Advancement of CFD-based Tools for Design and Optimization of Energy Devices

NATIONAL ENERGY TECHNOLOGY LABORATORY

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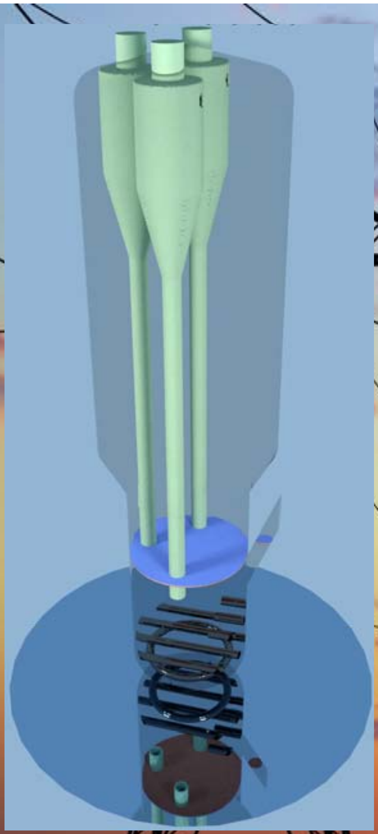
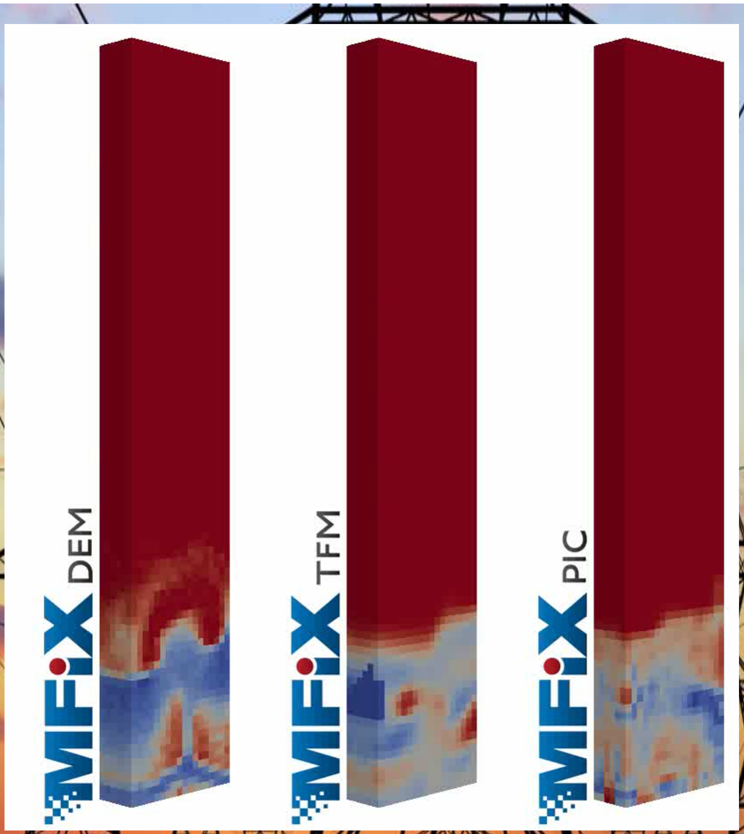
March 22, 2017





Solutions for Today | Options for Tomorrow

U.S. DEPARTMENT OF ENERGY

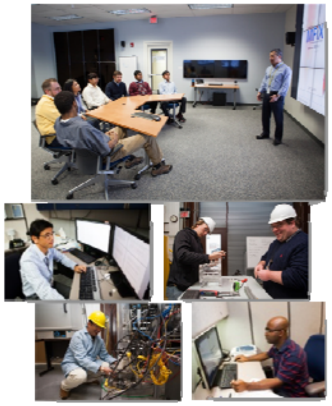
Outline

- **Advanced Reaction Systems Program**
  - MFiX Suite Multiphase Code Development and Validation
    - Code Development and Improvement
      - MP-PIC
      - DEM
      - GUI
    - Software Quality Assurance and Validation with UQ
    - Multiphase Experimentation for Model Development and Validation

NETL Multiphase Flow Science Team

31 years of Multiphase R&D

- **Development, Validation, Application and Support of Practical Multiphase Flow Simulation Tools**
  - Tools to guide the design, operation, and troubleshooting of multiphase flow devices
  - Emphasis on Fossil Fuel Technologies (e.g., coal gasifiers, CO_2 capture devices, Chemical Looping)
- **30+ Engineers and Scientists on the team**
  - Open-source Software Tools
    - **MFiX Suite** of Multiphase CFD Software
    - **C3M** Multiphase Chemistry Management Software
    - Optimization Toolset
  - Multiphase experimentation for model development and validation
    - High quality data made available to the public



MFS Team

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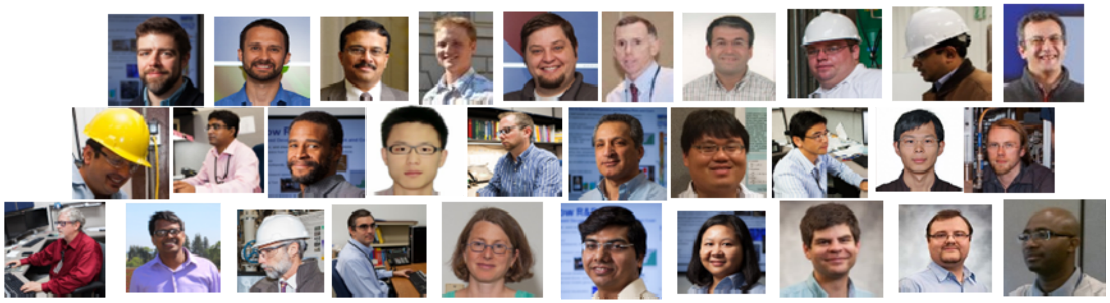


NETL Multiphase Flow Science
Home of the MFiX Software Suite

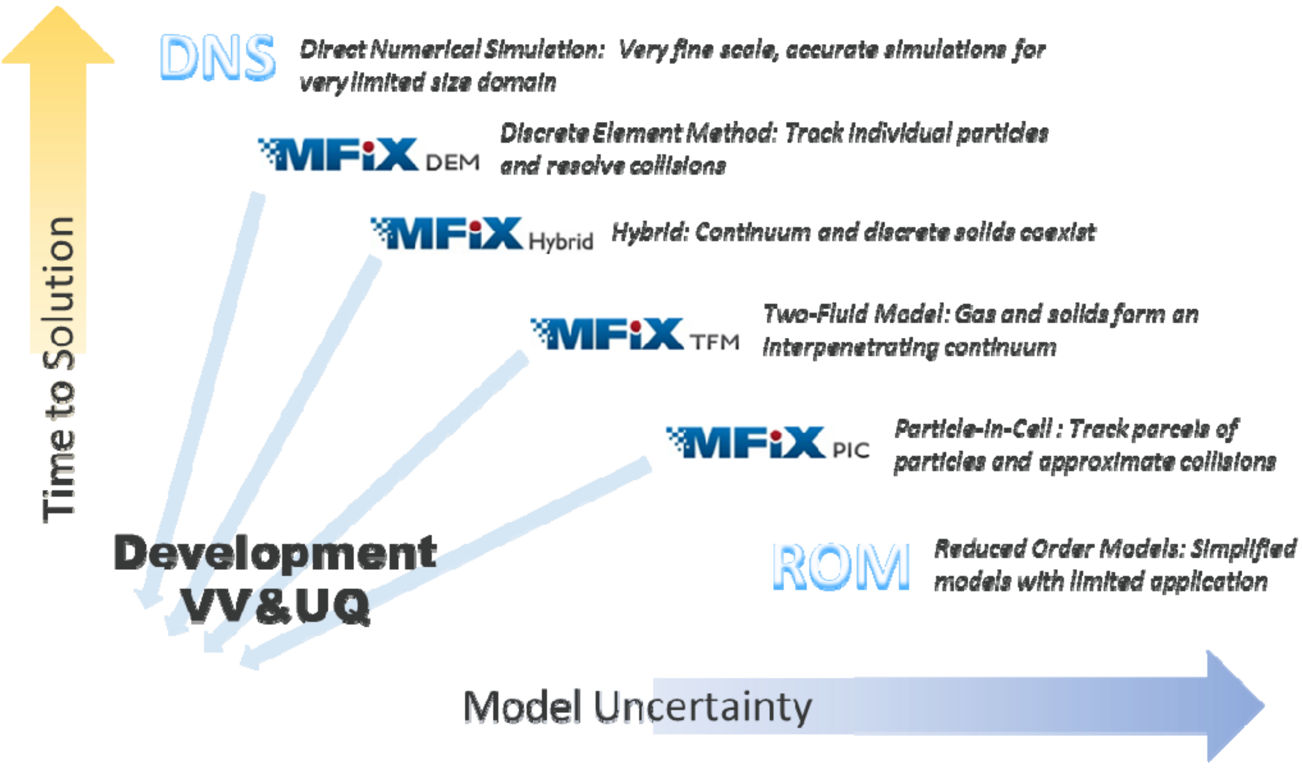
https://mfix.netl.doe.gov

MFiX Model Overview

NETL's multiphase CFD suite MFiX

- Open source, two decades of development
- Three distinct solids modeling capabilities
  - Different degrees of model complexity
  - Varying levels of development maturity

https://mfix.netl.doe.gov



DNS *Direct Numerical Simulation: Very fine scale, accurate simulations for very limited size domain*

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

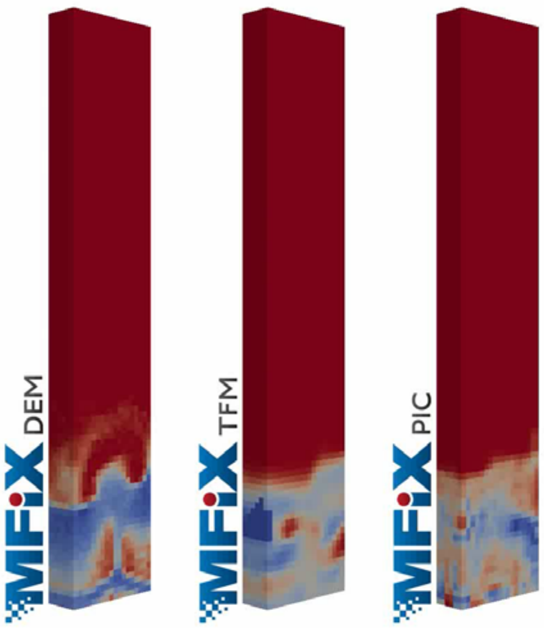
MFiX Hybrid *Hybrid: Continuum and discrete solids coexist*

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

MFiX PIC *Particle-in-Cell : Track parcels of particles and approximate collisions*

ROM *Reduced Order Models: Simplified models with limited application*

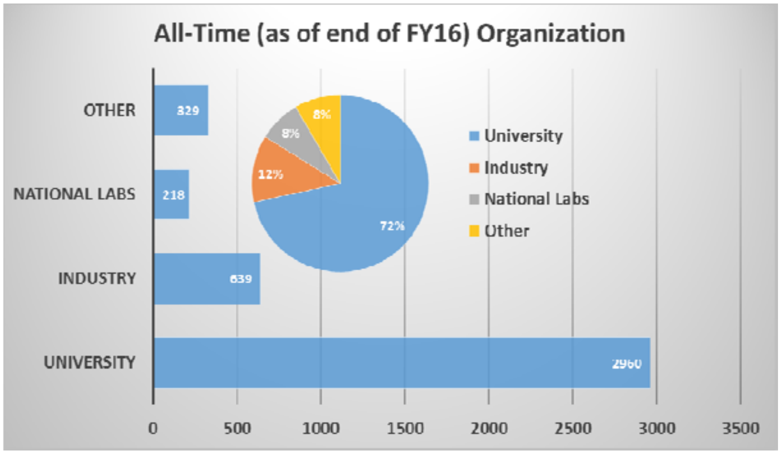
Managing the tradeoff between accuracy and time-to-solution

