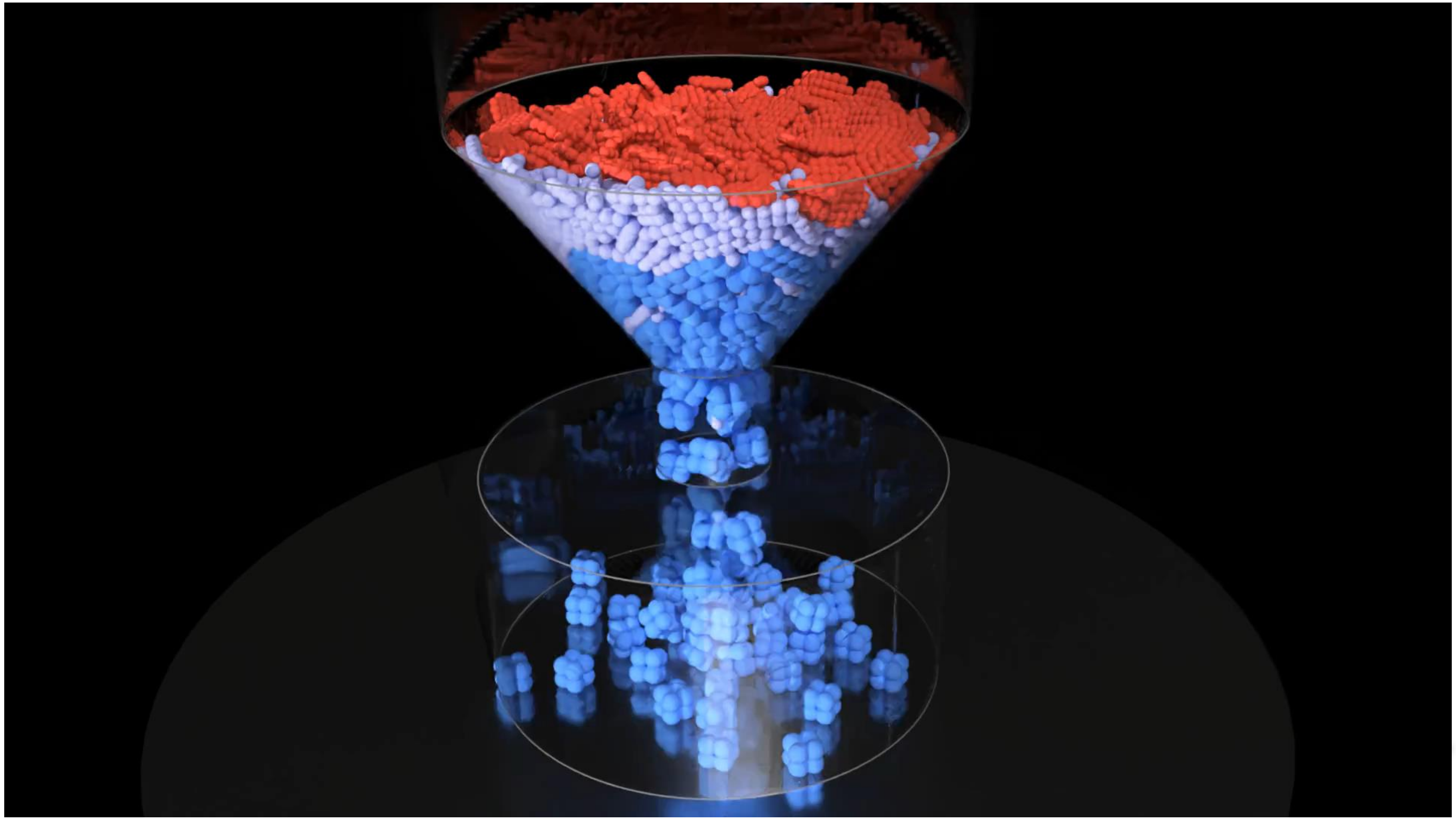
MFiX Development Updates

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

Jeff Dietiker
NETL Support Contractor



NETL 2024 Workshop on Multiphase Flow Science
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MFiX Suite of Multiphase Computational Fluid Dynamics Modeling Software

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Capabilities and Benefits

MFiX Multiphase Flow with Interphase eXchanges

3 Decades of development history

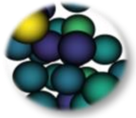
600+ downloads per month

8,800+ registered users

850 citations per year

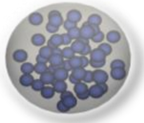
MFiX-TFM (Two-Fluid Model)

- Transport equations for both gas and solids phases
- Requires closure models



MFiX-DEM (Discrete Element Model)

- Uses first principles to account for particle interactions
- Computationally expensive



MFiX-PIC (Multiphase Particle In Cell)

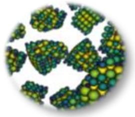
- Computationally efficient, tracks parcels
- Continuum stress model to approximate particle-particle interactions

MFiX-CGDEM (Coarse Grain DEM)

- Computationally efficient, tracks groups of particles
- Same contact mechanism as DEM

MFiX-SQP (Super Quadric Particle)

- Non-spherical particles, superquadric shapes
- Contact mechanism more expensive than DEM



MFiX-GSP (Glued Sphere Particle)

- Non-spherical particles, glued spheres
- Same contact mechanism as DEM

MFiX Suite of Multiphase CFD Software

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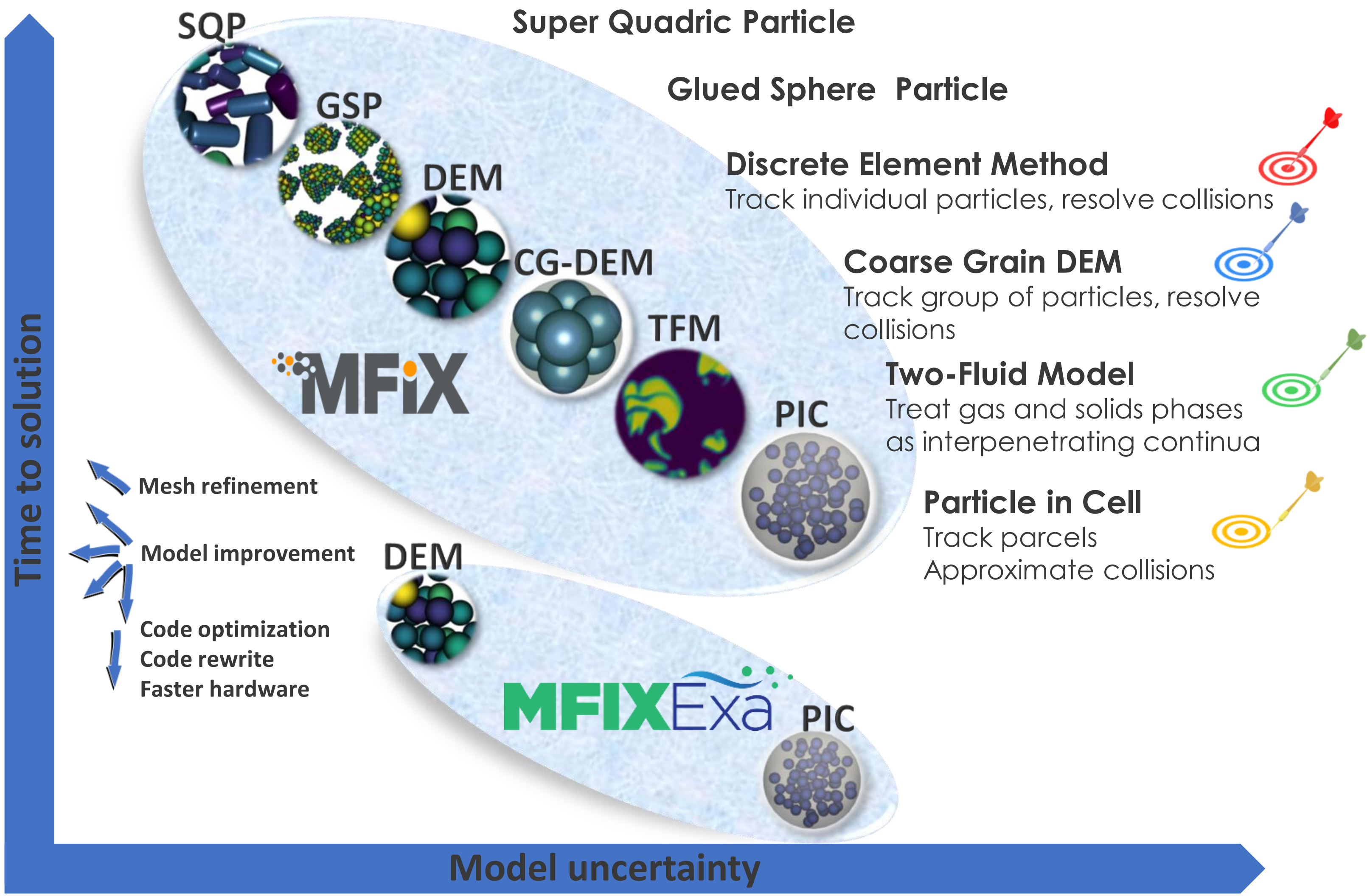
Managing the Tradeoff Between Accuracy and Time to Solution



