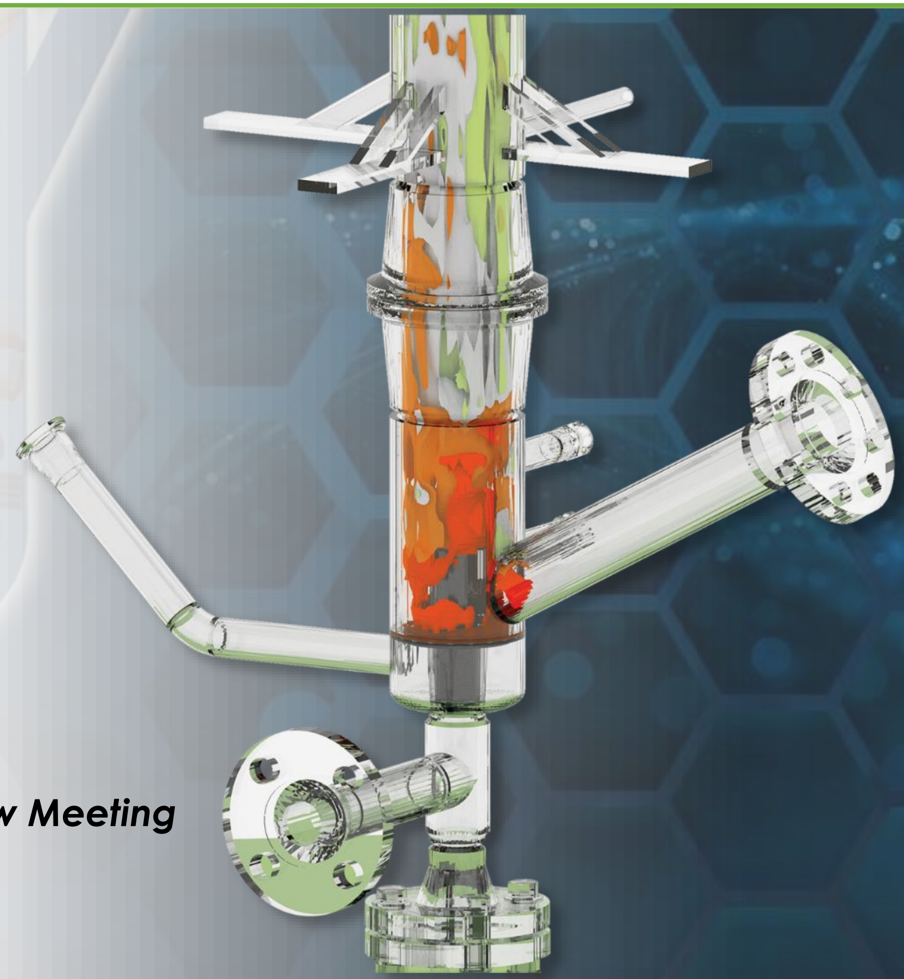
CARD: CFD for Advanced Reactor Design

Software Tools and Expertise to Address Multiphase Flow Challenges in Research, Design, and Optimization

Jeff Dietiker

NETL Support Contractor



2023 Spring FECM R&D Project Review Meeting

April 20, 2023

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CARD FWP – EY22 Task Structure

Task 2: MFiX Suite Multiphase Code Development, Validation and Enhancements

PI: Jeff Dietiker

- MFiX 22.3 release (Oct 2022) included force chain data visualization
- MFiX 22.4 release (Dec 2022) included new SuperDEM code and code acceleration features
- VVUQ: Bayesian statistical analysis of MFiX-PIC
- ML: Filtered drag model implementation

Task 3: Wafer Scale Engine Programming

PI: Dirk Van Essendelft

- First coupled single-phase CFD simulation completed
- Benchmark computational cycles timing report completed

Project Update

Task 2: MFiX Development, Validation, and Enhancements

- Graphical user interface (GUI)
    - Increase usability of the code
    - Minimize error in setup, execution, and post processing
- Additional models/physics required for challenging Fossil Energy and Carbon Management (FECM) applications:
    - Particle in cell
    - Coarse grain discrete element method
    - Non-spherical particles
    - Polydispersity
- Quality assurance (QA) program
    - Validation
    - Verification
    - Improved documentation, user guides, and validation experiments
- Machine learning integration
- Outreach capabilities through the MFiX web portal to better serve FECM and NETL stakeholders

MFiX Suite of Multiphase CFD Software

Capabilities and Benefits

MFiX Multiphase Flow with Interphase eXchanges

NETL flagship (CFD) code

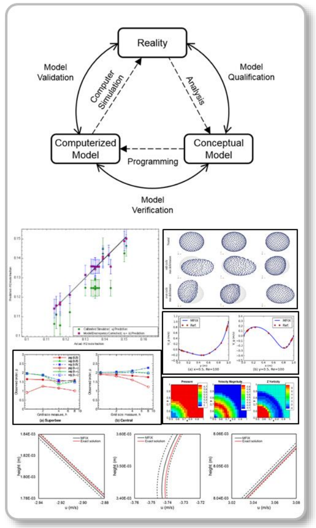
3 Decades
of development history

7,500+
registered users

300+
downloads per month

650
citations per year

- **Versatile toolset** (hydrodynamics, heat transfer, chemical reactions)
- **Gas/solids flows**
    - Gas: transport equations (continuity, momentum energy species)
    - Solids: transport equations or particle tracking
- **Open source**
    - Developed at NETL, in-house expertise
    - Runs on large High-Performance Computing (HPC) systems
- **Accelerate development and reduce cost**
- **Optimizes performance**
- **Reduces design risks**

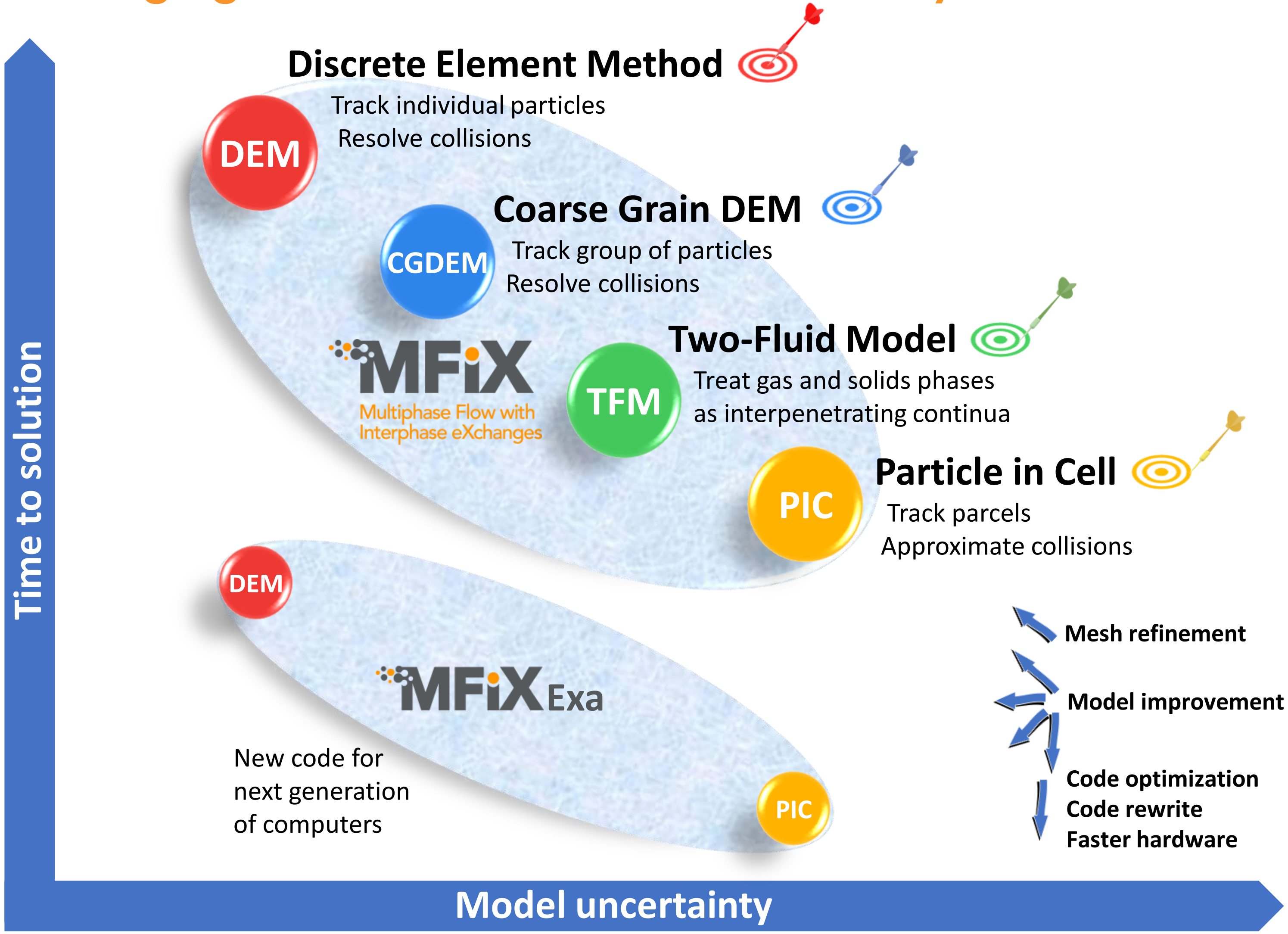


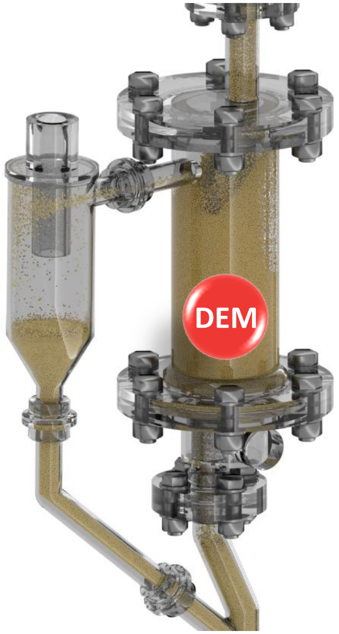
- **MFiX-TFM (Two-Fluid Model)**
- **MFiX-DEM (Discrete Element Model)**
- **MFiX-PIC (Multiphase Particle-In-Cell)**
- **MFiX-CGDEM (Coarse Grain DEM)**
- **MFiX Exa (Exascale) – Under Development**
- **C3M Multiphase Chemistry Management Software**
- **Nodeworks: Optimization and UQ Toolsets**
- **Tracker: Object Tracking in Videos/Image Stack**

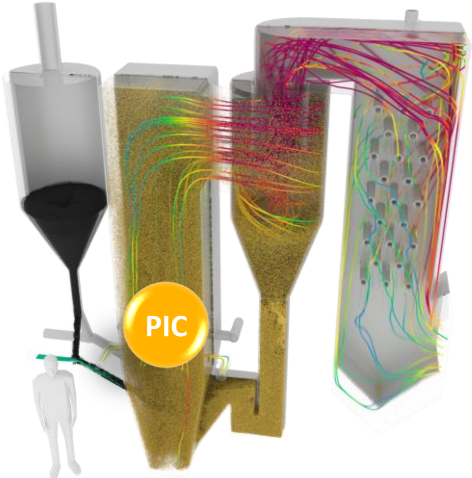
Multiphase Flow Science Software Portfolio

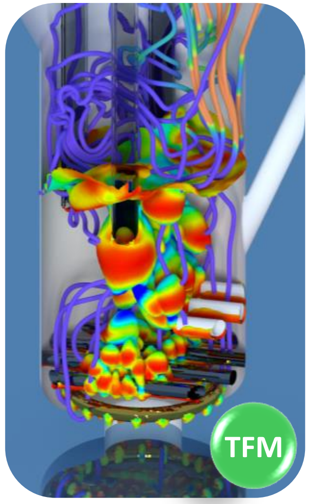
MFiX Suite of Multiphase CFD Software

Managing the Tradeoff Between Accuracy and Time to Solution

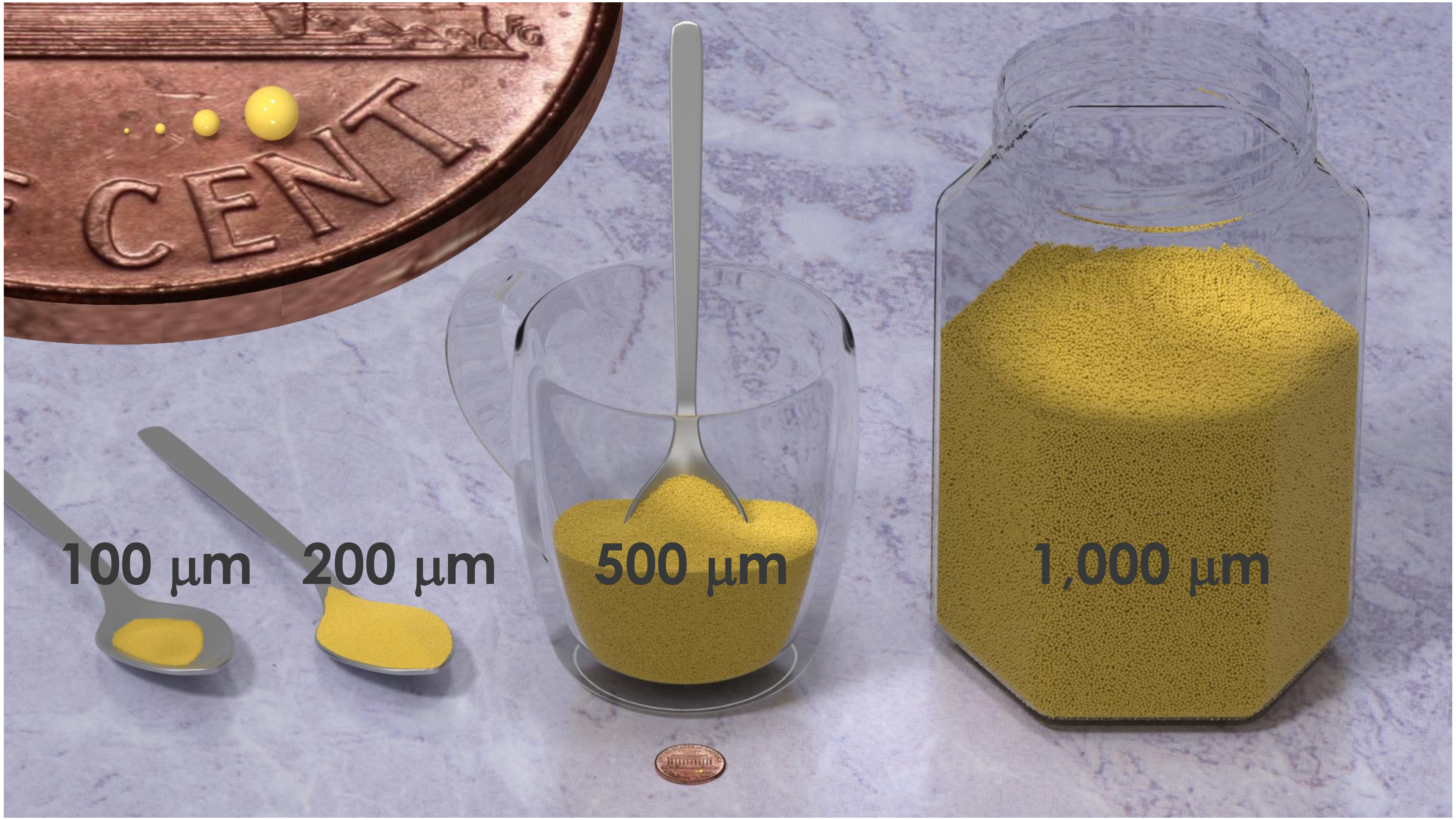








What can be Modeled with 1 Million Particles?



Enabling Large-Scale Simulations

Enabling Large-Scale Simulations

DEM example

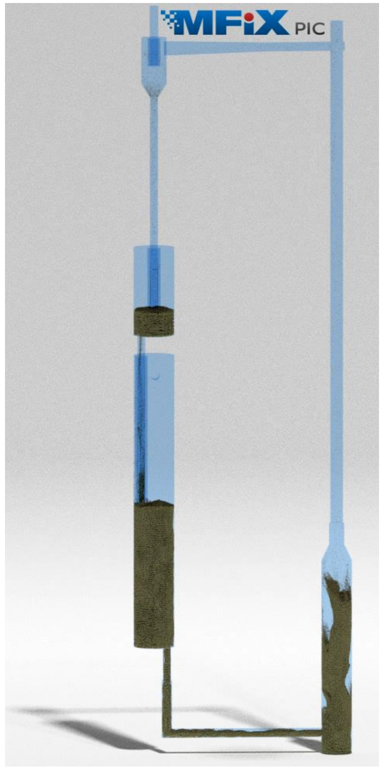
- Height = 0.68 m
- Particle diameter = 800 microns
- Particle count = 500,000 particles

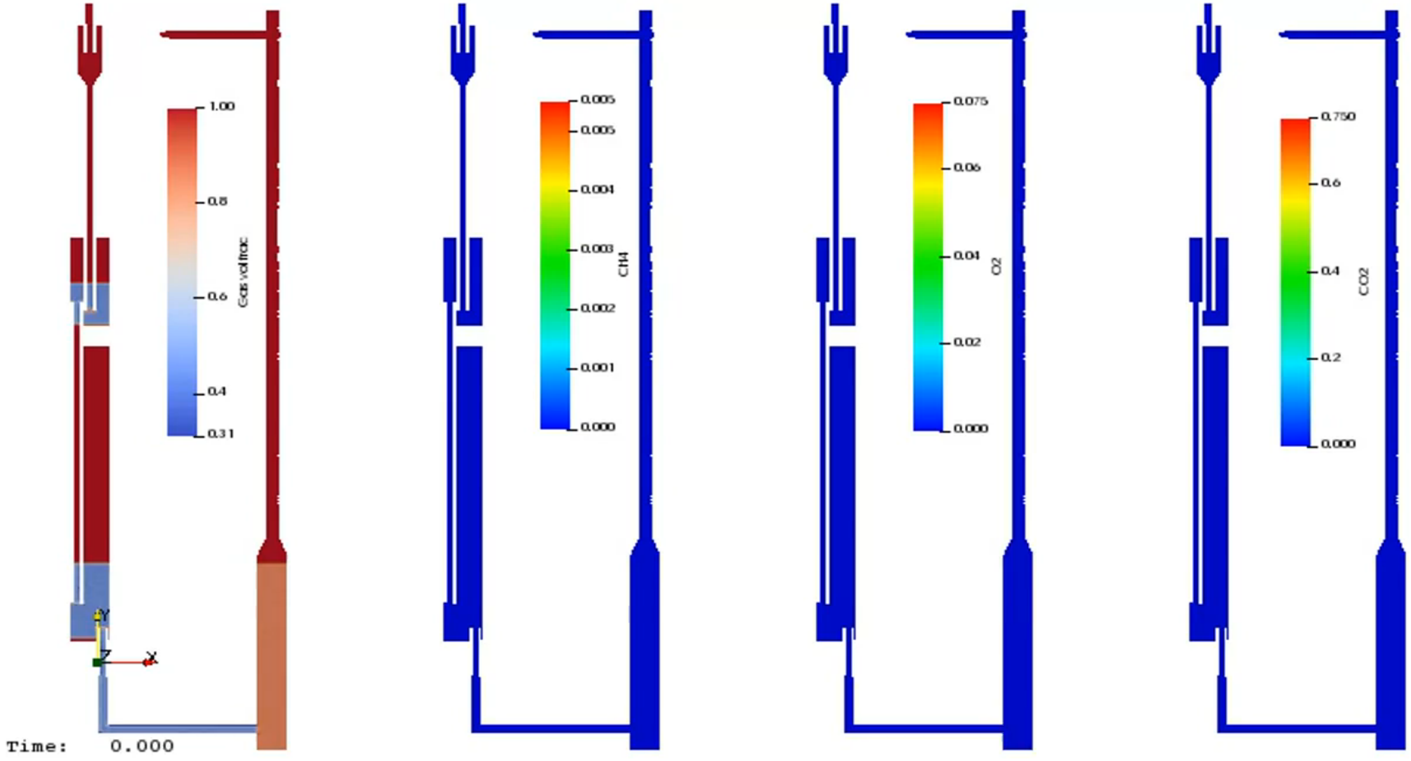
Enabling Large-Scale Simulations

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)