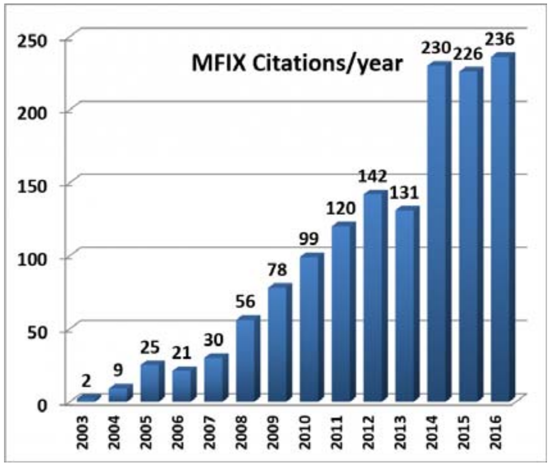


NETL Small Scale Challenge Problem

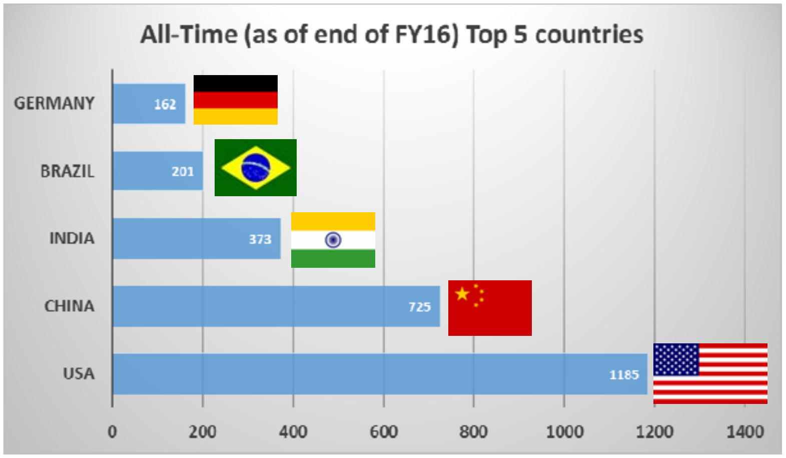
MFiX User Community Statistics

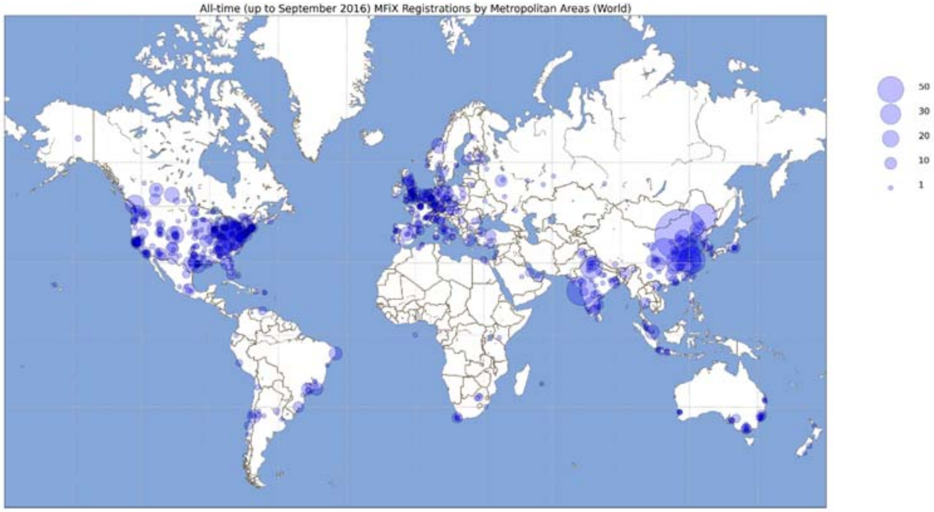
All-time Users as of end of FY16





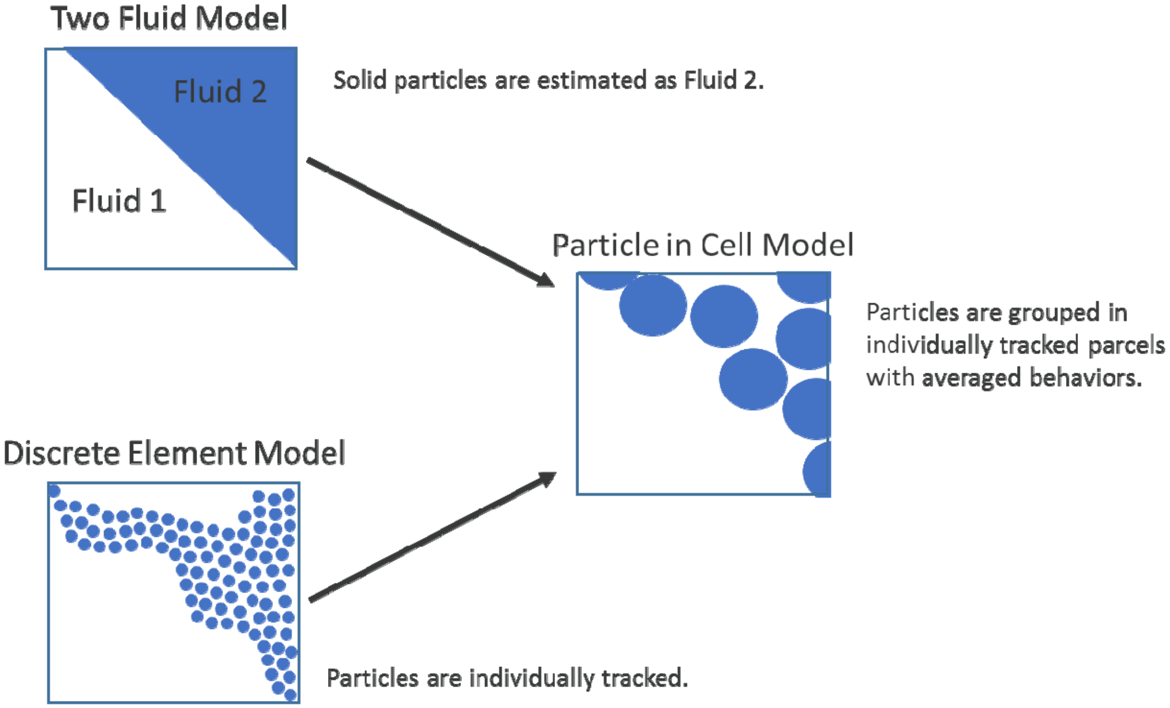
4000+ all-time MFiX registrations





Development of the MFiX-PIC code

- **Objective: Development of large scale reacting MFiX-PIC model**
  - Complex boundaries
  - Robustness
  - DMP generalization
  - Code optimization



Two Fluid Model

Solid particles are estimated as Fluid 2.

Particle in Cell Model

Particles are grouped in individually tracked parcels with averaged behaviors.

Discrete Element Model

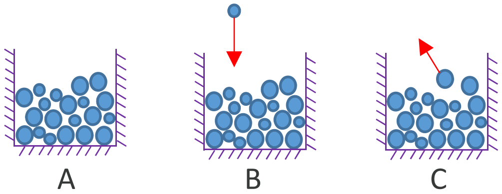
Particles are individually tracked.

Development of the MFiX-PIC code

Translating the theories of Snider and O'Rourke into MFiX code:

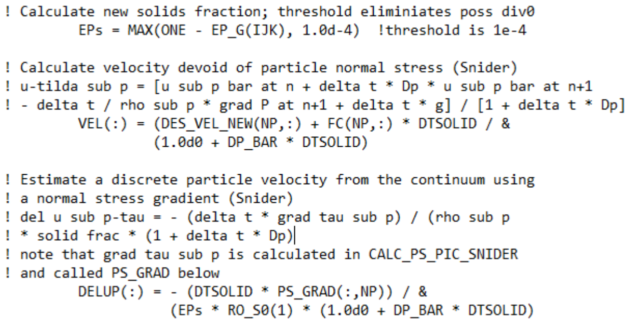
- Snider, D.M., "An Incompressible Three-dimensional multiphase Particle-in-Cell model for dense particle flows," Journal of Computational Physics, Vol 170, pp. 523-549.
- O'Rourke, P.J., et. al, "A model for collisional exchange in gas/liquid/solid fluidized beds," Chemical Engineering Science, Vol 64, pp. 1784-1797.

Examine gradients of particle contact stress (τ) to allow the PIC code to better model parcel behavior near areas of close-pack (θ_{cp}).



A: Parcels part of a close-pack region
B: Parcels approaching a close-pack region
C: Parcels leaving a close-pack region

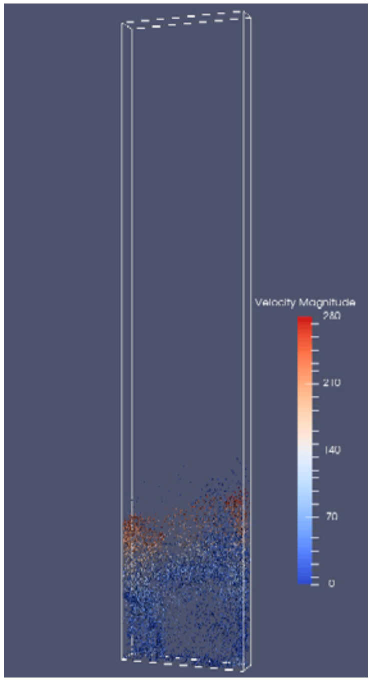
$$\tau = \frac{P_s \theta_s^{\beta}}{max\left[\theta_{cp} - \theta_s, \varepsilon(1-\theta_s)\right]} \longrightarrow$$



```
! Calculate new solids fraction; threshold eliminiates poss div0
         EPs = MAX(ONE - EP_G(IJK), 1.0d-4)  !threshold is 1e-4

! Calculate velocity devoid of particle normal stress (Snider)
! u-tilda sub p = [u sub p bar at n + delta t * Dp * u sub p bar at n+1
! - delta t / rho sub p * grad P at n+1 + delta t * g] / [1 + delta t * Dp]
         VEL(:) = (DES_VEL_NEW(NP,:) + FC(NP,:) * DTSOLID / &
                  (1.0d0 + DP_BAR * DTSOLID)

! Estimate a discrete particle velocity from the continuum using
! a normal stress gradient (Snider)
! del u sub p-tau = - (delta t * grad tau sub p) / (rho sub p
! * solid frac * (1 + delta t * Dp)|
! note that grad tau sub p is calculated in CALC_PS_PIC_SNIDER
! and called PS_GRAD below
         DELUP(:) = - (DTSOLID * PS_GRAD(:,NP)) / &
                    (EPs * RO_S0(1) * (1.0d0 + DP_BAR * DTSOLID)
```



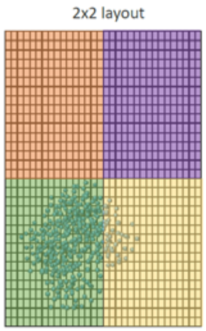
Managing the MFiX calculations at particle collision time scales translates to capturing better particle physics in both dilute and close-pack regions.