Multiphase Models

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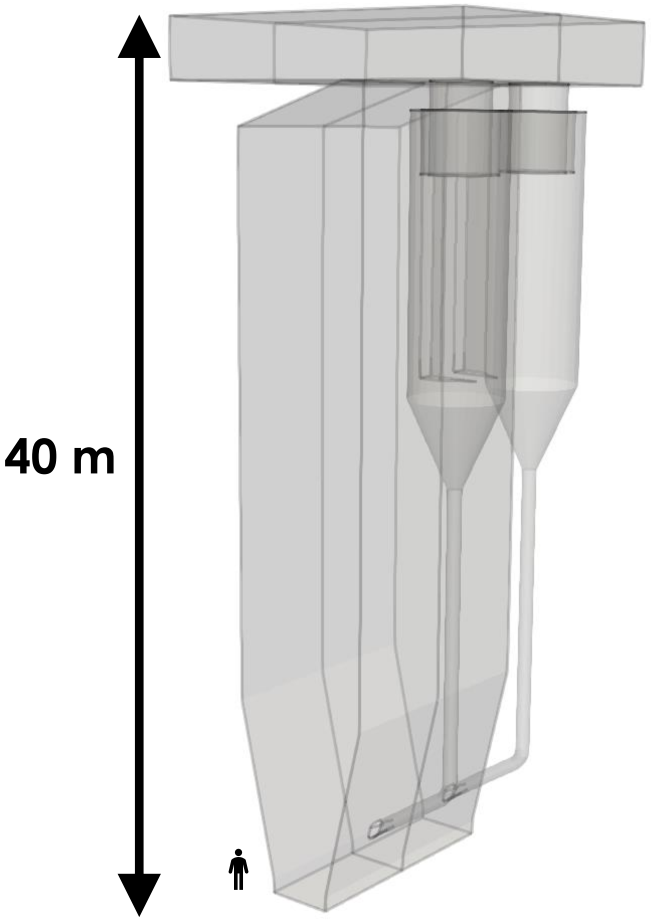
Example:10 MWth Industrial-Scale Circulating Fluidized Bed (CFB) Furnace

Miao Yang et al. (2023) **CFD Simulation of Biomass Combustion in an Industrial Circulating Fluidized Bed Furnace**, Combustion Science and Technology, 195:14, 3310-3340

- 40 m tall CFB furnace
- 60 tons of sand + biomass
- OpenFoam
- Coarse Grain DEM and PIC

Fine mesh:

- 600K cells
- 989K sand parcels
- 100K biomass parcels

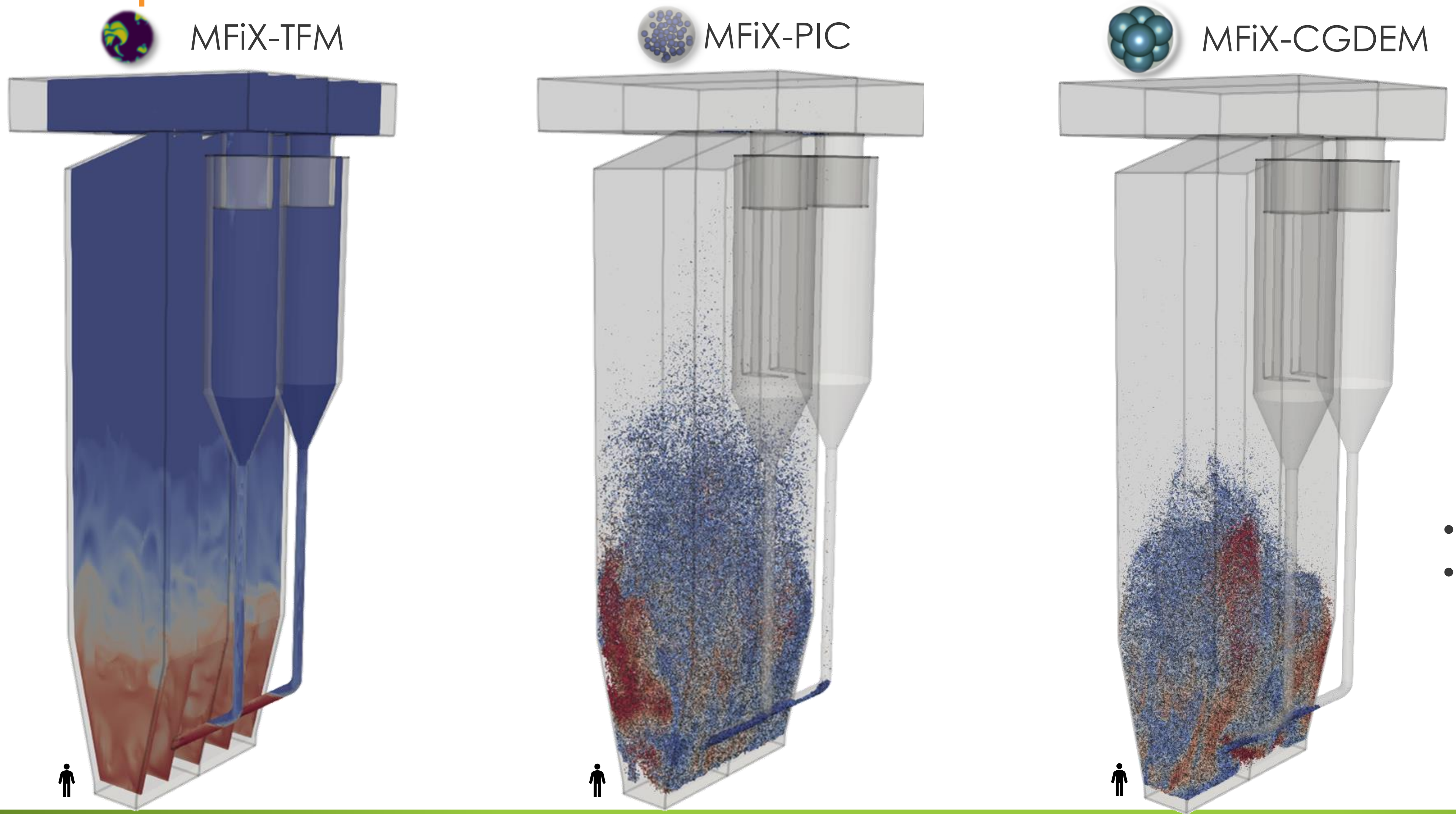


Refs	Scale	D	Model	subModel	H	T	R
Gu et al. (2020)	12 MWth	3D	E-L	MP-PIC	✓	✓	✓
Kong et al. (2020)	lab-scale	3D	E-L	MP-PIC	✓	✓	✓
Lin et al. (2022)	1 MWth	3D	E-L	MP-PIC	✓	✓	✓
Yang et al. (2020)	0.3 MWth	3D	E-L	MP-PIC	✓	✓	✓
Li and Shen (2021)	lab-scale	3D	E-E	TFM	✓	✓	✓
Cai et al. (2022)	lab-scale	3D	E-E	TFM	✓	✓	✓
Ghadirian, et al. (2019)	lab-scale	3D	E-E	TFM	✓	✓	✓
Wang et al. (2018)	lab-scale	3D	E-L	MP-PIC	✓	✓	✓
Wang et al. (2017)	600 MWth	3D	E-L	DEM	✓	✕	✕
Luo et al. (2015)	lab-scale	3D	E-L	DEM	✓	✕	✕
Lee et al. (2022)	550 MWth	3D	E-L	MP-PIC	✓	✕	✕
Tu and Wang (2018)	lab-scale	3D	E-L	MP-PIC	✓	✕	✕
Kadyrov, et al. (2019)	lab-scale	3D	E-L	MP-PIC	✓	✕	✕
Yang and Wang (2020)	lab-scale	3D	E-L	MP-PIC	✓	✕	✕
Muhammad et al. (2019)	lab-scale	3D	E-L	MP-PIC	✓	✕	✕
Ma et al. (2017)	lab-scale	3D	E-L	MP-PIC	✓	✕	✕
Li et al. (2021)	lab-scale	3D	E-L	MP-PIC	✓	✕	✕
Liu et al. (2002)	lab-scale	3D	E-E	TFM	✓	✕	✕
Lu et al. (2018)	lab-scale	2D	E-E	TFM	✓	✕	✕
Deng et al. (2021)	350 Mw	1D	×	×	✓	✓	✓

H- Hydrodynamic, *T*- thermo., R- gasification/combustion

Multiphase Models

Example:10 MWth Industrial-Scale CFB Furnace



MFiX:

- 1.7M cells
- 1.4M parcels/CGP

MFiX Development

4 Releases in EY23 (See mfix.netl.doe.gov for Full Release Note)

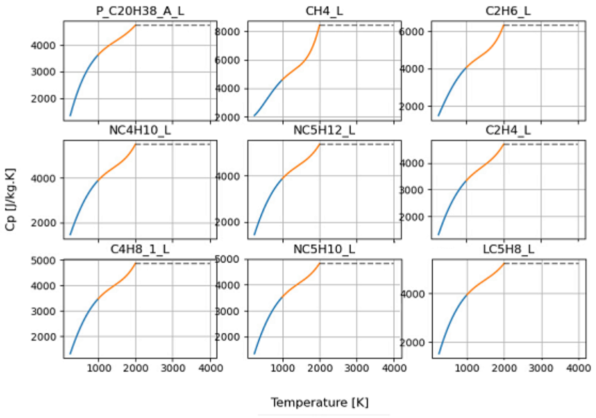
- **23.2:** - Support for Chemkin thermodynamic data
  - Chemical species and reaction equation import