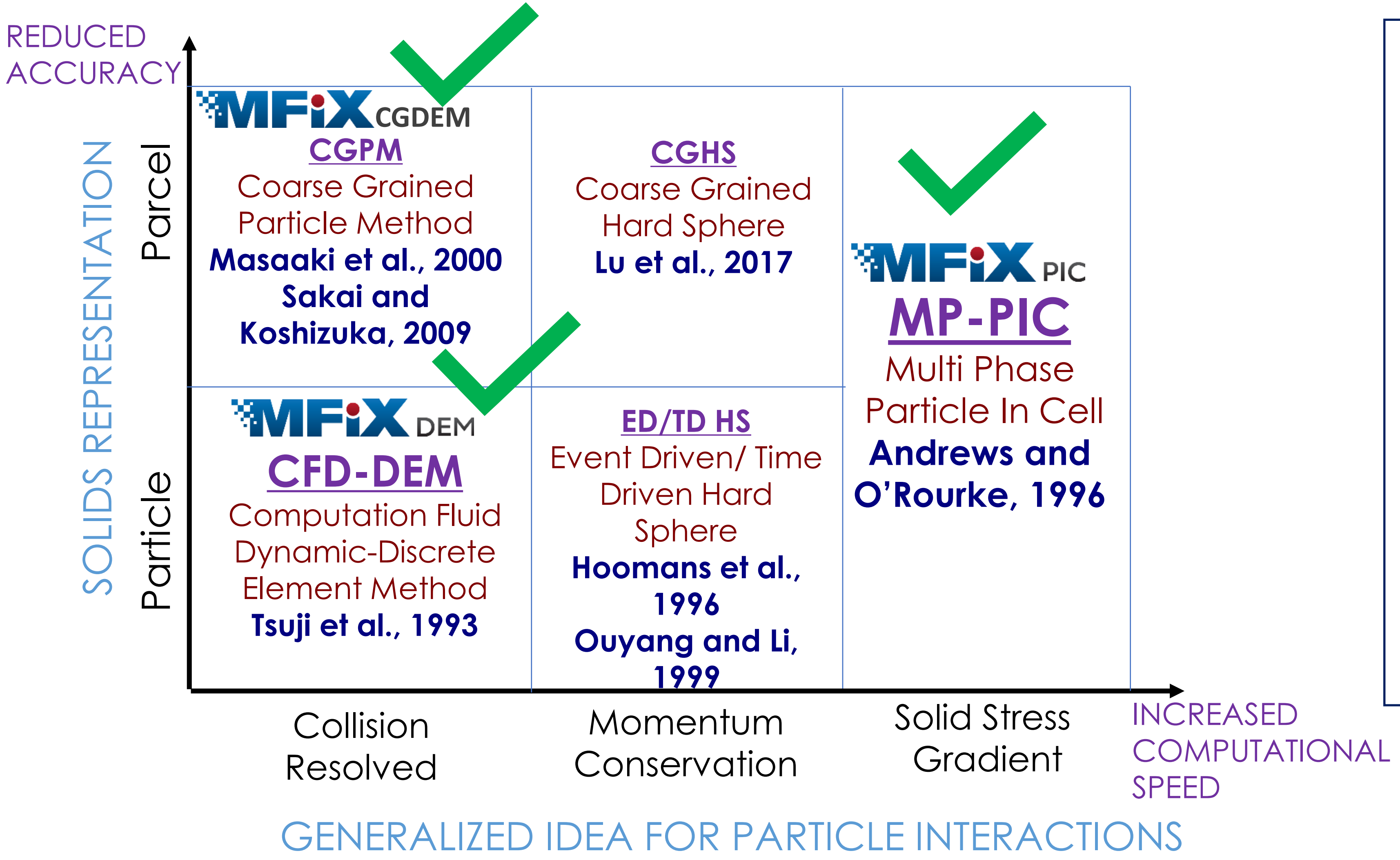
Simulation of industrial scale multi-phase flow devices is within MFiX's grasp!

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, with tractable time to solution.

Multiphase Particle In Cell (MP-PIC)

Use MP-PIC for Computational Speed and Averaged Accuracy



Particle Flow in Cyclone

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

MFiX Development

PIC Collision Damping

- Collision of gas–solid jets
- Two jets colliding
- Solids fraction = 0.1, velocity = 20 m/s
- No energy loss at walls (e_w = 1)
- Statistical weight = 1
- Polydisperse system, particle diameter:
    - Mean=650 μm, σ=25 μm, clipped at mean±2σ
    - Mean=350 μm, σ=25 μm, clipped at mean±2σ
- Without collision damping, the two jets do not interact

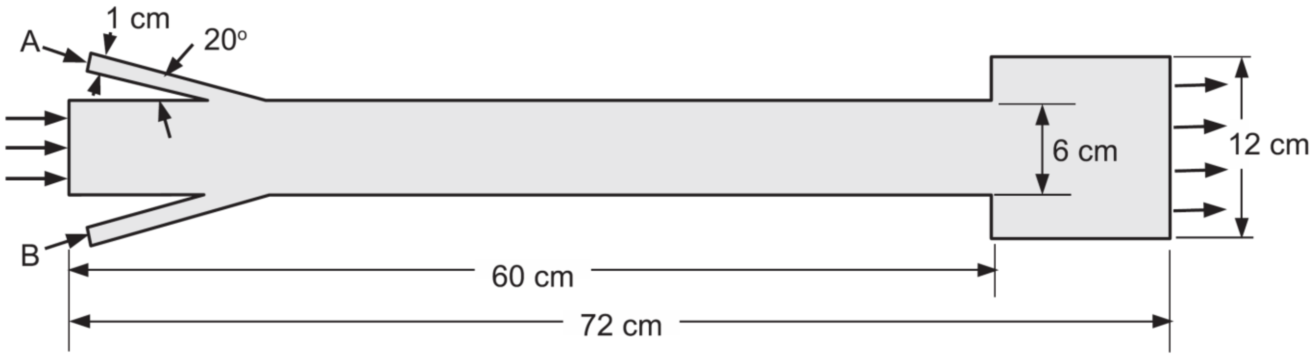
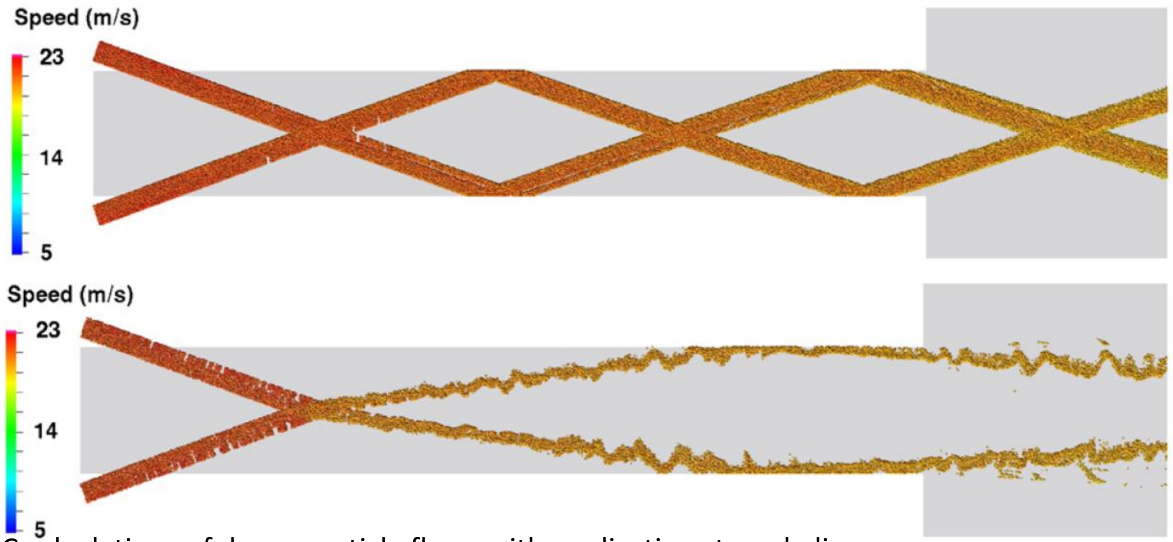


Fig. 5. Channel geometry used for the calculations of two impinging gas-particle jets.



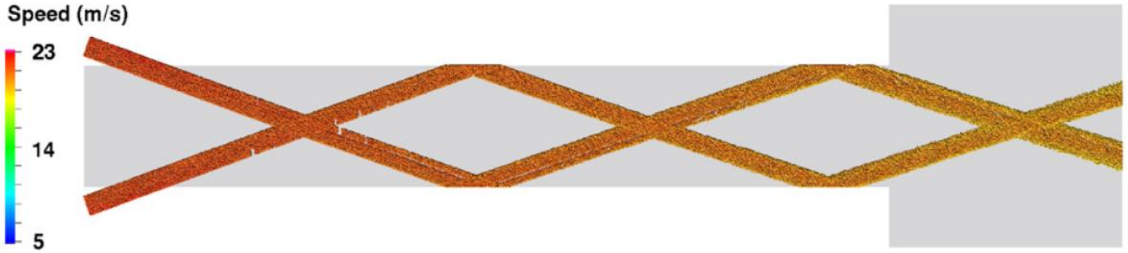
Peter J. O'Rourke, Dale M. Snider,"An improved collision damping time for MP-PIC calculations of dense particle flows with applications to polydisperse sedimenting beds and colliding particle jets", Chemical Engineering Science,Volume 65, Issue 22, 2010, https://doi.org/10.1016/j.ces.2010.08.032.

MFiX Development

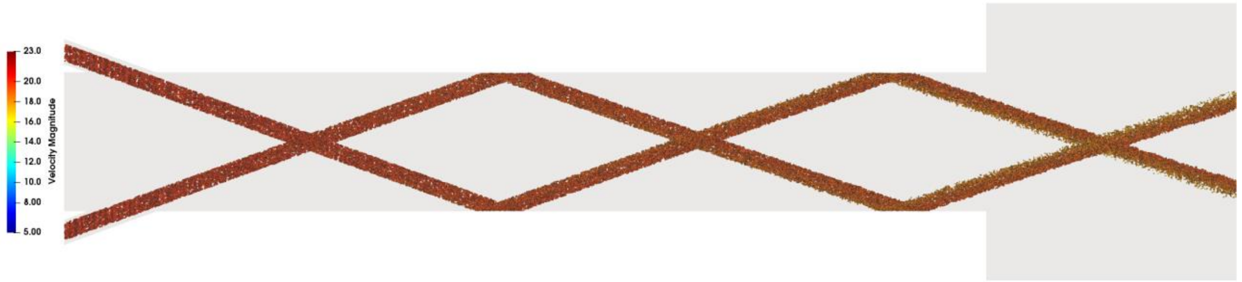
NATIONAL ENERGY TECHNOLOGY LABORATORY

Mean=650 μm, σ=25 μm, Clipped at Mean±2σ

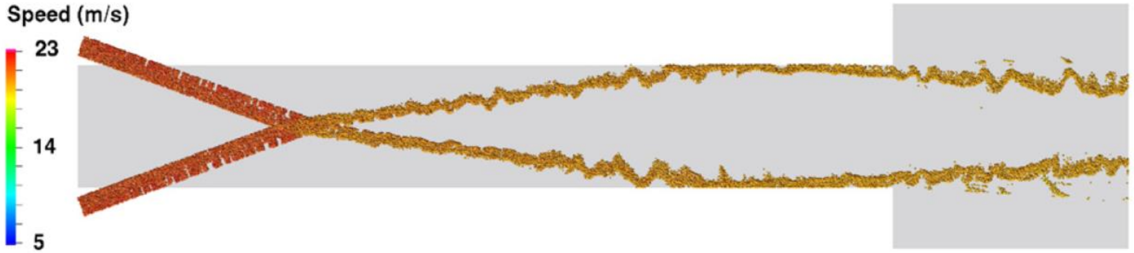
No damping



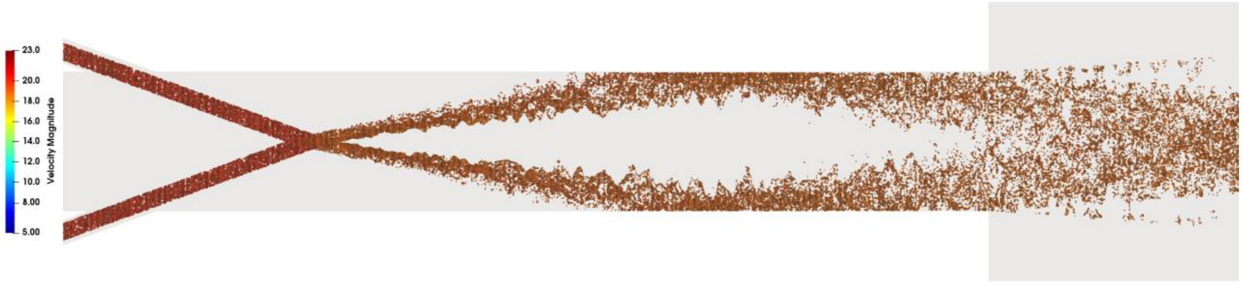
No damping



With damping, ep=0.8



With damping, ep=0.8

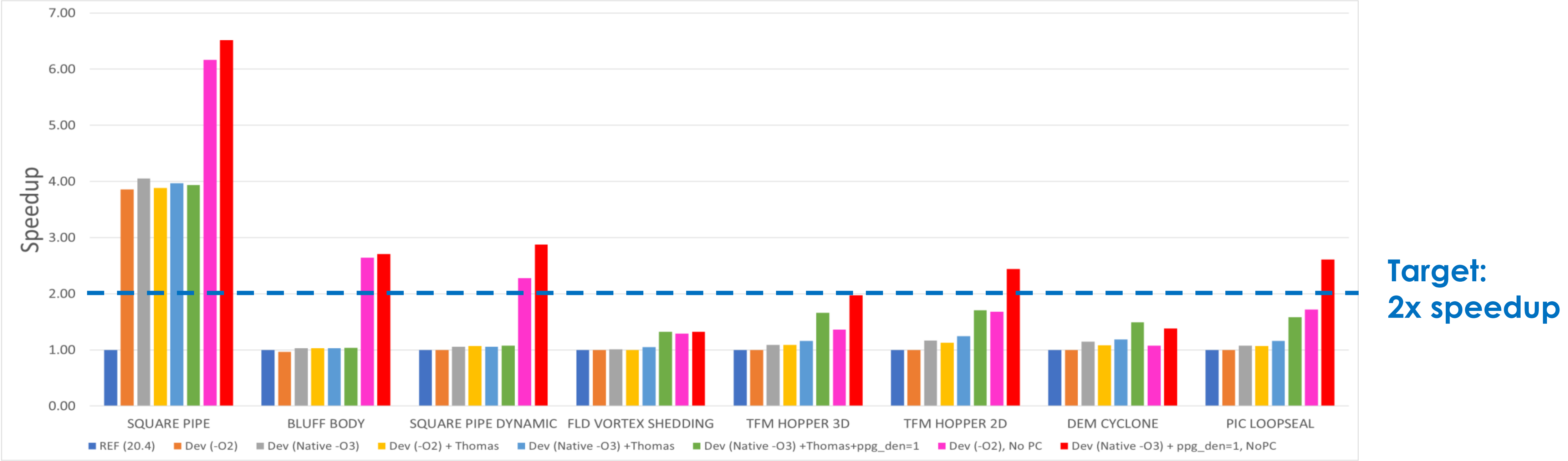


Barracuda
(Paper)

MFiX

Fluid Solver Acceleration

- New convergence criteria for Steady State: ~ 4x speedup
- "march=native –O3": 3 to 14% faster
- Optimized Thomas algorithm: 3 to 11% faster
- Lowering ppg_den from 10 to 1: up to 25% faster (helps when ppg is dominant residual)
- Turning off the PC: ~ 2x speedup (fluid solver)
  - May fail to converge if DT=cst with bad initial conditions (need to set adaptive time step)
- Best combination: No PC, "march=native –O3" flag, ppg_den=1

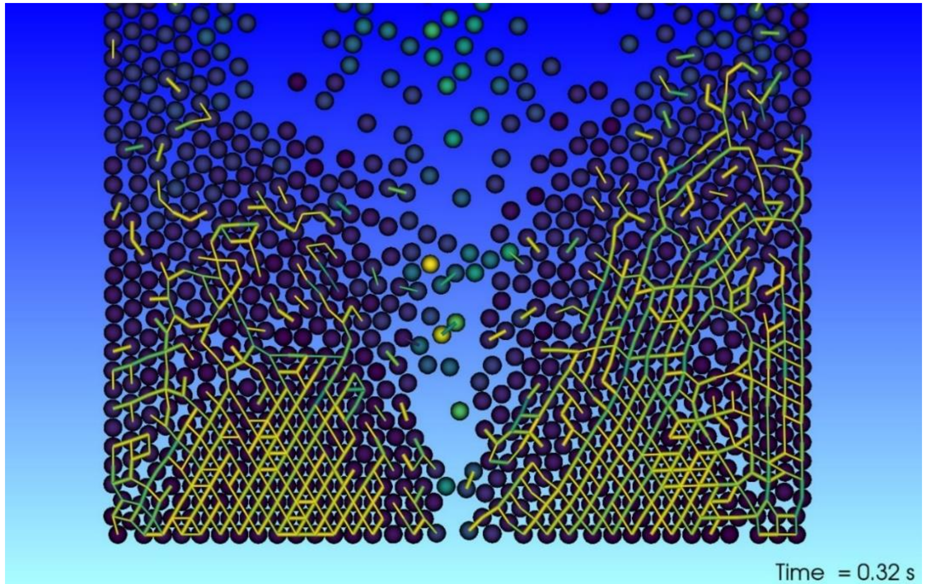


MFiX Development

MFiX 22.3 (Oct 2022) Release

Force Chain Data Visualization

What is it and why do we care? A force chain data visualization allows a researcher to examine areas where groups of particles are held together by compressive forces. Think about how bricks, without mortar, are held into an arch.