Development of the MFiX-DEM code

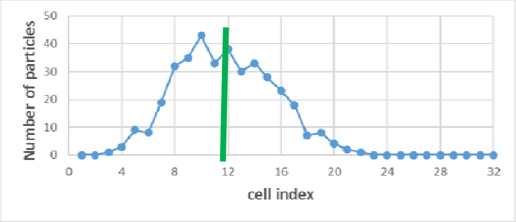
- **DEM simulations suffer from large load imbalance**
- **Bottleneck is most heavily loaded processor**
- **As of 2016-1 Release:**
  - Specify the partition layout as input (ex: 4x4x4 for 64-core run)
  - Choice of partition layout affects simulation speed
  - Option to manually specify a partition at the beginning of the run (static decomposition) in gridmap.dat
  - Not efficient when particles circulate or when inventory changes in time
- **Provide a minimally invasive Dynamic Load Balance (DLB) option for MFiX-DEM Simulations**
  - No major code modification
  - Low overhead
  - Use existing partition scheme (gridmap)
  - Can be used in future if DEM gridmap is modified
  - Work with all Lagrangian approaches

Technical Approach

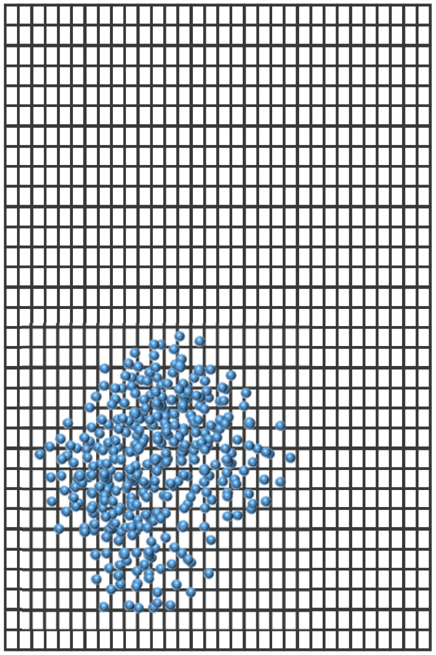
Dynamic Load Balance Implementation



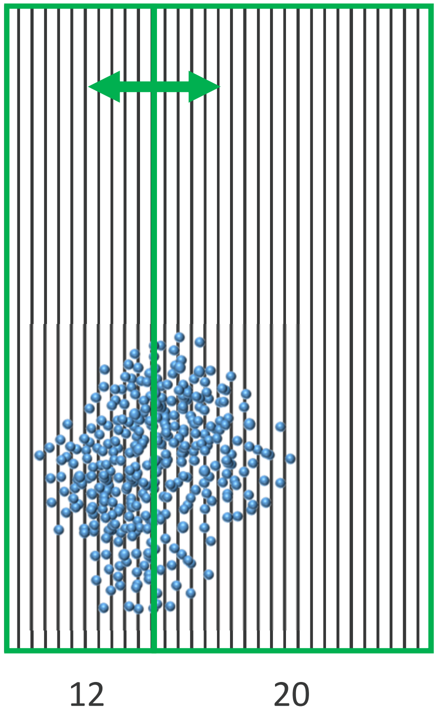
- **Find best partition by moving PE boundary planes in each direction, individually, then combine**



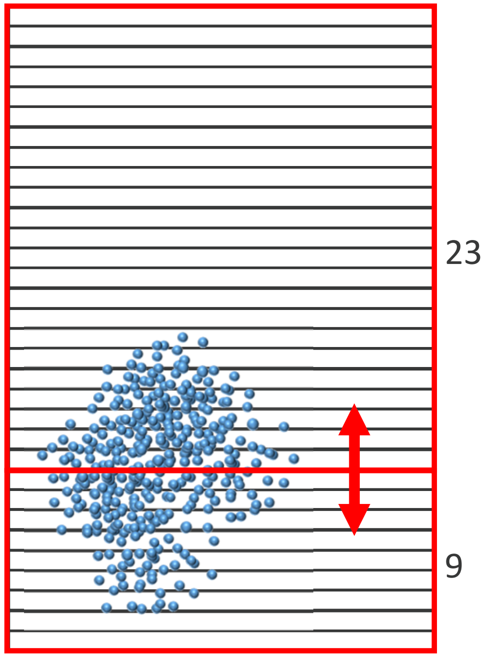
- Need to gather number of particles as 1D arrays
- Adjustment done on Head node
- Partition snaps on grid, ("All or Nothing")



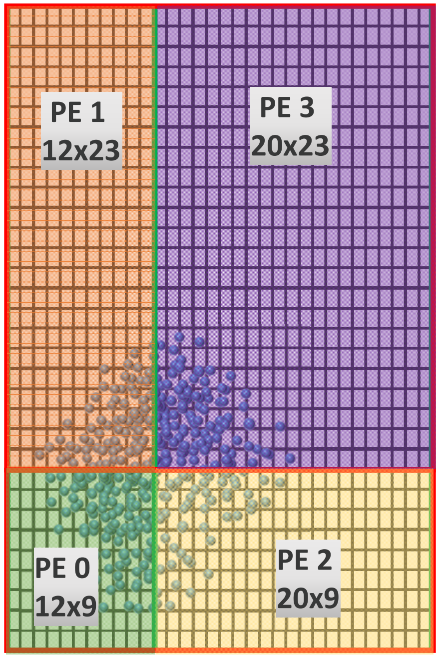
Example: 4 Pes, 2x2 layout
Mesh size is 32x32



Adjust size in x-direction



Adjust size in y-direction

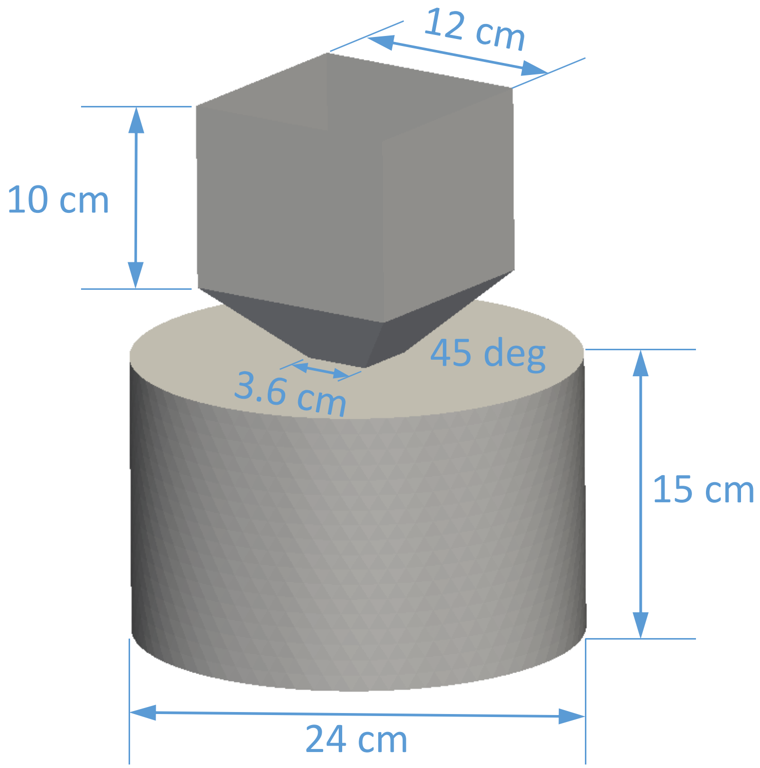


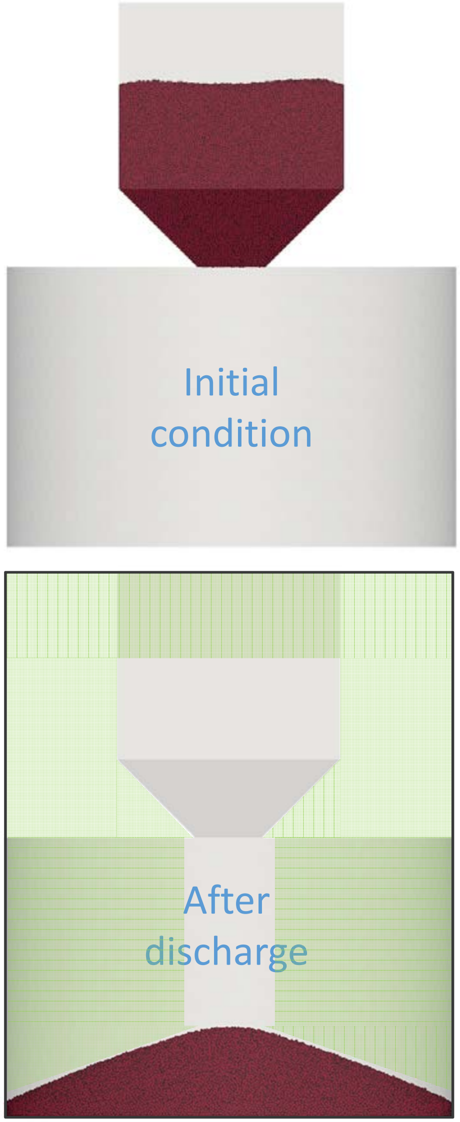
Combine

Results – Hopper – Granular Flow

Simulation setup

- Density= 2,300 kg/m^3
- Diameter=1.6 mm
- 300,000 particles





Granular flow

Run for 5 seconds

64 cores

DLB_DT = 0.025 s

Grid size = 56x64x56

Reference (No DLB): 4x4x4 Layout

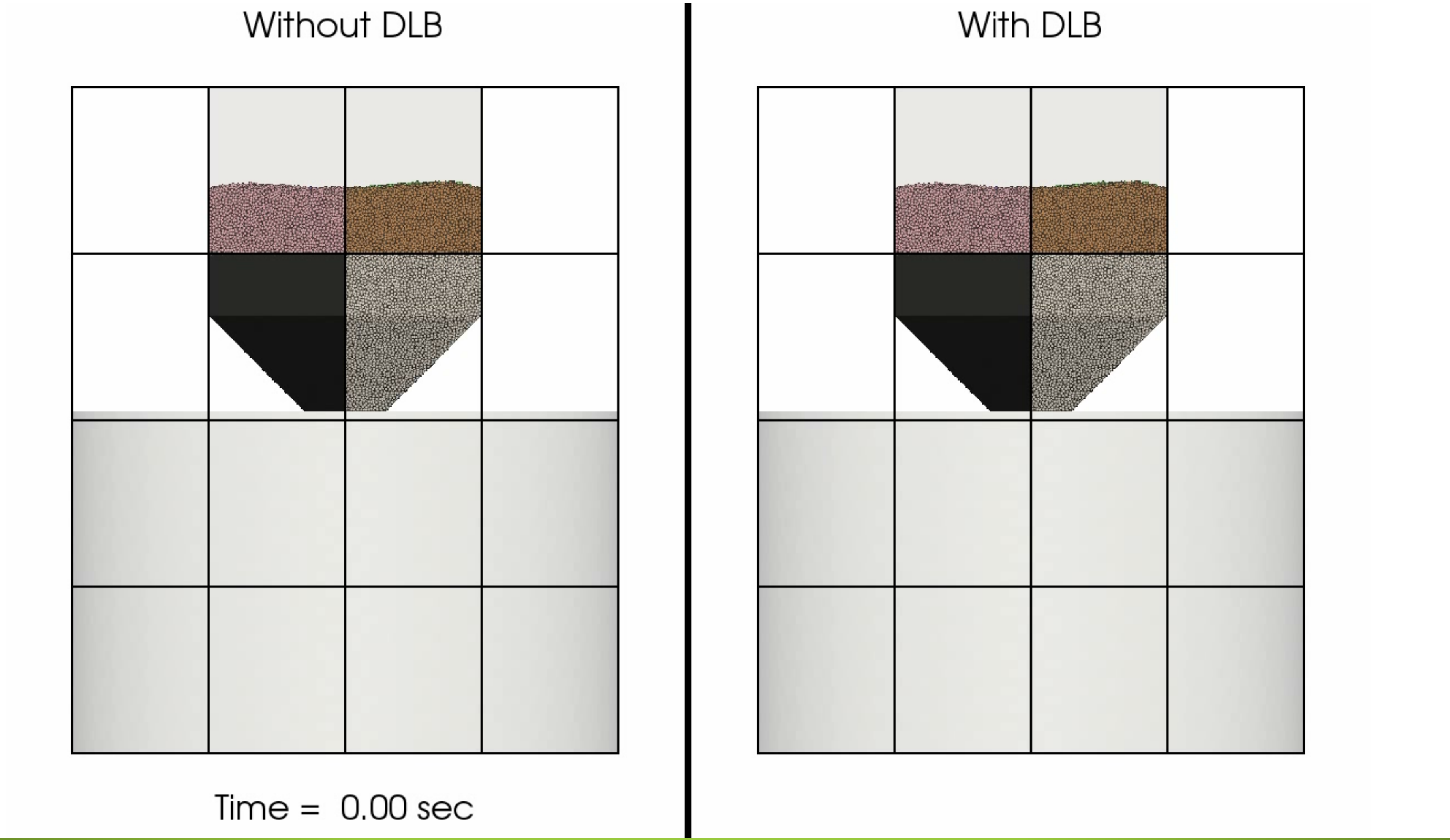
Dynamic Load Balance Layouts:

- 2x16x2
- 4x4x4
- 8x1x8

Cut-cell preprocessing can be turned off (no IC nor MI/MO BC)

