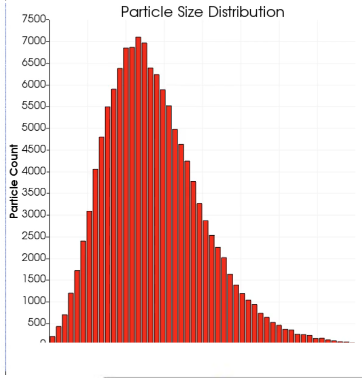
Polydispersity (DEM)

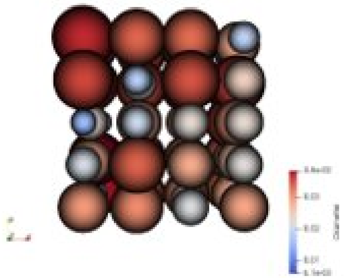
- Available in 20.3 Release (September 2020)
- Merge and complement ASU implementation
- Initial and Boundary (mass inflow) conditions
- DEM Particle size distribution
  - Normal
  - Log-normal
  - Custom (user-defined)
- Improvement in IC seeding
  - Robust
  - Lattice
  - Spacing
  - Flexibility in input
    - Volume fraction
    - Solid inventory
    - Particle count



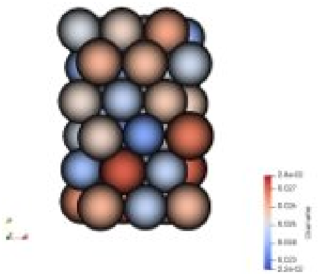




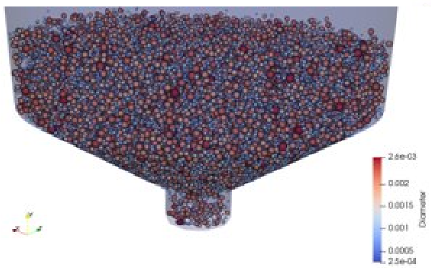


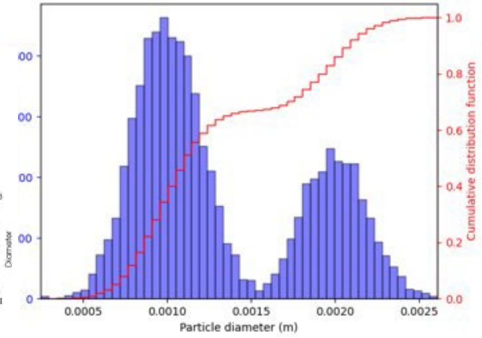


Cubic lattice



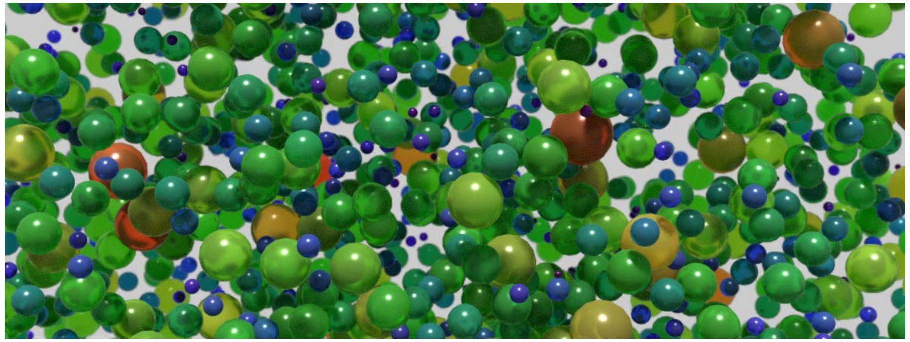
Hexagonal lattice

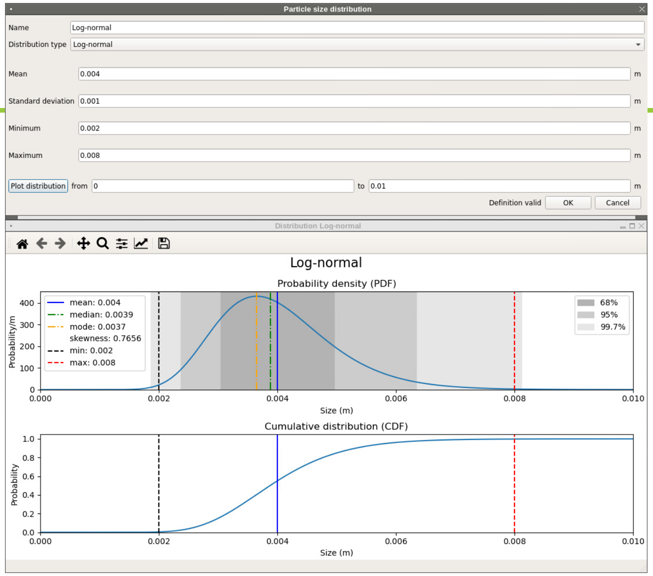


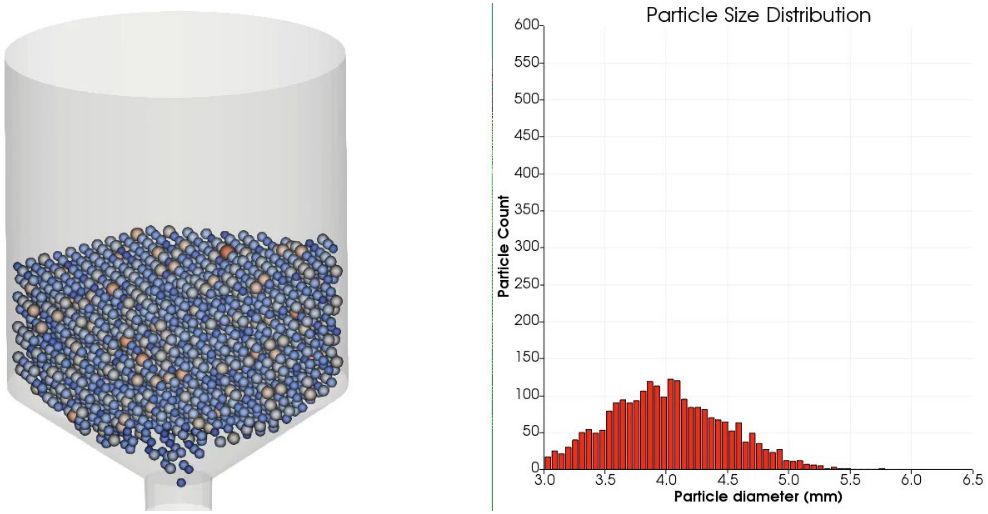


Polydispersity (DEM)

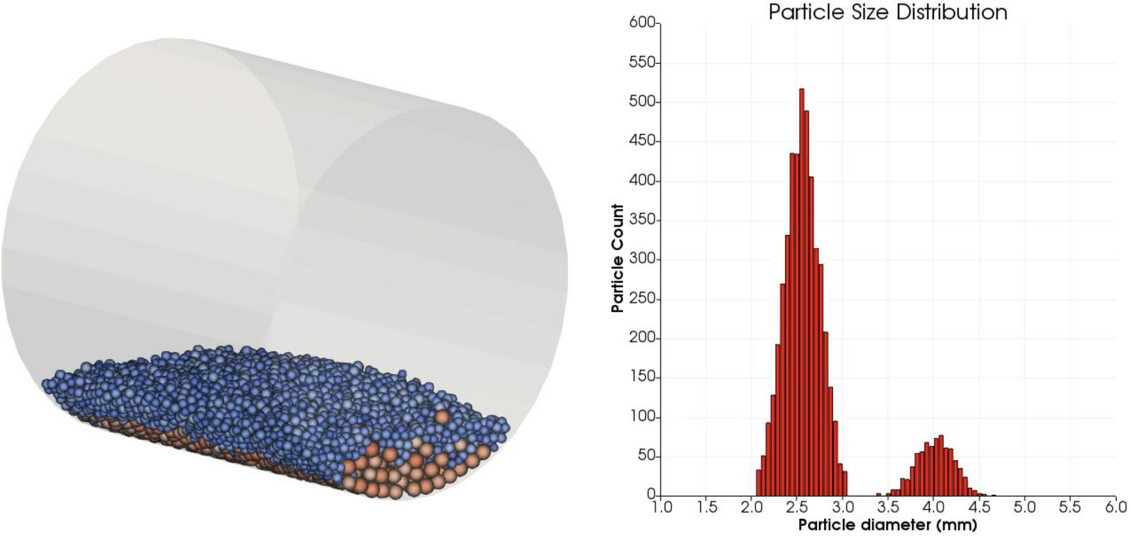
Polydispersity examples







Initial + Boundary Conditions



Particle coating

Non-spherical particles (SuperDEM)

NATIONAL ENERGY TECHNOLOGY LABORATORY

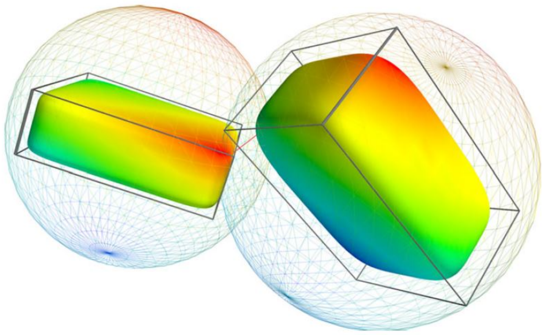
- Superquadrics are a family of geometric shapes defined as

$$\left[\left(\frac{x}{a_1}\right)^{\frac{2}{\varepsilon_2}} + \left(\frac{y}{a_2}\right)^{\frac{2}{\varepsilon_2}}\right]^{\frac{\varepsilon_2}{\varepsilon_1}} + \left(\frac{z}{a_3}\right)^{\frac{2}{\varepsilon_1}} = 1$$

- Can represent ~ 80% of all shapes by varying **five parameters**

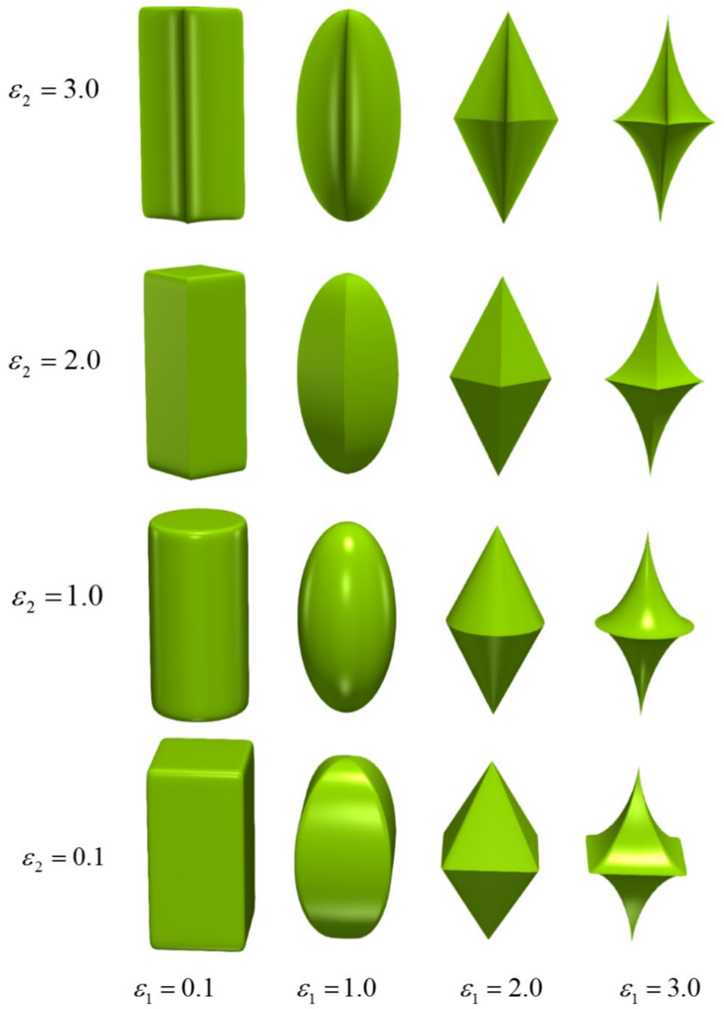
$$[a_1, a_2, a_3, \varepsilon_1, \varepsilon_2]^T$$

Semi-axis — roundness parameters



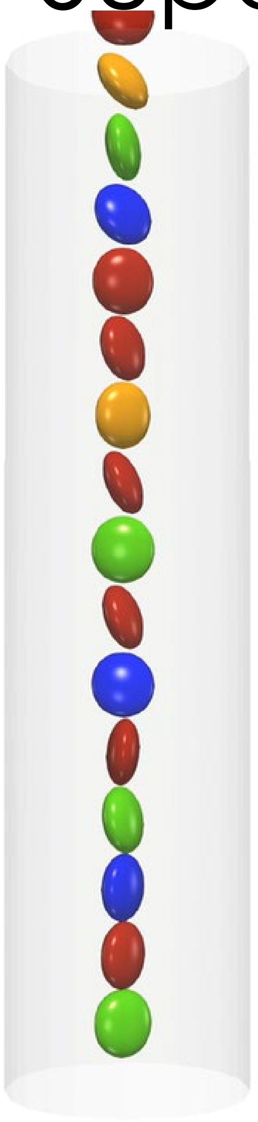
Bounding spheres and oriented bounding boxes