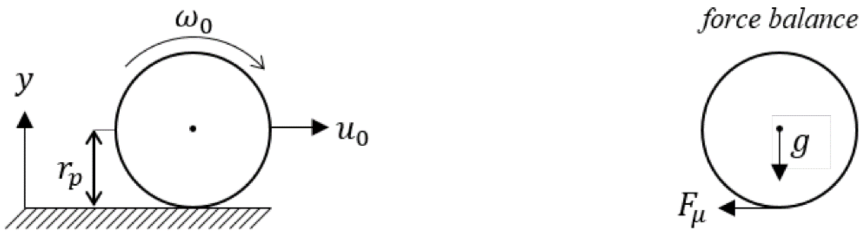
Still image from MFiX-GUI

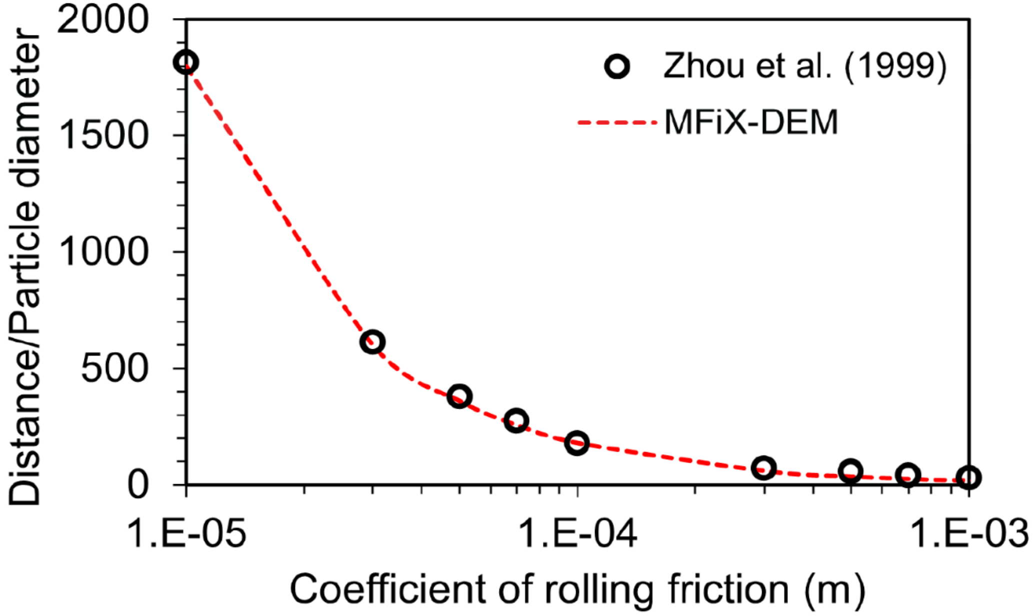
The MFiX GUI now allows a user to see how forces connect static particles at a given point in time.

Impact: CFD models of granular solids, where force chain data is characterized, inform reactor designers of solids stagnation points. This information can be used to eliminate these dead areas in reactors and in discharge configurations where bridging can be catastrophic.

MFiX Development

22.1 DEM Rolling Friction





Y.C. Zhou, B.D. Wright, R.Y. Yang, B.H. Xu, A.B. Yu, "Rolling friction in the dynamic simulation of sandpile formation", Physica A: Statistical Mechanics and its Applications, Volume 269, Issues 2–4, 1999, Pages 536-553, ISSN 0378-4371, https://doi.org/10.1016/S0378-4371(99)00183-1.

Non-Spherical Particles (SuperDEM)

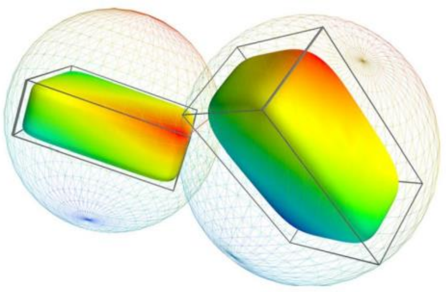
- Superquadrics are a family of geometric shapes defined as

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

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

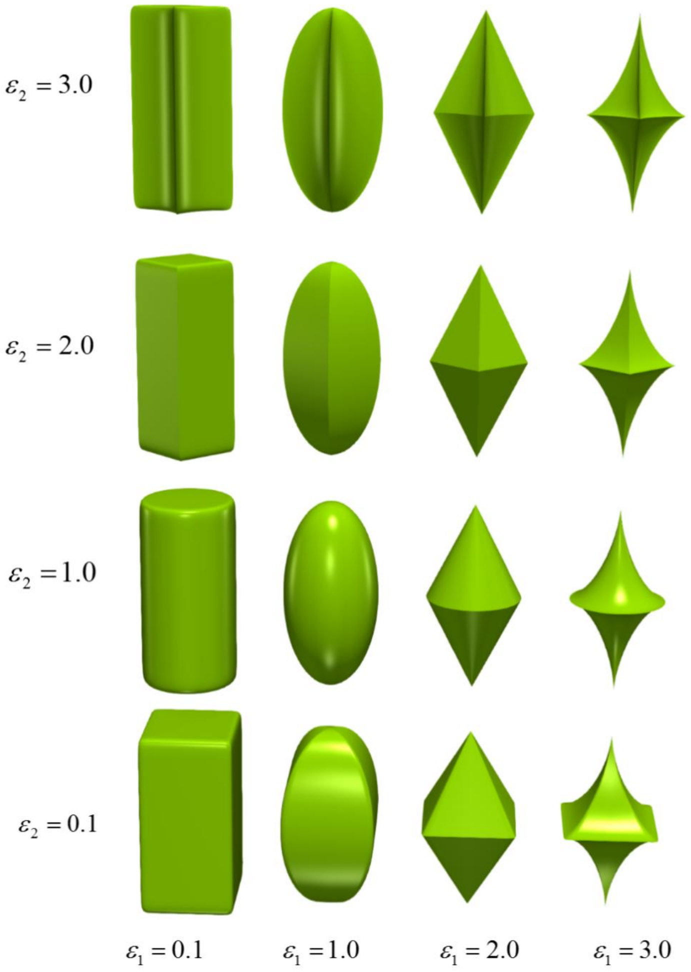
$$[a_1, a_2, a_3, \varepsilon_1, \varepsilon_2]^T$$

Semi-axis (a_1, a_2, a_3)   Roundness parameters ($\varepsilon_1, \varepsilon_2$)



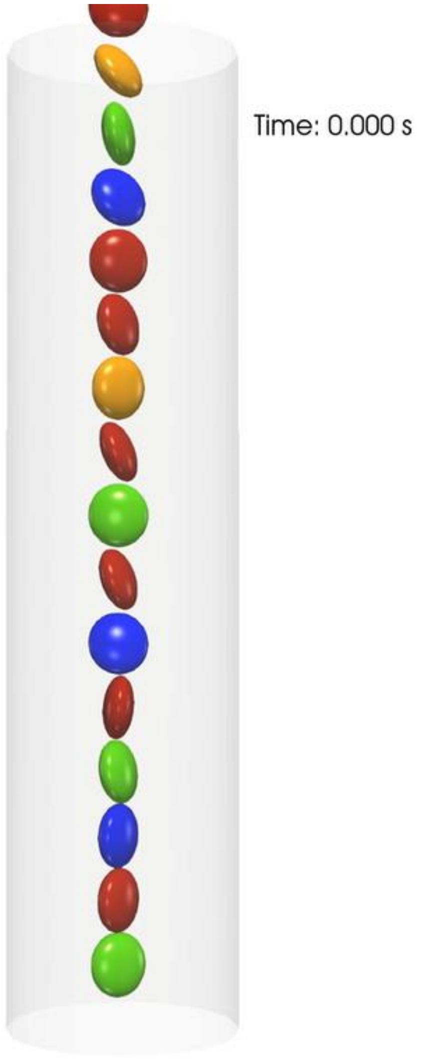
Bounding spheres and oriented bounding boxes

Superquadric particles

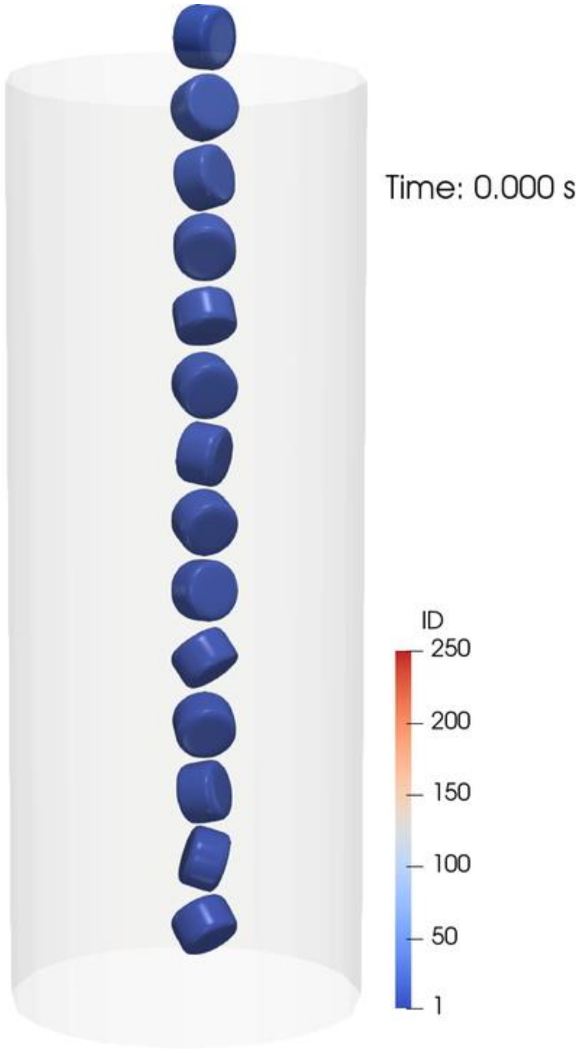


a1=2
a2=2
a3=4

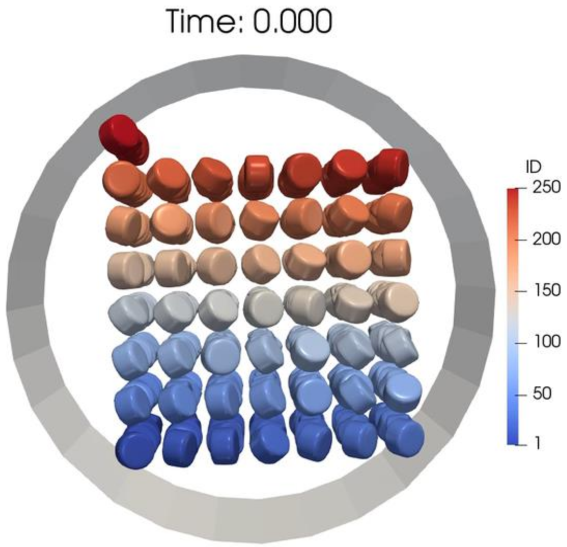
SuperDEM Examples



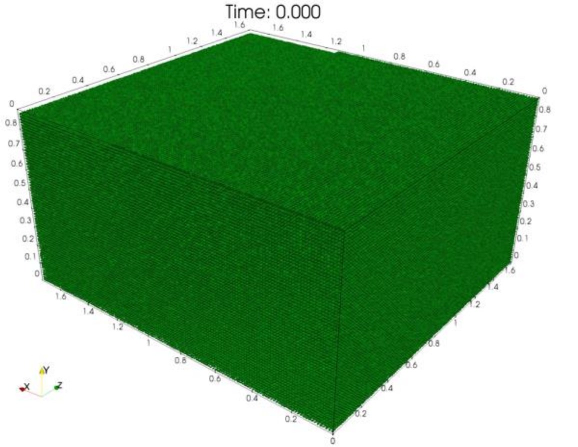
M&M candy static packing



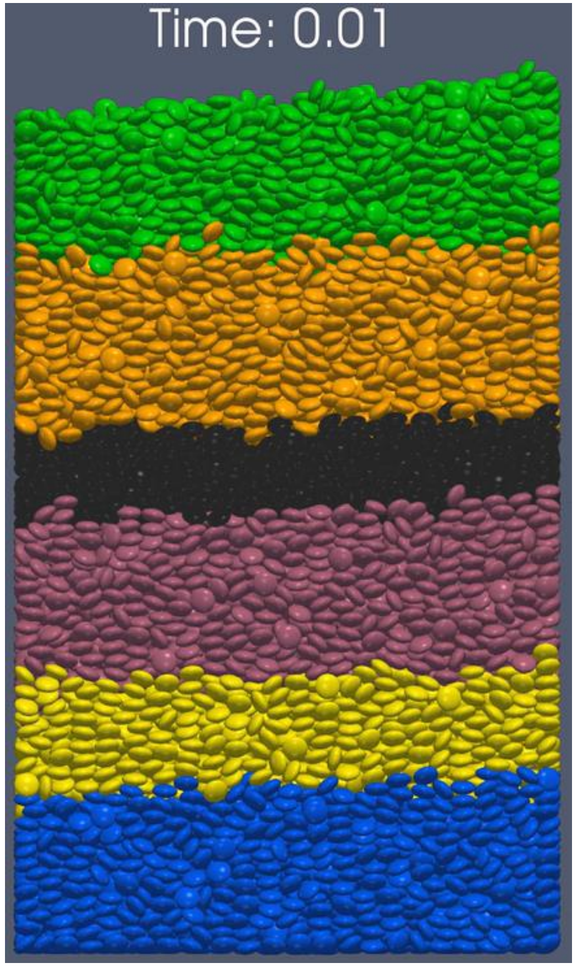
Cylinder candy static packing



Cylinder rotating drum

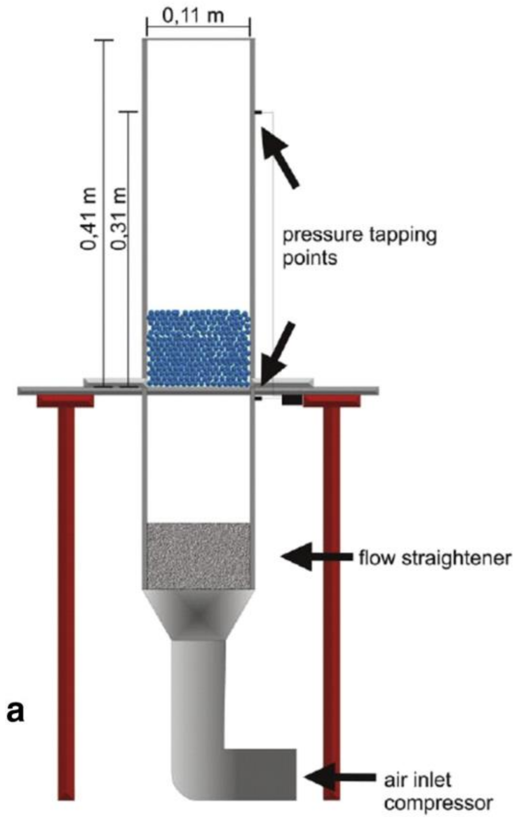


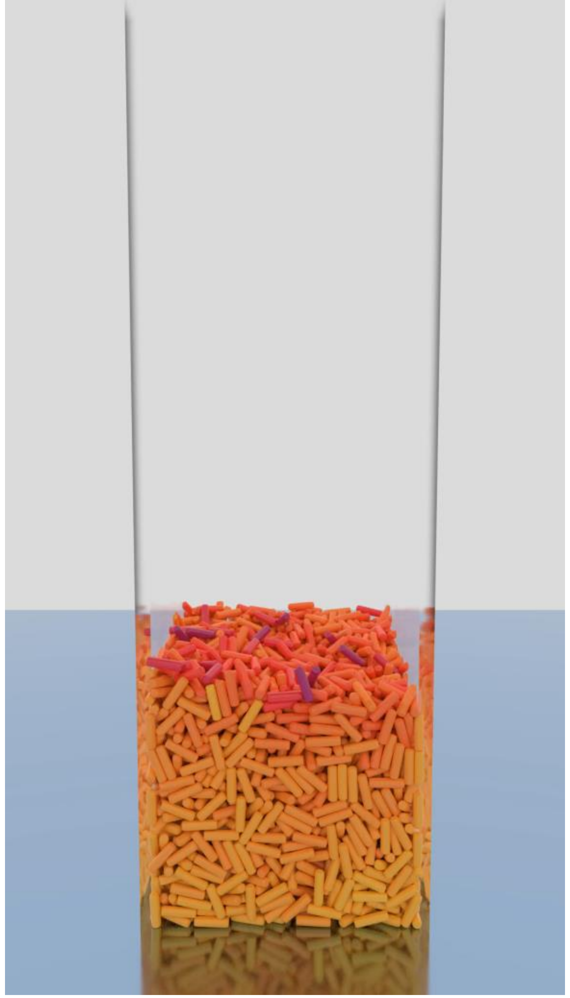
1 million non-spherical particles



M&M candy hopper discharge

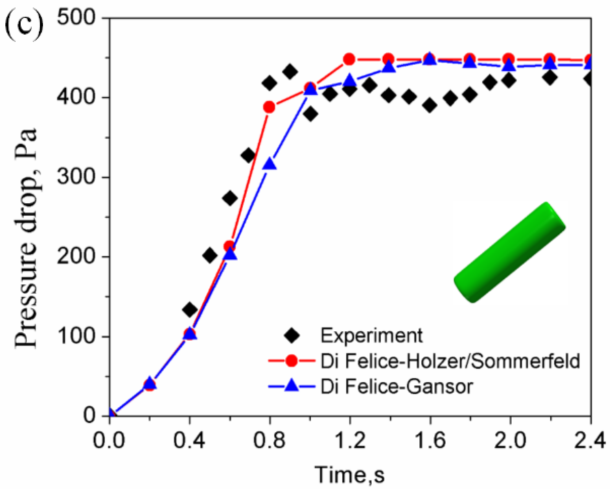
Validation Experiment





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			



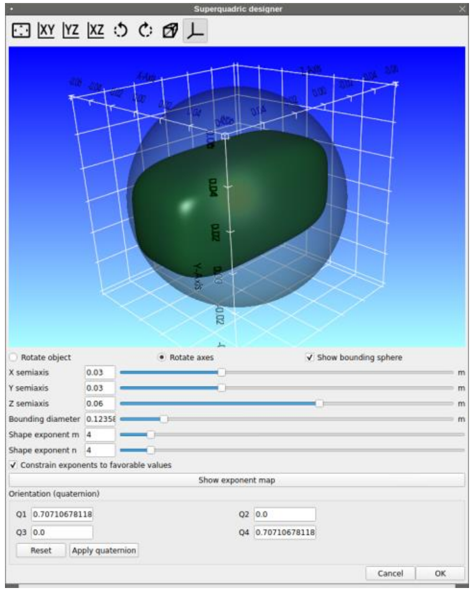
Experiment: Vollmari K, Jasevičius R, Kruggel-Emden H. Experimental and numerical study of fluidization and pressure drop of spherical and non-spherical particles in a model scale fluidized bed. Powder Technology. 2016;291:506-521.