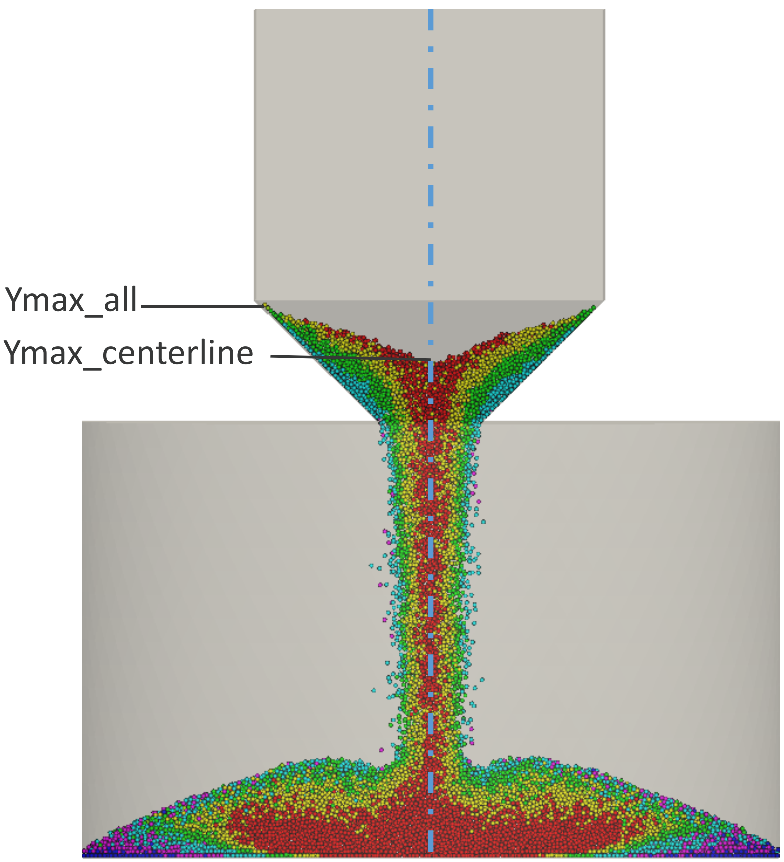
Results – Hopper – Granular Flow

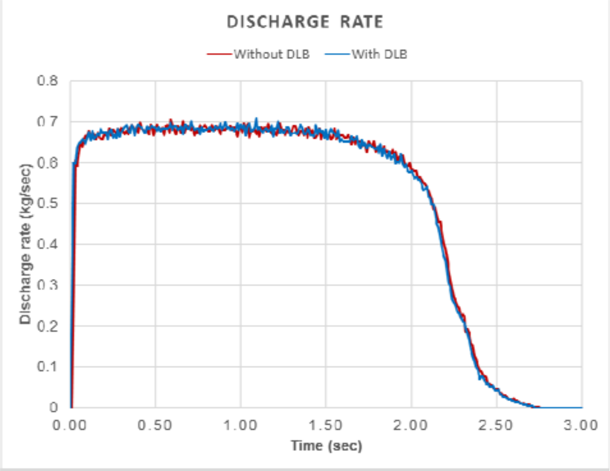
Particles colored by rank

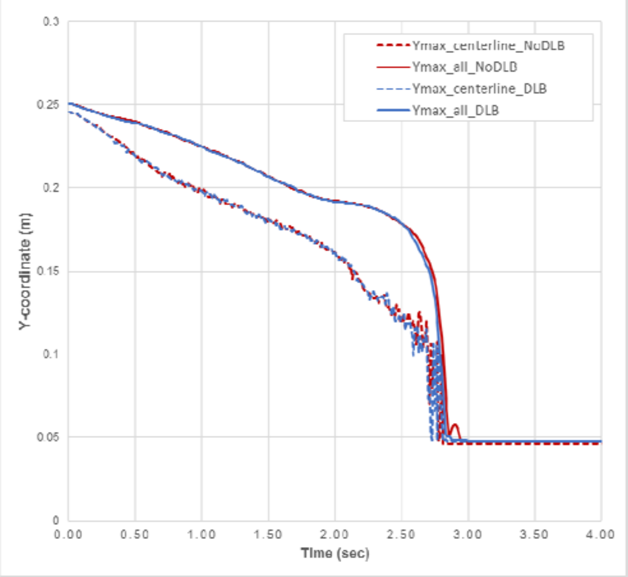


Results – Hopper – Granular Flow

Comparison between Static and Dynamic decomposition



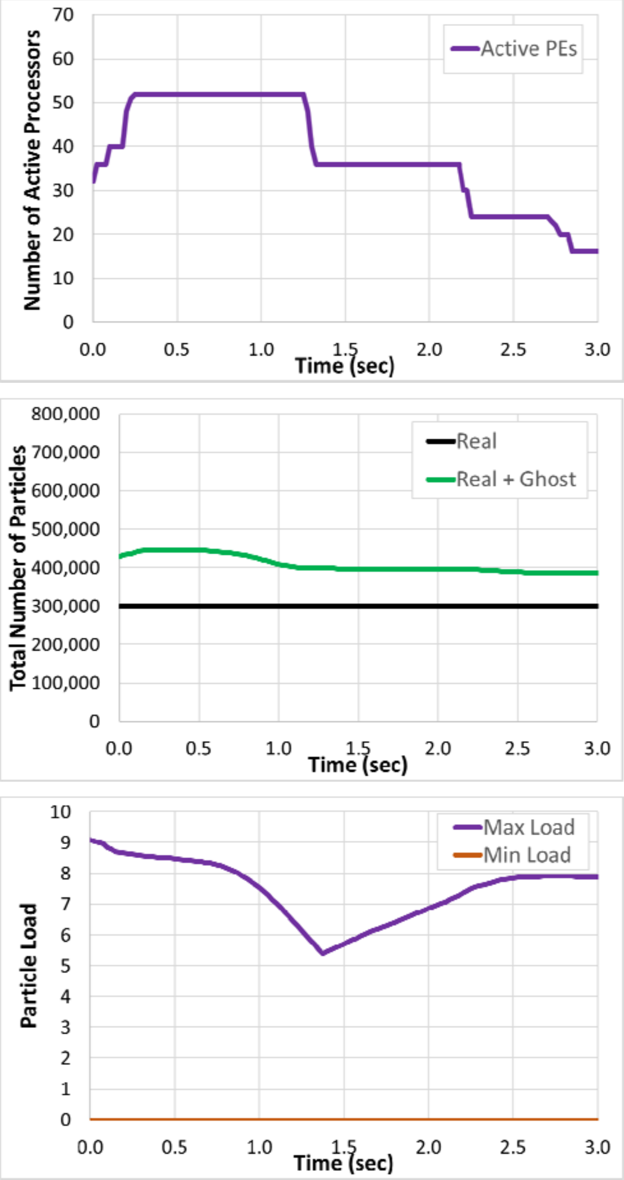




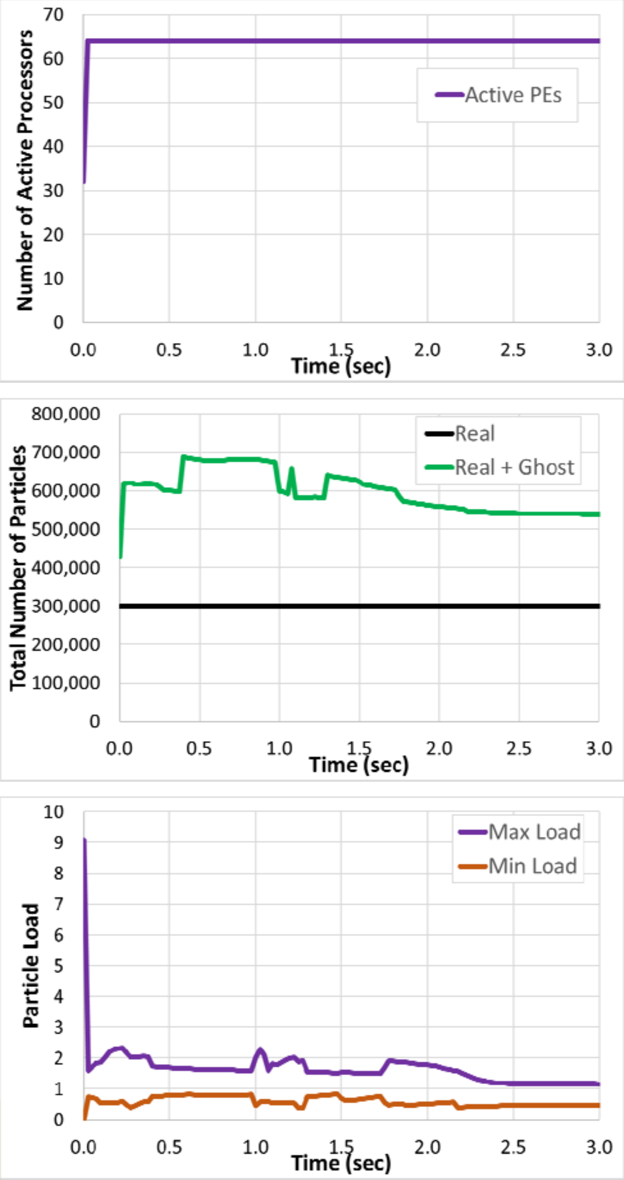
- **Same discharge rate**
- **Same angle of repose (21 deg)**

Results – Hopper – Granular Flow

Reference (No DLB,4x4x4 layout)



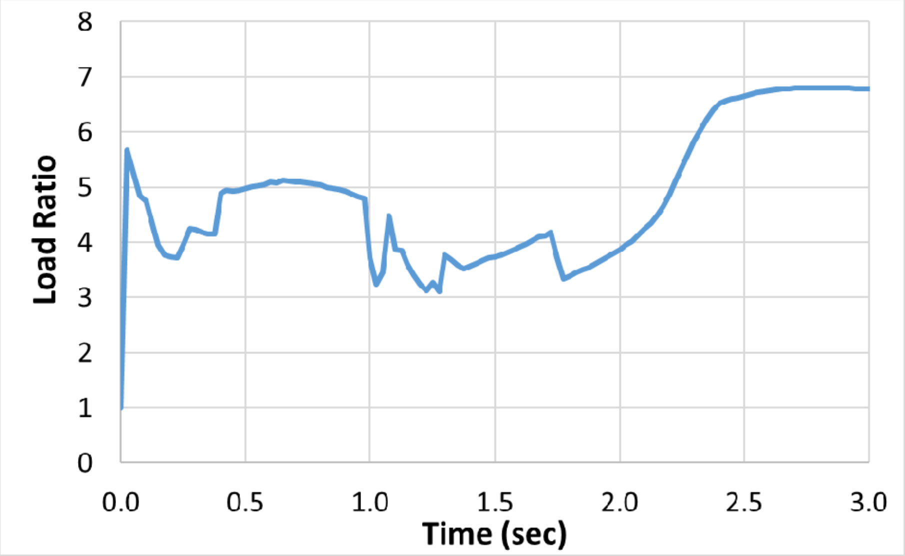
DLB, Minimize Load (Mixed layout)