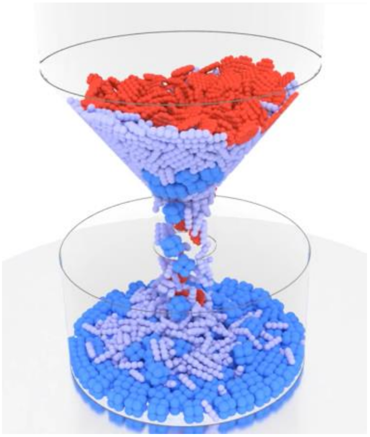
- **23.3:** - Stiff solver for DEM simulations
  - Default Shared Memory and Distributed Memory solvers
  - Keyword control of floating-point exception handling

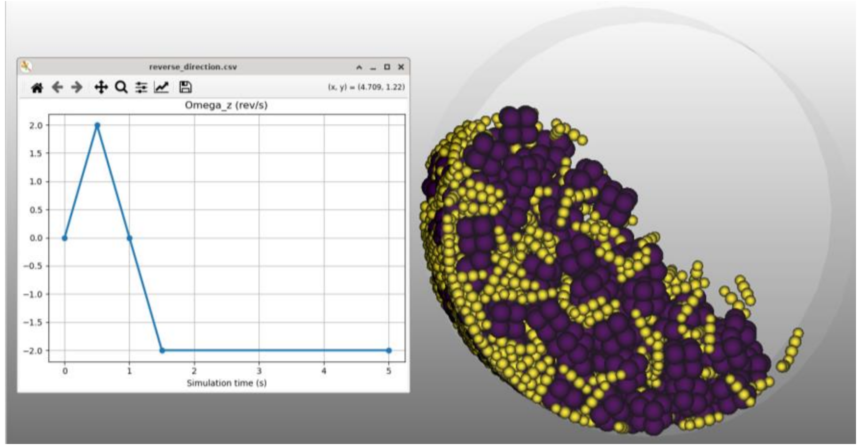
- **23.4:** - New adaptive time step option (nice dt)

- **24.1:** - Glued Sphere Particle model
  - Non-Newtonian viscosity model (Herschel-Bulkley)
  - Mass inlet ramps