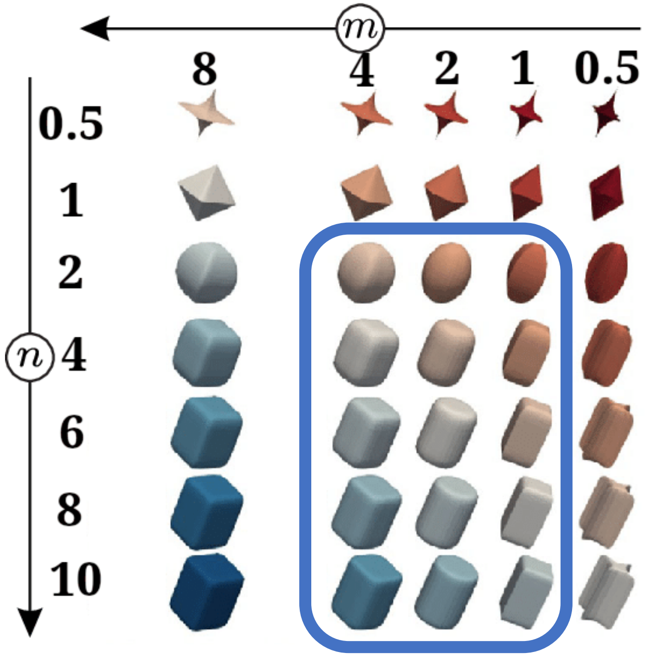
SuperDEM

Non-Spherical Particles Code Acceleration

$$\left(\left|\frac{x}{a}\right|^{m} + \left|\frac{y}{b}\right|^{m}\right)^{n/m} + \left|\frac{z}{c}\right|^{n}$$

- Need to compute x^y for non-integer x and y
- Range $0 \le x \le 2$ and $y \ge 1.$
- 70% code spent on exponentiations
- Integer powers and square roots are computationally inexpensive
- We can compute certain powers quickly, e.g., $x^{2.5}$ is x*x*sqrt(x) (not an approximation)
- Constrain m and n to be integers or dyadic rationals
- Developed new function xpow
- **6x speedup** compared with built-in math library
- Overall speedup on hopper benchmark is about **2.1x**





SuperDEM

MFiX 22.4 (Dec 2022) Release

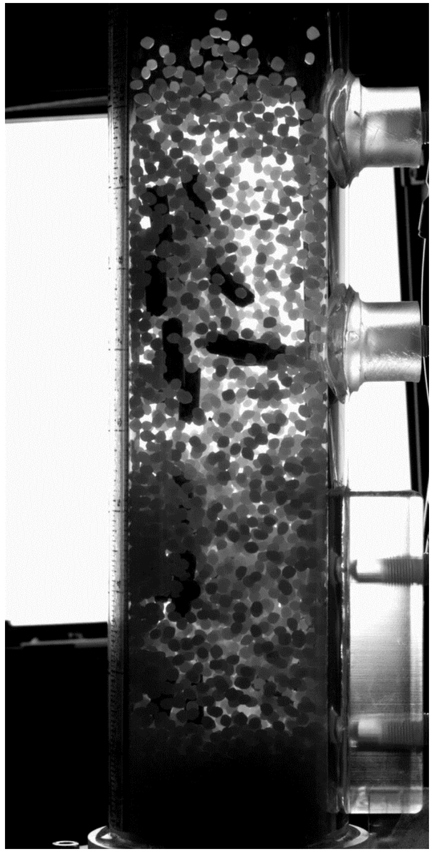
Superquadric Discrete Element Model (SuperDEM)

Impact: Realistic CFD simulation captures realistic physical outcomes.

LDPE particles
Dp = 3.755 mm
ρ = 930 kg/m^3
N=5788

Woody biomass
Dp = 6 mm
Length=12 mm
ρ = 1158 kg/m^3
N=100

CARD continues to advance CFD tools to better support FECM mission to minimize environmental impacts of fossil fuels while working towards net-zero emissions.

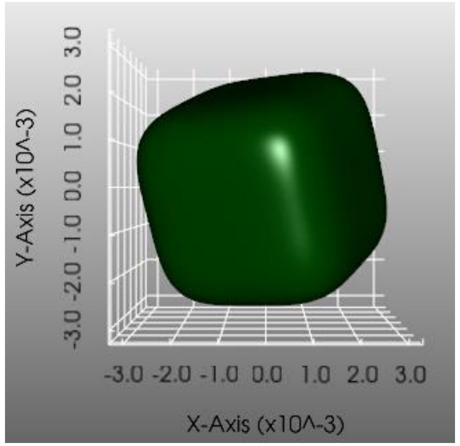


Impact Application: H_2 production by co-firing biomass and plastic

Application of SuperDEM on the Dice-Alignment Problem

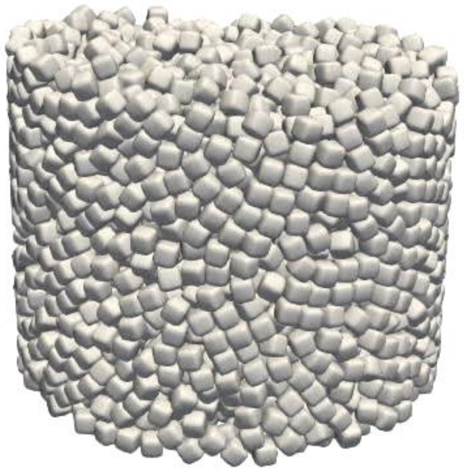
(a) Initial state

(b) Final state



- ~4000 Particles
  $R_{\text{particle}} = 0.25\ cm$
- $R_{\text{container}} = 5\ cm$

Time: 0 s



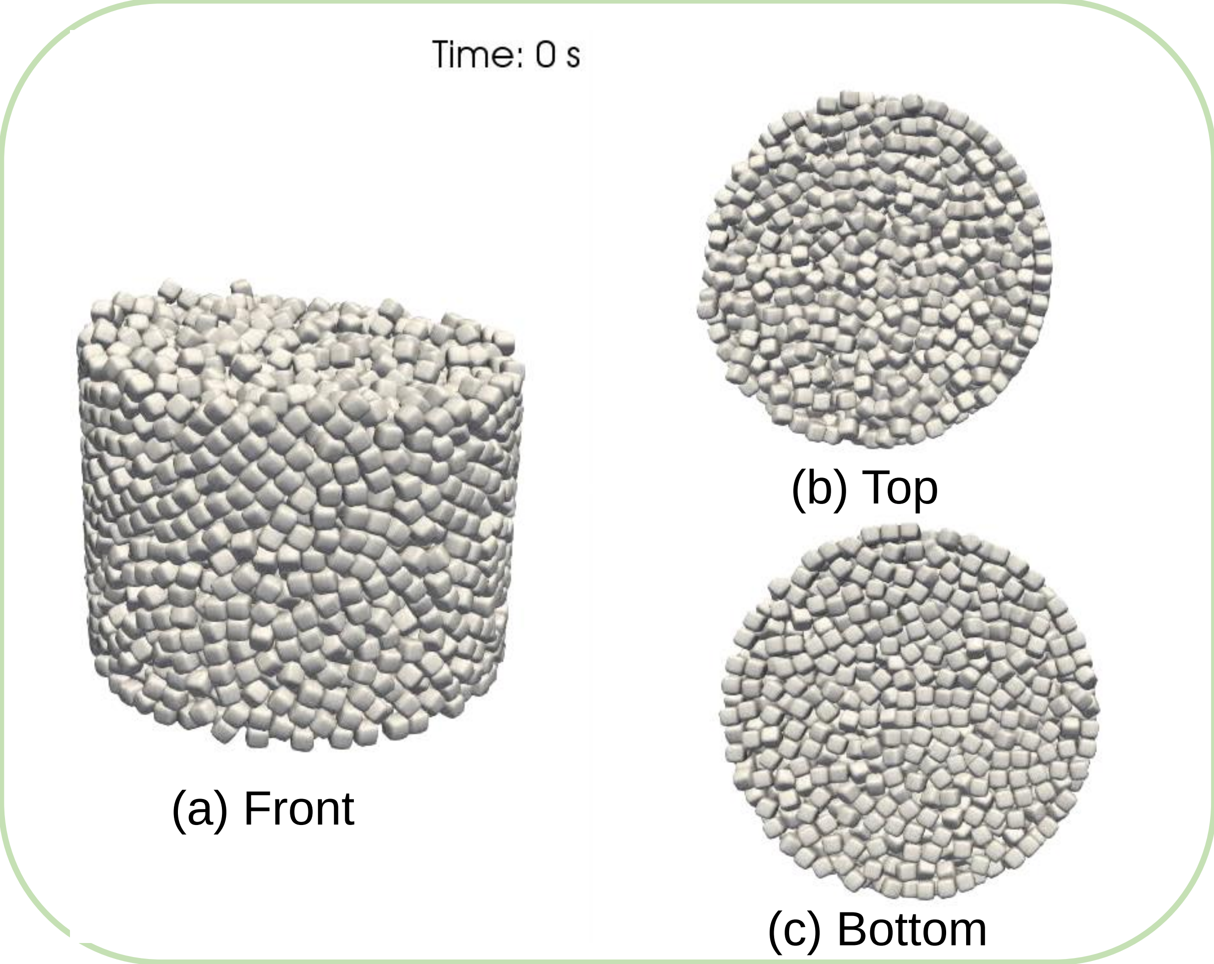
(a) 25,000 cubic particles are packed randomly in the container

Alternating rotations ("Twists") are applied to the container

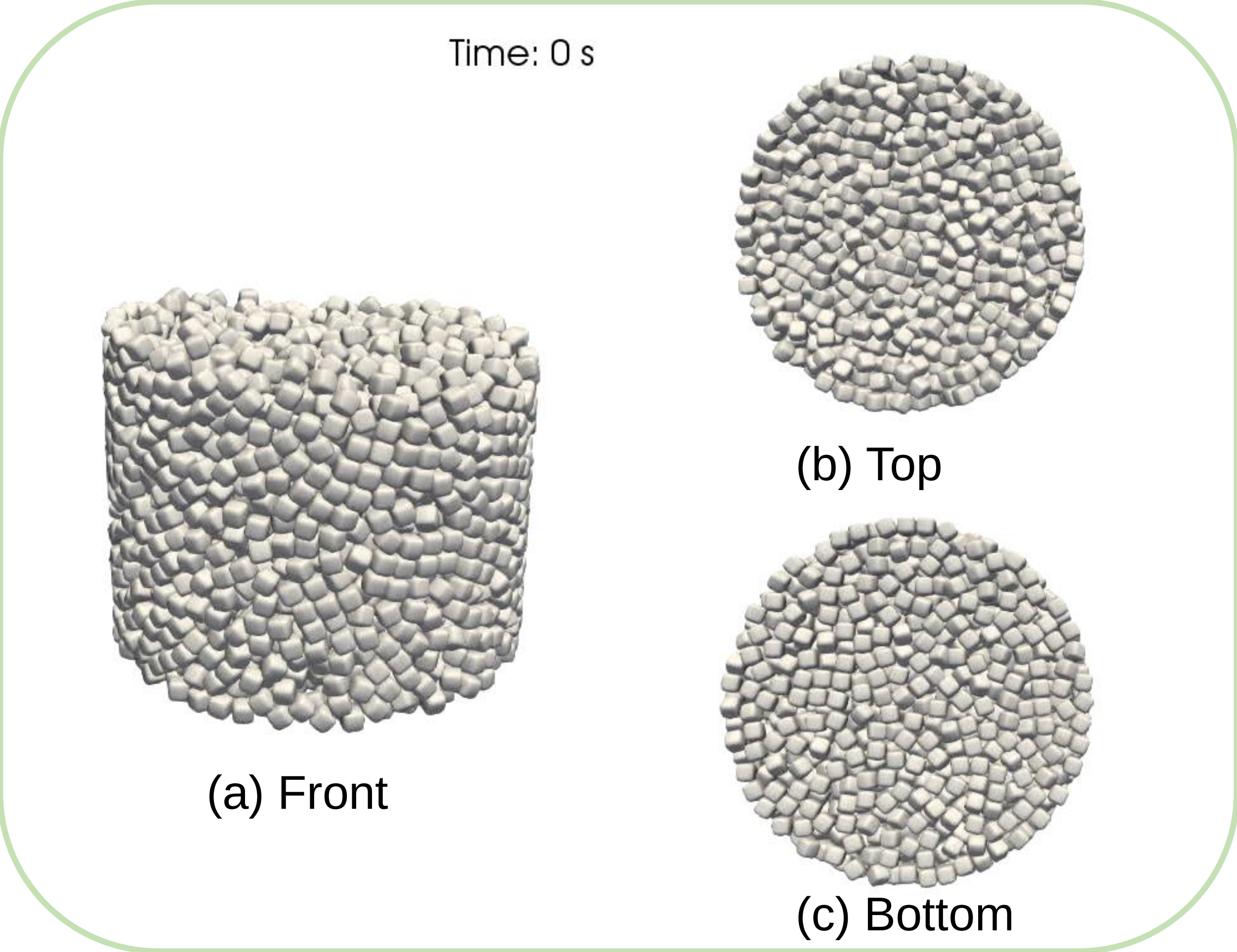
(b) A densest limit is reached: concentric rings of horizontally aligned cubes are superimposed in the vertical direction

- Asencio, K., Acevedo, M., Zuriguel, I., & Maza, D. (2017). Experimental study of ordering of hard cubes by Shearing. *Physical Review Letters*, *119*(22).

Dice Alignment under Various Tangential Accelerations

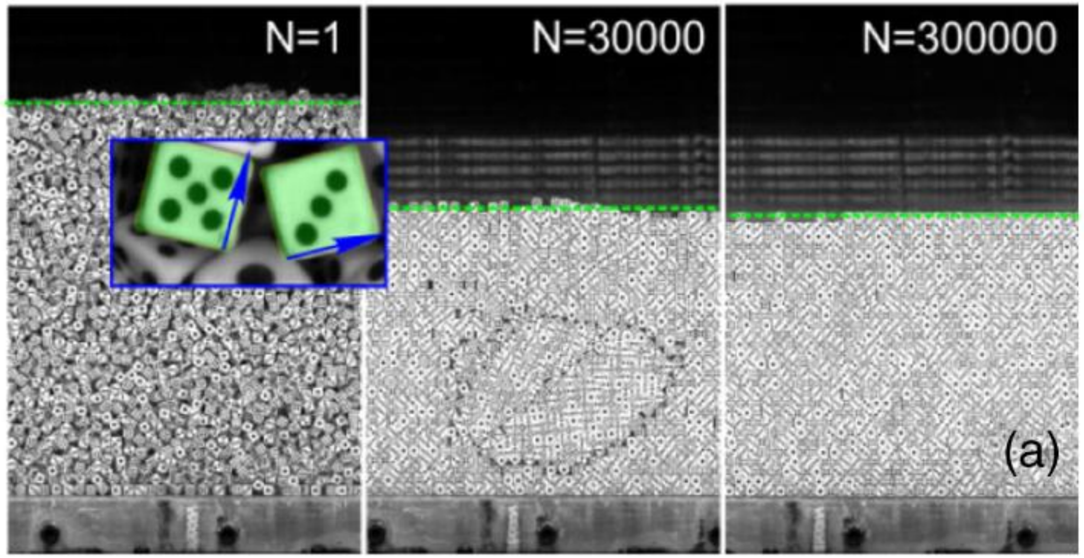


Case (a): Slow Acceleration



Case (b): Fast Acceleration

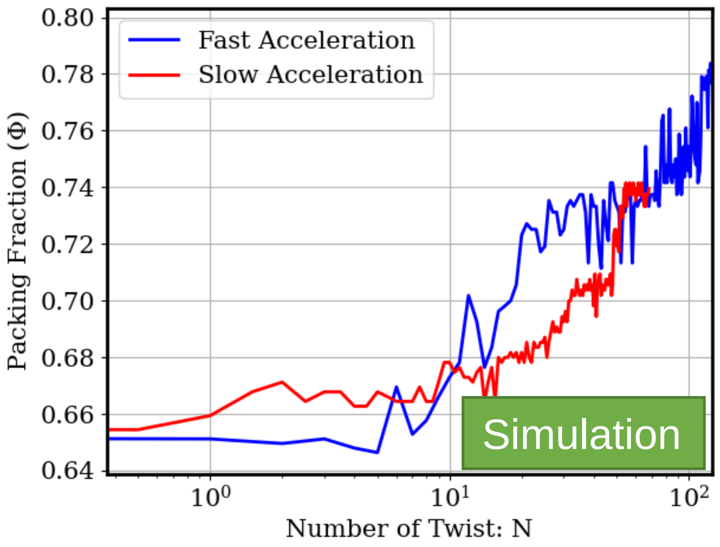
Quantitative Analysis of Dice Alignment

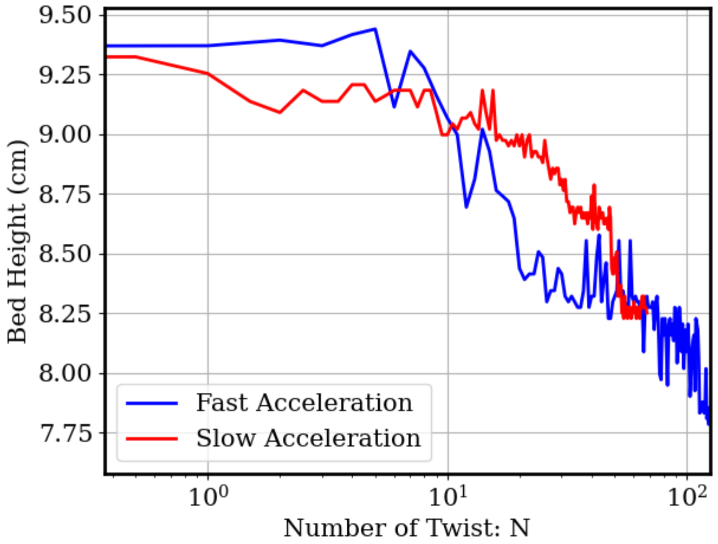


- Bed height, H_{bed}, decreases with the number of twist due to the packing of particles

$$\phi = \frac{V_{dice} N_{dice}}{A_{reactor} H_{bed}}$$

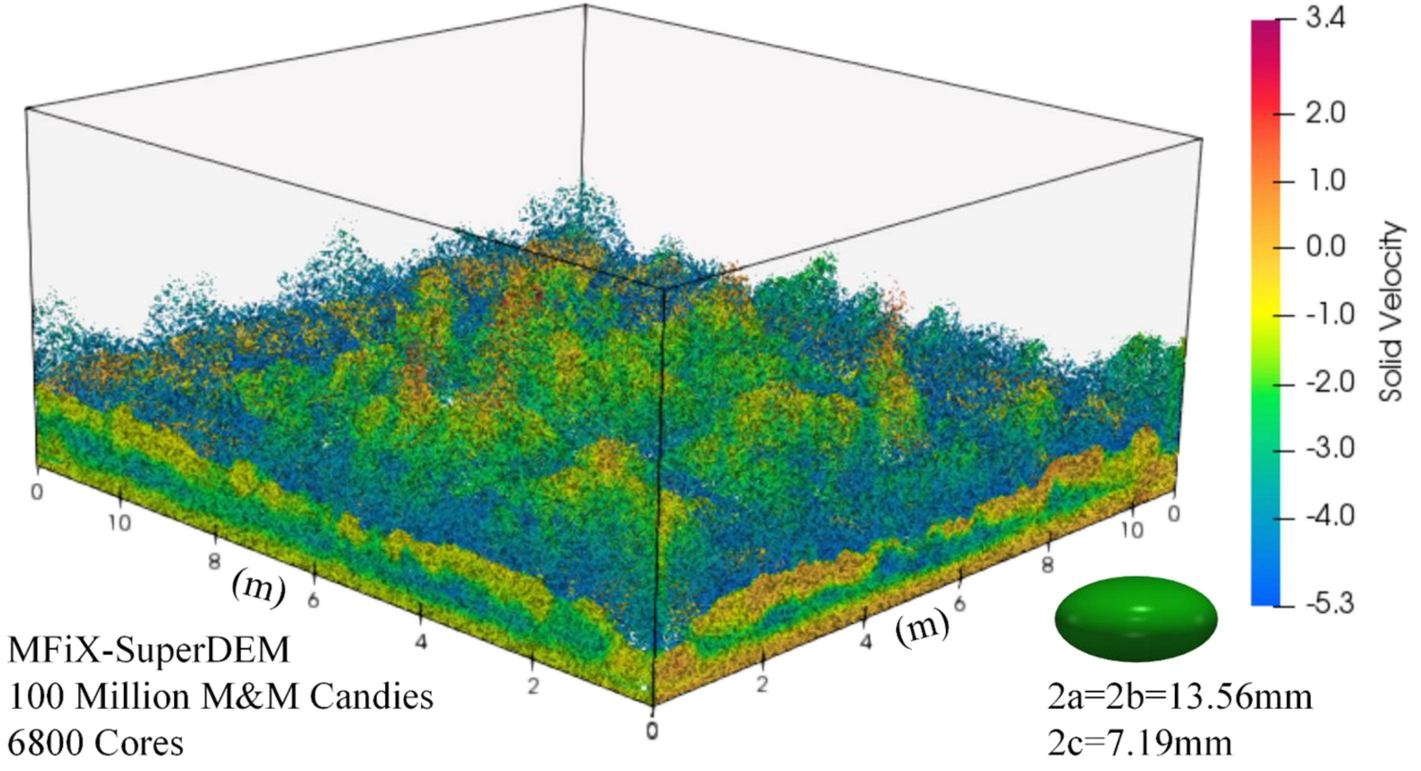
  - V_{dice}: volume of one dice
  - N_{dice}: number of dice
  - $A_{reactor}$: cross-area of container