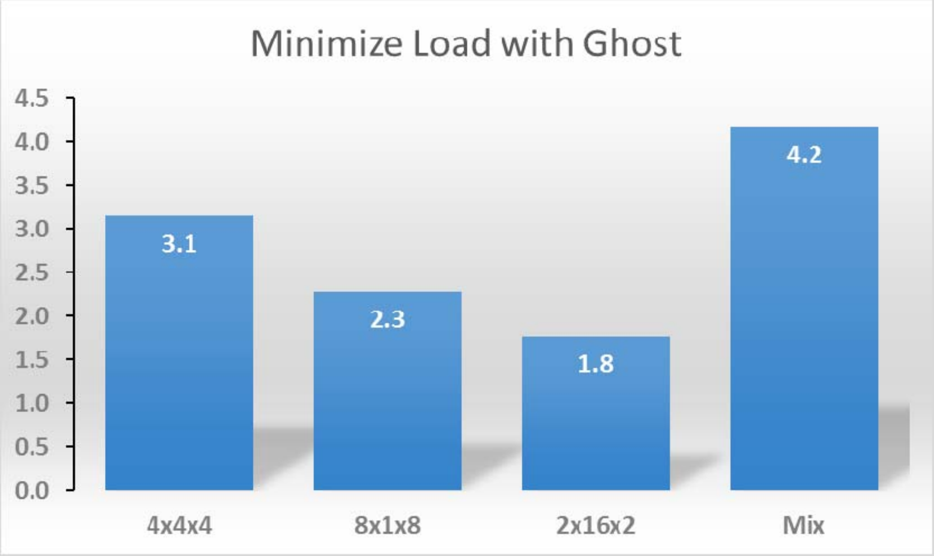


Results – Hopper – Granular Flow

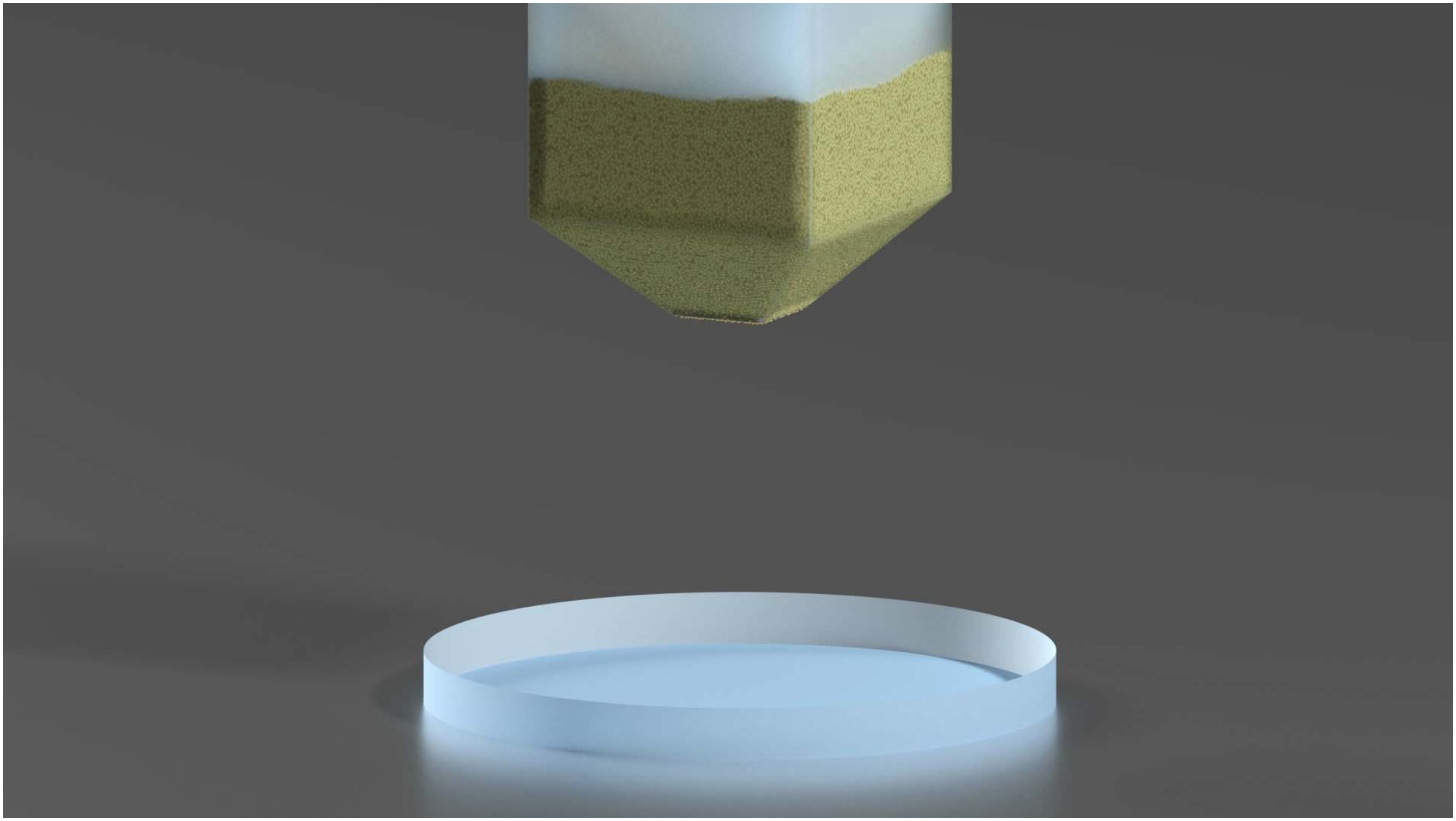
Code Performance

- Particle load ratio (static 4x4x4 / Mixed layout)
- Speedup is 4.2



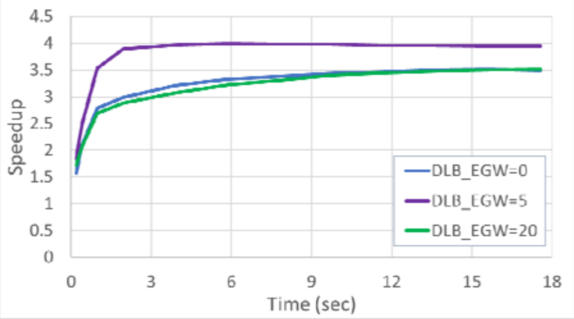


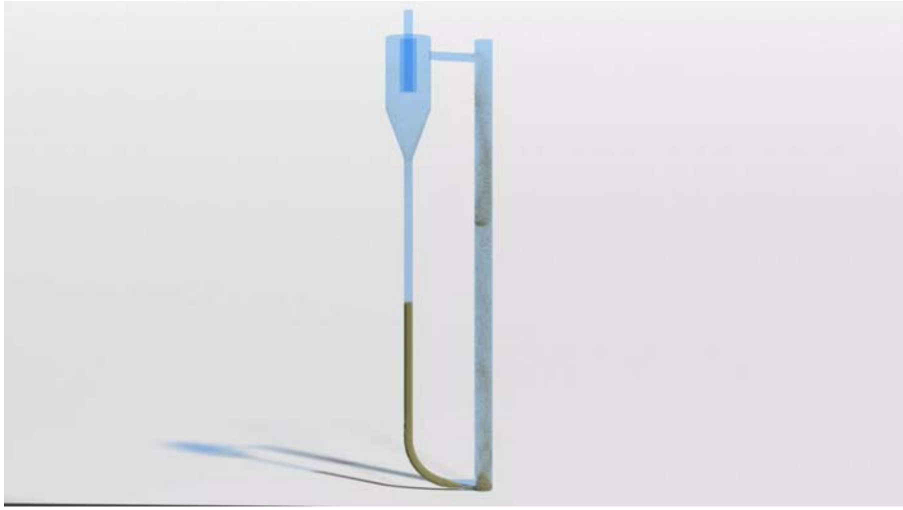
Results – Hopper – Granular Flow

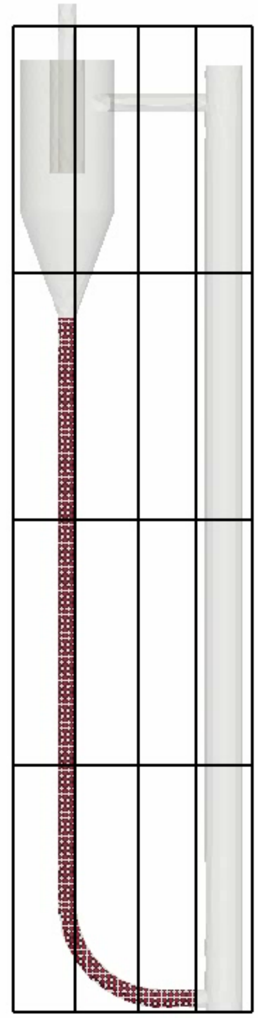


Results – Mini CFB

- minicfb benchmark
- 673K Particles, Diameter = 800 µm
- 64 cores, Reference layout=4x4x4
- DLB with Mixed layout
- Speedup changes with time
- Speedup between 3.5 and 4
- Need compromise between balancing DEM and Eulerian meshes
- Improve speedup by tuning DLB_EGW







Time = 0.00 sec

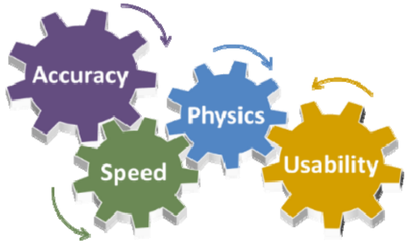
MFiX Development Activities

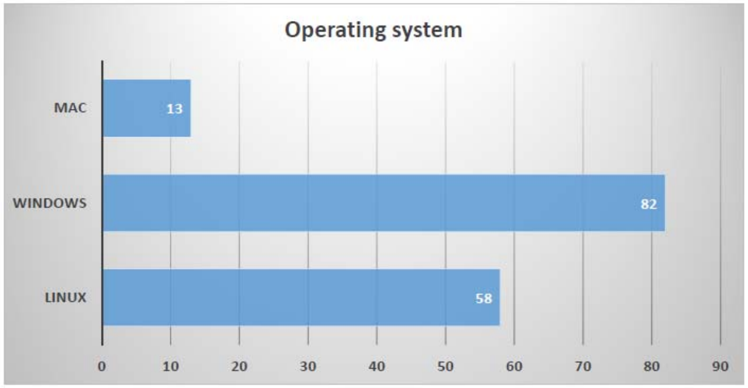
Graphical User Interface
- Guided creation of setup
- Interactive runtime control
- Basic visualization

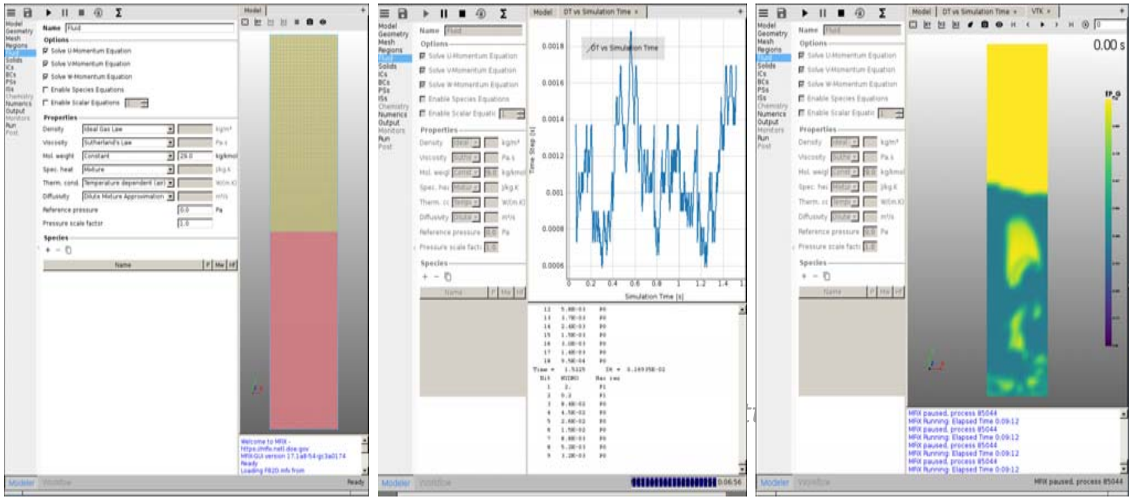
Beta release expected in Spring, 2017

Official release in Summer 2017

Optimization toolset later in 2017



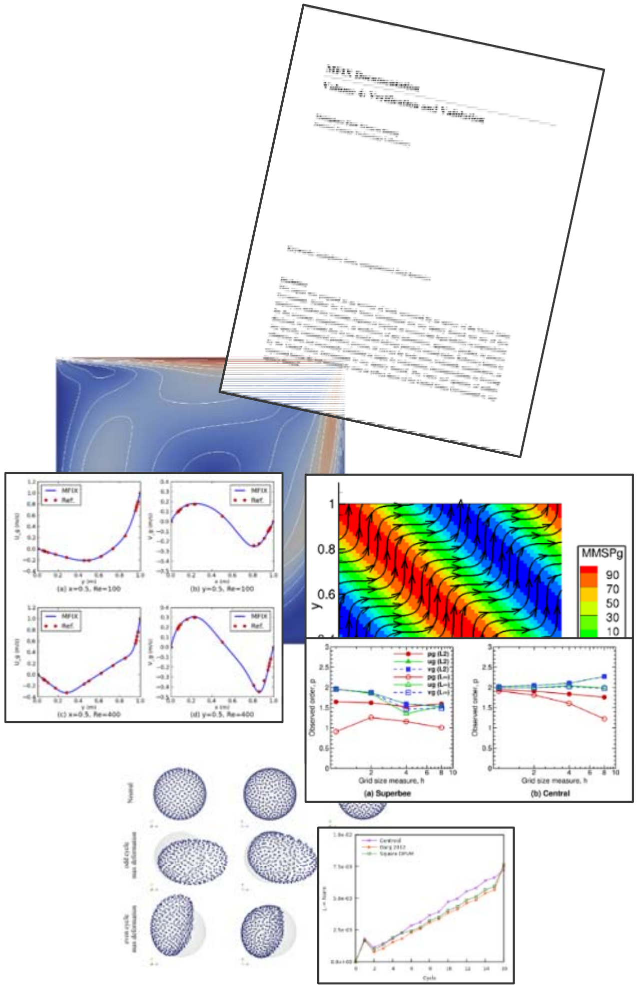




MFiX Software Quality Assurance (SQA)