- **24.2:** - New keyframe data workflow
  - DEM rigid motion



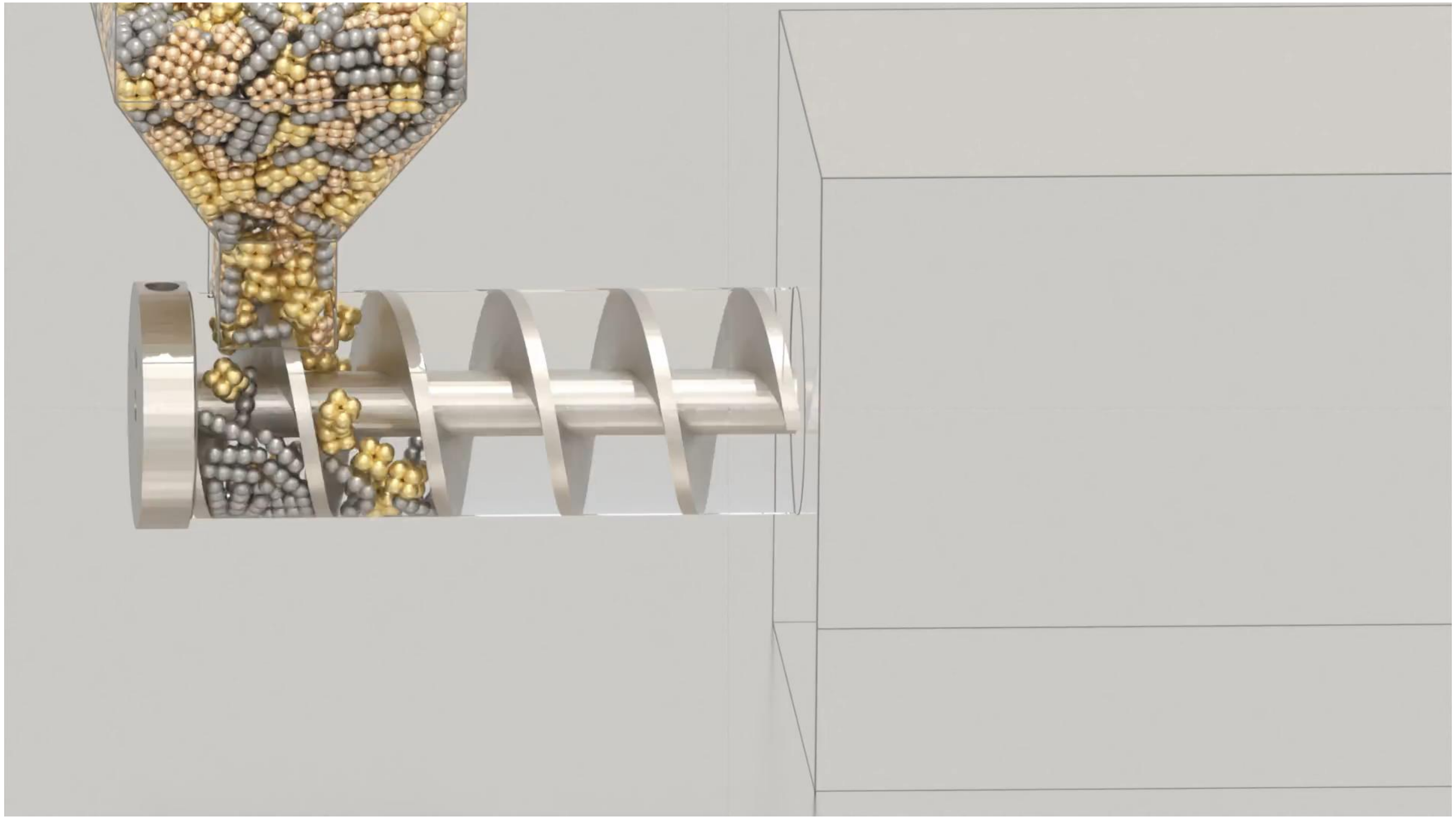




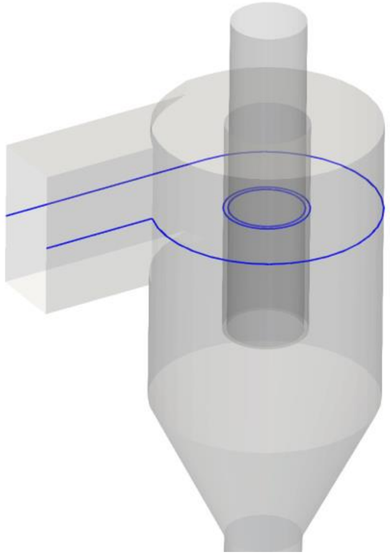
MFiX Development

23.2 Example

- **Screwfeeder**
    - Glued sphere DEM
    - Moving STL
    - Keyframe data

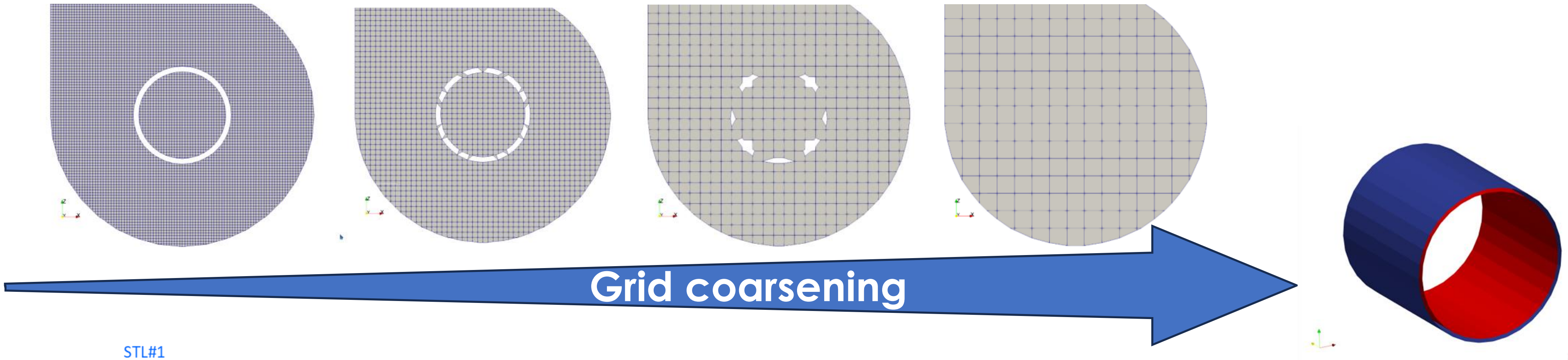


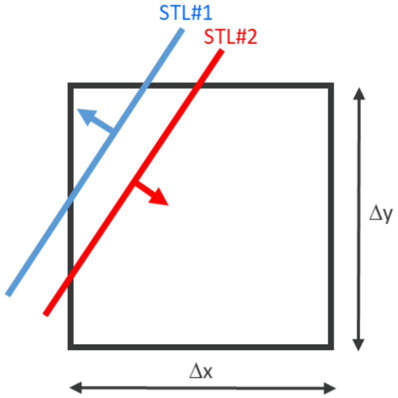
Thin Wall Boundary Conditions

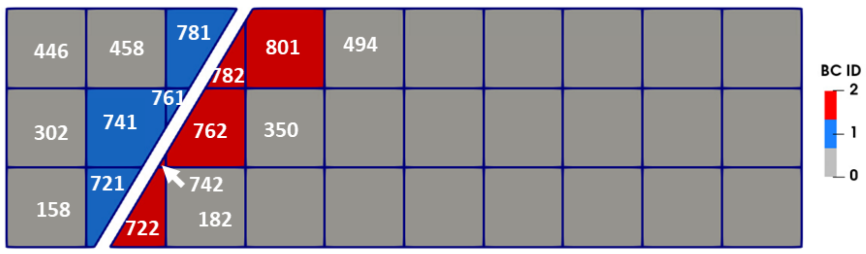


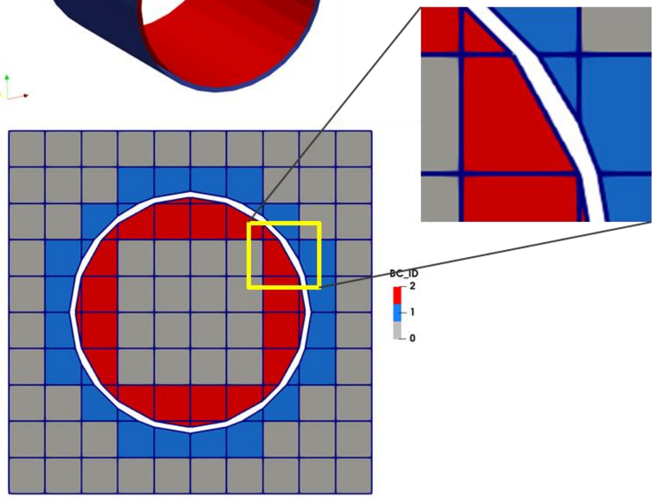
Motivation

- Cut cell approach cannot resolve geometric details smaller than cell size
- Internal walls must be at least 2-3 times thicker than cell size
- Not always feasible to refine the mesh



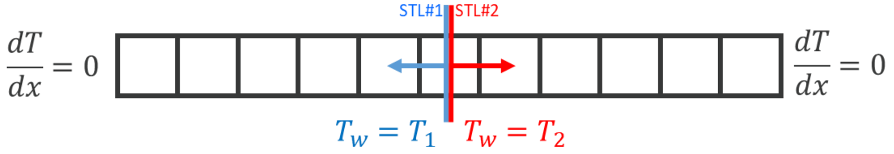


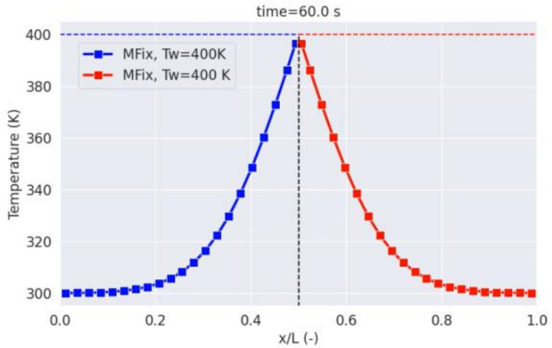




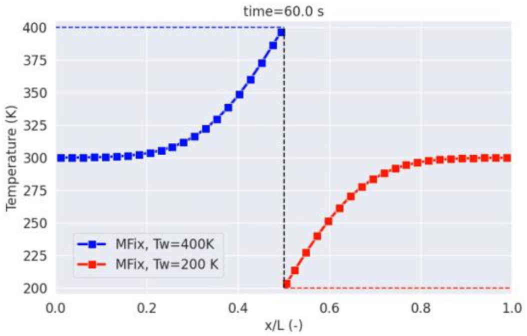
Thin Wall Boundary Conditions

- Scalar cell meshing
- Test with simple Heat Transfer

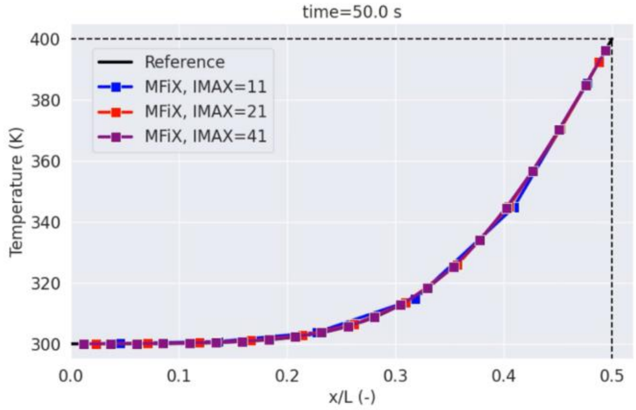


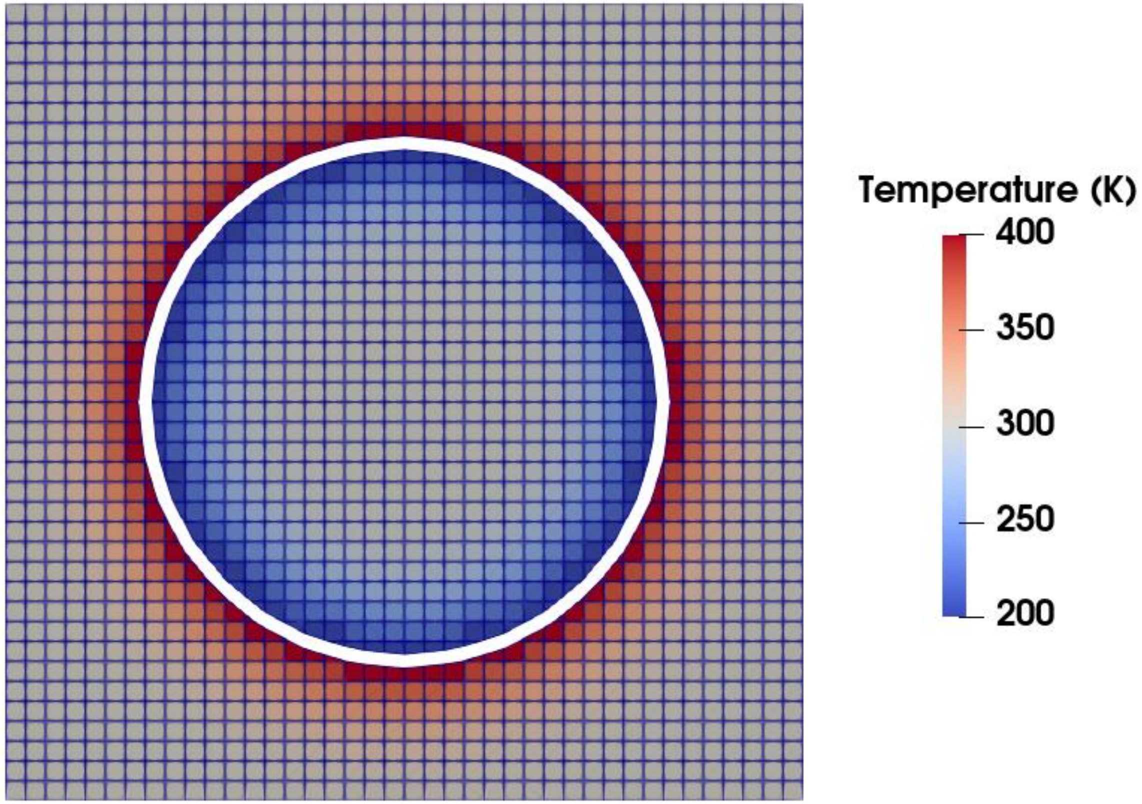


T_1=400K, T_2=400K



T_1=400K, T_2=200K





Glued Sphere Model (Non-Spherical Particles)