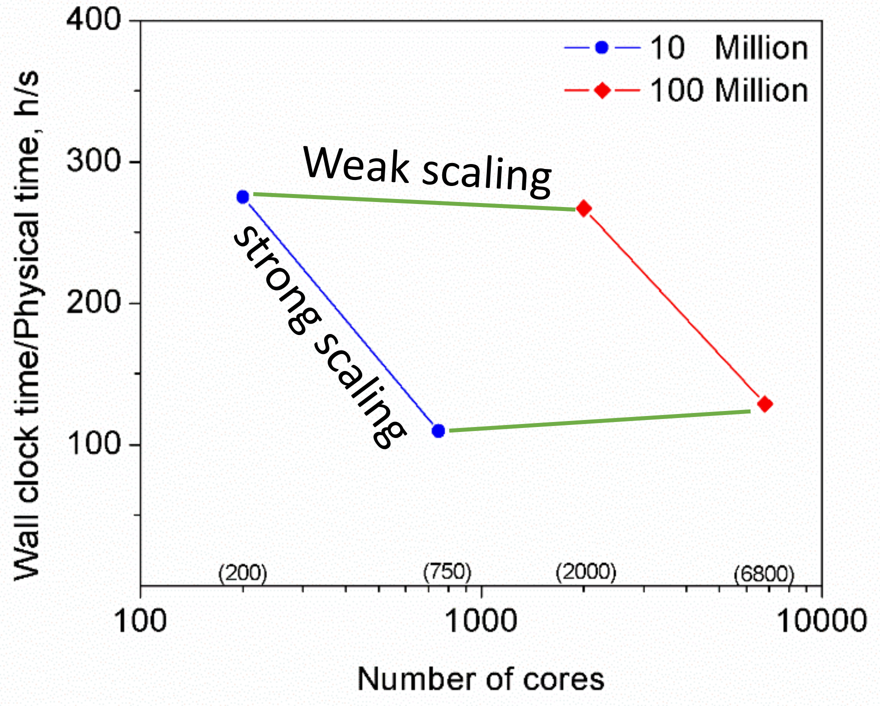




- Same varying trend is obtained in experiment and simulations
- Fast acceleration can accelerate particle packing
- One-to-one comparison is hard to obtain due to the random initial packing and different container size and number of particles

Massively Parallel SuperDEM Simulation





- The solver was parallelized using Message Passing Interface (MPI)
- Simulation on NETL supercomputer Joule 2 (80 K cores), World Top 60, 2020
- Non-spherical particles fluidization simulation, 100 million (6,800 cores)

NETL Multiphase Flow Science
Home of the MFiX Software Suite

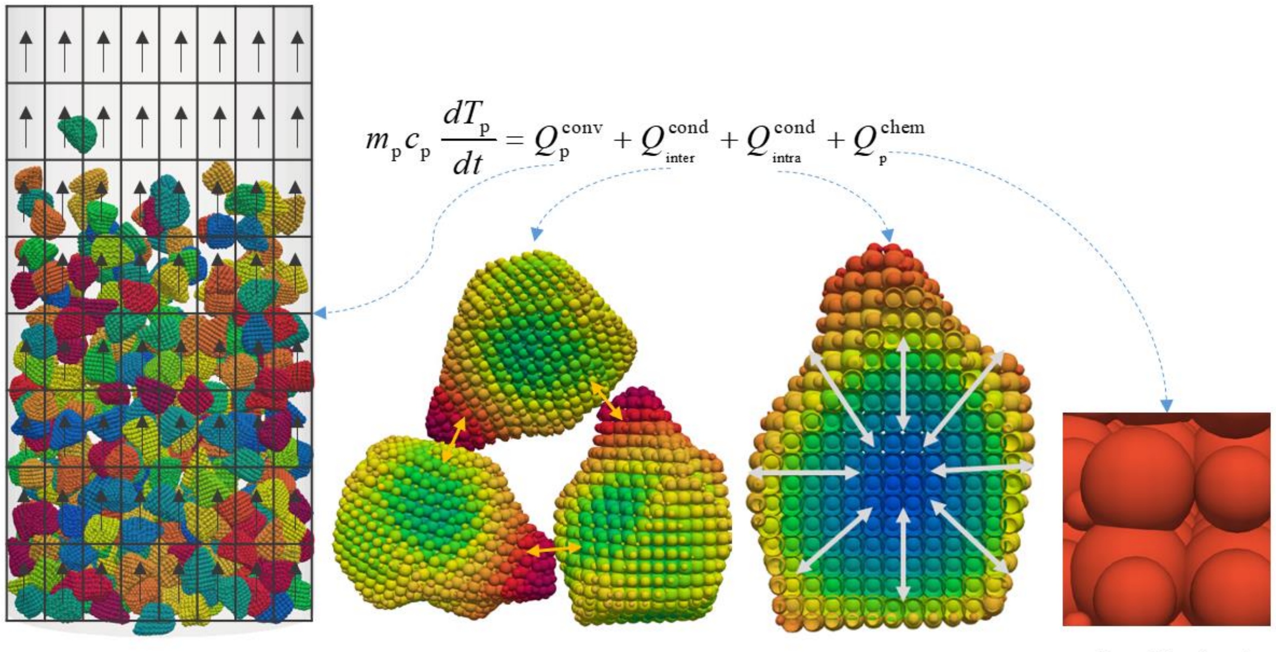
U.S. DEPARTMENT OF ENERGY

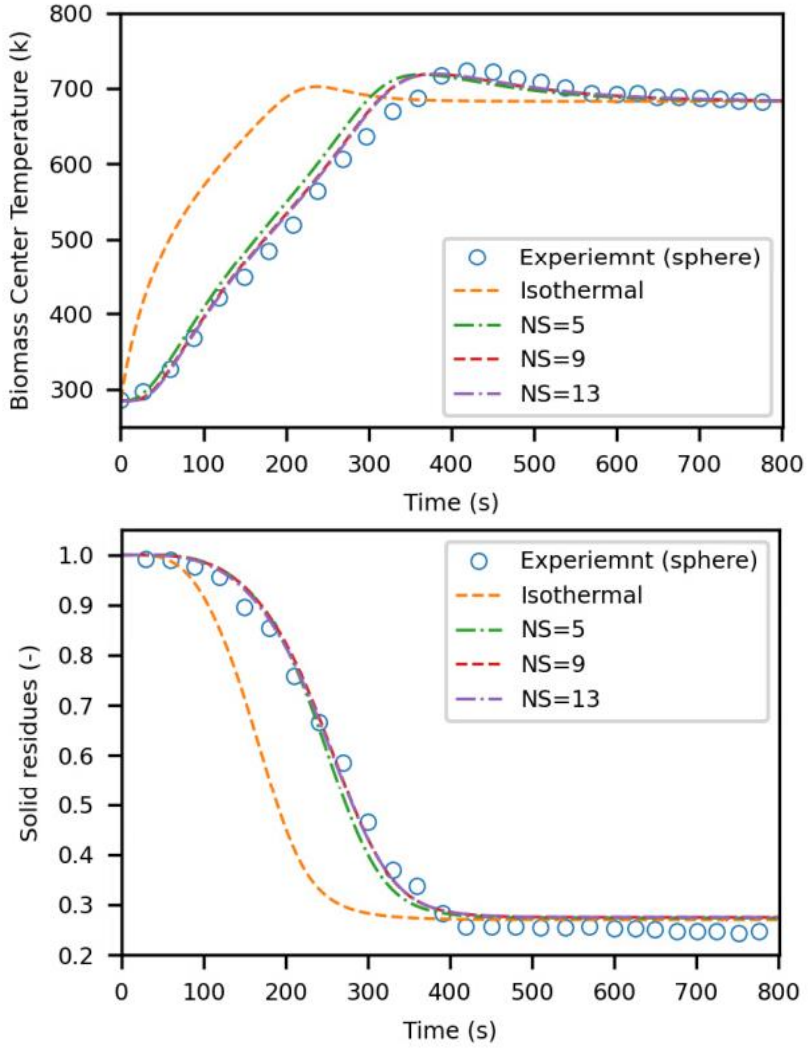
Glued-Sphere DEM

Irregular Shape of Particles

- Composite spheres
- Intra-particle temperature distribution

$$m_p c_p \frac{dT_p}{dt} = Q_p^{conv} + Q_{inter}^{cond} + Q_{intra}^{cond} + Q_p^{chem}$$

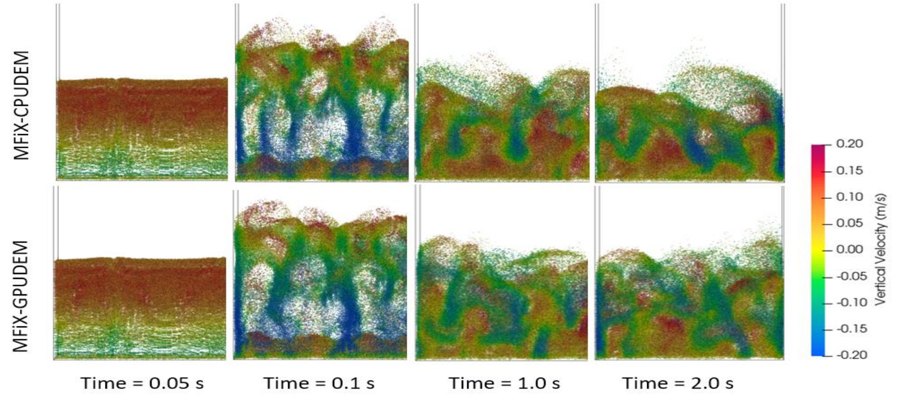


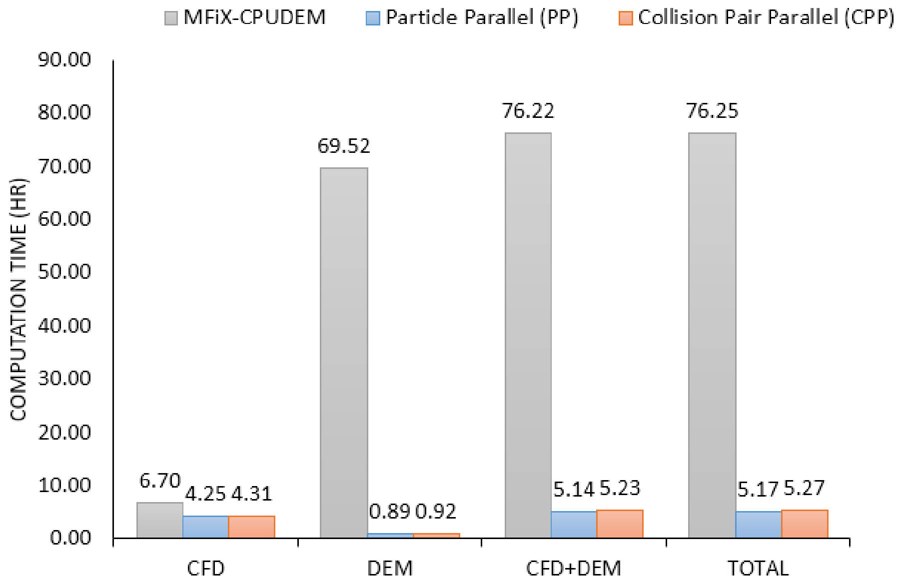


Hundredfold Speedup of MFiX-DEM Using GPU

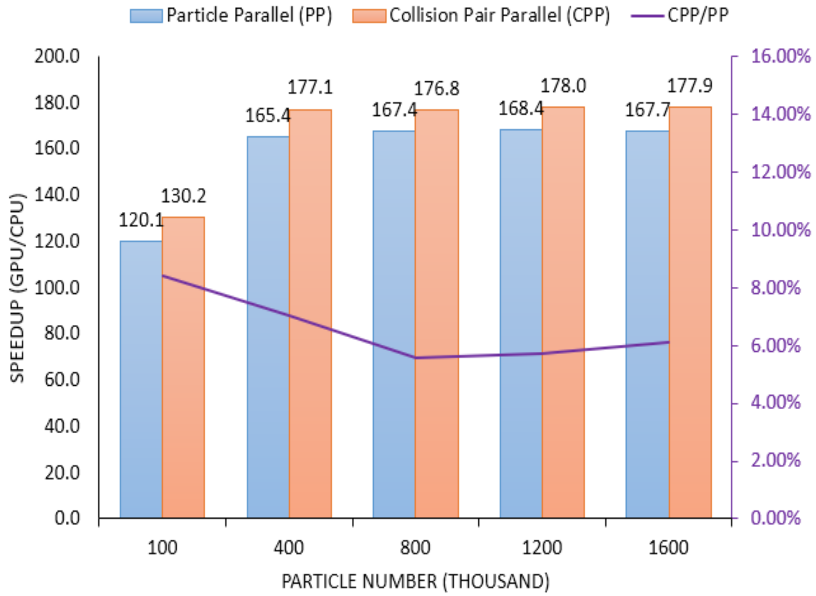
DEM Solver was Ported to GPU (Prototype)

- 170-fold speedup with double precision, 243-fold with single precision
- Re-use CFD, interphase coupling, and chemical reaction modules in MFiX

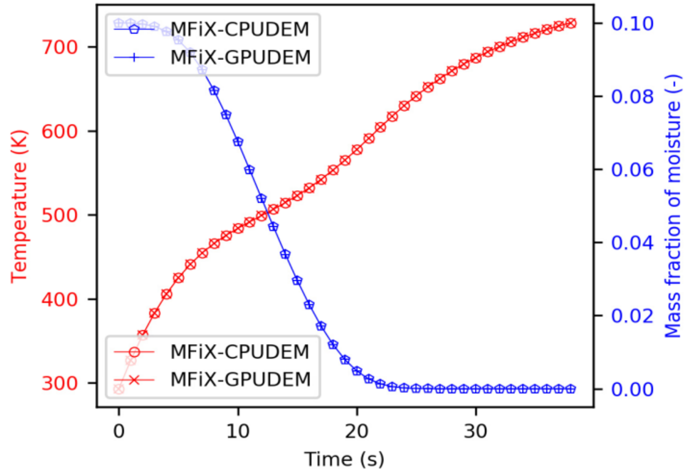




Fluidized Bed Speedup



Particle Packing Speedup

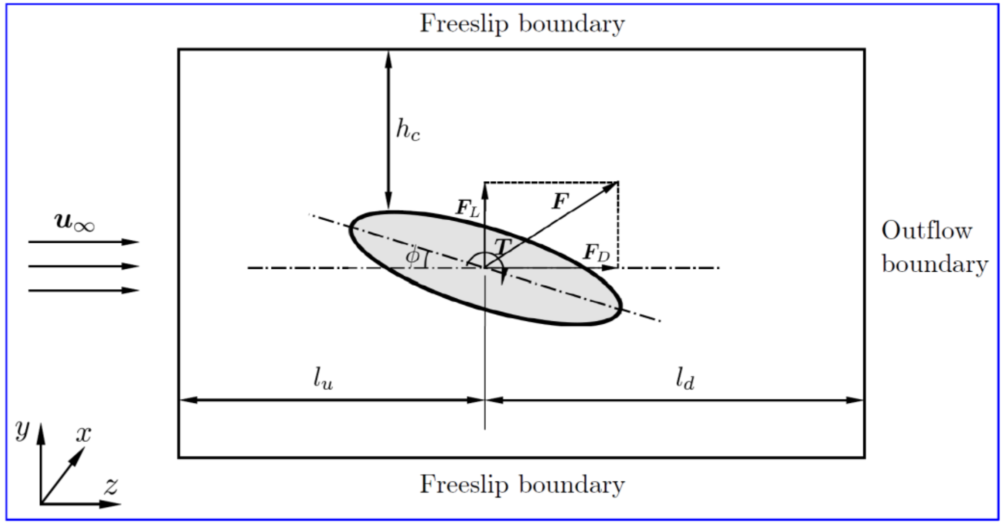


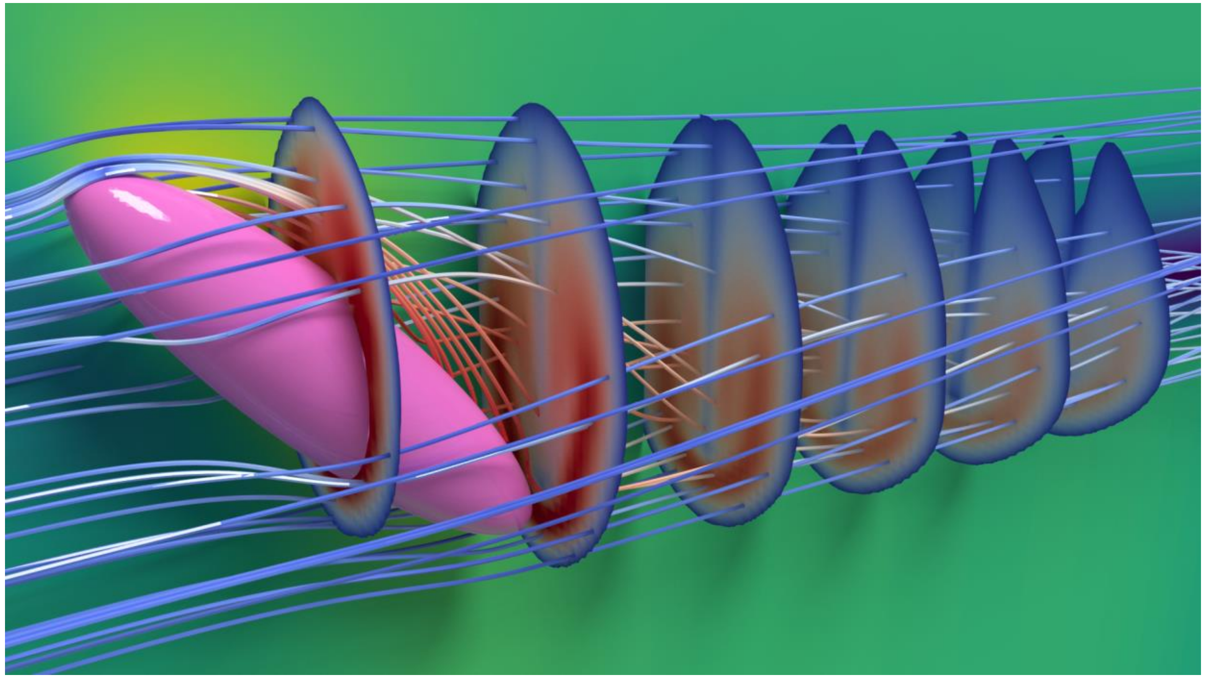
Heat Transfer & Chemical Reactions (Biomass Drying)

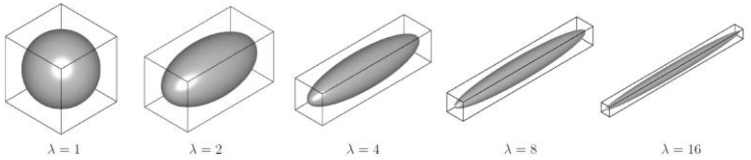
Non-Spherical Particle Drag

Non-Spherical Particle Drag Law

- Detailed simulations of flow around prolate spheroids
- Lattice Boltzmann method (LBM)
- Reynolds numbers range 0.1 ≤ Re ≤ 2000
- Incident angles 0° ≤ Φ ≤90°
- Aspect ratios 1 ≤ λ ≤ 16
- Accurate correlations for average drag, lift and torque coefficients are proposed







Sathish Sanjeevi, Jean-F. Dietiker, and Johan T. Padding, "Accurate hydrodynamic force and torque correlations for prolate spheroids from Stokes regime to high Reynolds numbers ", accepted for publication, Chemical Engineering Journal.