MFIX SQA performs systematic verification of MFIX features for correctness and numerical accuracy

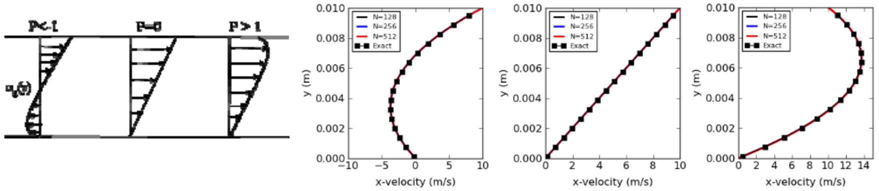
- **Documented in MFIX Verification and Validation Manual** **(https://mfix.netl.doe.gov/download/mfix/mfix_current_documentation/MDV3-VVUQ-v0.5.pdf)**
- **Test cases (1) exercise one or more sub-models, (2) are computationally inexpensive, and (3) strive for maximum code coverage with minimal test overlap.**
- **Source code managed in NETL hosted GitLab repository.**
- **GitLab repository is monitored by Jenkins, a continuous integration (CI) server:**
  - Executes verification test suite after every commit
  - Reports results via email and archives daily ‘snapshots’ of test case performance

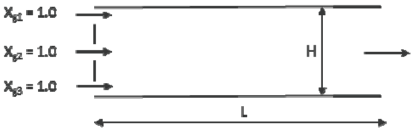


VVUQ

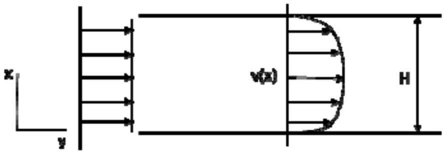
- **Verification and Validation (V&V)**
  - Documenting additional cases to include more physical models

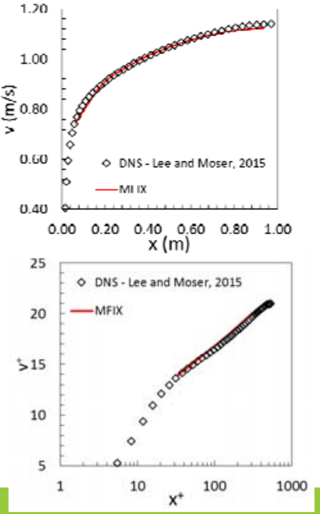
Case	Description	Momentum	Thermal energy	Species	Turbulence
FLD01	Poiseuille flow	X			
FLD02	Heat conduction		X		
FLD03	Lid-driven cavity	X			
FLD04	Gresho vortex problem	X			
FLD05	Couette flow	X			
FLD06	Species mixing	X		X	
FLD07	Turbulent flow in a channel	X			X
FLD08	Turbulent flow in a pipe	X			X
FLD09	Turbulent round jet	X			X

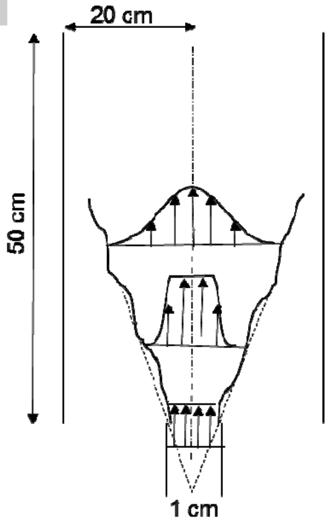


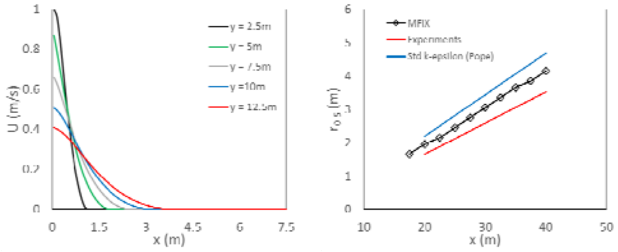


Species	MW (kg/kmol)	MFIX-X_{gi}	L_2 error
1	1	0.027778	5.86e-7
2	10	0.277776	2.07e-6
3	25	0.694446	1.48e-6





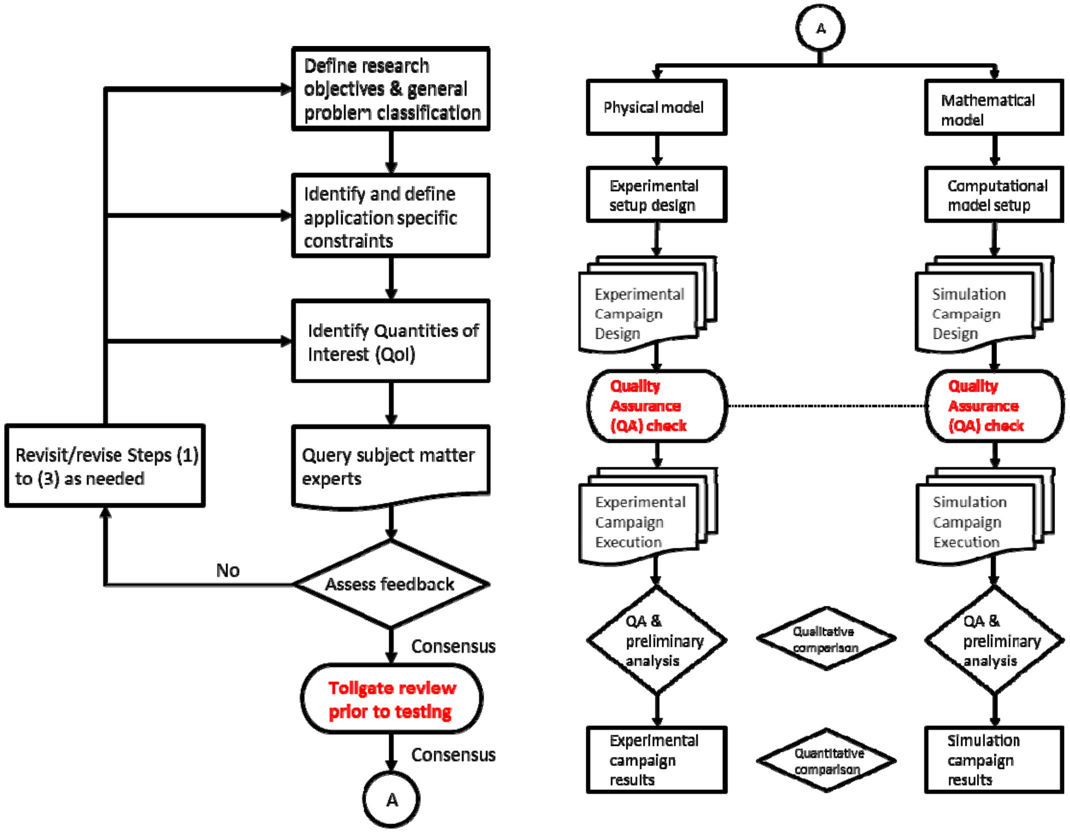




Source	Spreading rate
Experiments	0.094
MFIX - std. k-ε	0.122
Pope (1978) - std. k-ε	0.125

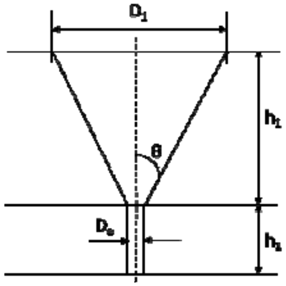
VVUQ

- **Development and application of VVUQ roadmap**
  - Systematic VVUQ approach for multiphase flows
  - Conical hopper discharge experiments
    - Particle jamming observed in previous experiments at NETL
    - Design criteria to ensure mass flow operation mode
  - MFIX-DEM simulation campaign
    - Validation of MFIX-DEM linear spring dashpot model
    - Sensitivity analysis of model parameters on the quantities of interest

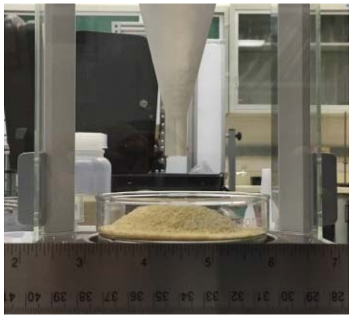


VVUQ roadmap application

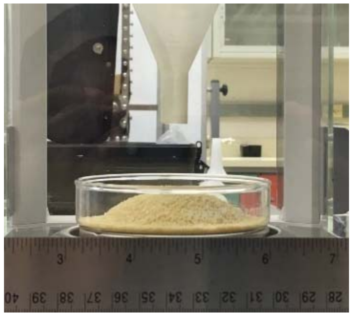
- **Objectives**
  - Validation of MFIX-DEM spring dashpot model
  - Assess sensitivity of collision model parameters on QoI
- **Control variables**
  - Orifice diameter
  - Apex angle
- **Quantities of interest (QoI)**
  - Discharge flow rate
  - angle of repose
- **Material: High density polyethylene (HDPE)**
  - Mean particle diameter: **848 μm**
  - Density: **884 kg/m^3**



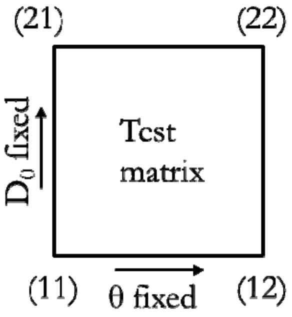
Hopper 11



Hopper 22

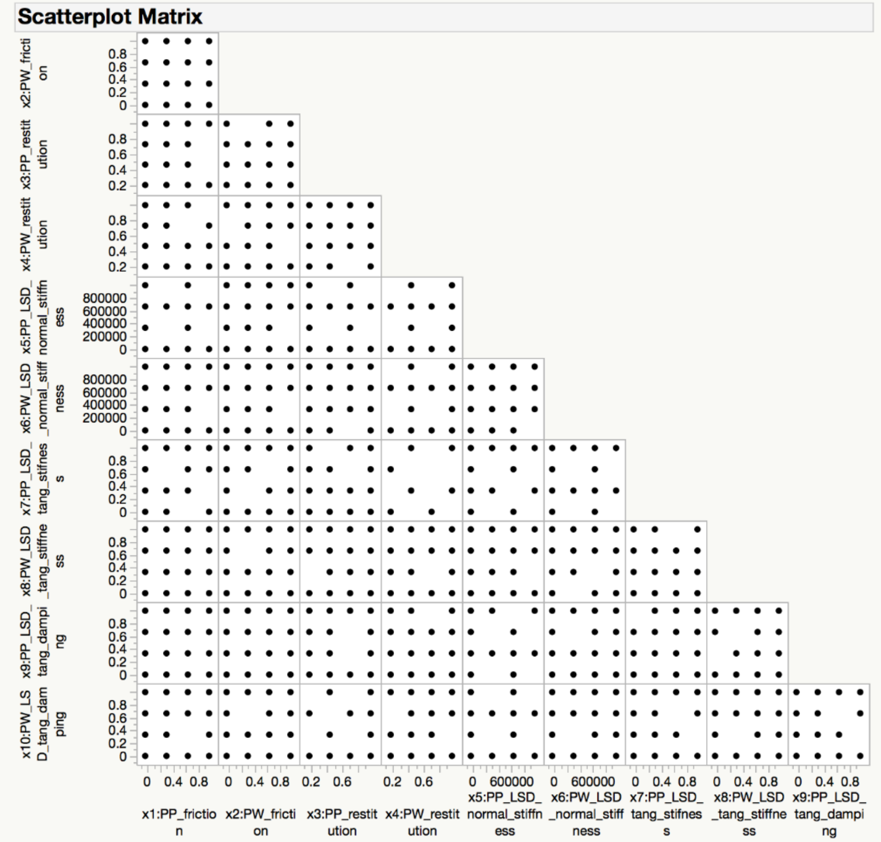


Index	θ (deg)	h_1 (cm)	h_2 (cm)	D_o (mm)	D_1 (cm)
11	13.44	10	2.5	5.8	5.36
12	13.12	10	2.5	7	5.36
21	23.63	10	2.5	5.8	9.33
22	23.34	10	2.5	7	9.33