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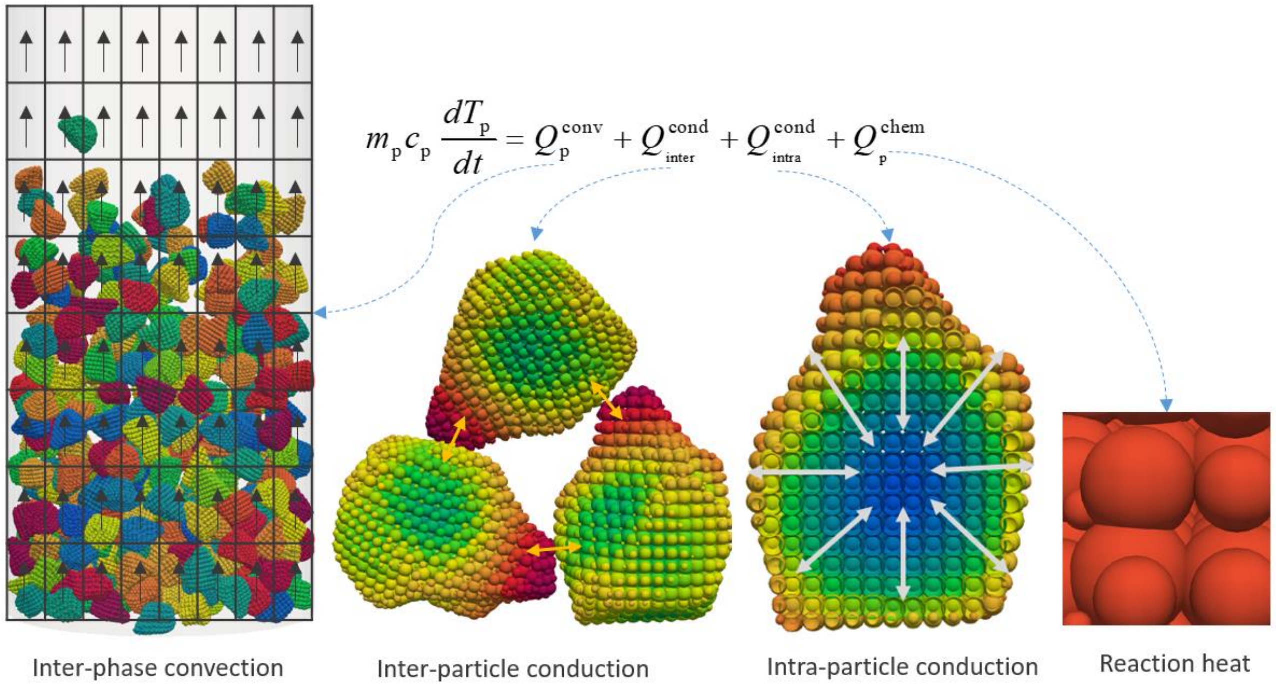
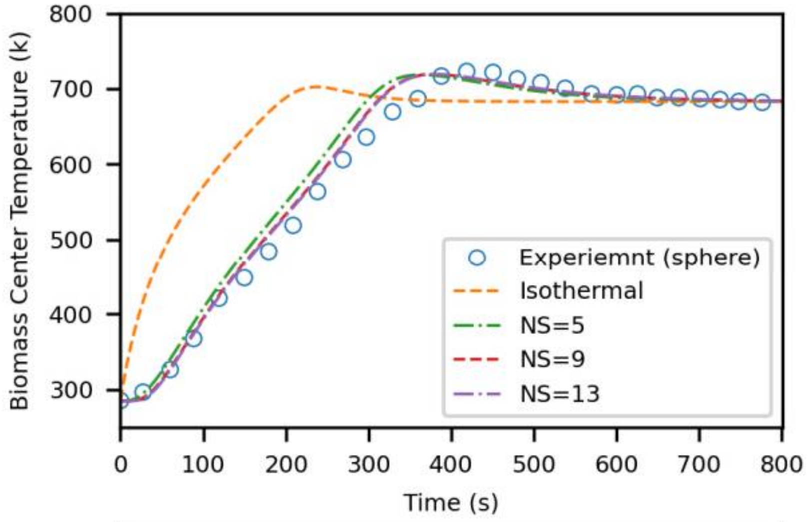
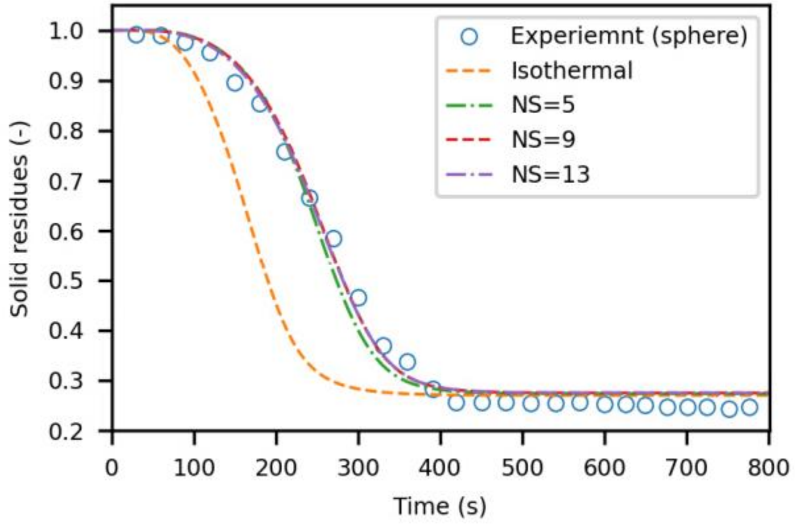
Irregular Shape of Particles

- Composite spheres
- Intra-particle temperature distribution

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





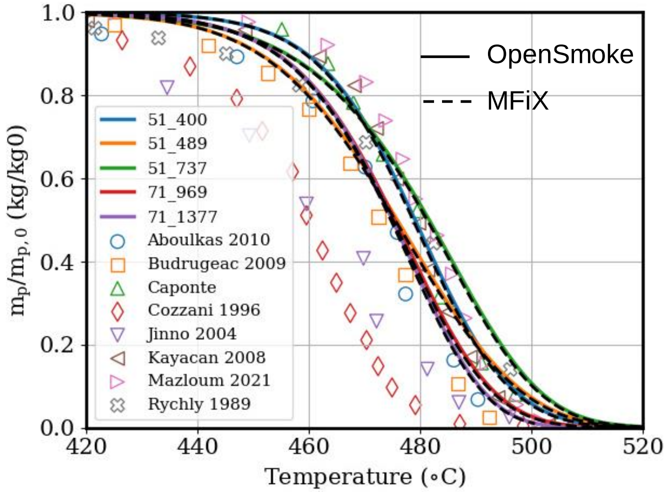


NETL Multiphase Flow Science
Home of the MFiX Software Suite

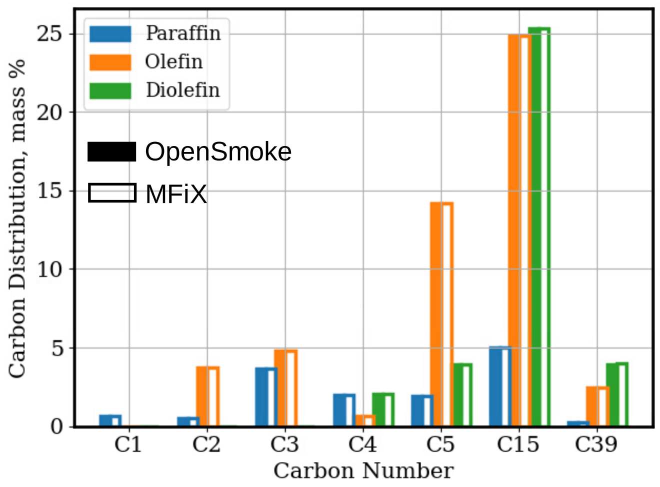
Chemistry Management

DEM Stiff Solver (10x to 100x Speedup)

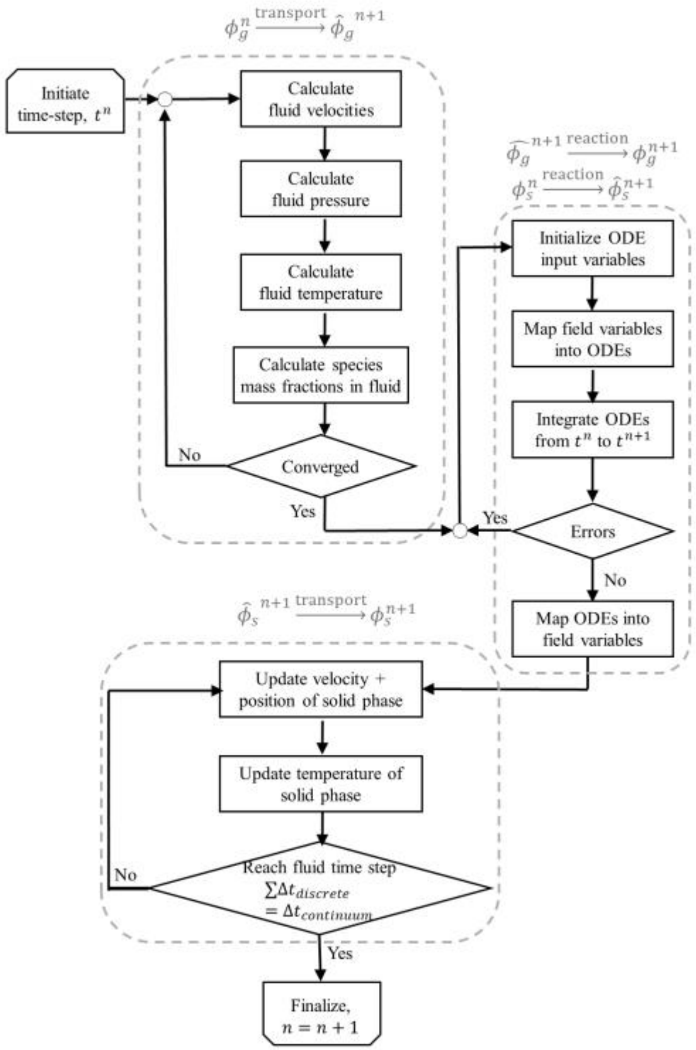
- Stiff solver (fractional-step method) was extended to all discrete particle models (DEM, GSP, SQP, CGP, PIC)
- Improves the ability to deal with detailed chemical mechanisms
- Separates chemical reactions from transport phenomena
- Tested with pyrolysis mechanism from Politecnico di Milano (400 to 1,377 reactions)
- MFiX predicts the same particle mass change and species productions as OpenSMOKE and experimental data