Superquadric particles

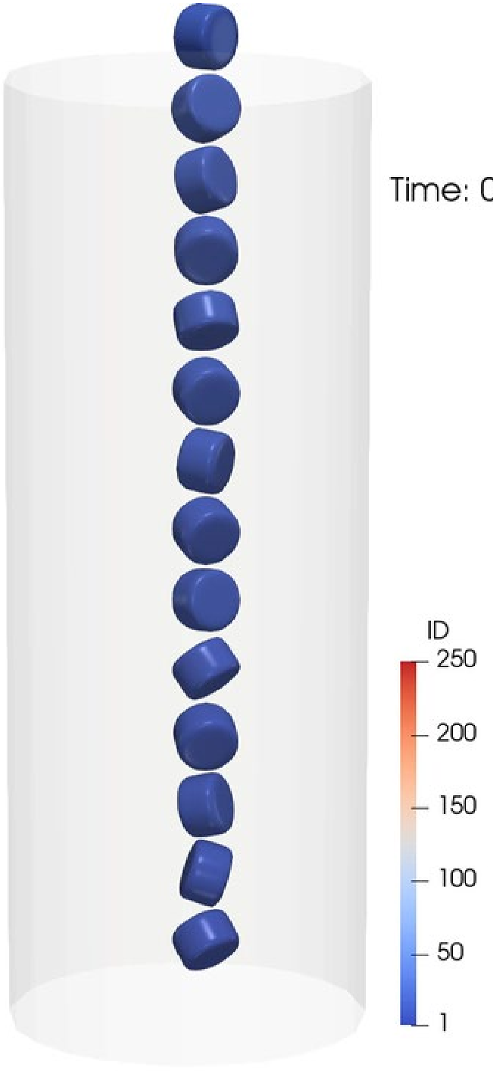


a1=2
a2=2
a3=4

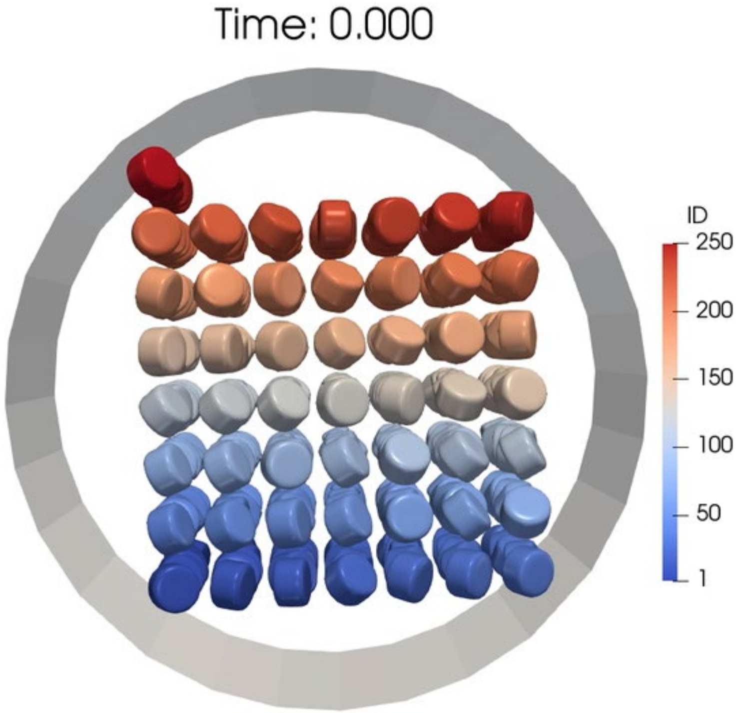
SuperDEM examples



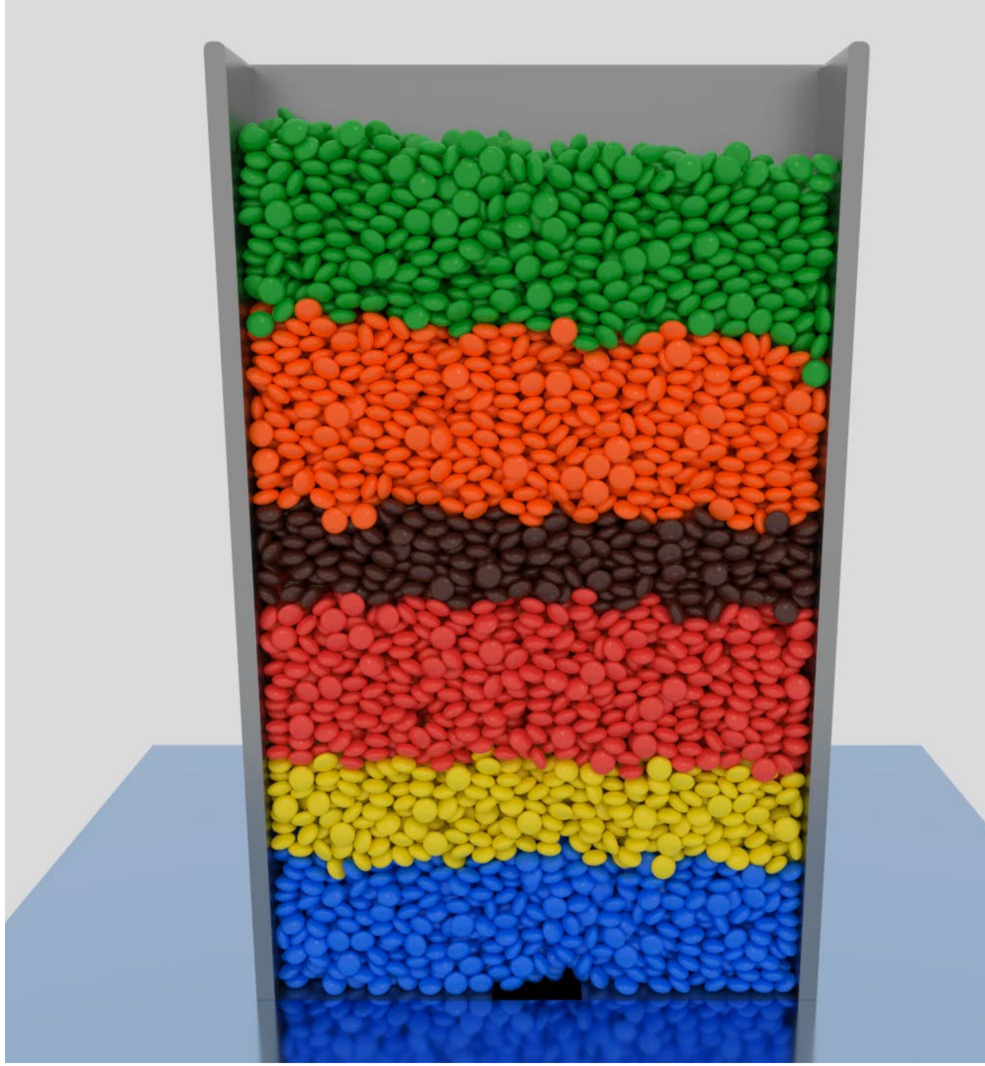
M&M candy static packing



Cylinder candy static packing

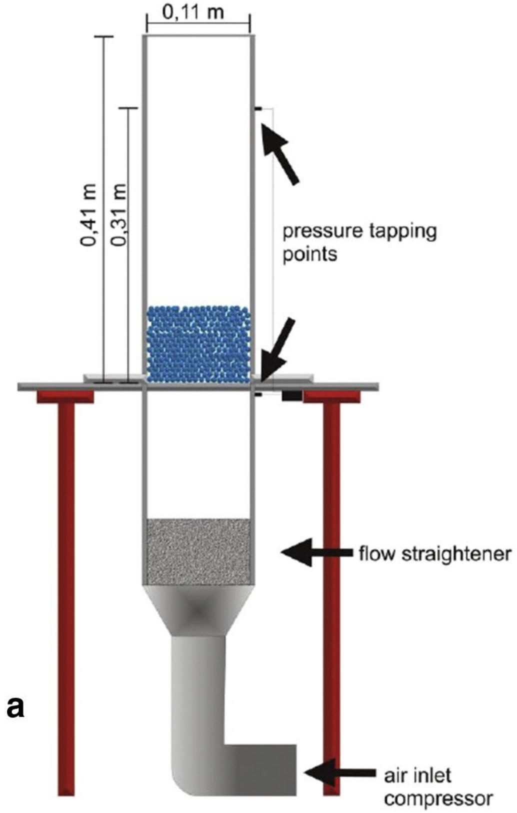


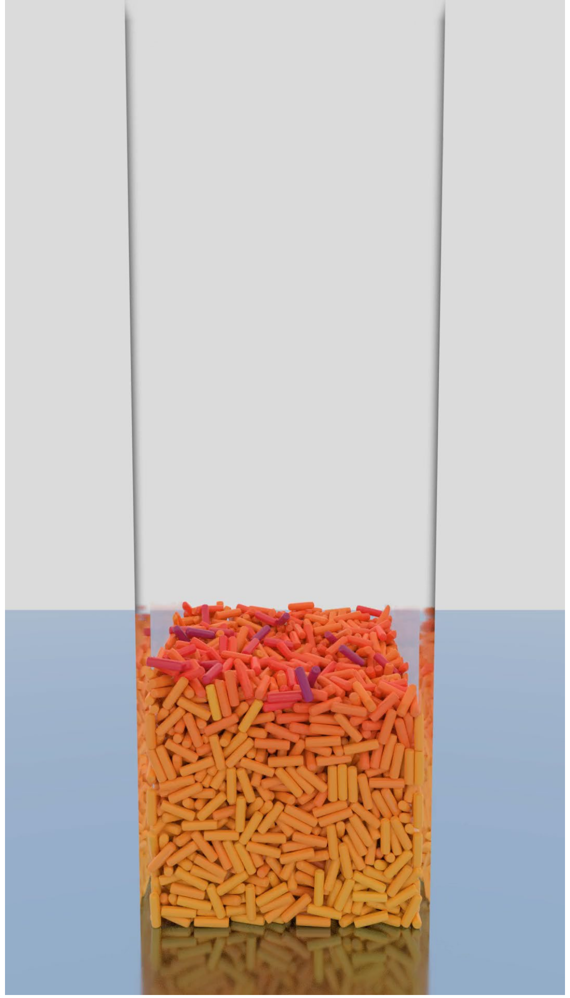
Cylinder rotating drum



M&M candy discharging from a hopper

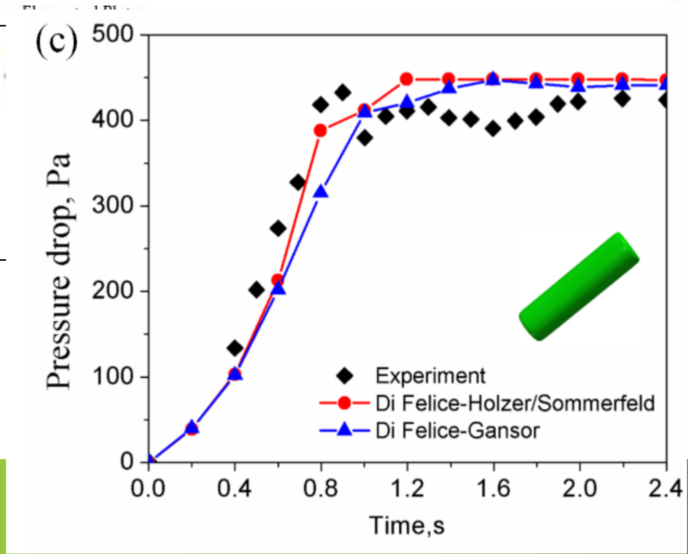
Validation experiment





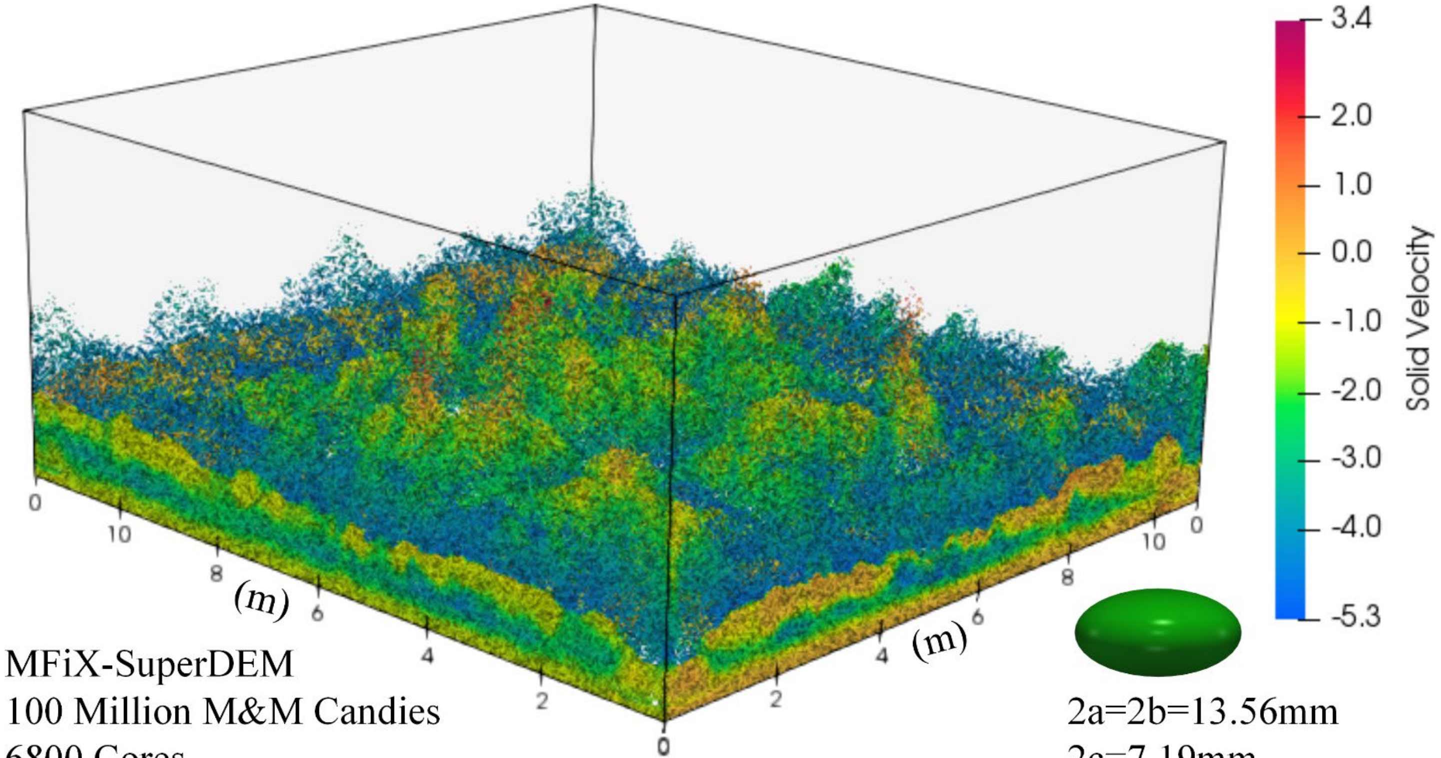
Particle properties including the volume equivalent diameter d_e-class, the particle dimensions, the sphericity ϕ, the particle density ρ_p, the bed height L and the averaged porosity ε for the initial, unfluidized setup.

Shape	Sphere	Sphere	Ideal Cylinder	Cube	Cube
d_e–class [mm]	7	5	7	5	7
Size [mm]	7.2	5	6.1 6.2	4.2 4.3 4.5	5.2 6.3 6.3
ϕ [–]	1.00	1.00	0.87	0.81	0.80
ρ_p [kg/m³]	772.5	823.0	708.5	639.7	746.9
L_{fb} [mm]/ $\bar{\varepsilon}$ [–]	95 0.40	88 0.40	98 0.36	98 0.37	103 0.43
Shape	**Elongated Cylinder**	**Elongated Cuboid**	**Elongated Cuboid**	**Plate**	**Elongated Plate**
d_e–class [mm]	7	5	7	5	5
Size [mm]	3.9 14.0	3.0 3.0 7.1	4.2 4.2 11.4	2.0 4.9 6.0	2.0 4.0 8.0
ϕ [–]	0.75	0.75	0.73	0.71	0.69
ρ_p [kg/m³]	764.4	745.6	639.7	754.1	756.6