VVUQ roadmap application - Screening

Screening Experiment Method : Morris Method (MOAT)
# of Input Parameters : 10
Preferred Sample Size: 110
Most conservative Sample Size : 44



Revised bounds for consideration Uncertain Input Parameters/Factors:		Parameter Type	Lower Bound	Upper Bound
Factor 1	PP coefficient of friction (sliding)	Numerical	0	1
Factor 2	PW coefficient of friction (sliding)	Numerical	0	1
Factor 3	PP restitution coefficient	Numerical	0.2	0.99
Factor 4	PW restitution coefficient	Numerical	0.2	0.99
Factor 5	PP LSD normal spring stiffness coefficient	Numerical	1.00E+02	1.00E+06
Factor 6	PW LSD normal spring stiffness coefficient	Numerical	1.00E+02	1.00E+06
Factor 7	PP LSD tangential spring stiffness coefficient	Numerical	0.1	0.9
Factor 8	PW LSD tangential spring stiffness coefficient	Numerical	0.1	0.9
Factor 9	PP LSD tangential damping factor	Numerical	0.1	0.9
Factor 10	PW LSD tangential dampeing factor	Numerical	0.1	0.9

- Morris One-at-a-time (MOAT): Computationally efficient for sensitivity analysis involving a large parameter space. Consider r trajectories and m parameters:
- Elementary effect:

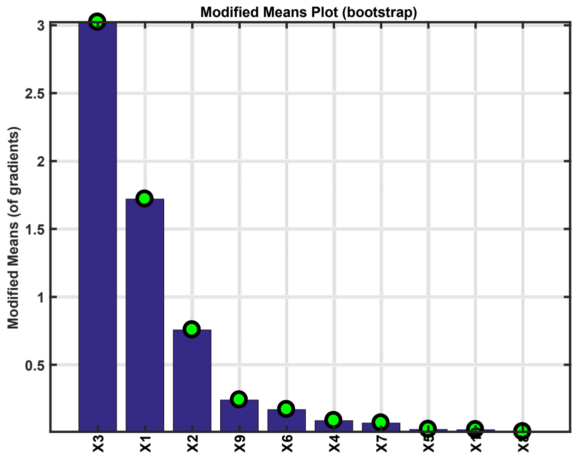
$$d_{ij} = \frac{c_i(k_1,k_2,\ldots,k_{j-1},k_j+\Delta,k_{j+1},\ldots,k_m) - c_i(k_1,k_2,\ldots,k_{j-1},k_j,k_{j+1},\ldots,k_m)}{\Delta}$$

- Global effect:

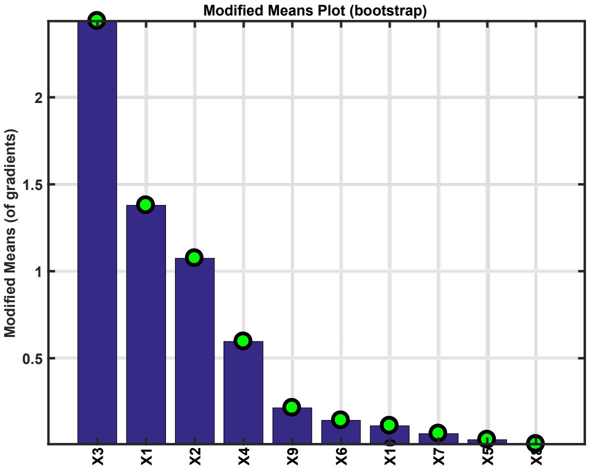
$$\mu_{ij} = \frac{\sum |d_{ij}|}{r}, \quad \sigma_{ij}^2 = \frac{r\sum (d_{ij})^2 - \left(\sum d_{ij}\right)^2}{r(r-1)}$$

- Larger mean, μ_{ij} → more sensitive, larger variance, σ_{ij}^2 → more non-linearity/interactive effects

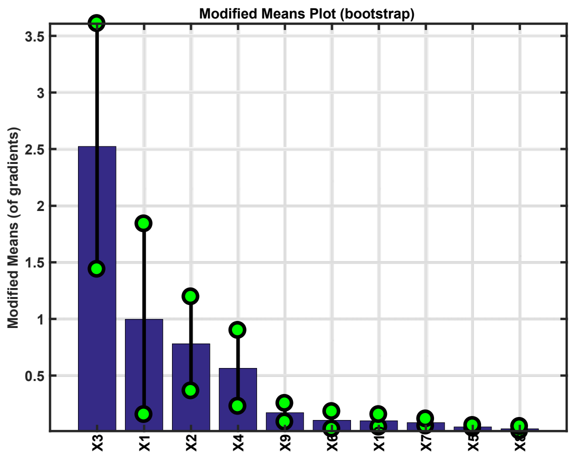
VVUQ roadmap application - Screening



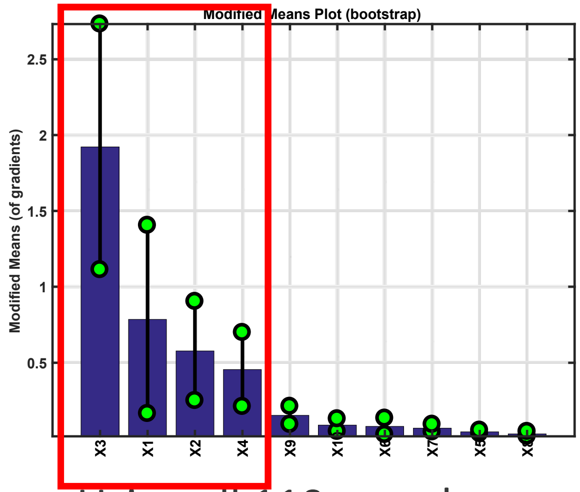
Using first 44 samples



Using first 55 samples



Using first 77 samples



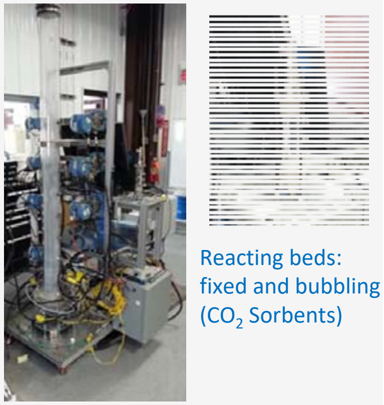
Using all 110 samples

Rank	N=44	N=55	N=77	N=110
1	x3	x3	x3	x3
2	x1	x1	x1	x1
3	x2	x2	x2	x2
4	x9	x4	x4	x4
5	x6	x9	x9	x9
6	x4	x6	x6	x10

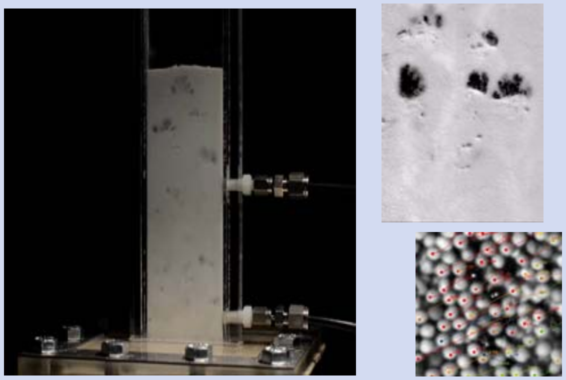
Multiphase Flow Analysis Laboratory

MFAL supporting model development and validation

- **Experimentation for Model Development and Validation**
  - Operation of Small-Scale Fixed, Bubbling, and Circulating Fluidized Beds for Validation
    - Small Fixed Bed for heat transfer, kinetics (1in Dx 6 in H)
    - Bubbling Fluidized Bed (4in D x 72in H)
    - Rectangular 2-D bed (2in x 0.125in x 18in H)
    - Small Scale Circulating Bed (1in D x 48in H)
  - Pilot-Scale Cold Flow Circulating Bed (12in D x 60 ft H)
  - Flow control, measurement, diagnostics
    - High Speed PIV
    - LDV
    - Low and High Speed Pressure
    - High Speed video
    - Image analysis
    - Tracer gas



Reacting beds: fixed and bubbling (CO_2 Sorbents)

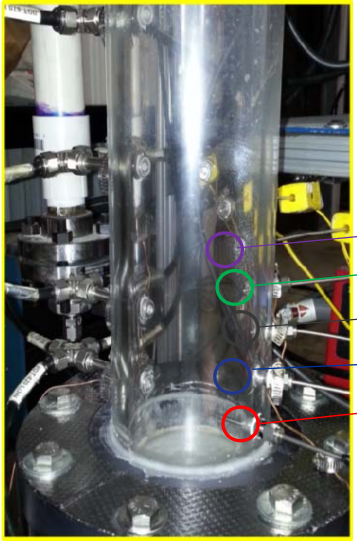


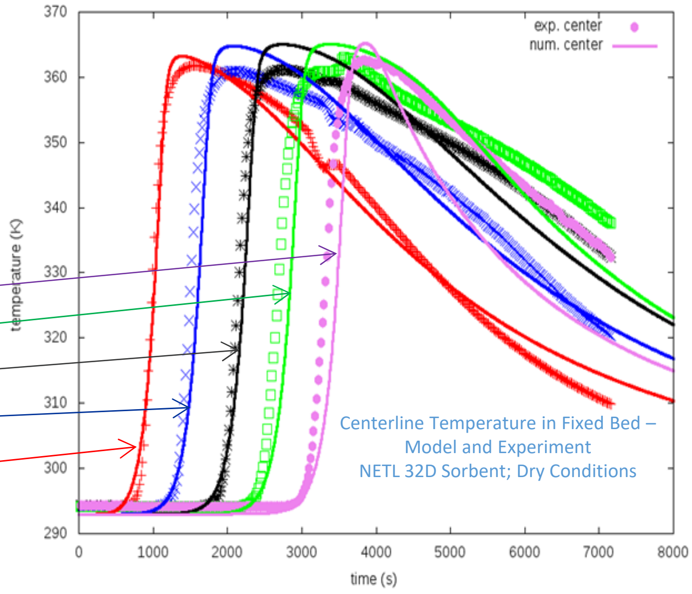
Small bubbling beds with image analysis

Multiphase Flow Analysis Laboratory

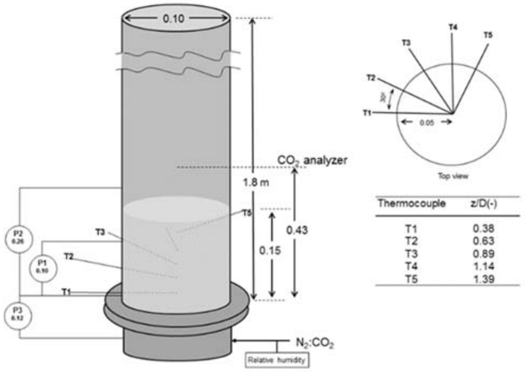
MFAL supporting model development and validation

- **Small-Scale Bubbling Bed experiments performed with NETL CO_2 Sorbent Particles to validate MFiX-TFM**
  - excellent agreement with fixed bed tests