(a) Particle Mass Change



(b) Gas Species Production



Chemistry Management

Implementation of CHEMKIN Mechanism in MFiX

```
# Chemical reaction section
@(RXNS)
Reaction_1 {
      chem_eq = "A + B --> 2*C + 3*D"
      dh = 1e3
      fracdh(0) = 1
      arrhenius_coeff =  1000 0.0 2e3
      reverse_calc = fromForwardRateConstant
      rxn_order = A:2 B:1.5
      third_body_param = M_all "A:2 E: 0.5"
      press_rxn_param = Troe_coeff "press_coeff: 0.1 0.2 0.3 &
                               Arrhenius_press: 100 -2.0 3e5"
       lt_coeff = 200 500
       fit_coeff = JAN  "coeff: 1 2 3 4 5 6"
}
@(END)

@(DES_RXNS)
Reaction_DES_1{
      chem_eq = "F + 2*G --> H + 3*J"
      dh = 2e3
      fracdh(0)  = 0.5
      fracdh(1)  = 0.5
      arrhenius_coeff = 1e3 -1.0 3e5
      reverse_calc = fromForwardRateConstant
      rxn_order = F: 0.3 G: 2.0
}
@(DES_END)
```

```
ARRHENIUS_RATES_FLUID = .True.
ARRHENIUS_RATES_DES = .True.
```

Two ways to give the reaction rates:

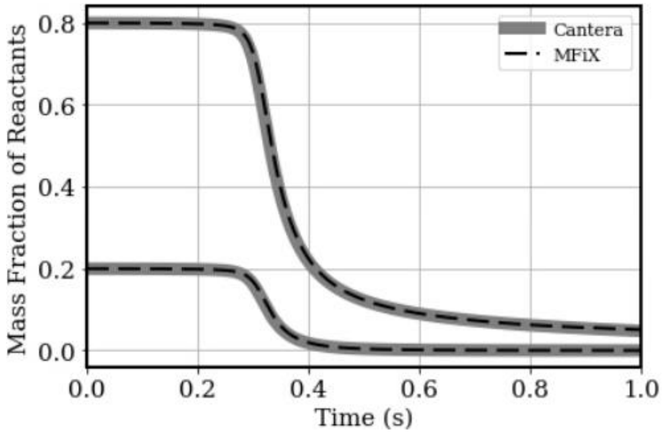
1. User-defined functions (UDF): usr_rates.f and usr_rates_des.f
2. Give parameters used for reaction rates in the input file (no UDF is required):
   1) Input the CHEMKIN mechanism file
   2) Add the parameters manually using the corresponding keywords

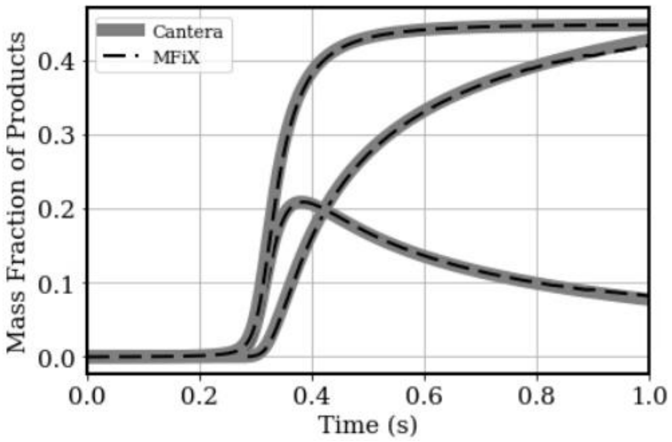
It could be applied to single gas phase and multiphase models in MFiX, like TFM, DEM, CGDEM, and PIC.

It is helpful when the users want to use CHEMKIN mechanisms directly, especially for detailed chemical mechanisms.

CH_4 combustion in a batch reactor using CHEMKIN ***GRI-30 mechanism***:

- Constant temperature: $T_0 = 1000K$
- Initial composition: CH_4: 20 wt.%, O_2: 80 wt.%





Integrating Machine Learning into MFiX

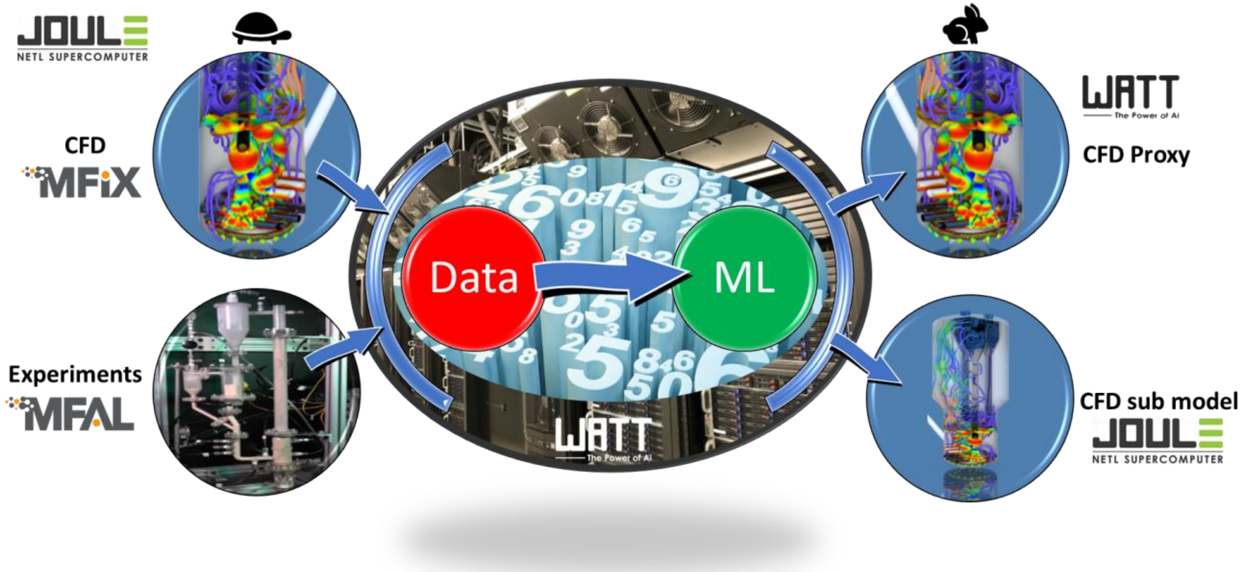
CFD & Machine Learning Workflow

- 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
- User-Defined Function (UDF) hook to use ML During Simulation
  - Call ML model at run time

Python scripting

or

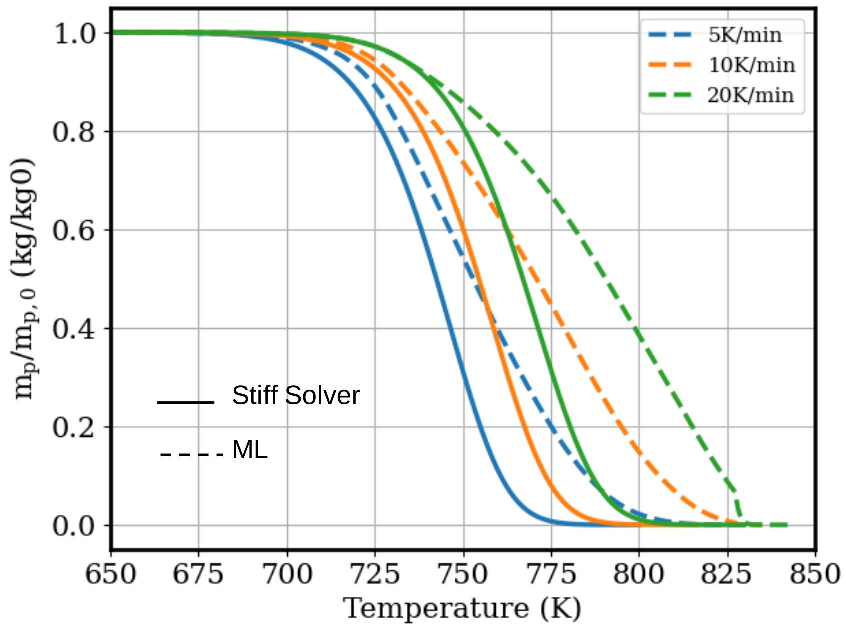
In-house ML tools



Chemistry ML acceleration

Stiff Solver ML Proxy

- ML model is integrated into MFiX to replace the stiff solver
- The mechanism for the pyrolysis of high-density polyethylene (HDPE) from Politecnico di Milano is applied to develop and test the ML model
- Data generated by MFiX
- Timing for the reaction terms are compared under three heating rates of particles. Two time-steps are tested
- Current preliminary ML model gives reasonable predictions of particle mass change
- ML model is much faster than the stiff solver, especially with high heating rate and smaller time steps