L_{fb} [mm]/ $\bar{\varepsilon}$ [–]	103 0.44	103 0.42	115 0.40	102 0.43	108 0.46
Shape	**Elongated Cuboid**	**Plate**			
d_e–class [mm]	5	7			
Size [mm]	2.0 3.0 11.0	2.2 9.0 9.8			
ϕ [–]	0.64	0.63			
ρ_p [kg/m³]	728.1	672.8			
L_{fb} [mm]/ $\bar{\varepsilon}$ [–]	117 0.48	121 0.46			



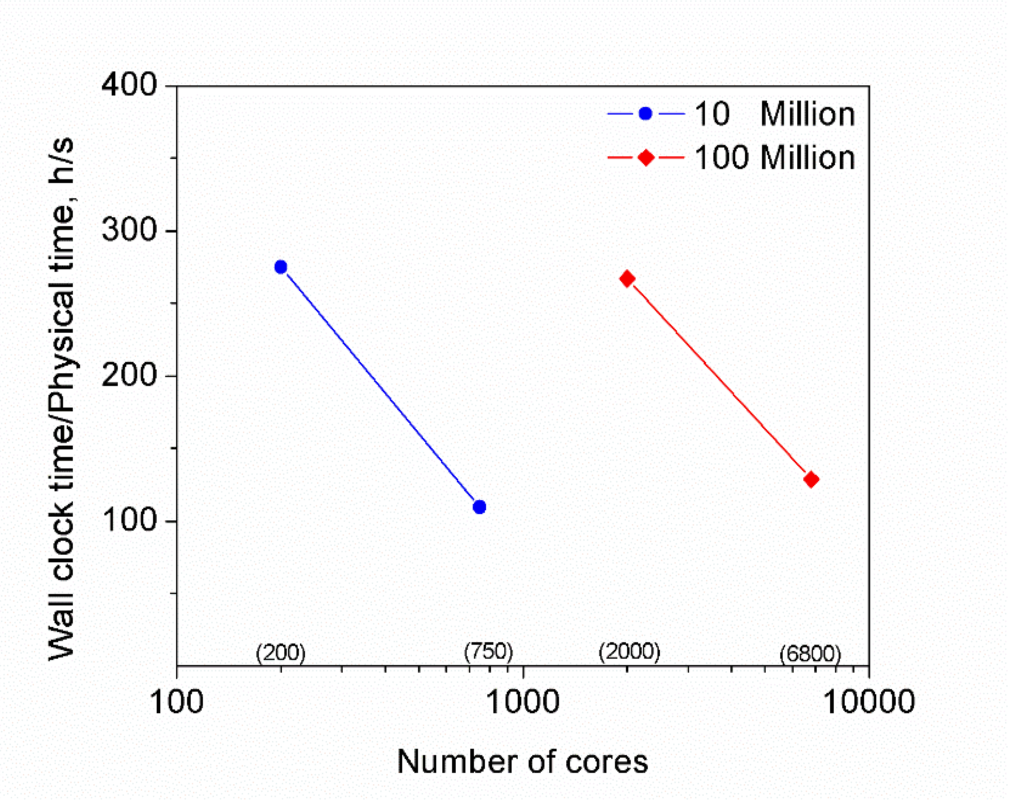
Experiment: Vollmari K, Jasevičius R, Kruggel-Emden H. Experimental and numerical study of fluidization and pressure drop of spherical and non-spherical particles in a model scale fluidized bed. Powder Technology. 2016;291:506-521.

Massively Parallel SuperDEM Simulation



MFiX-SuperDEM
100 Million M&M Candies
6800 Cores

2a=2b=13.56mm
2c=7.19mm

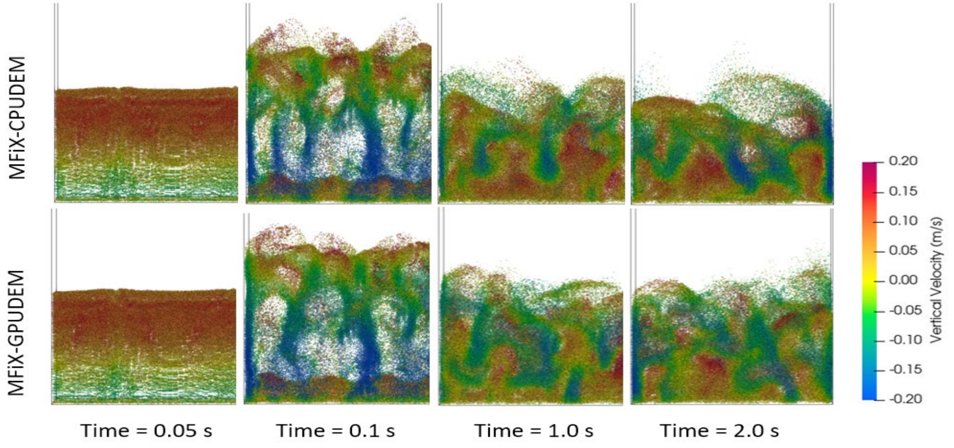


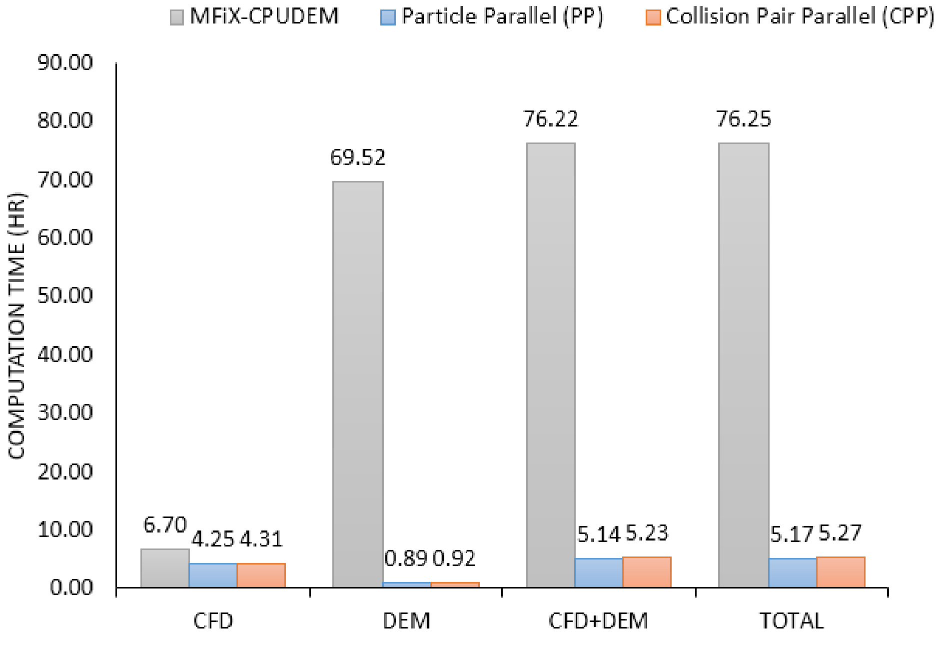
- The solver was parallelized using MPI.
- Simulation on NETL supercomputer Joule 2 (80K cores) , World Top 60, 2020
- Non-spherical particles fluidization simulation, 100 million (6800 cores)

Hundredfold Speedup of MFiX-DEM using GPU

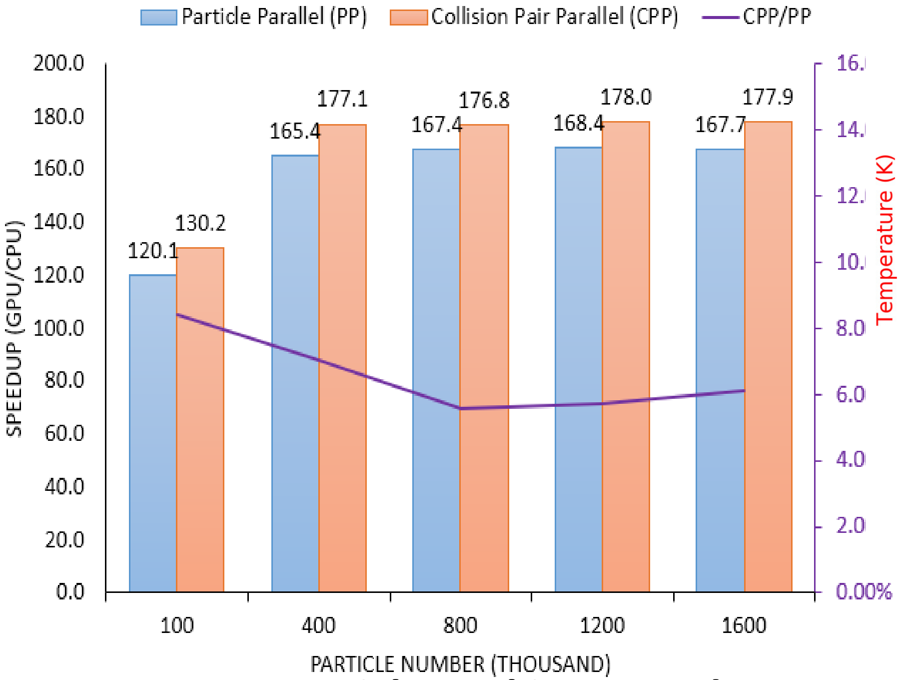
NATIONAL ENERGY TECHNOLOGY LABORATORY

- DEM solver was ported to GPU (prototype)
- 170 fold speedup with double precision, 243 fold with single precision
- Re-use CFD, interphase coupling, and chemical reaction modules in MFiX