NETL Multiphase Flow Science
Home of the MFiX Software Suite

Non-Spherical Particle Drag

Non-Spherical Particle Drag Law

Lift and Drag

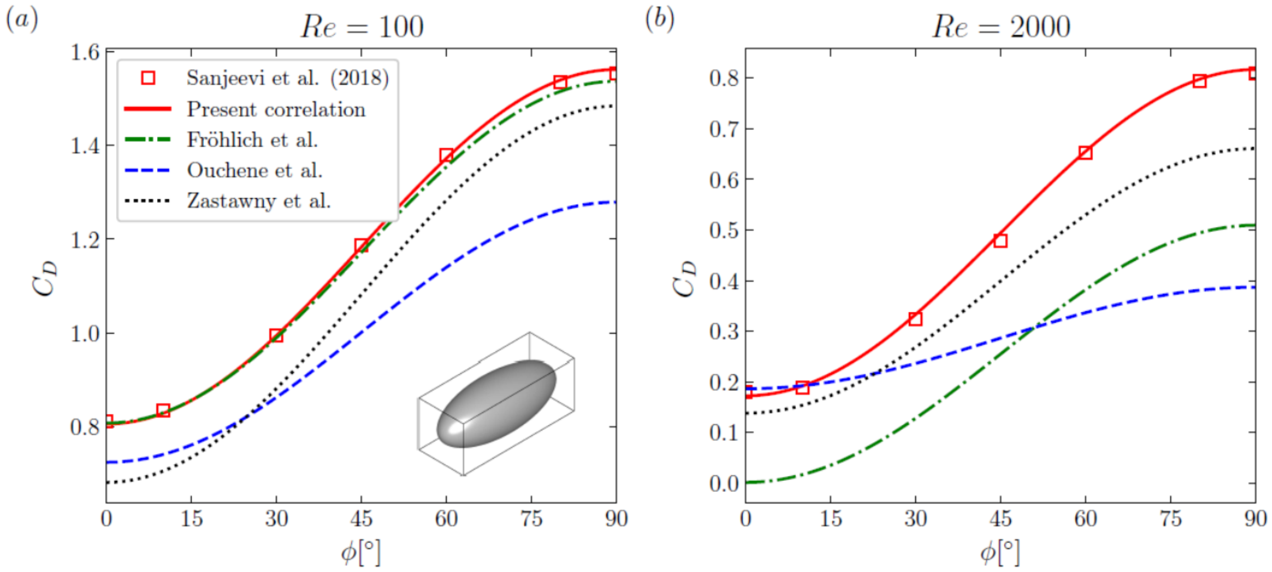


Figure 12: Comparison of C_D against ϕ for $\lambda = 2.5$ at (a) $Re = 100$ and (b) $Re = 2000$.

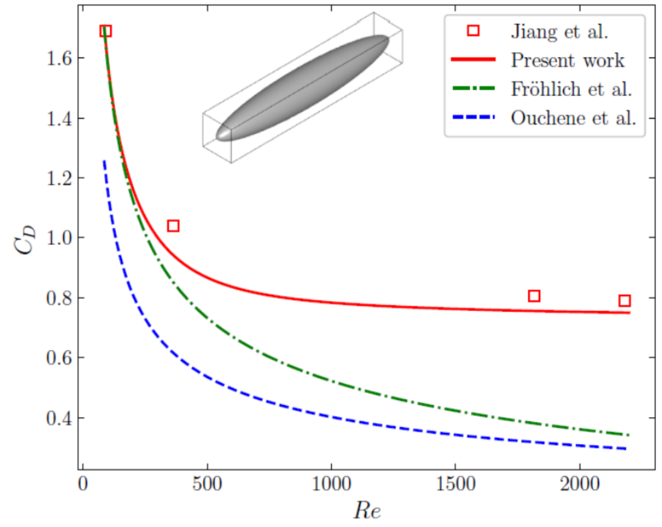


Figure 13: Comparison of C_D for a particle of $\lambda = 6$ at $\phi = 45°$ from different correlations with the DNS data of Jiang et al. [21, 22].

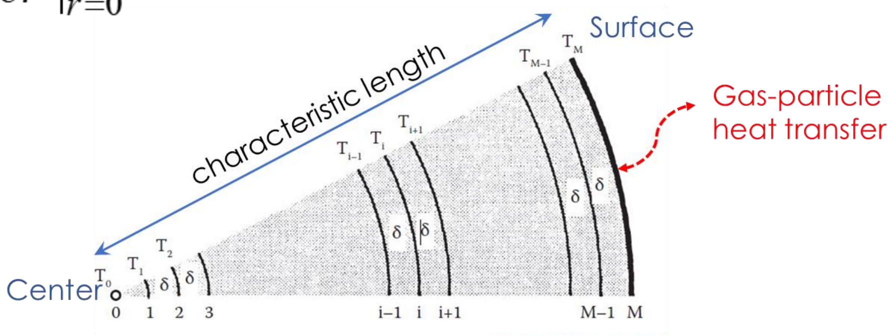
Single-Particle Pyrolysis

$$\frac{\partial}{\partial t}\left(\rho_s c_{p,s} T_s\right) = \frac{1}{r^b}\frac{\partial}{\partial r}\left(k_{s,eff} r^b \frac{\partial T_s}{\partial r}\right) + \sum\left(-\Delta H_i R_i\right)$$

Boundary conditions:

$$k_{s,eff}\left.\frac{\partial T_s}{\partial r}\right|_{r=r_0} = f_c h_{conv}(T_f - T_s) + \sum Q_{i,j,cond} / A_p + Q_{i,wall} / A_p$$

$$\left.\frac{\partial T_s}{\partial r}\right|_{r=0} = 0$$



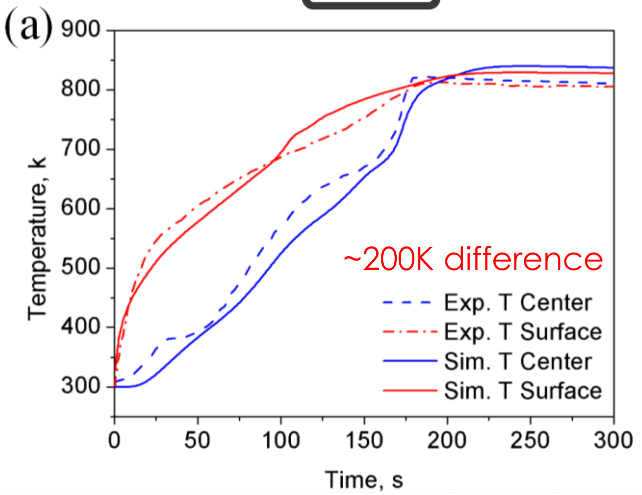
Discretize into several layers (T, species, properties, rates, etc)

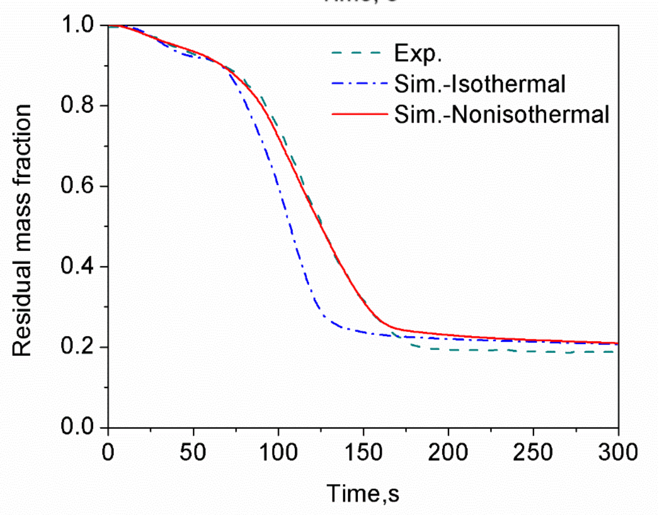
L=19 mm

D=8 mm

biomass spruce pellet

44% CELL, 26% HCE, 17.5% LIG-C, 9.5% LIG-H, 3% LIG-O





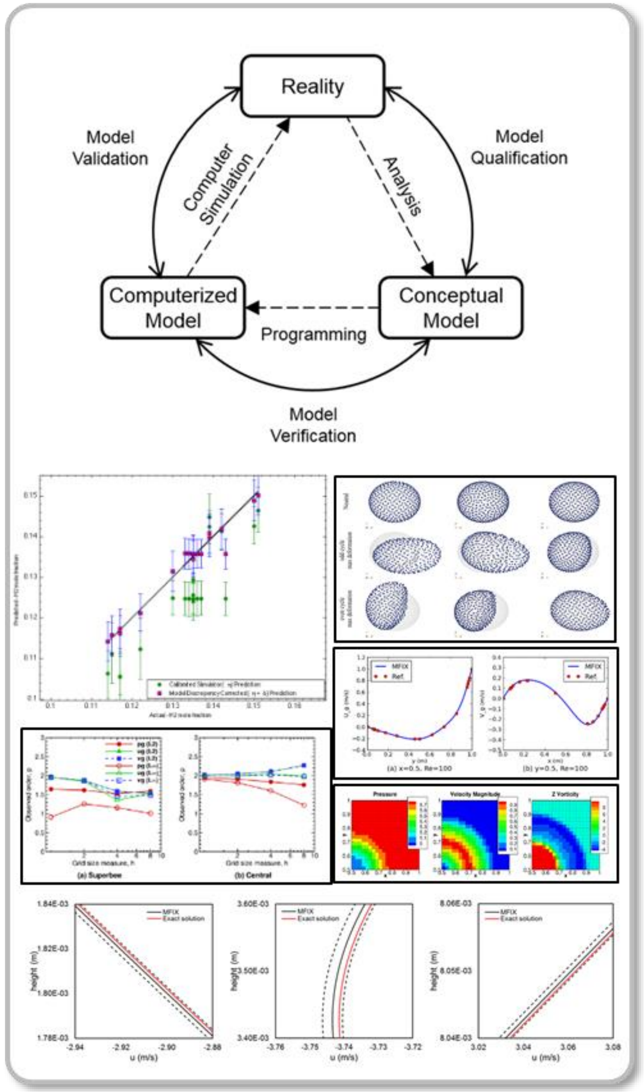
Isothermal model overpredicted the reaction rate!

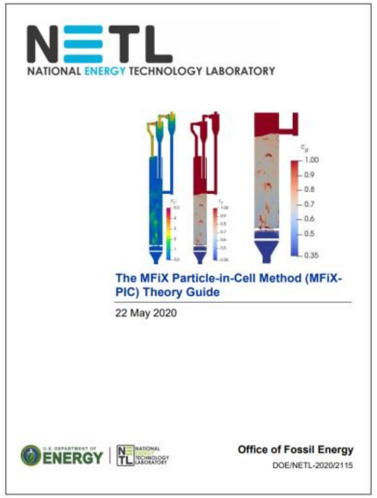
Experiment reference: Andrés Anca-Couce, Peter Sommersacher, Robert Scharler, Journal of Analytical and Applied Pyrolysis, 127, 2017, 411-425

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?

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The MFiX Particle-in-Cell Method (MFiX-PIC) Theory Guide

22 May 2020

Office of Fossil Energy

DOE/NETL-2020/2115

Accomplishments

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

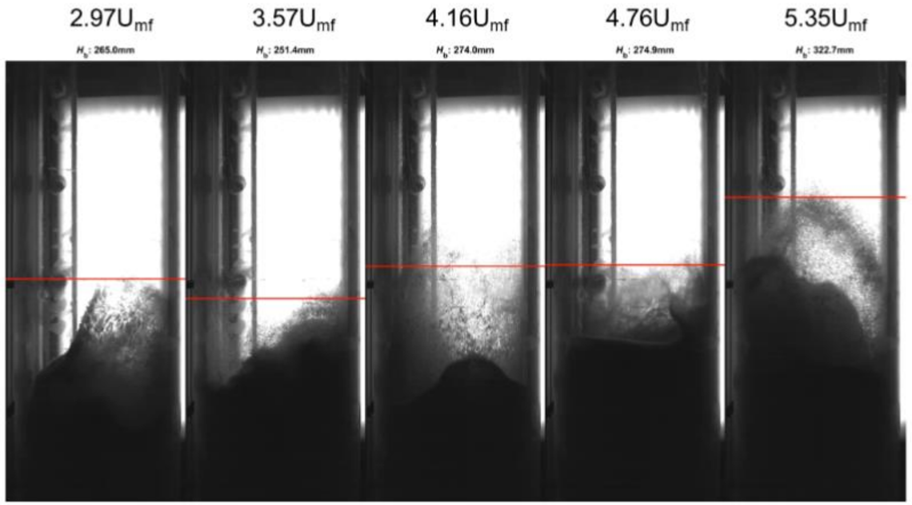
MFiX Quality Assurance

VVUQ: Bayesian Statistical Analysis of MFiX-PIC

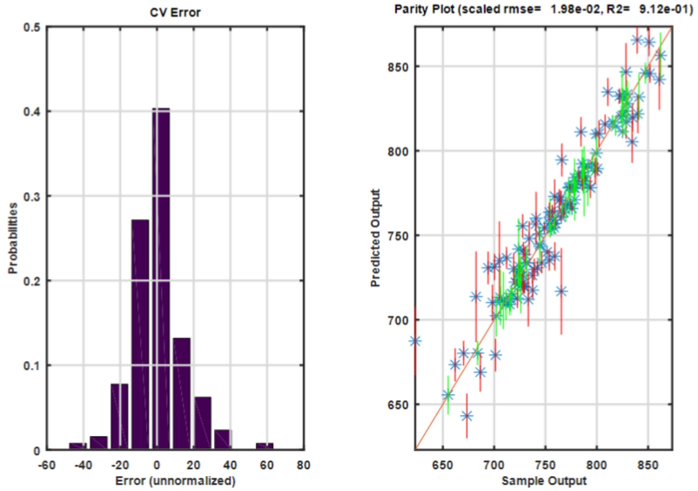
Bayesian Statistical Analysis (BSA)

- parameter sensitivity: which input parameters influence a solution the most)
- parameter calibration: the best value range for an input parameter to match an experimental observation
- Using BSA on input settings in low-fidelity simulation, like MFiX-PIC, can improve simulation accuracy over an entire flow regime.

Real Data



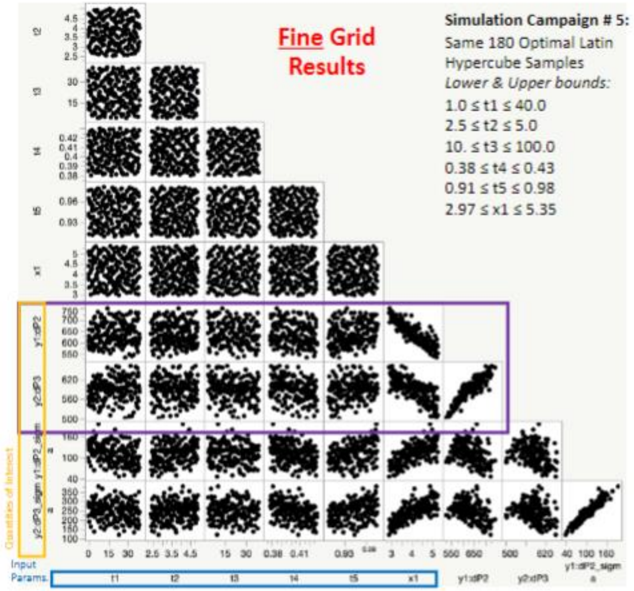
Surrogate Data



MFiX Quality Assurance

VVUQ: Bayesian Statistical Analysis of MFiX-PIC

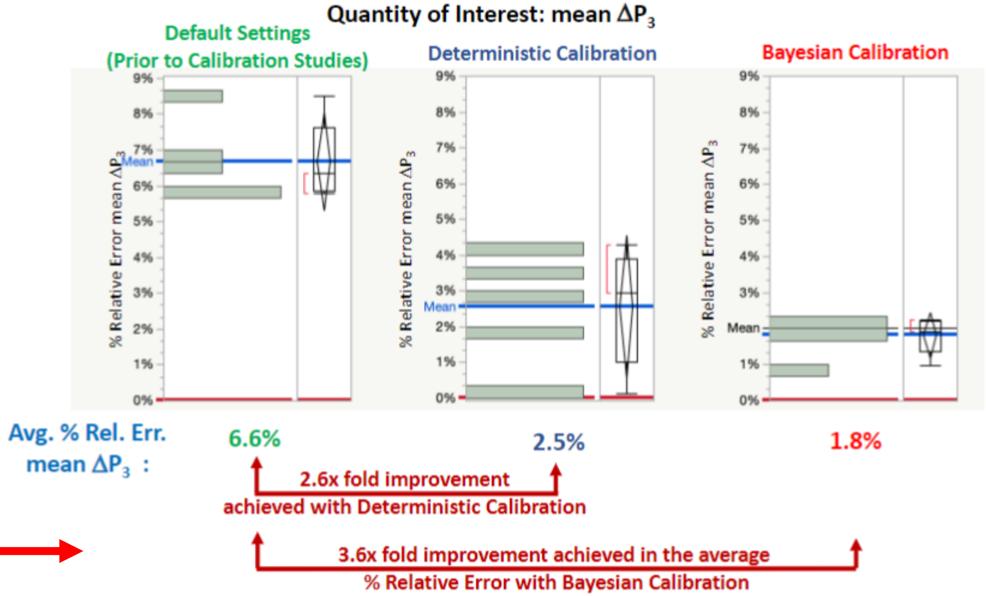
Bayesian Statistical Analysis (BSA)
Using lower fidelity modeling with well-defined input settings produces more accurate simulation results, without additional CFD tuning.