Time step: $dt = 0.5s$

	5K/min	10K/min	20K/min
Stiff Solver	276 min	217 min	132 min
ML Model	18 min	10 min	5 min
Speedup	**15.3**	**21.7**	**26.4**

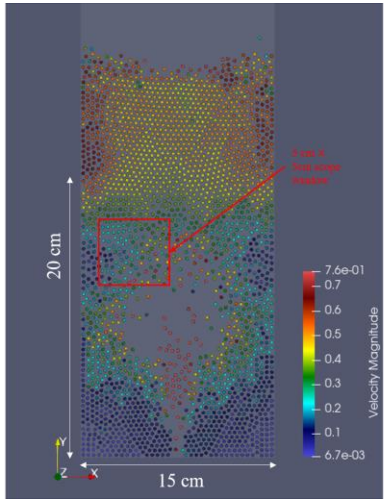
Time step: $dt = 0.01s$

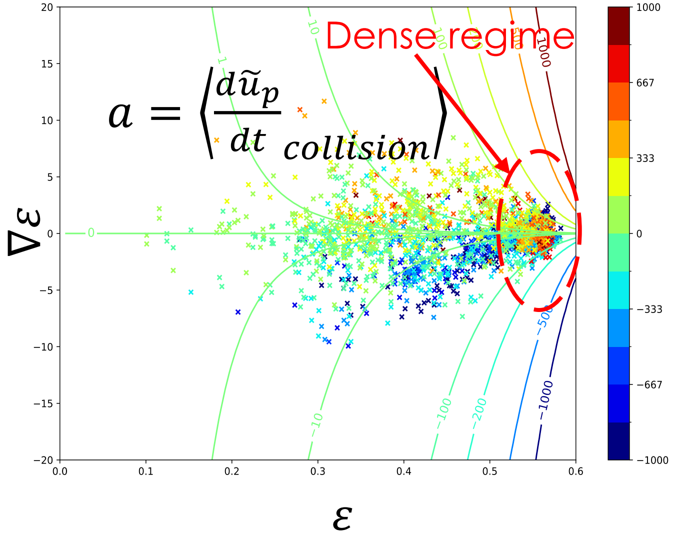
	5K/min	10K/min	20K/min
Stiff Solver	882 min	441 min	227 min
ML Model	24 min	12.5 min	8 min
Speedup	**36.8**	**35.3**	**28.4**

PIC Stress ML Modeling Using DEM Data

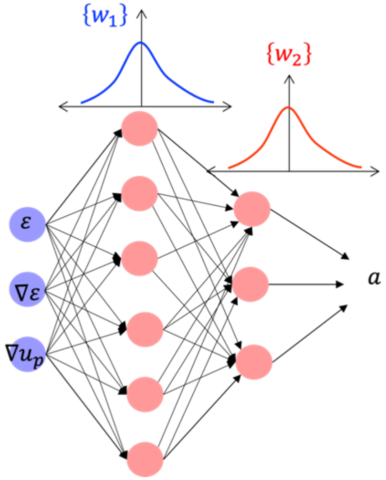
Data Collection

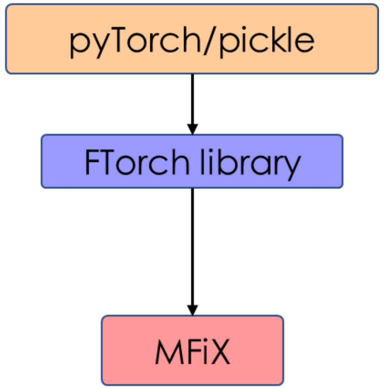
- DEM fluidized bed with various inlet velocities
- Spatially sample average particulate properties:
- Volume fraction (ε), Gradient of volume fraction ($\nabla\varepsilon$), Granular temperature (θ)
  - Average particle velocity (u_p), its gradient (∇u_p), Deceleration due to collisions (a)
- Temporal averaging of the spatially sampled data is performed over 50 DEM timesteps





- Distinct dense and dilute regimes are observed. Compaction of particles in the dense region and high deceleration magnitudes
- Sampled DEM deceleration term is different from the Harris and Crighton (1994) model used in PIC approach
- Combining Harris & Crighton criteria with sampled datapoints using Bayesian approach
- Incorporating trained BNN model in MFiX code





Outreach: MFiX Stats

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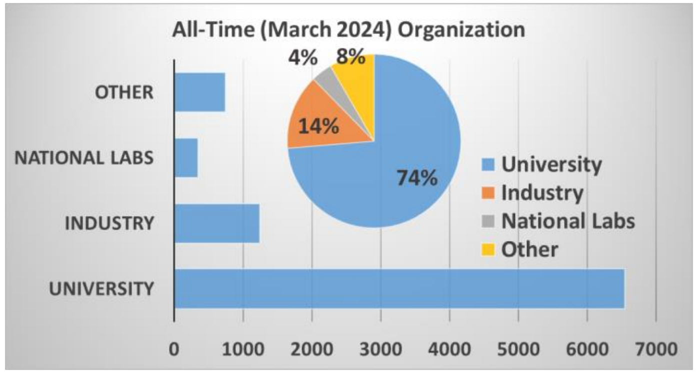
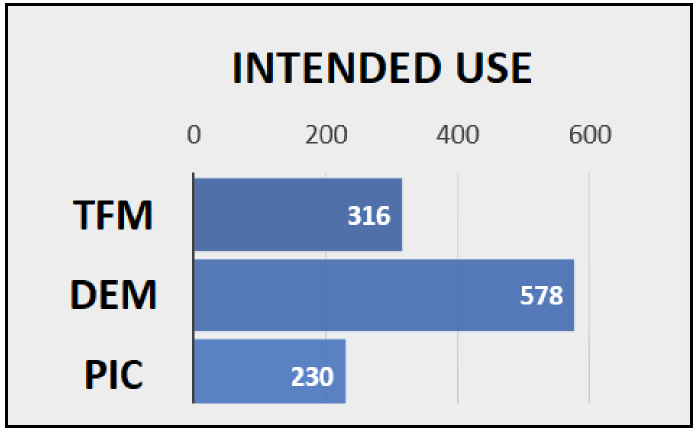
Stakeholders and Technology Transfer

All-time MFiX registrations = **8,800+**

EY23 Registrations = 725

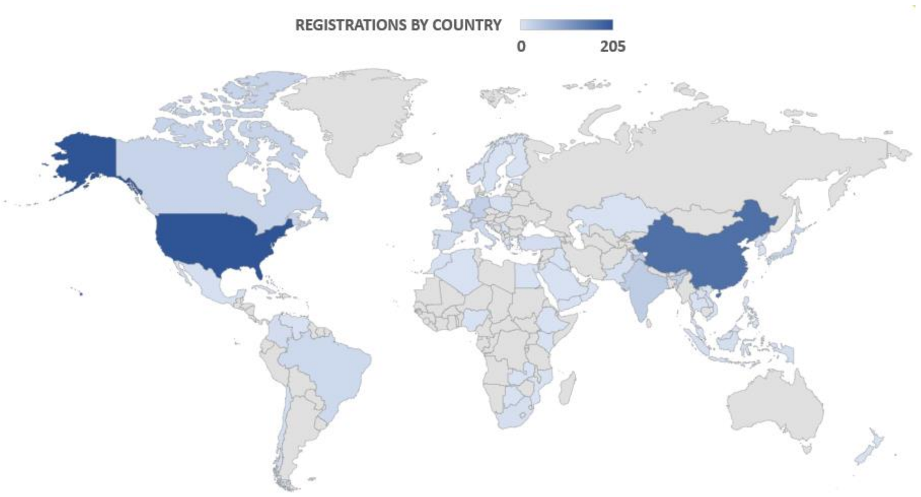
EY23 Downloads = 9,200

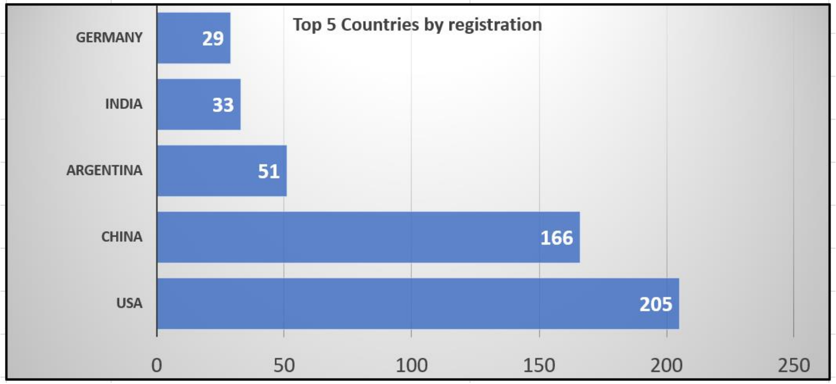




Universities using MFiX in their curriculum:

- Arizona State University
- Pennsylvania State University
- Hamburg University of Technology, Germany
- Universidad de La Serena, Chile
- Universidad Nacional de La Plata, Argentina

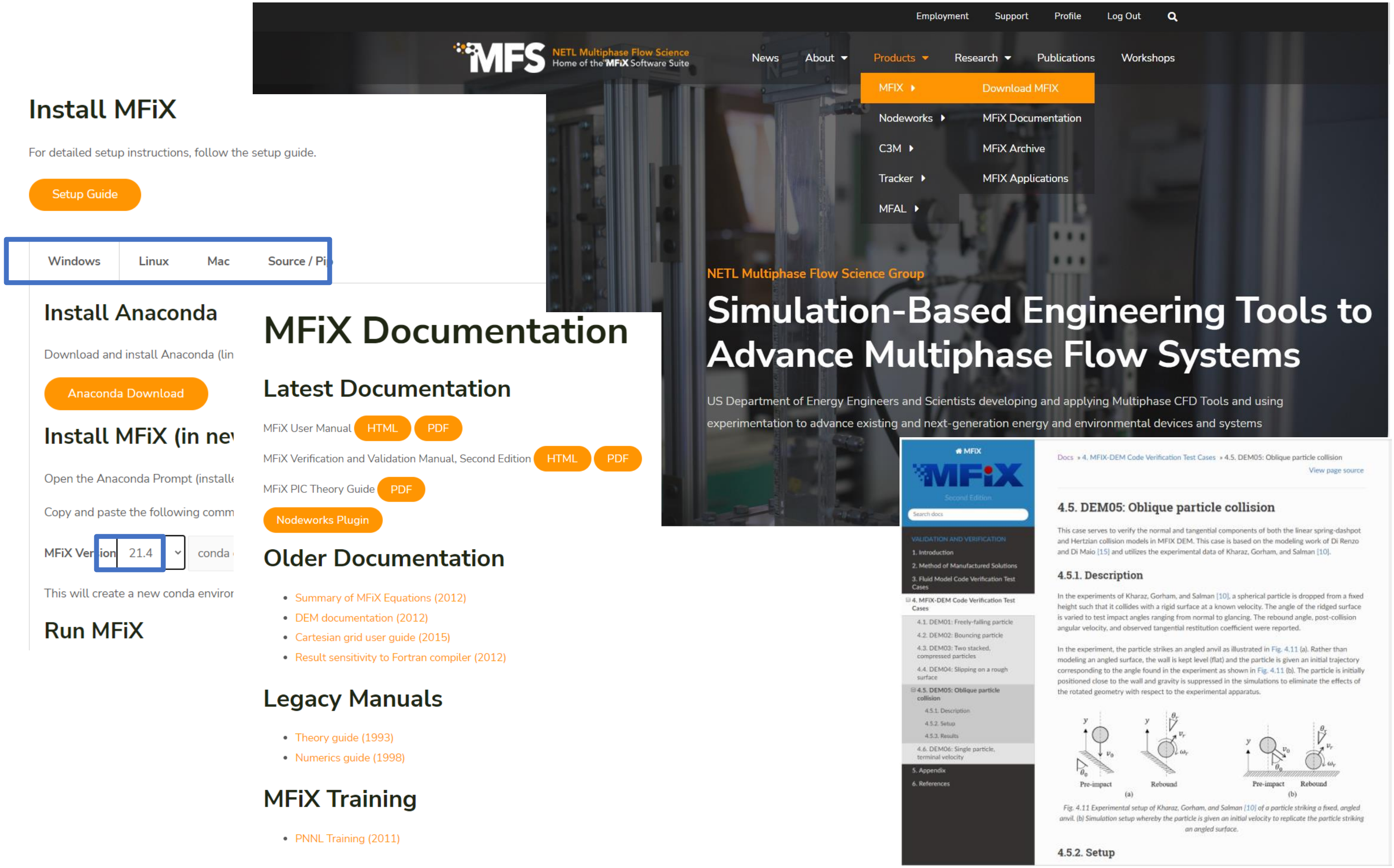


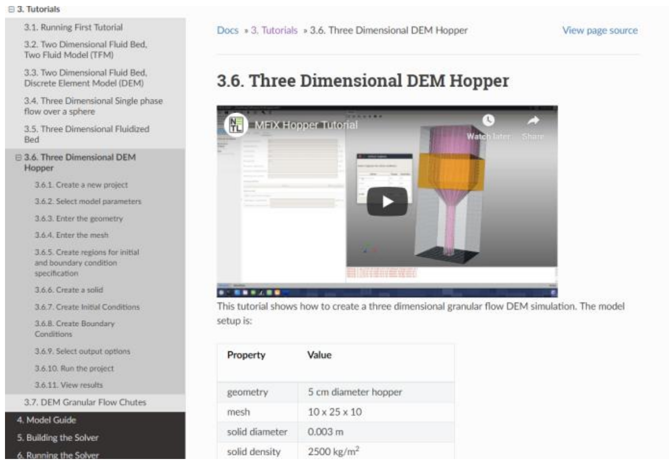


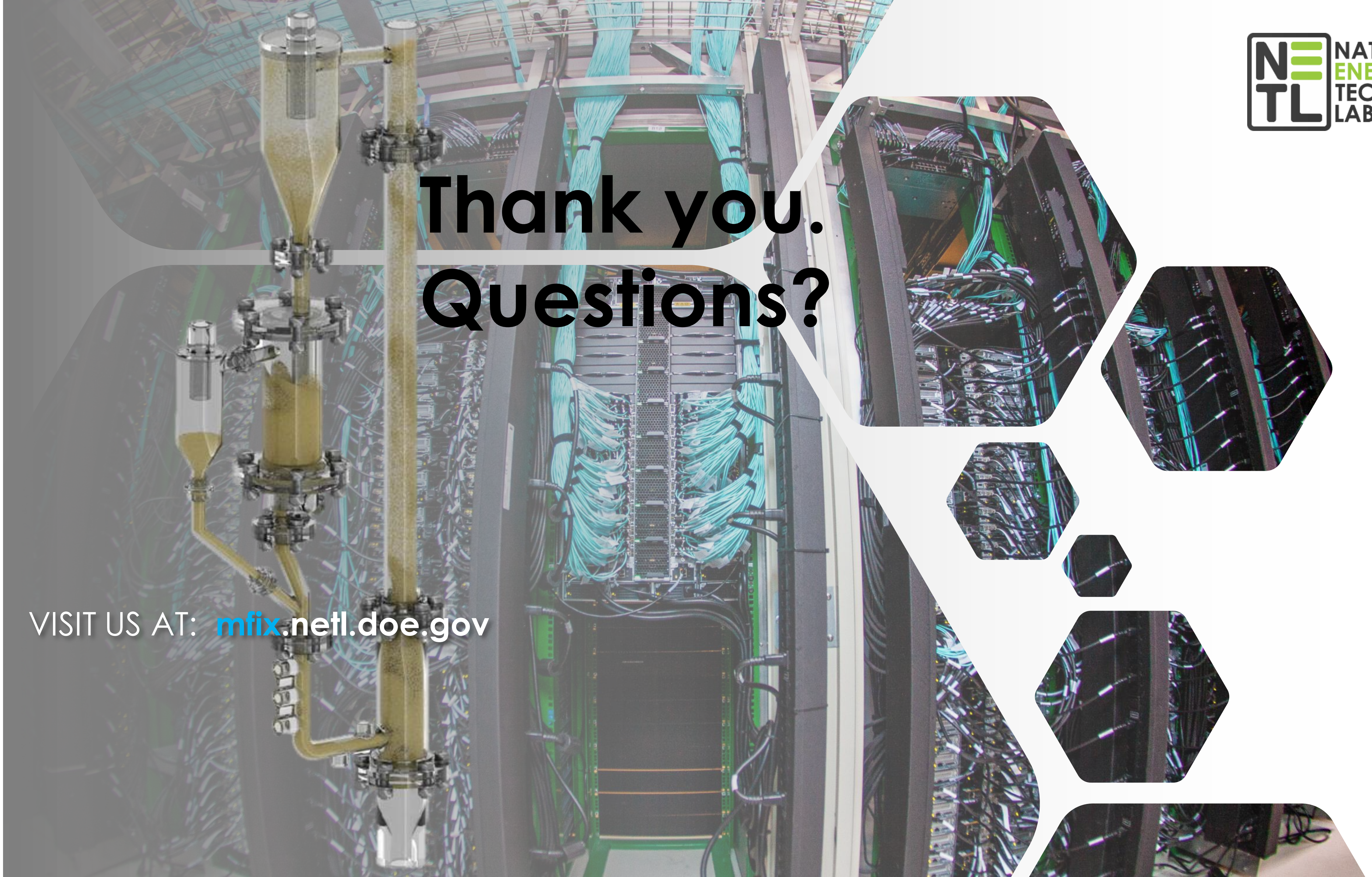
Resources – MFiX Website

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

https://mfix.netl.doe.gov







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