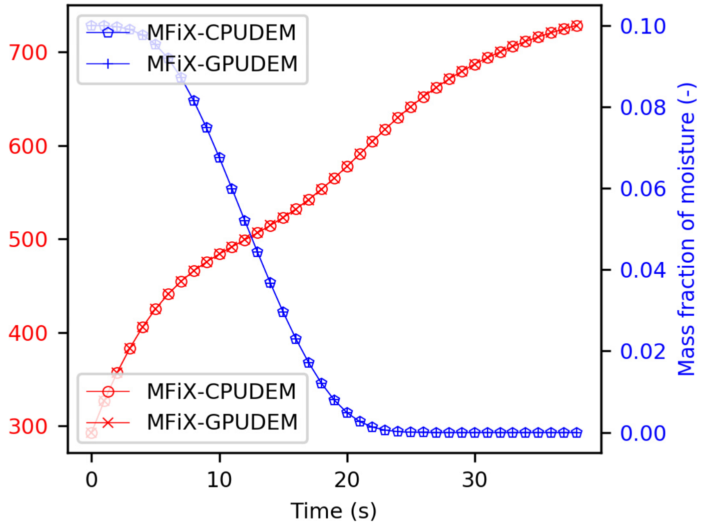




Fluidized bed Speedup



Particle packing Speedup

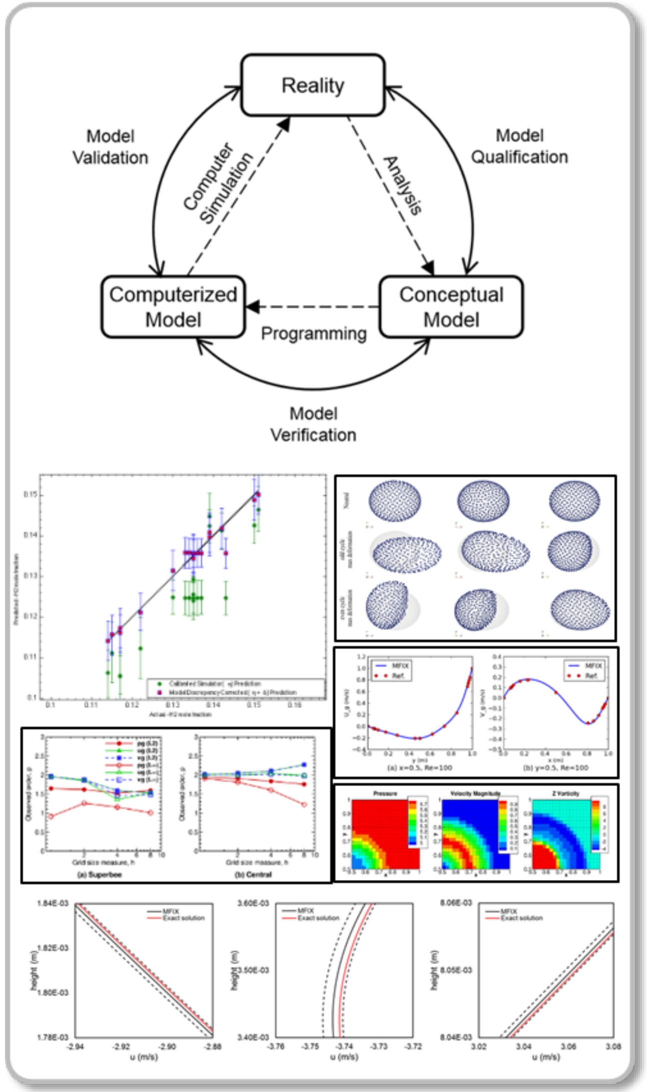


Heat transfer & chemical reactions (biomass drying)

MFiX Quality Assurance

Building Confidence in Simulation Results

- **Verification**
  - Code verification – Does the code do what we expect?
  - Solution verification – Is the answer any good?
- **Validation -** How does the answer compare to the real world?
- **Uncertainty Quantification**
  - Where is the error in my solution coming from?
  - What happens to my answer when I change an input to my model?



Accomplishments

- MFiX Verification and Validation Manual 2nd Ed. (PDF & html)
- PIC theory guide (May 2020)

MFiX Quality Assurance

Building Confidence in Simulation Results

- **PIC parameter sensitivity and calibration**
  - How sensitive are PIC simulations to PIC model parameters?
  - Recommend parameter values for a given type of application

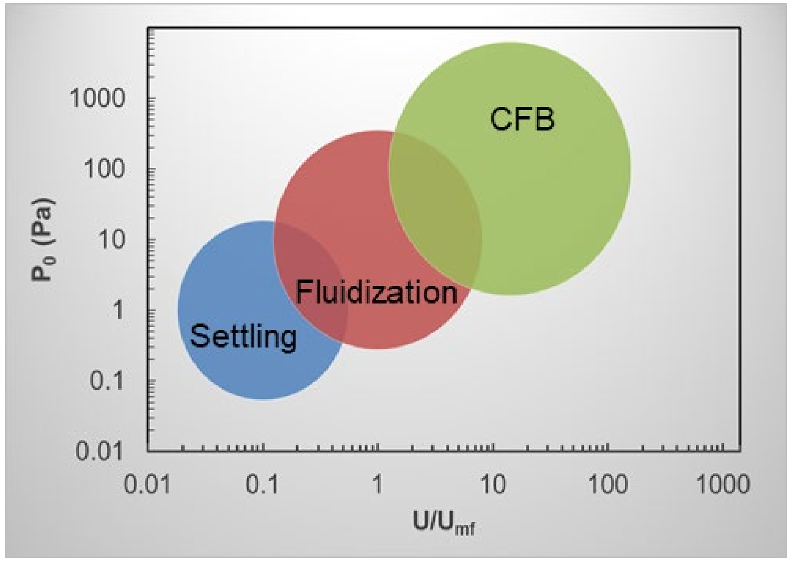
Parcel momentum equation

$$\frac{d\vec{V_p}}{dt} = \beta(\vec{U_g} - \vec{V_p}) - \frac{1}{\rho_p}\nabla p - \frac{1}{\varepsilon_p \rho_p}\nabla \tau_p + \vec{g}$$

$$\tau_p = \frac{P_0 \varepsilon_p^{\beta}}{\max\left(\varepsilon_{cp} - \varepsilon_p, \delta(1-\varepsilon_p)\right)}$$

Cases selected to cover a broad range of flow conditions

- Particle Settling: $U/U_{mf} < 1.0$ ($P_0 \sim 1$) (Analytical solution)
- 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:

	t1 Pressure linear scale factor	t2 Volume fraction exponential scale factor	t3 Statistical weight	t4 Volume fraction at maximum packing	t5 Solid slip velocity factor
C1: Particle Settling	[1,20]	[2,5]	[3,20]	[0.35,0.5]	[0.5,1.0]
C2: Fluidization	[1,100]	[2,5]	[10,100]	[0.4,0.5]	[0.85,0.98]
C3: Circulating Fluidized Bed	[1,250]	[2,5]	[4]	[0.4,0.5]	[0.85,0.98]

*Parameters selected based on prior sensitivity study

C1: Particle settling

Problem setup

Control variable: Initial solids concentration

Range: [0.05,0.25]

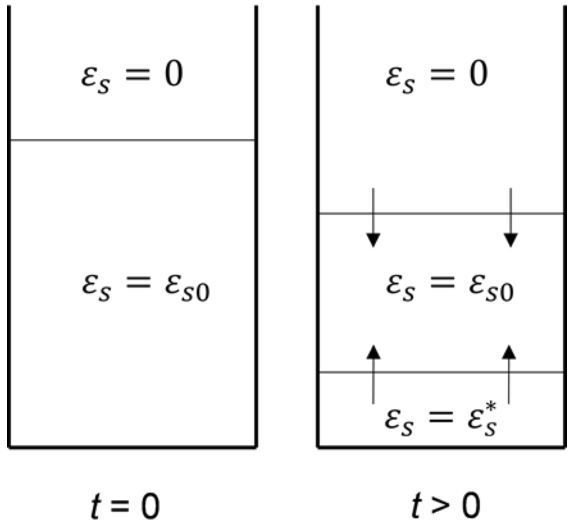
	x1 Initial solids concentration
C1: Particle Settling	[0.05,0.25]

Response variable: Location of filling shock (y2)

CFD results are compared with analytical solutions

Control variables: CFD (PIC parameters)

	t1 Pressure linear scale factor	t2 Vol. fraction exponential scale factor	t3 Statistical weight	t4 Vol. fraction at maximum packing	t5 Solid slip velocity factor
C1: Particle Settling	[1,20]	[2,5]	[3,20]	[0.35,0.5]	[0.5,1.0]



Analytical Solution:

Location of shock $x(t) = -t\left(\frac{\varepsilon_s^* \varepsilon_g^* u_r^* - \varepsilon_{s0}\varepsilon_{g0}u_{r0}}{\varepsilon_s^* - \varepsilon_{s0}}\right)$

Rel. velocity (Stokes' drag) $u_r = \frac{g\Delta\rho d_p^2}{18\mu_g}\varepsilon_g^{3.65}$

C1: Particle settling

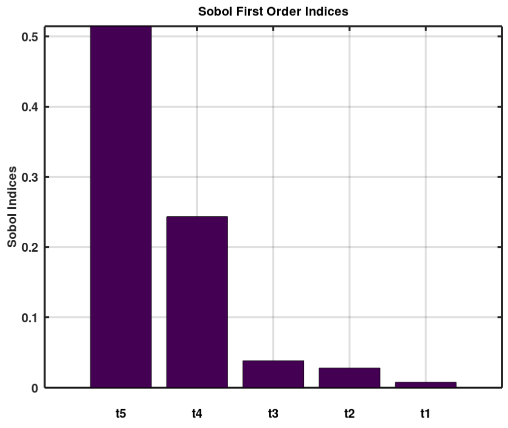
Sensitivity analysis and Deterministic calibration

Response surface constructed from 55 samples

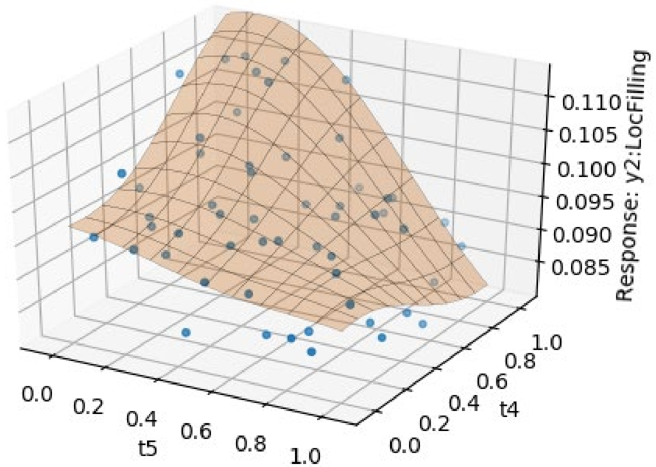
Sobol indices show the following:

- main effects (first oder)
- interactive effects (second order)

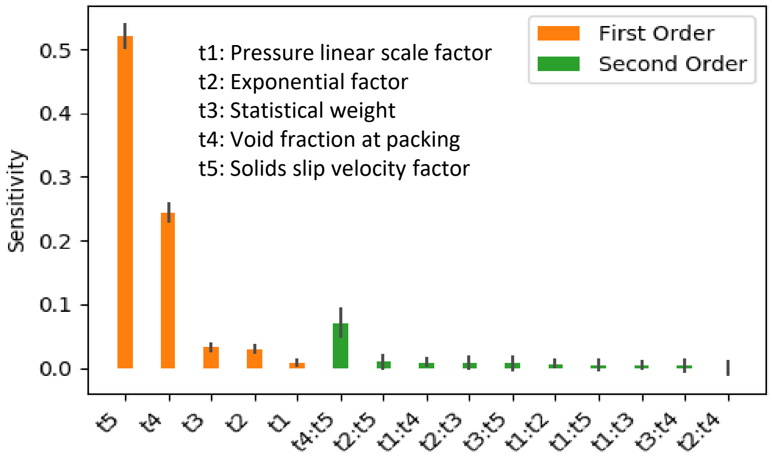
Code-to-Code comparison with PSUADE



3D plot of the data-fitted surrogate model



Sensitivity Analysis using Sobol Indices



Parameters obtained through deterministic calibration

Parameter	Default	Range	Calibrated
t1 Pressure linear scale factor	100	[1,20]	14.309
t2 Vol. fraction exponential scale factor	3.0	[2,5]	2.165
t3 Statistical weight	5.0	[3,20]	12.241
t4 Vol. fraction at maximum packing	0.42	[0.35,0.5]	0.399
t5 Solid slip velocity factor	1.0	[0.5,1.0]	0.828