Sensitivity identifies parameter importance

AND

Calibration improves simulation accuracy



Impact: Less computational resource needed for accurate simulation.

Demonstrated ML in MFS Portfolio

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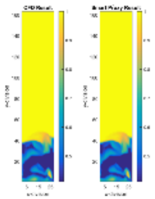
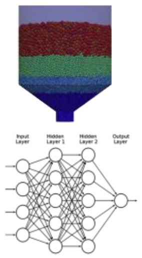
2015
MFiX CFD Proxy



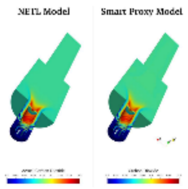
Data from MFiX was used to train a neural network based digital twin, that reproduces the CFD data at a fraction of the time. [1,2,3,4]

2018
Hopper Classification



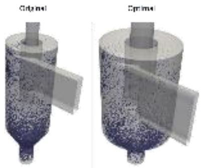
DEM Data was used to train CNN and reconstruct initial packing from hopper discharge data. [5]

2019
ANSYS FLUENT Proxy



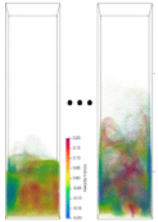
Data from ANSYS FLUENT was used to train and construct a digital twin, for a natural gas combustor. [6,7]

2020
Nodeworks Workflow



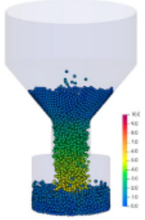
ML in Nodeworks workflow to generate response surfaces that can be used to perform optimization and sensitivity analysis. [8]

2021
ML Filtered drag



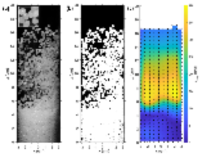
MFiX was used to generate high resolution data and an ML filtered drag was developed and used back in MFiX on coarser mesh. [9]

DEM acceleration



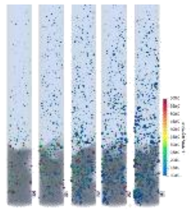
ML was used to accelerate contact detection in DEM simulations. Proof of concept was performed using MFiX. [10]

2022
Image Analysis

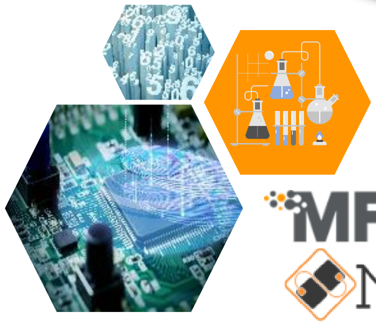


ML image processing was used to measure binary fluidization of non-spherical and spherical particles. [11]

Intra-particle model



ML was used to derive intra-particle model for biomass detailed pyrolysis kinetics. [12]



MFiX MFAL Nodeworks

7+ years experience with ML in software development and experimental data analysis
14 publications and presentations

Prior to 2015, ROM [13] and UQ [14], used methods similar to ML

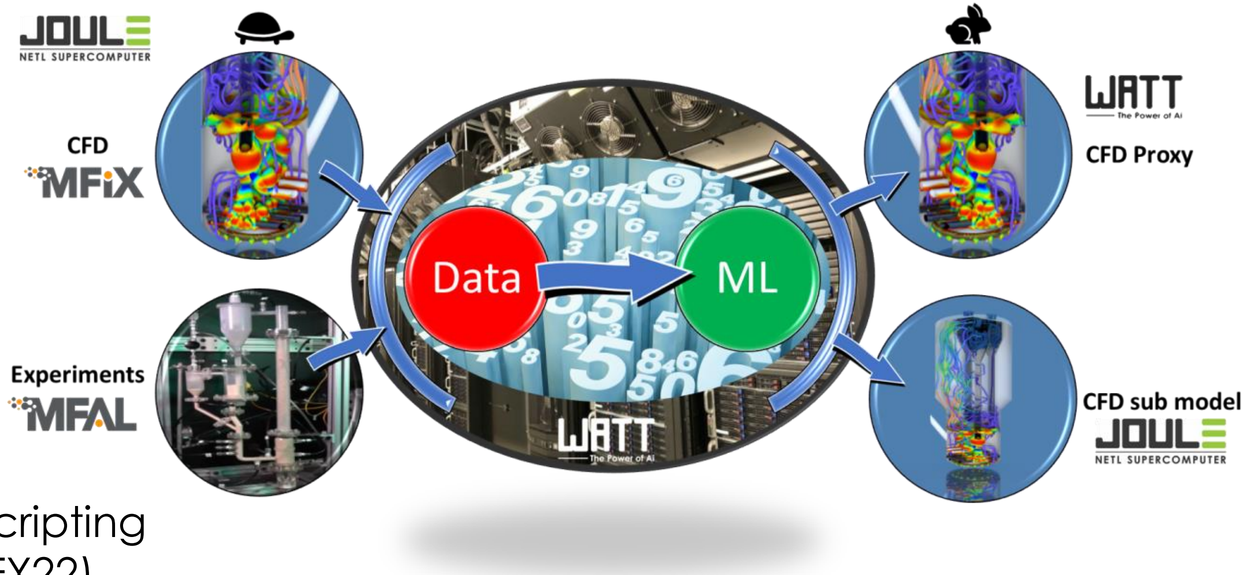
MFS NETL Multiphase Flow Science
Home of the MFiX Software Suite

ML Plan

CFD & Machine Learning Workflow

- Data Generation
  - Setup
  - Customize output
  - Run CFD
  - Archive/transfer data
- Data Preparation
  - Data cleanup
  - Data compression/dim. reduction
  - Data labeling
  - Remove outliers
  - Normalization
  - One-hot encoding
- ML Training
  - Feature selection and engineering
  - Model + hyperparameters
  - Hyperparameter optimization
  - Training
  - Cross validation
- UDF Hook to use ML During Simulation (CARD EY22)
  - Call ML model at run time

Python scripting (CARD EY22) or Nodeworks



Machine Learning Plan

Potential Areas of Development

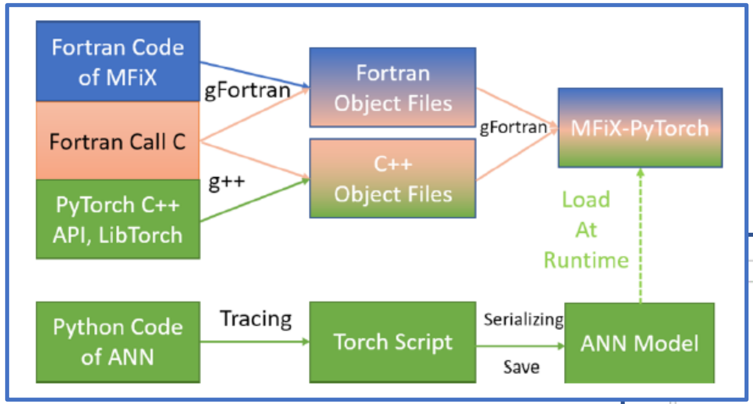
- Filtered drag model
  - Develop a filtered drag model from high resolution CFD
  - Run coarse CFD with filtered drag to improve accuracy
  - Benefit: Enables large-scale simulation at better accuracy
- Chemistry model
  - Represent complex kinetics with a fast ML model
  - Benefit: Faster reactive simulations
- Intra-particle model
  - Account for intra-particle effect (temperature, chemistry)
  - Benefit: Improved accuracy for large or non-spherical particles
- Drag laws for non-spherical
  - Effect or shape and orientation on drag
  - Crowding effect in assembly
  - Benefit: Improved accuracy for non-spherical particles
- PIC stress model
  - Use DEM data to train PIC stress model
  - Benefit: Improved PIC accuracy on wide flow regimes
- DEM collision detection
  - Accelerate particle collision algorithm
  - Benefit: Faster high-fidelity DEM simulations
- On-the-fly model training
  - Train model while simulation is running
  - Avoid storing large data set

ML Integration into the Solver

ML: Filtered Drag Model Implementation

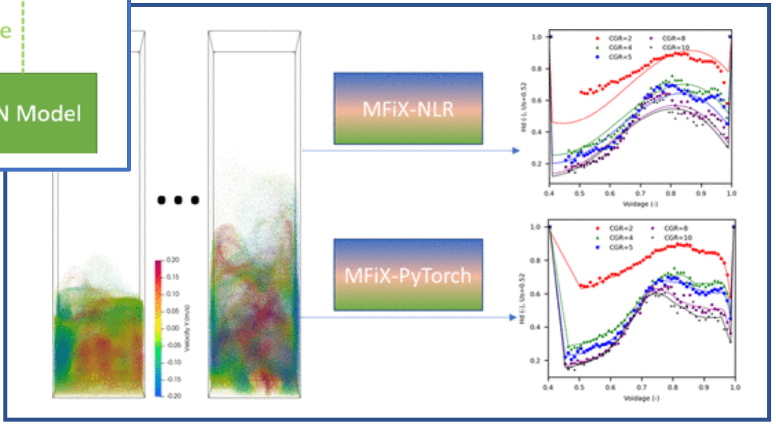
<u>Machine-Learned Filtered-Drag</u>

What is it and why do we care? Drag is fluid resistance, a force that acts in the opposite direction of particles moving through a fluid. In CFD, drag laws are related to the size, shape, and velocity of the particles being carried by the fluid, as well as the fluid itself. It is an evolutionary value that must be recalculated constantly.



ML-methods coupled to MFiX

An artificial neural network (ANN) is compared to non-linear regression (NLR) ML-techniques.



Machine-learned drag from high-fidelity modeling can be applied to low-fidelity models (like PIC and CG-DEM) to improve solution accuracy and computational speed.

Development of a Filtered CFD-DEM Drag Model with Multiscale Markers Using an Artificial Neural Network and Nonlinear Regression, Liqiang Lu, Xi Gao, Jean-François Dietiker, Mehrdad Shahnam, and William A. Rogers, *Industrial & Engineering Chemistry Research* **2022** *61* (1), 882-893; DOI: 10.1021/acs.iecr.1c03644.

Outreach: All-Time MFiX Stats

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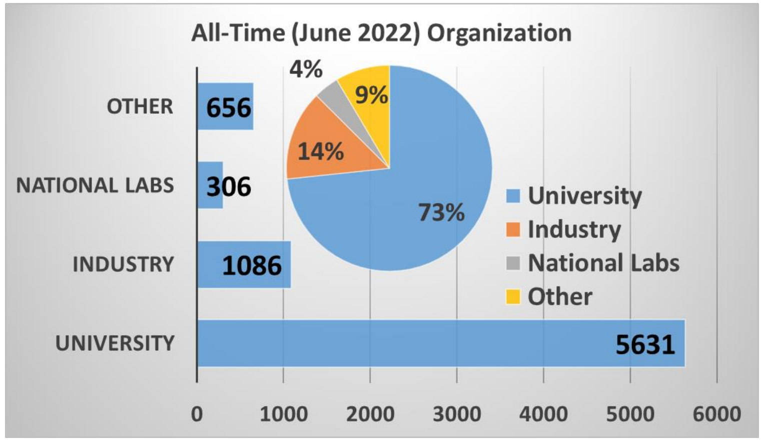
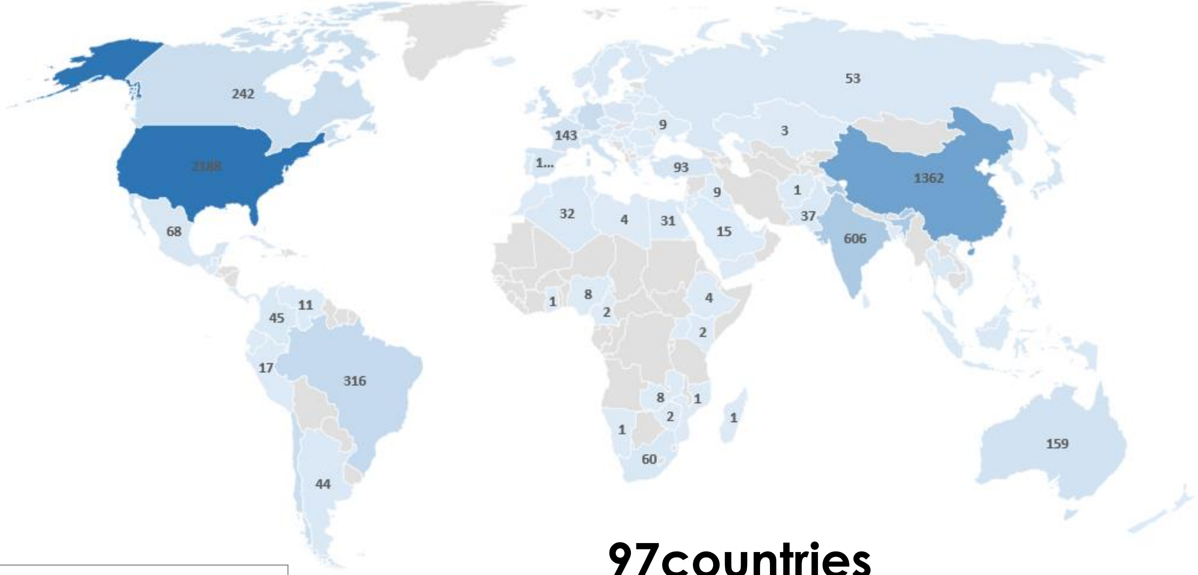
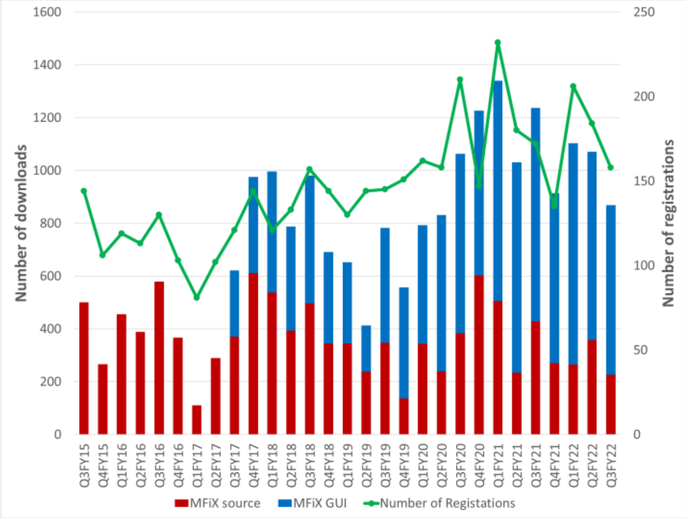
Stakeholders and Technology Transfer

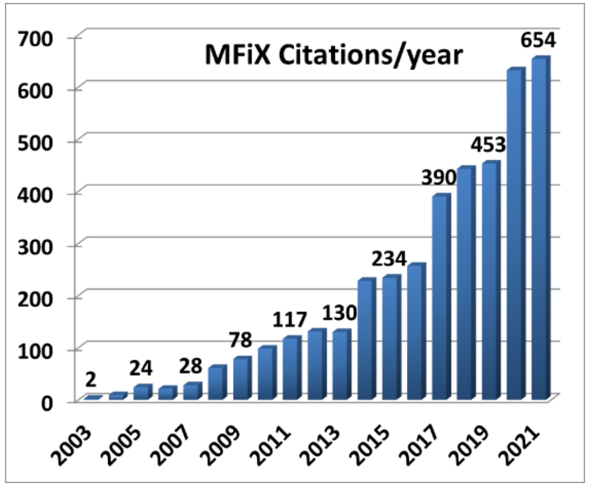
All-time MFiX registrations = **7,500+**

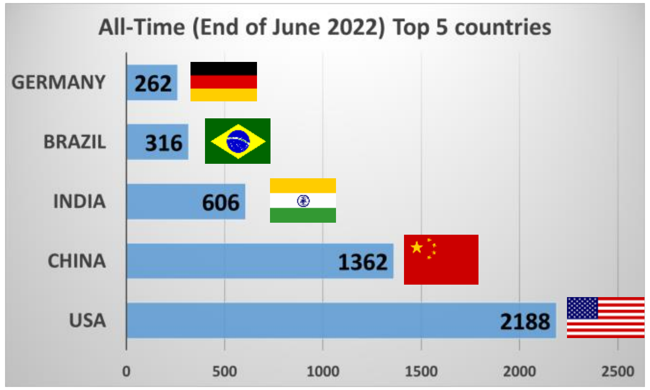




97countries



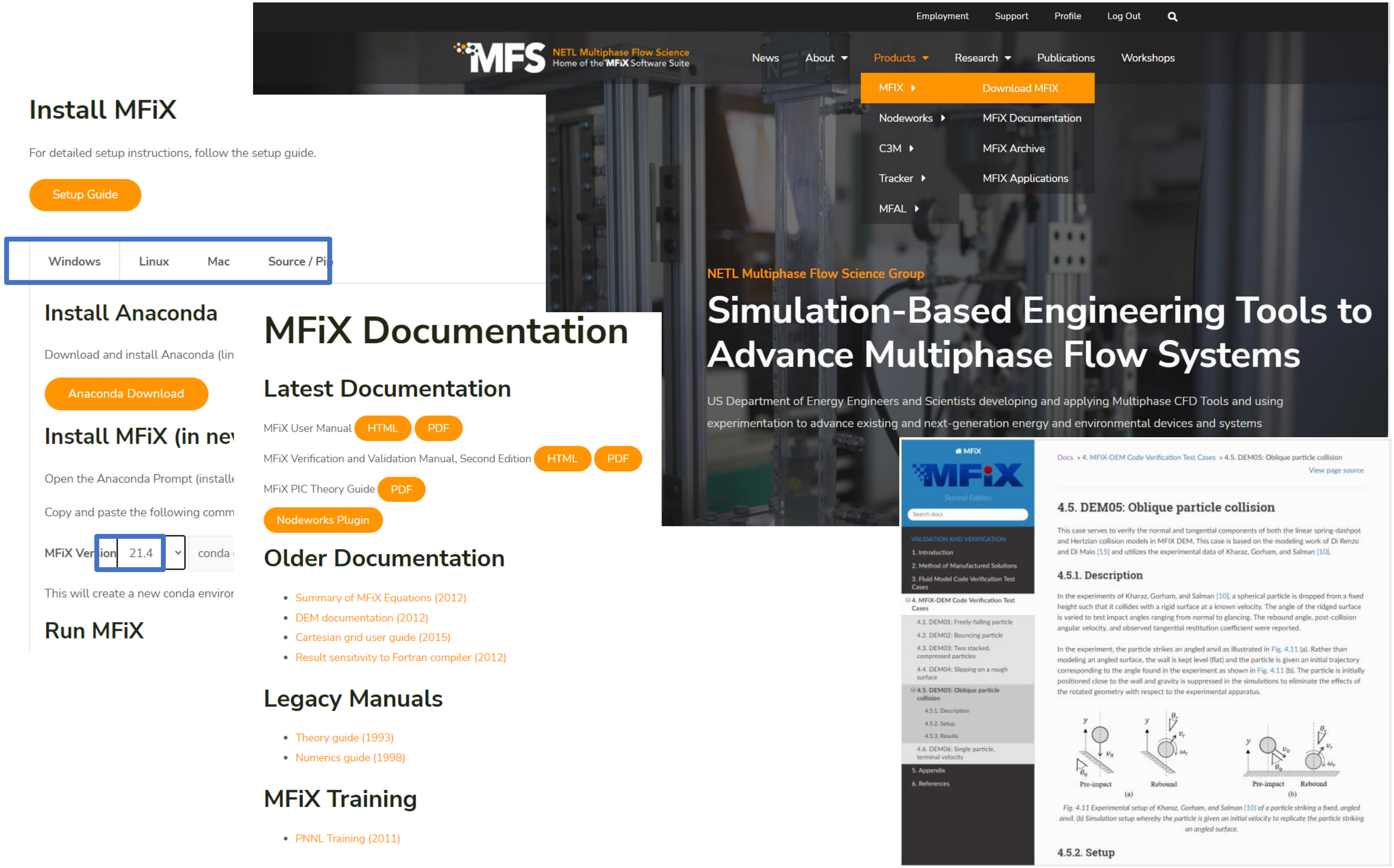


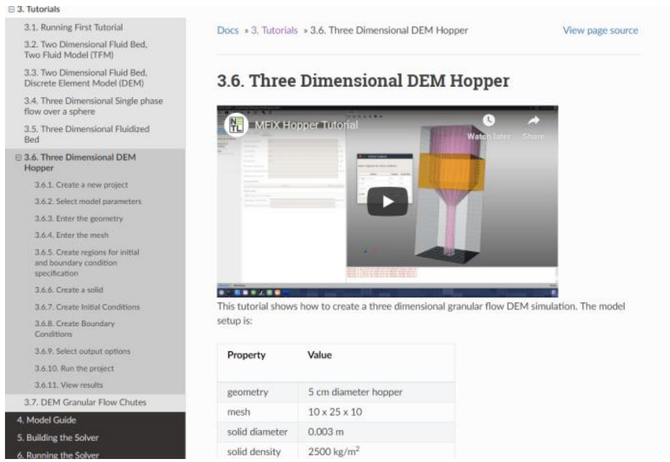


Resources – MFiX Website

- Showcase NETL's Multiphase Flow Science (MFS) team
  - MFS software
  - Documentation
  - Forum
  - Experimental data (challenge problem)
  - Publications
  - Workshop proceedings
  - News, announcements