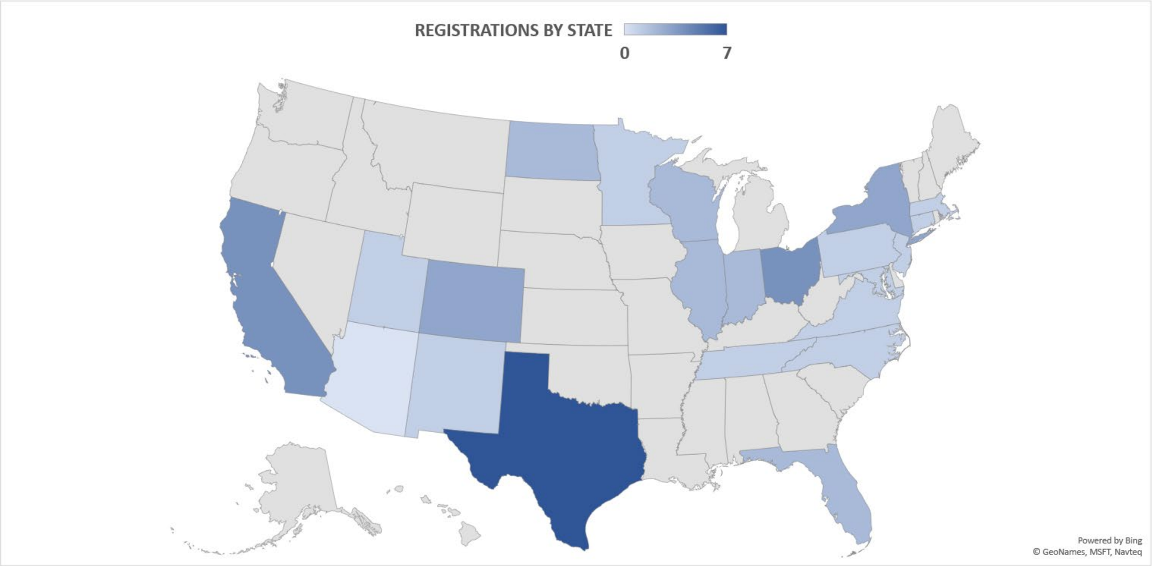
Outreach: User base

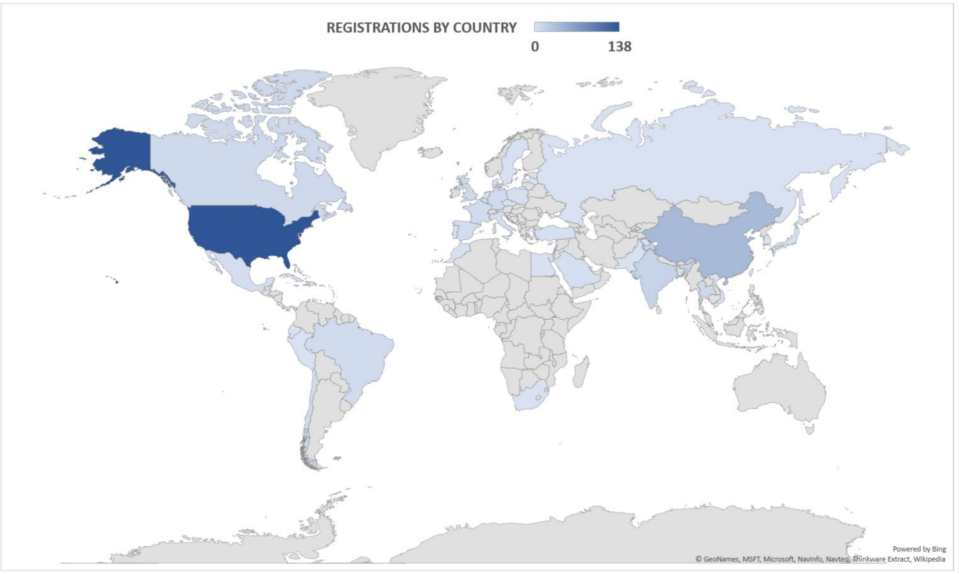
Still going strong amid pandemic crisis

Q2FY20 (Jan-March 2020) : 158 registrations, 831 MFiX Downloads

Q3FY20 (April-June 2020) : 161 registrations, 815 MFiX Downloads

All-time registrations = **6,264** (June 30th 2020)



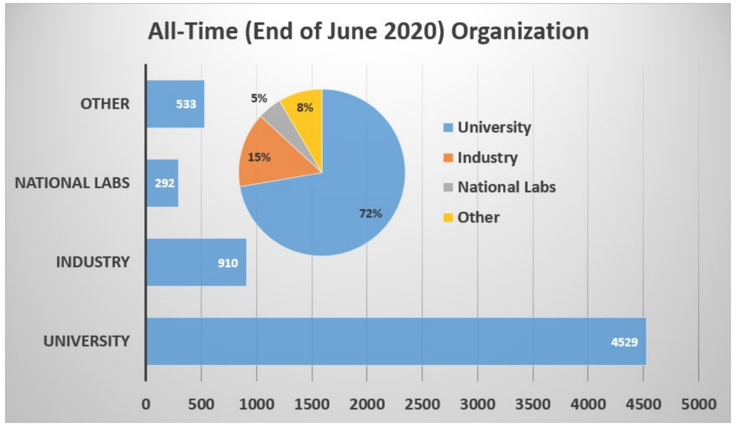


Registrations location (Q2FY20 + Q3FY20)

Outreach: All-time MFiX Stats

Stakeholders and Technology Transfer

- All-time MFiX registrations = **6,264**
  - University = 4,529
  - Industry = 910
  - Nat. Labs = 392
  - Other = 533



- **81 countries, Top 5:**

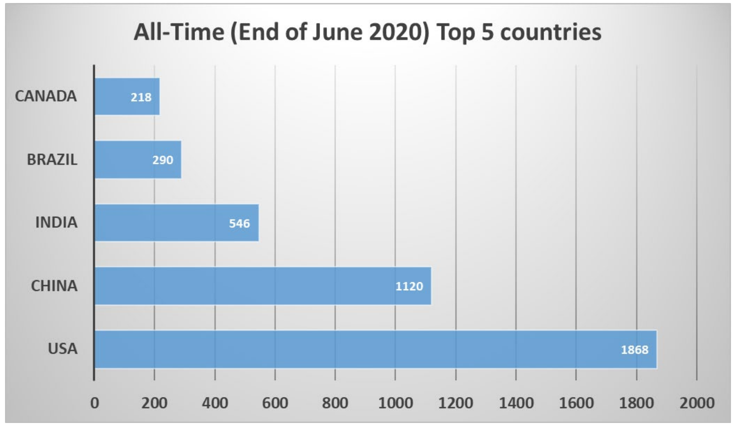
 USA : 1,632

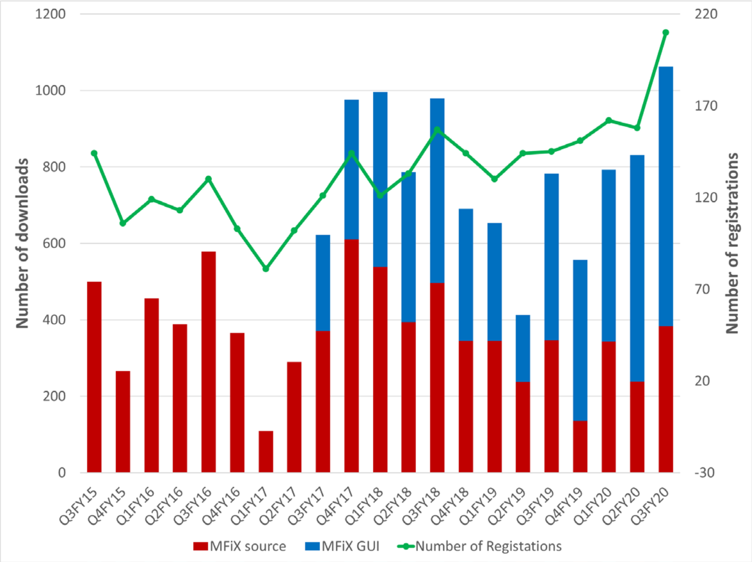
 China : 1,020

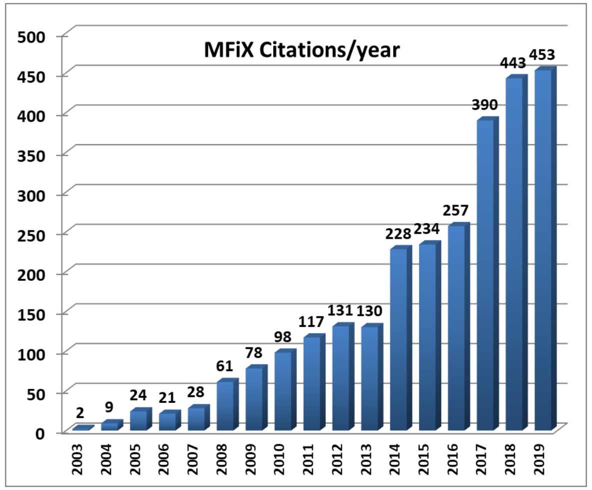
 India : 509

 Brazil : 268

 Canada : 196



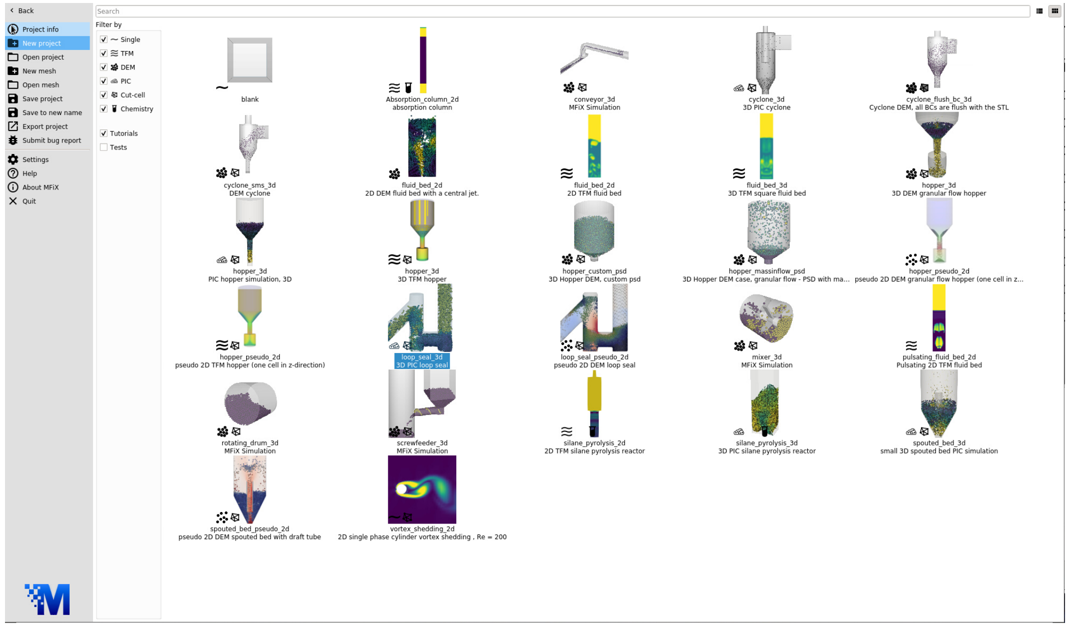




MFiX-How to get started?

NETL Multiphase Flow Science
Home of the MFiX Software Suite.

- Website: https://mfix.netl.doe.gov
- Register
- Download / Install MFiX
- Read documentation
- Run tutorials / templates
- Decide best modeling approach for chosen application
- Review questions / Submit questions / report issues on the Forum
- New users are encouraged to use the GUI
- Advanced users/developers can use command line



MFiX Documentation

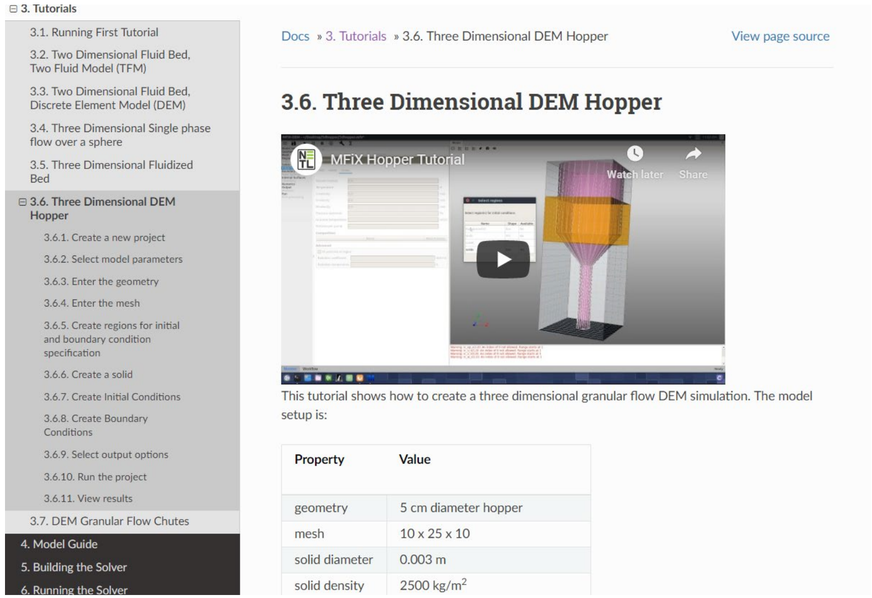
https://mfix.netl.doe.gov/doc/mfix/19.2.0

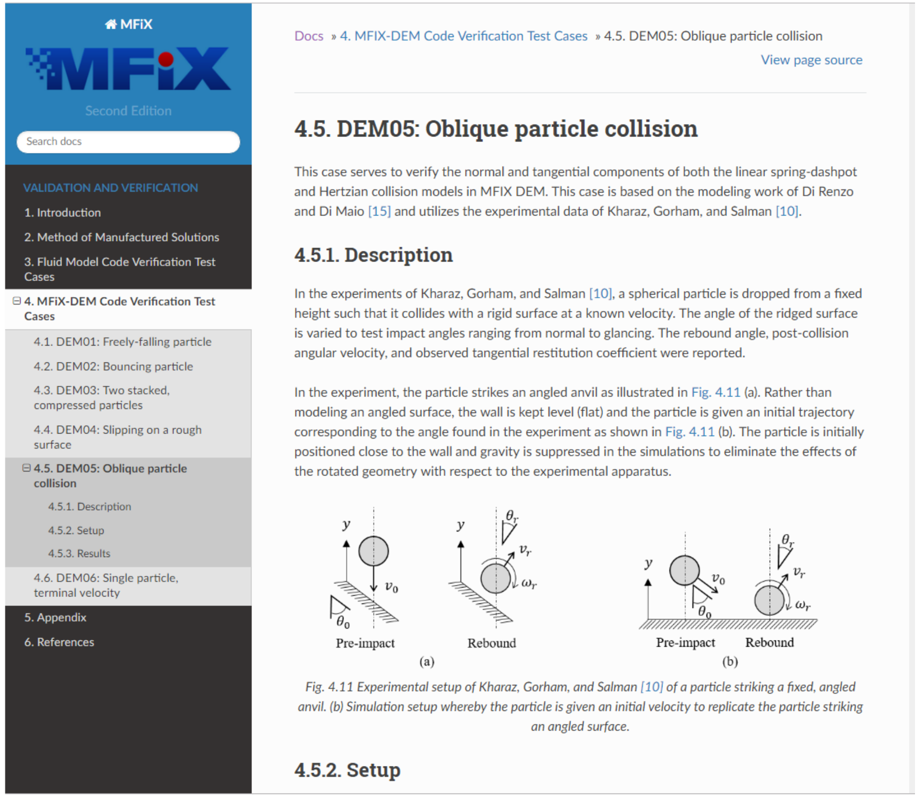
User manual

V&V manual

Html and pdf

Text and video tutorials





MFiX Forum

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

User support

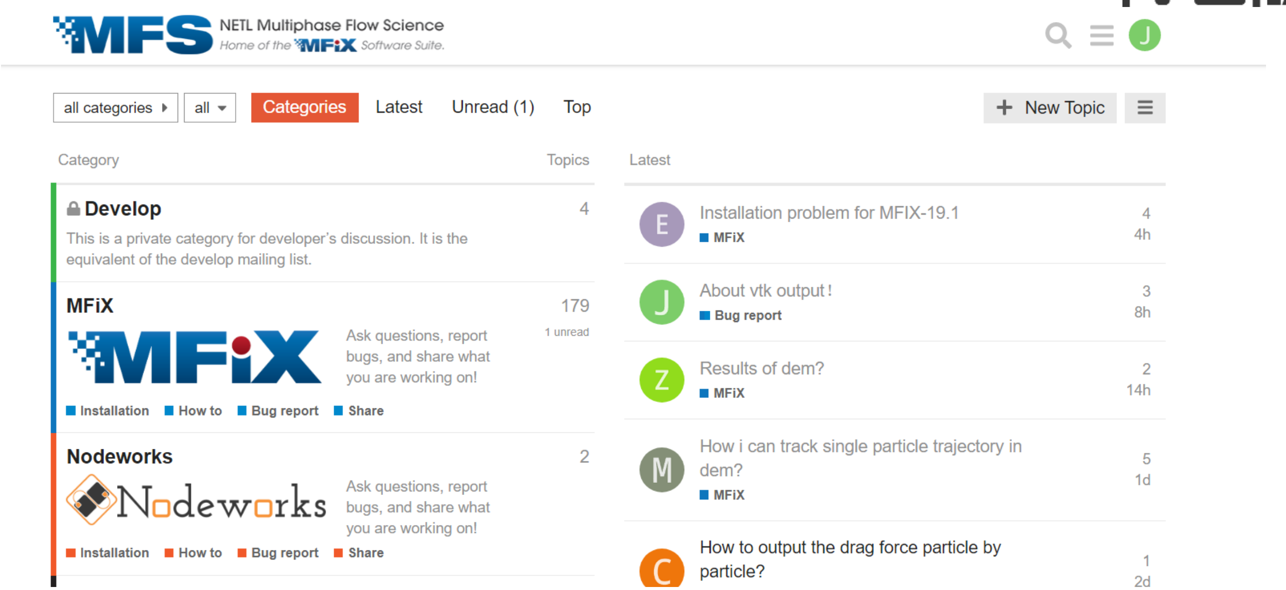
Categories

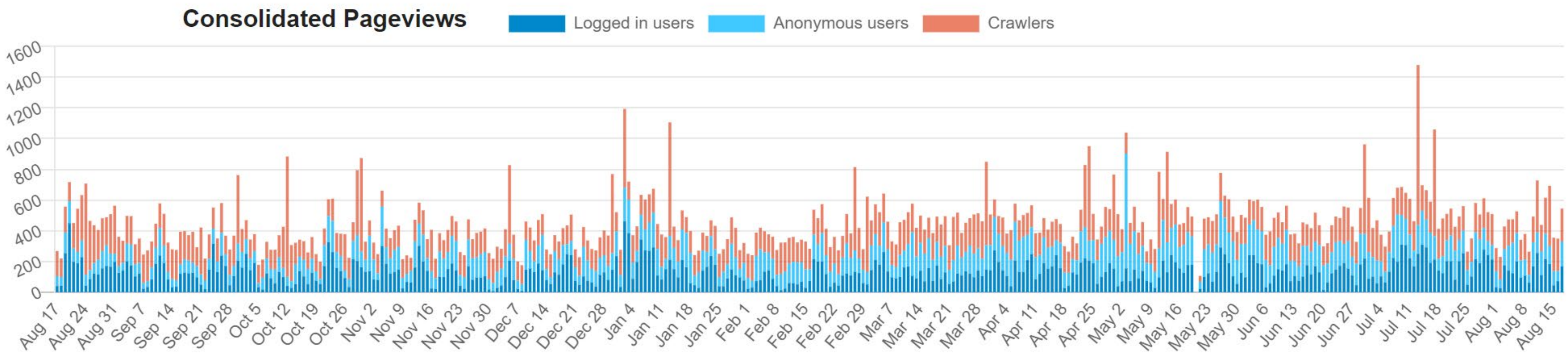
- Installation
- How to
- Bug report
- Share

Topics (threads)

File attachment

Searchable





Acknowledgment

This work was performed in support of the US Department of Energy's Fossil Energy Crosscutting Technology Research Program. The Research was executed through the NETL Research and Innovation Center's Advanced Reaction Systems. Research performed by Leidos Research Support Team staff was conducted under the RSS contract 89243318CFE000003.

Disclaimer

NATIONAL ENERGY TECHNOLOGY LABORATORY

This work was funded by the Department of Energy, National Energy Technology Laboratory, an agency of the United States Government, through a support contract with Leidos Research Support Team (LRST). Neither the United States Government nor any agency thereof, nor any of their employees, nor LRST, nor any of their employees, makes any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

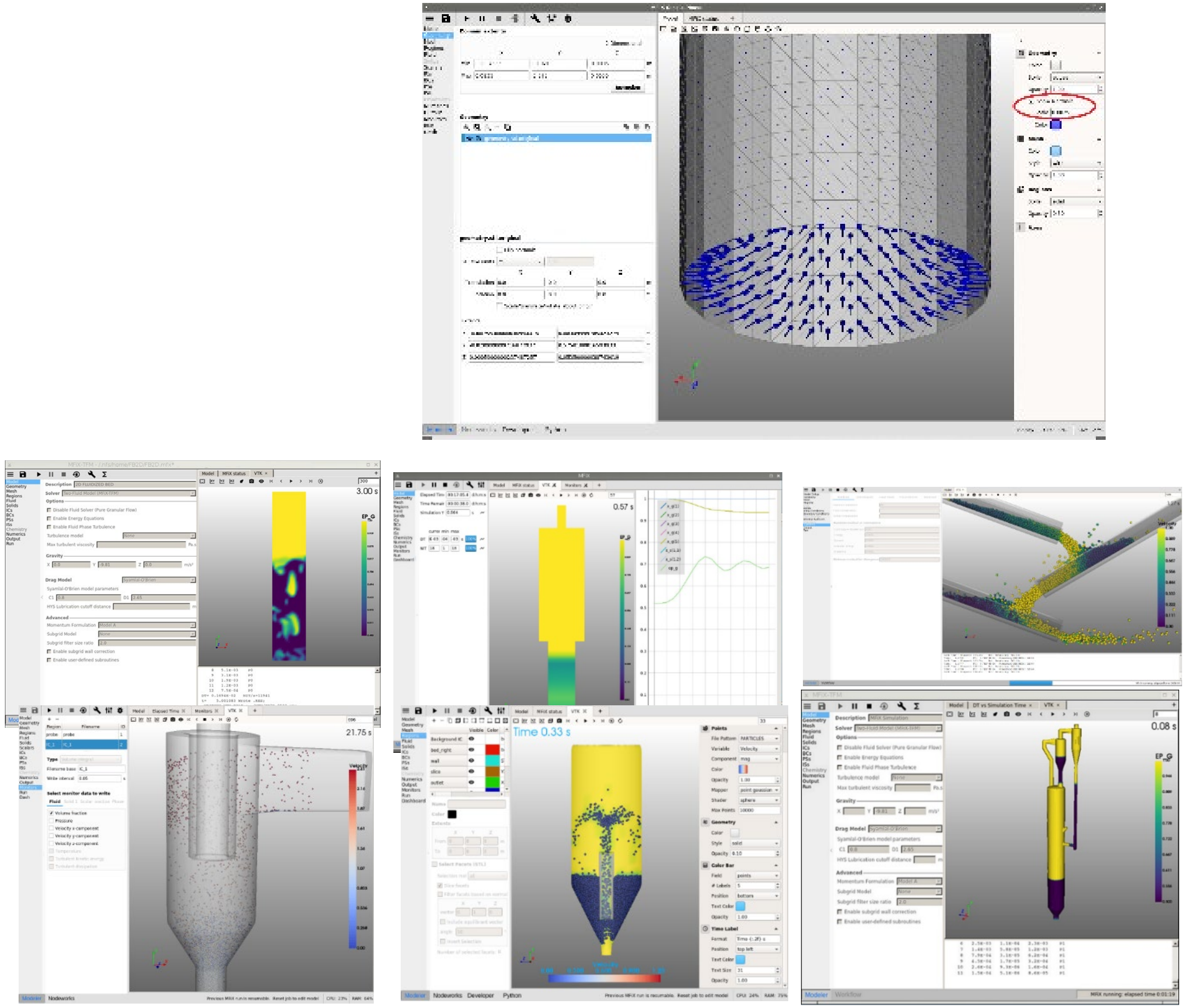
Preprocessor development

User setup (.mfx file) greatly improved by GUI

Increased demand for complex geometry

Mesh generation

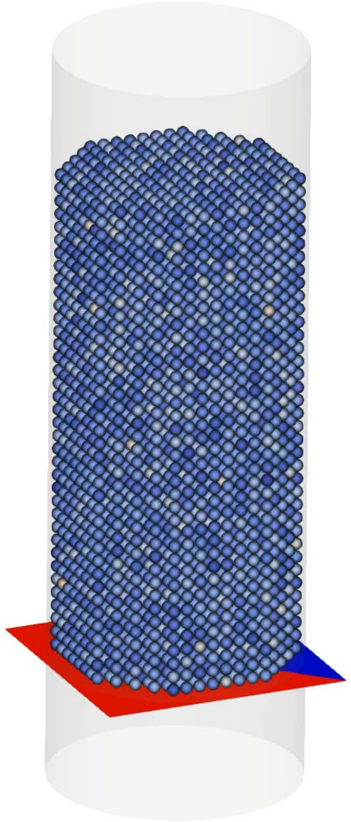
- Workflow challenge
- Geometry input (STL file)
- Preprocessing (cut cells)
- Mesh quality
- Difficult to troubleshoot
- Specific constrains for TFM, DEM and PIC