https://mfix.netl.doe.gov

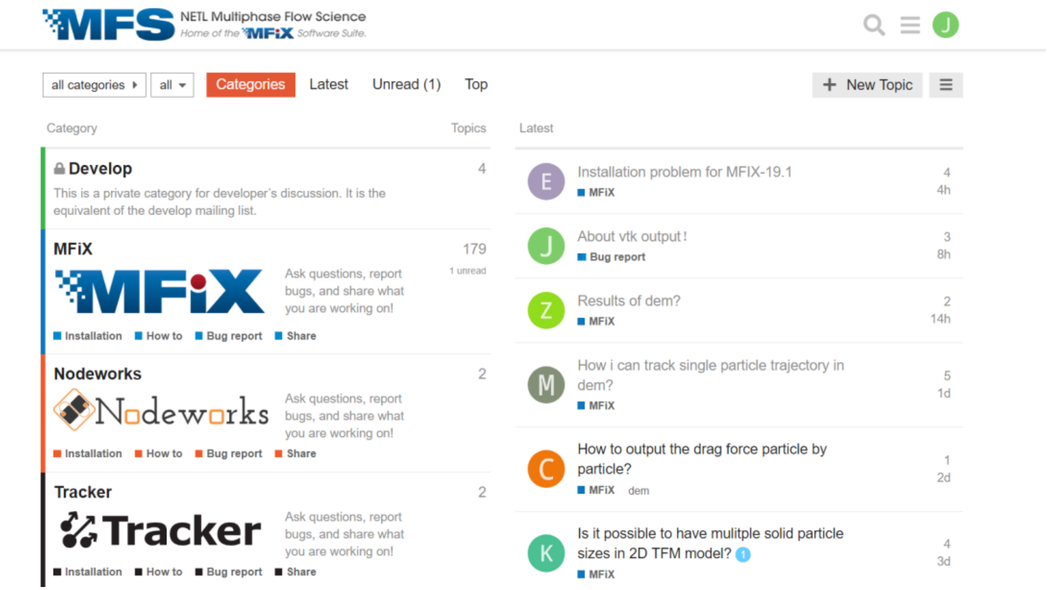


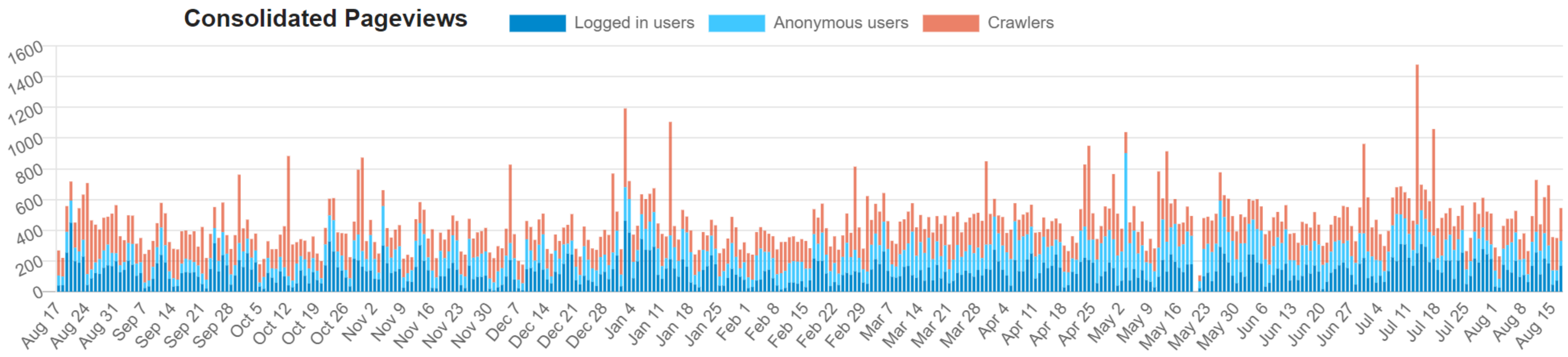


MFiX Forum

- User support
- Categories
  - Installation
  - How to
  - Bug report
  - Share
- Topics (threads)
- File attachment
- Searchable

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





Task 2: MFiX Suite Multiphase Code Development, Validation and Enhancements

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EY23 Plans

Continue to develop new capabilities for MFiX and engage our user community's CFD application needs

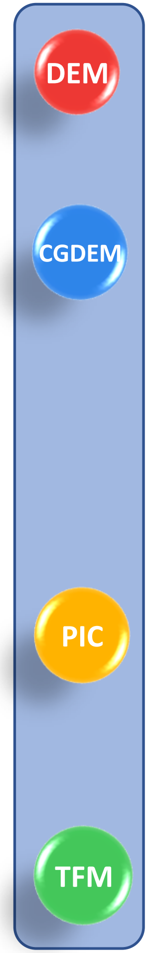
Planned Activities:

- Incorporate ML-based drag model
- Formal release of glued-sphere DEM
- ML-training for PIC stress model
- Incorporate thin-wall boundary condition
- Radiation model VVUQ (from U Wyoming)
- Agglomeration model development
- ML intra-particle model pre-planning
- GPU acceleration in MFiX-Classic (DEM)
- Bridging scales Atomistic->Reactor modeling

Planned Milestones:

- Three official releases of updated MFiX software
- Technical Report update to include VVUQ results

- 19.2 Text editor, keyword browser, Advanced pane
- 19.3 Monitor support for PIC, Keyframe data
- 20.1 SMS workflow, TPKKV drag
- 20.2 PIC CFL, moving STL, Improved GTSH kinetic theory
- 20.3 DEM polydispersity, DEM seeding
- 20.4 Coarse Grain DEM, PIC collision damping
- 21.1 2x fluid solver speedup. Procedural STL, 6 new drag laws, 3 new Nusselt correlations
- 21.2 CGDEM specify statistical weight per phase, Force chain visualization, Reaction rate output, Filtering of particle_input.dat/output.dat
- 21.3 Guo-Boyce friction model, Residence time output, Create animation from GUI
- 21.4 Polydispersity for PIC
- 22.1 DEM Rolling friction
- 22.2 Time-averaged monitors
- 22.3 New visualization pane
- 22.4 Super-DEM



(VVUQ: Verification, validation and Uncertainty Quantification)

Task 3: Wafer Scale Engine Programming

Advantaging next generation hardware

A single chip carries 1.2 - 2.6 trillion transistors.

Early challenges:
- making the chip (expense and QA)
- programming the chip
- interfacing I/O with the chip
- only one user at a time

The possibilities:
- incredible calculation speed
- reduced electrical load
- ideal format for AI

Cerebras Wafer Scale Engine CS-2

Figure 3: Front view of the CS-2, with doors open. Fans in the bottom half move air; pumps in the top right move water, power supplies and I/O in the top left provide power and data.

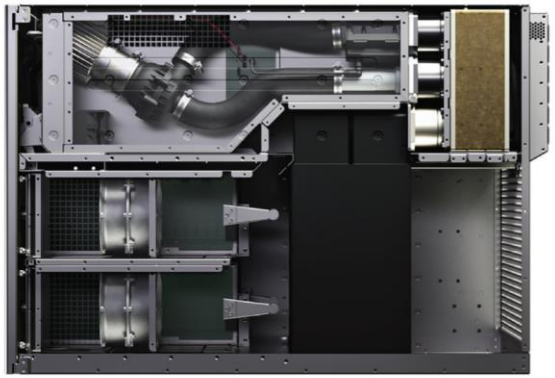


Figure 4: This side view shows the water movement assembly (top), and the air movement infrastructure — fans and a heat exchanger (bottom half).

*

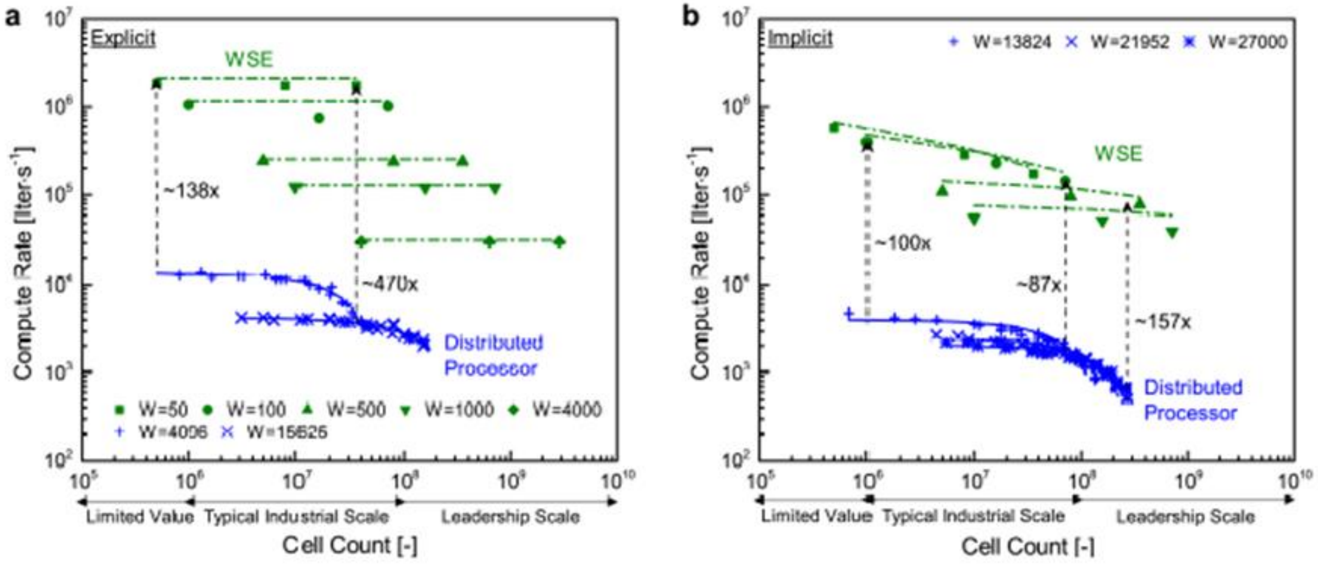
* Cerebras Wafer Scale Engine Is A Massive AI Chip Featuring 2.6 Trillion Transistors & Nearly 1 Million Cores (wccftech.com)

Task 3: Wafer Scale Engine (WSE) Programming

WSE-Field Equation API

- Field equations (stencil problems) are generally memory bound (performance is limited by memory access rates)
- Full featured linear equation system within the WFA
- Up to 470x improvement in solution speed over traditional computing techniques
- Explicit and implicit solution of the heat equation
- The WFA outperformed OpenFOAM on Joule by ~2 orders of magnitude

```python
from WSE_FE.WSE_Interface import WSE_Interface
from WSE_FE.WSE_Array import WSE_Array
from WSE_FE.WSE_Loops import WSE_For_Loop
import numpy as np

# Instantiate the WSE Interface
wse = WSE_Interface()

# define constants
c = 0.1
center = 1.0 - 6.0 * c

# Create the initial temperature field and BC's
T_init = np.ones((102, 102, 102))*500.0
T_init[1:-1, 1:-1, 0] = 300.0
T_init[1:-1, 1:-1, -1] = 400.0

# Instantiate the WSE Array objects needed
T_n = WSE_Array(name='T_n', initData=T_init)

# Loop over time
with WSE_For_Loop('time_loop', 40000):
    T_n[1:-1, 0, 0] = center * T_n[1:-1, 0, 0]\
        + c * (T_n[2:, 0, 0] + T_n[:-2, 0, 0]
               + T_n[1:-1, 1, 0] + T_n[1:-1, 0, -1]
               + T_n[1:-1, -1, 0] + T_n[1:-1, 0, 1])

wse.make_WSE(answer=T_n)
```

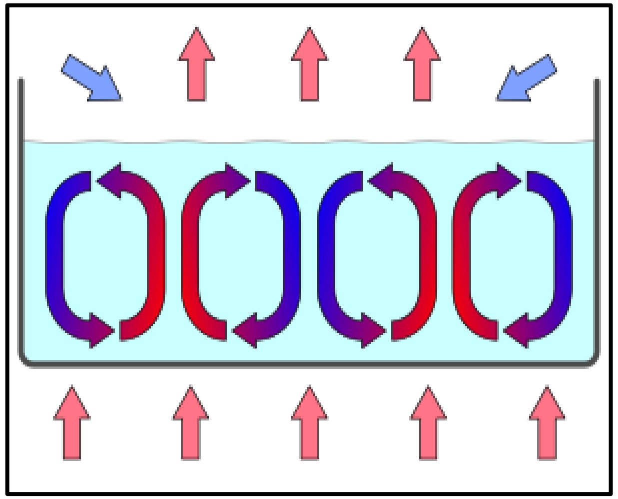


Task 3: Wafer Scale Engine (WSE) Programming

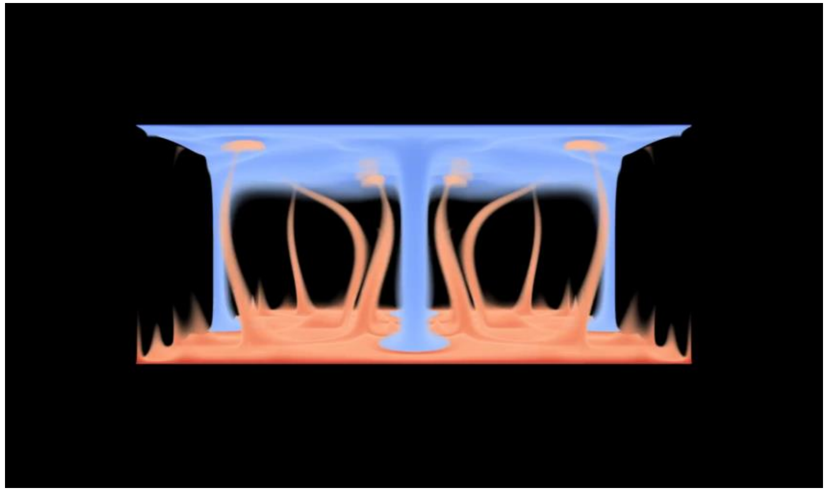
First Coupled Single-Phase CFD Simulation Completed

Rayleigh-Bénard Convection

What is it and why do we care? R-B convection occurs when a lower hot plate interacts with an upper cold plate to create predictable rolling fluid features in between. Gravity and buoyancy drive the effect. This is a calculable single-phase CFD feature that can be directly compared to simulation results.



WSE offers an alternate computing architecture to HPC. Still in its infancy, NETL is positioning itself to advantage an emerging technology to support FECM goals.



Impact: NETL offers proof-of-concept on a new hardware architecture

Task 3: Wafer Scale Engine Programming

EY23 Plans

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Planned Activities:

- Develop at least one mapping strategy to map a generic CFD problem with any mesh type the WSE.
- Translate the mapping to a routing plan and kernel layout.
- Evaluate mapping strategy for several complex geometries using a performance model to check for bottlenecks.
- Integrate new strategy in existing **WSE Field Equation API (WFA).**

Planned Milestones:

- Technical Report detailing the developed mapping strategy and any impacts on performance (end of EY23).

Task 4: MFIX-Exa: Code Development, Validation and Enhancements

New Task for EY23

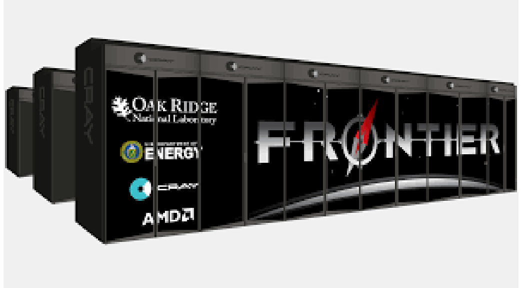
- Plan: Q4 Integration into CARD; transition from Office of Science ECP Project

[(2022): MFIX-Exa – Exascale Supercomputing to Model Chemical Looping Reactors for Industrial Carbon Capture - Exascale Computing Project (exascaleproject.org)]
[(2021): MFIX-Exa leverages CFD-DEM strengths to modernize reactor simulations - Exascale Computing Project (exascaleproject.org)]

- MFIX-Exa already contains PIC and DEM multiphase modeling codes which are used for gas-solids simulations

Next big steps:

- Lay groundwork for volume of fluid (VOF) code to incorporate gas-liquid-solids simulation
- Create a GUI to make the code more accessible to users



EXASCALE COMPUTING PROJECT

CARD FWP – EY23 Task Structure

Simulation Based Engineering Pushing Code Forward for Industrial Scale Systems

Task 2: MFiX Suite Multiphase Code Development, Validation and Enhancements
PI: Jeff Dietiker

- The home of MFiX-Classic CFD development, Nodeworks and Tracker

Task 3: Wafer Scale Engine Programming
PI: Dirk Van Essendelft

- A new computer chip architecture is investigated

Task 4: MFIX-Exa Code Development, Validation and Enhancements
PI: Jordan Musser

- Transitioning an Office of Science Exa-scale Computing Project to FECM advantage

Thank you
Questions?

VISIT US AT: mfix.netl.doe.gov