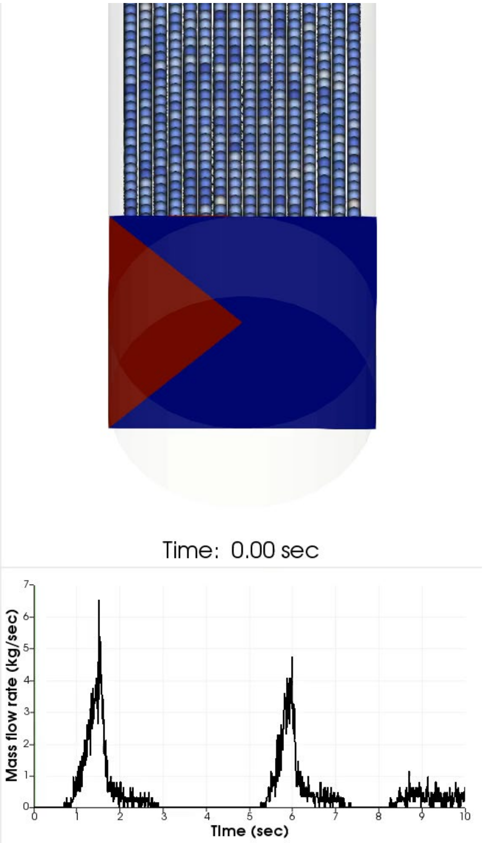


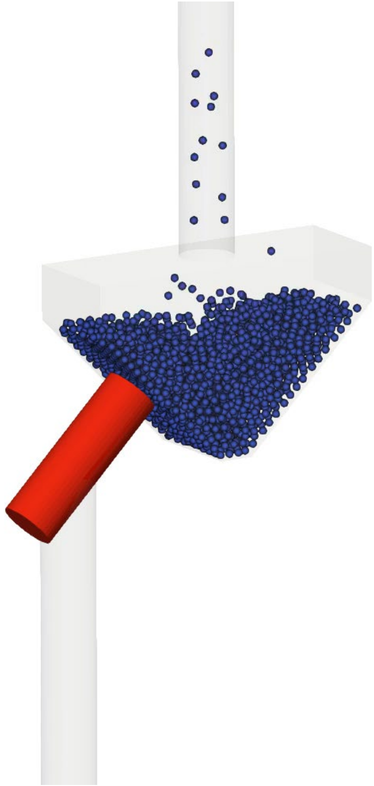
Moving geometry

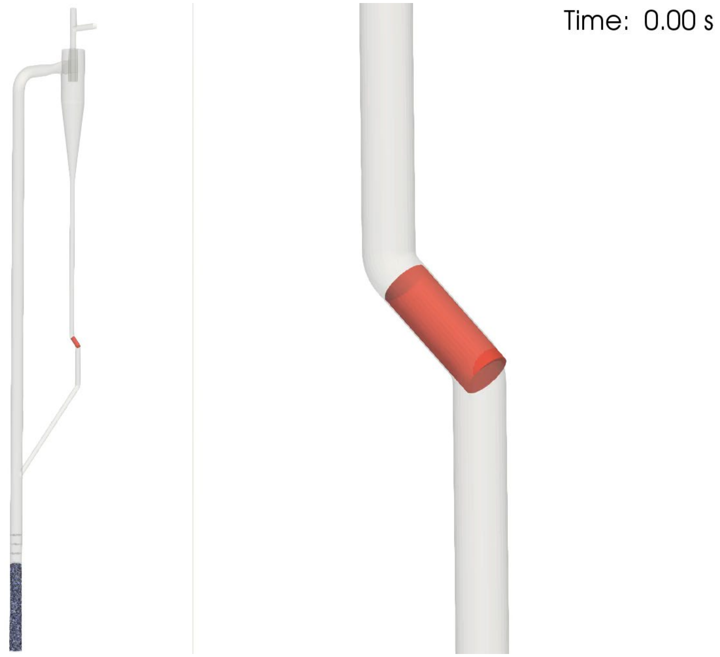
Several options to represent moving geometry

- Ability to control flow rate





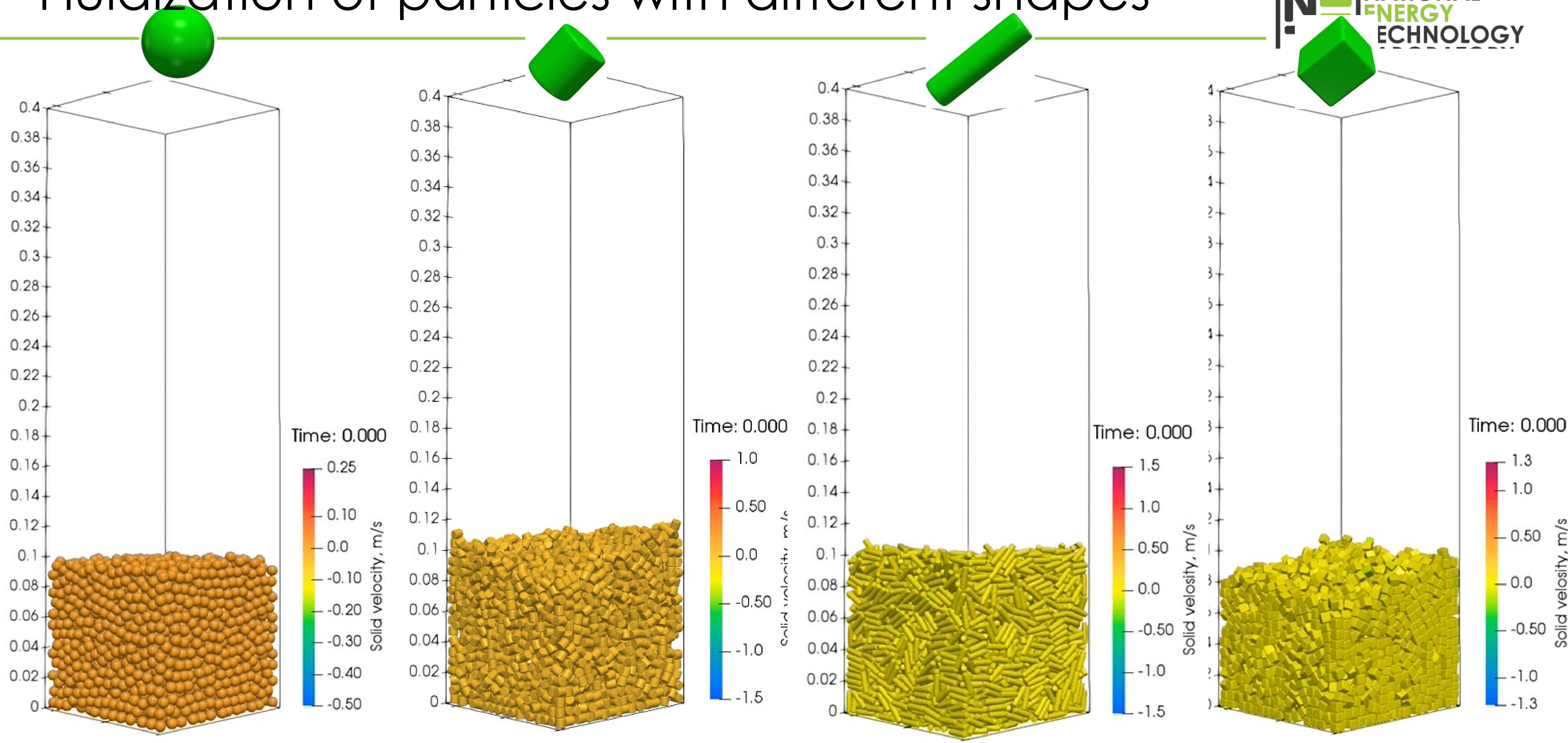




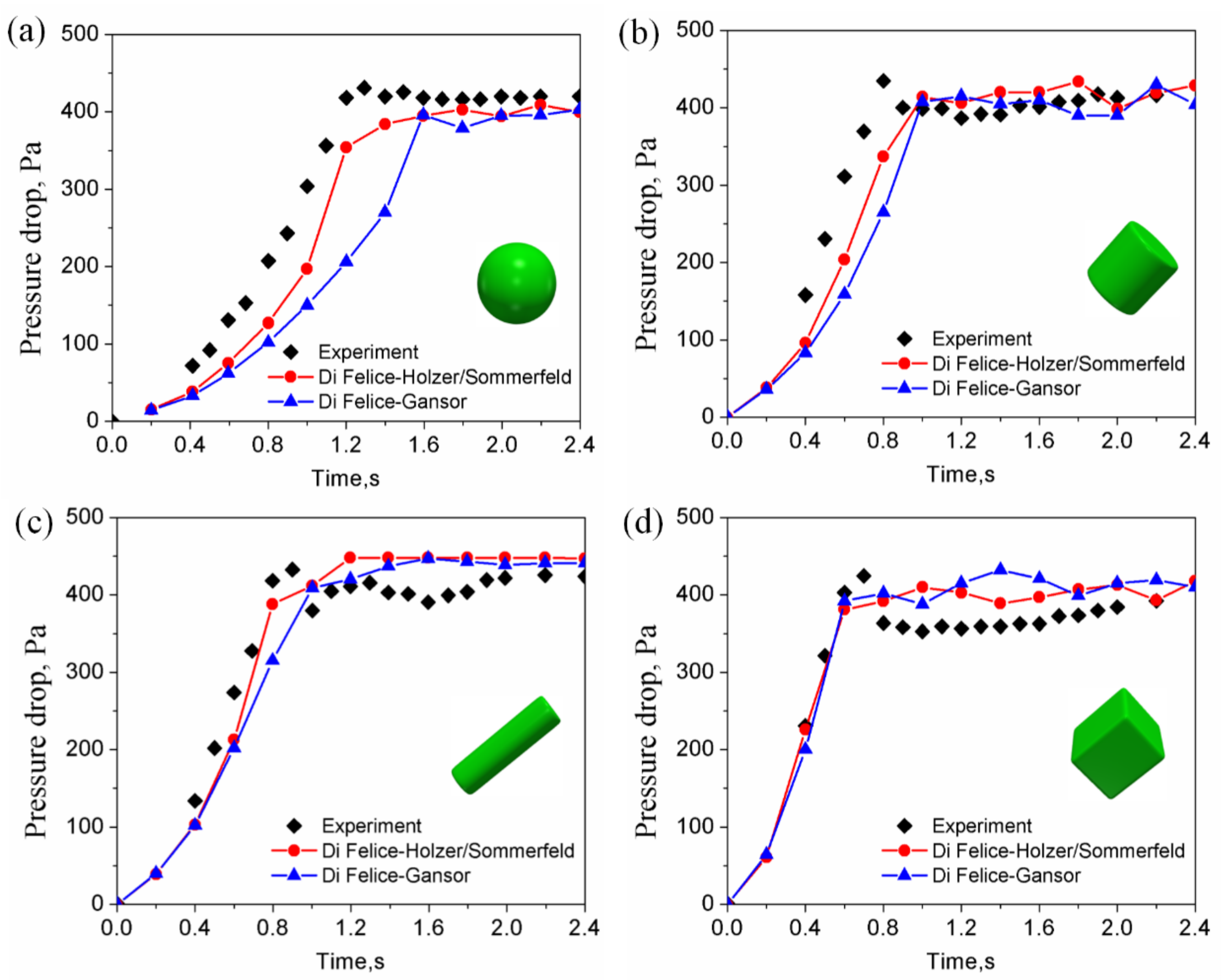
Fluidization of particles with different shapes

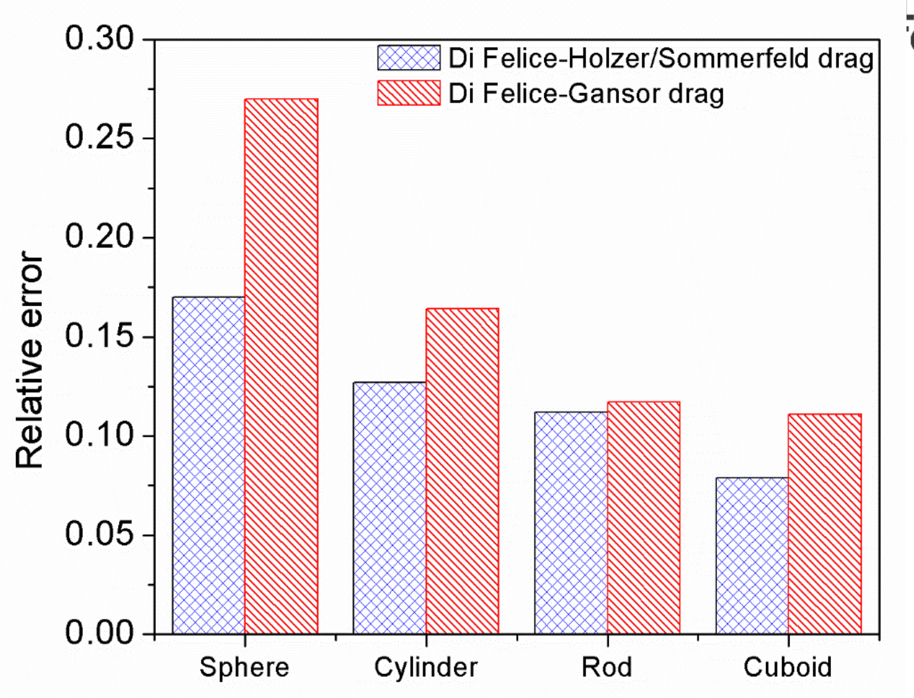
Ug=1.6 m/s

NATIONAL ENERGY TECHNOLOGY



Validation-Pressure drop





- Both drag models consider the effects of particle orientation and cell voidage
- Di Felice-Holzer/Sommerfeld drag correctly capture the pressure in both fixed bed and fluidized bed regimes for each shape particles.
- Unresolved SuperDEM-CFD can not capture the channeling flow. Particle-resolved DEM-CFD may be tested in the future.

SuperDEM development progress

- **Summary**
  - Oriented bounding box (OBB) algorithm has been implemented and verified
  - Superquadric contact algorithm has been implemented and verified
  - Quaternion theory for object orientation (rotation between local and global) has been implemented and verified
  - VTP (xml) was modified to output tensor for superquadric particle visualization
  - Superquadric particle collision with wall (plane, STL)
  - Non-linear forces between superquadric particles
  - Parallelization (MPI)
  - 100 million non-spherical particles large scale simulation on 6800 cores
  - A new interpolation scheme (DPVM-Satellites) was developed.
  - Non-spherical drag models (Di Felice-Gansor and Di Felice Holzter/SommerFeld) considering particle orientation and cell voidage were implemented
  - A new general scheme to calculate the projection area of non-spherical particle perpendicular to the flow was developed.
  - 100 million non-spherical particles fluidization simulation on 6800 cores

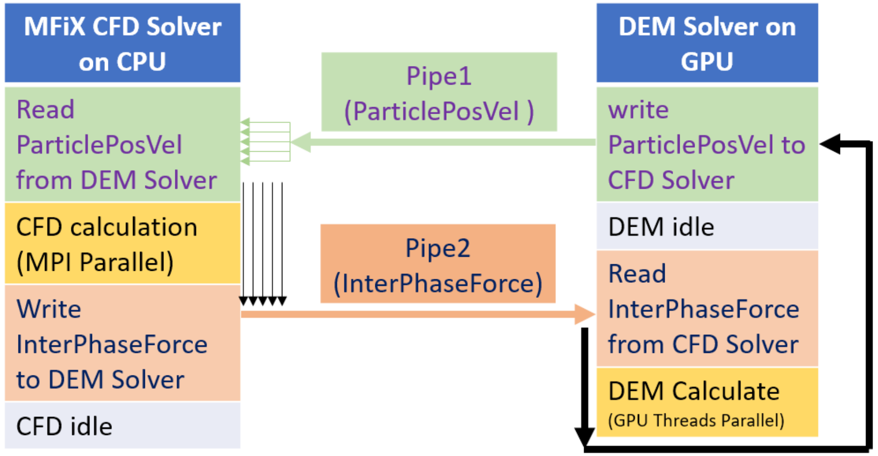
- **Future work**
  - Heat transfer, mass transfer, chemical reaction
  - Coupling with other sub-models
  - Multi-superquadric particles to model moving internals, such as baffle, moving wall, etc.
  - Advanced superquadric contact algorithm

Hundredfold Speedup of MFiX-DEM using GPU Computation

NATIONAL ENERGY TECHNOLOGY LABORATORY

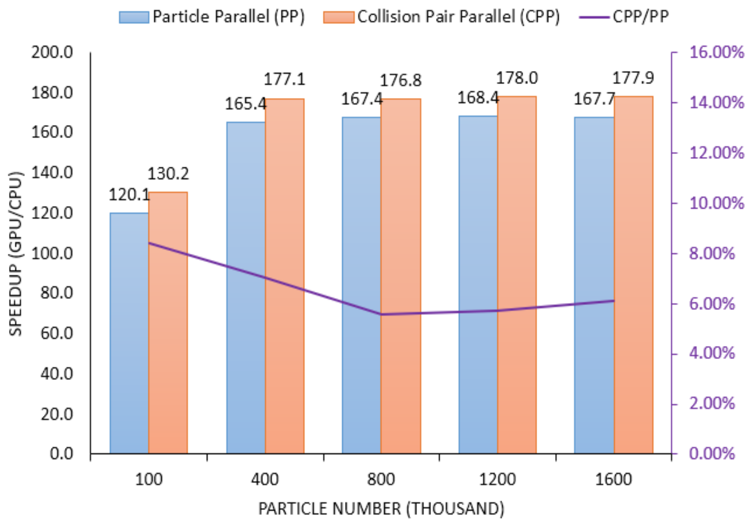
GPU Solver & MFiX coupled solver

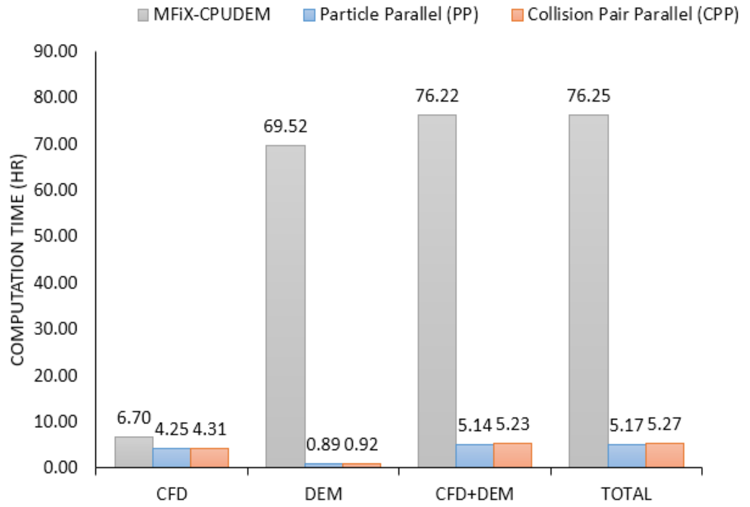
X	Start	Allocate memory, generate/read particles
Generate neighbor list	storeTOverlapToUnsortedArray	Store tangential overlap based on unsorted particle ID
	calcHash	Map particles into searching cells
	sortParticles	Sort particles based on ID of cells.
	reorderDataAndFindCellStart	1) Rearranging particle data into sorted arrays. 2) Mark the first and last particles in each cell
	generateNeighborList	1) For each particle, calcBinPos, loop over particles in each neighbor bin, store neighbor particles 2) copy tangential overlaps
	collide	1) collision with neighbor particles 2) collision with boundaries
	updatePosVelOmg	Update pos/vel/omega
X	End	Release memory



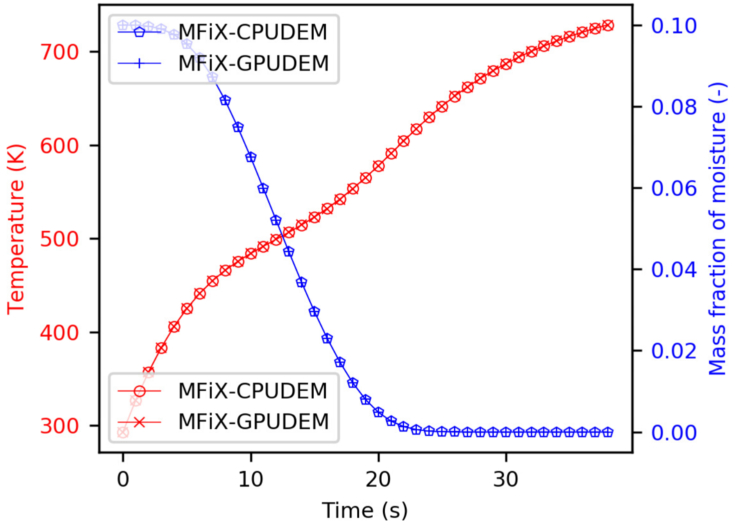
Algorithm of GPU-MFiX data exchange through pipes. Multiple small arrow lines on CPU side indicate MPI parallel processes. DEM is limited to one GPU card.

Speedup in Simulations of particle packing (up) & Fluidized bed (bottom)





Heat transfer & chemical reactions (biomass drying)

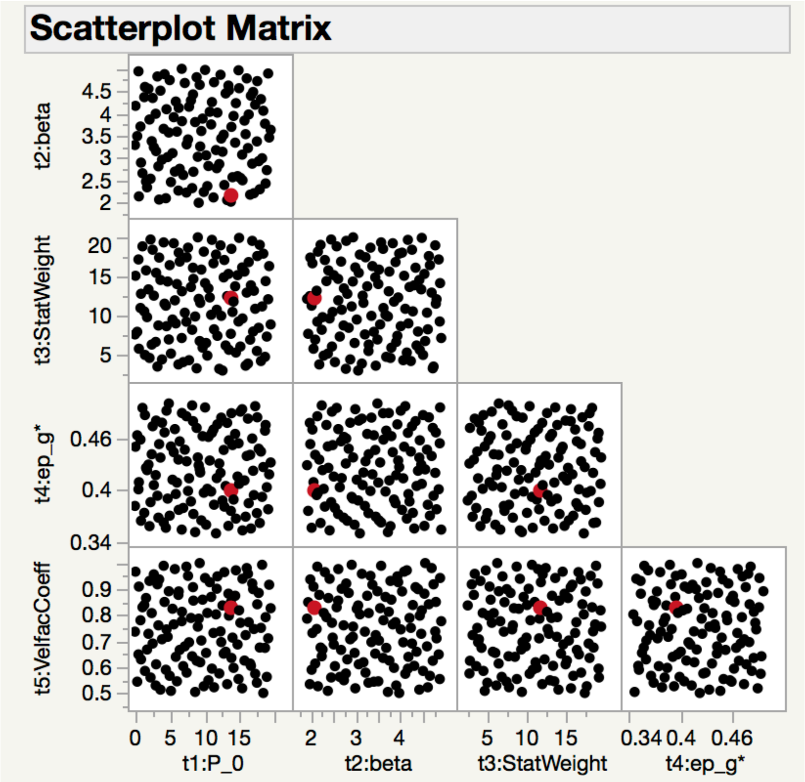


- ➢ DEM solver is ported to GPU
- ➢ 170 fold speedup with double precision, 243 fold with single precision
- ➢ Re-use CFD, interphase coupling, and chemical reaction modules in MFiX

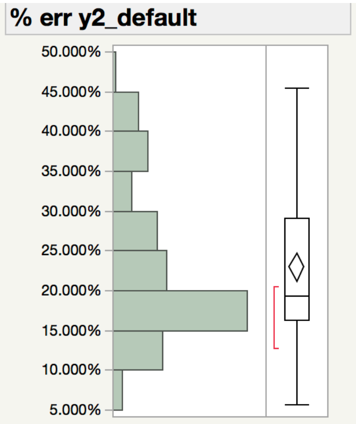
C1: Particle settling

Deterministic calibration (using 120 samples and PSUADE)

Testing calibrated parameters at “unseen” settings



Comparing Distribution of % Error (Default vs Calibrated Settings)

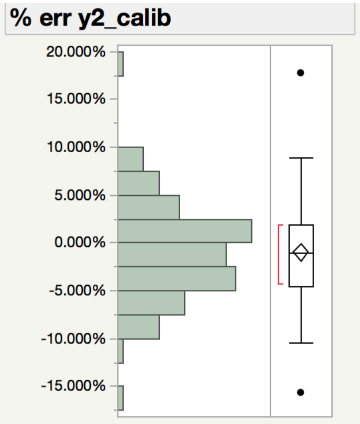


Quantiles

100.0%	maximum	45.450%
99.5%		45.450%
97.5%		44.450%
90.0%		38.590%
75.0%	quartile	29.090%
50.0%	median	19.390%
25.0%	quartile	16.340%
10.0%		13.190%
2.5%		9.080%
0.5%		5.620%
0.0%	minimum	5.620%

Summary Statistics

Mean	0.2299454
Std Dev	0.0950501
Std Err Mean	0.0087132
Upper 95% Mean	0.2471999
Lower 95% Mean	0.2126908
N	119

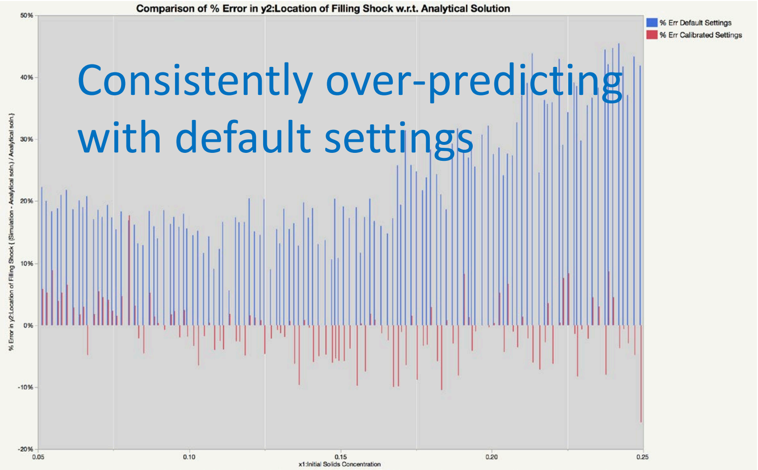


Quantiles

100.0%	maximum	17.730%
99.5%		17.730%
97.5%		8.670%
90.0%		5.250%
75.0%	quartile	1.850%
50.0%	median	-1.030%
25.0%	quartile	-4.530%
10.0%		-7.180%
2.5%		-9.960%
0.5%		-15.690%
0.0%	minimum	-15.690%

Summary Statistics

Mean	-0.009611
Std Dev	0.0500527
Std Err Mean	0.0045883
Upper 95% Mean	-0.000525
Lower 95% Mean	-0.018697
N	119



22.99% vs -0.96%

With calibrated settings for all 5 parameters both over-predicting with default settings