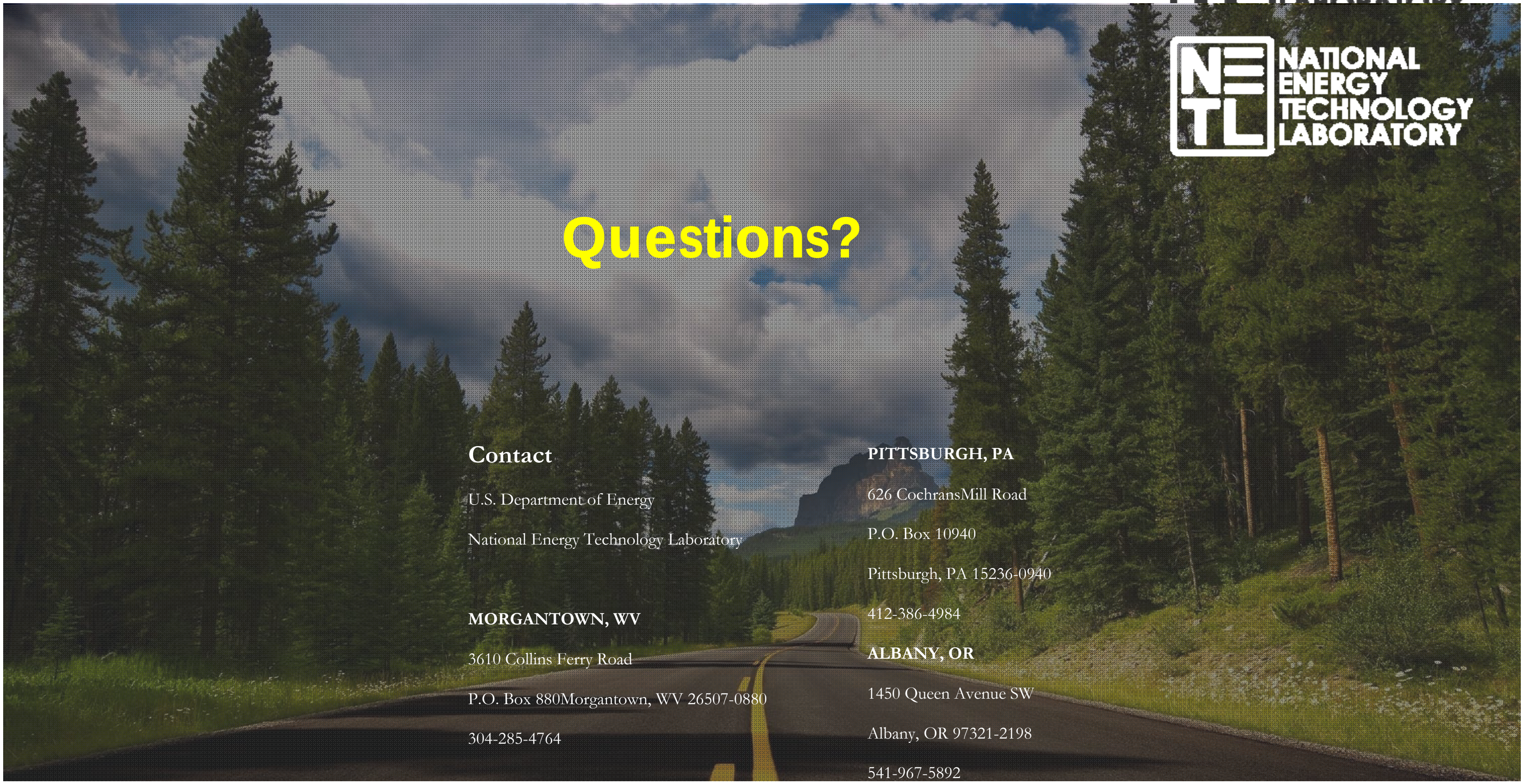
Centerline Temperature in Fixed Bed – Model and Experiment
NETL 32D Sorbent; Dry Conditions



Thermocouple	z/D(-)
T1	0.38
T2	0.63
T3	0.89
T4	1.14
T5	1.39

Conclusions

- **MFiX suite code development**
  - Continued support for TFM and DEM model (capabilities and speed)
  - Emphasis on gas/particle flows with chemical reactions
  - Development of large scale reacting MFiX-PIC model
  - Improved usability of the MFiX suite through redesigned GUI
- **Verification, Validation and Uncertainty Quantification (VV&UQ)**
  - Additional cases for MFIX V&V manual to include more physical models
  - VVUQ methodology
  - Preliminary experiments with 3-D printed geometries
  - Ranking of model parameters from screening studies
- **Multiphase Flow Analysis Laboratory (MFAL)**
  - Supports model development and validation
- **Milestones:**
  - Release of MFiX with improved GUI (07/31/2017)
  - Validation experiments and simulations for Circulating Fluidized Bed (06/30/2017)
  - Release of MFiX-PIC code (06/30/2018)



Questions?

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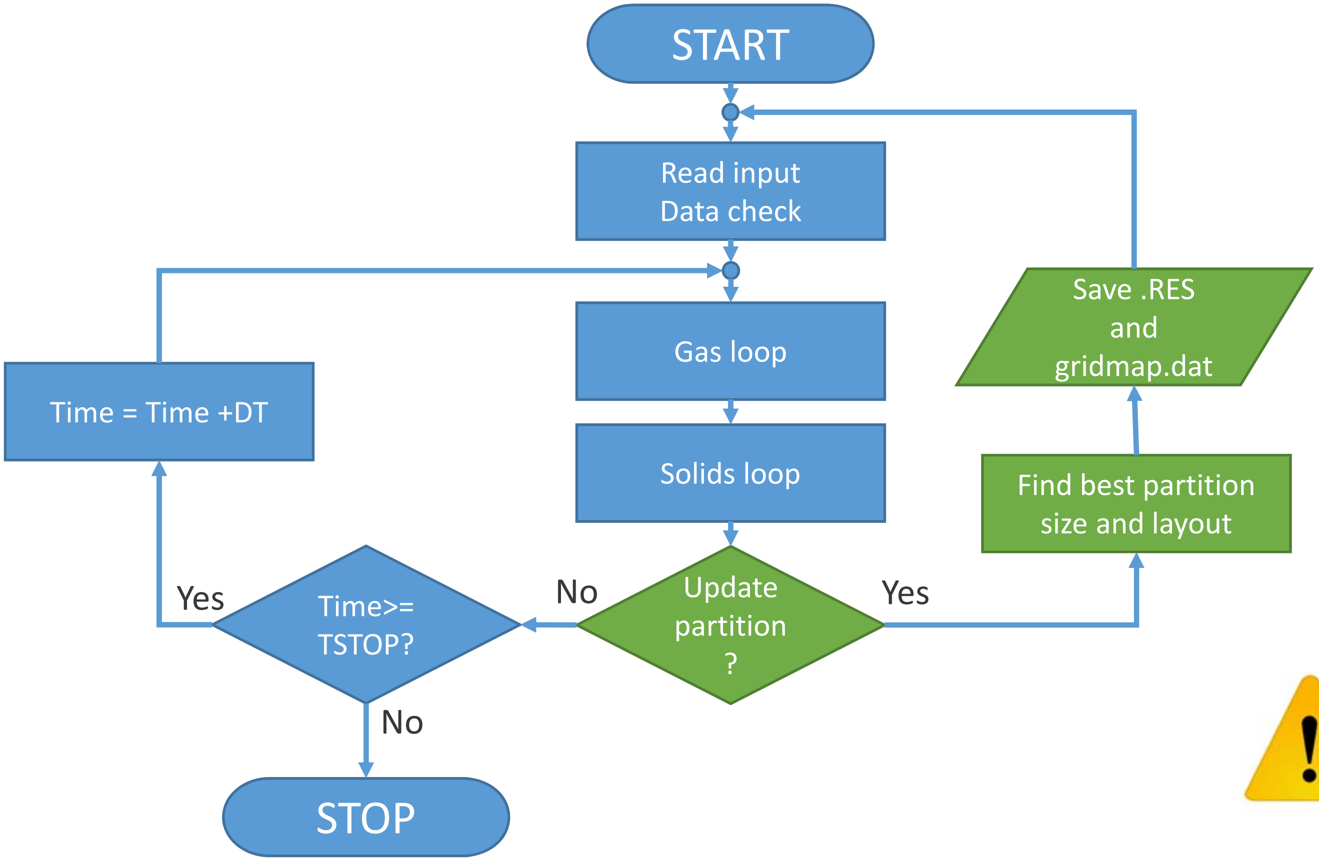
Additional slides

Technical Approach

Dynamic Load Balance Implementation

- After optimization, partition info saved in gridmap.dat
- Graceful termination is triggered, and MFiX does a RESTART_1



New keywords:

DLB_DT : controls how often partition is updated

DLB_NODESI(:) :List of layouts
DLB_NODESJ(:)
DLB_NODESK(:)

DLB_EGW: Eulerian grid weight

⚠ Relies on Serial IO to distribute particles upon restart

Results – Hopper – Granular Flow

Code Performance

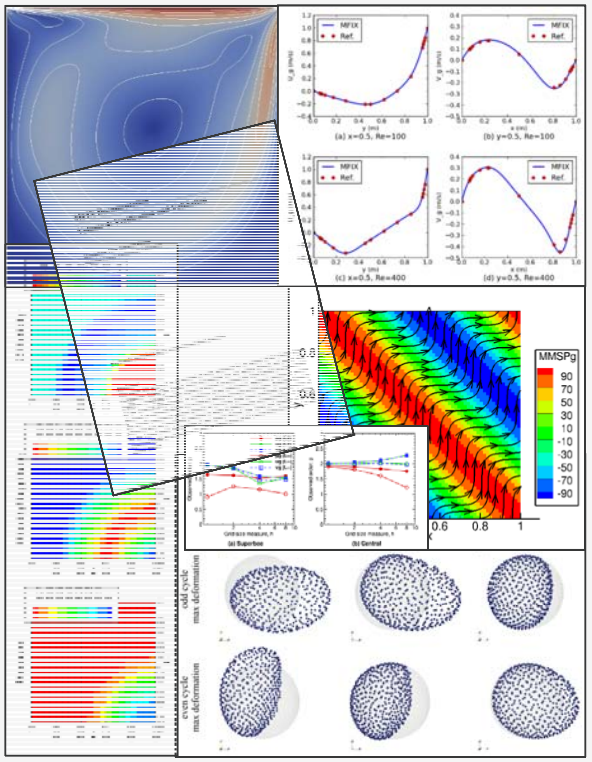
- **Bottleneck is most loaded processor**
- **Particle Load: PL= NPP/ INPP (Target = 1.0)**
  - NPP = Number of particles owned by a Processor
  - INPP = Ideal Number of particles per processor: INPP = TNP/ NumPEs
  - TNP = Total number of particles
  - NumPEs = Number of processors
- **Option to include Ghost particles or not in TNP and NPP**
- **Minimize**
  - Maximum PL value among processors (normalized quantity), or
  - Maximum number of particles among processors (absolute quantity)
- **Real life timing (time stamp of vtp files), 1000 vtp files over 5 secs**

VVUQ Summary

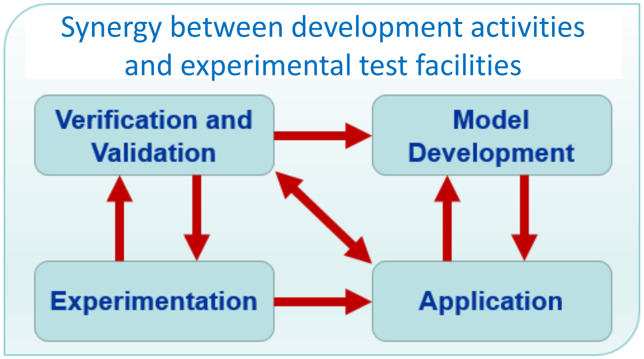
- **Additional cases for MFIX V&V manual to include more physical models**
- **Survey of subject matter experts for VVUQ methodology input**
- **Preliminary experiments with 3-D printed geometries**
- **Ranking of model parameters from screening studies:**
  1. Particle-particle coefficient of restitution
  2. Particle-particle coefficient of friction
  3. Particle-wall coefficient of friction
  4. Particle-wall coefficient of restitution
- **Things to do:**
  - Full-blown design of experiments and uncertainty quantification
  - Presentation of the VVUQ roadmap development and application activities at the ASME V&V 2017 summer meeting

MFiX Software Quality Assurance (SQA)

MFIX SQA performs systematic verification of MFIX features for correctness and numerical accuracy



Verification Test Suite



Synergy between development activities and experimental test facilities

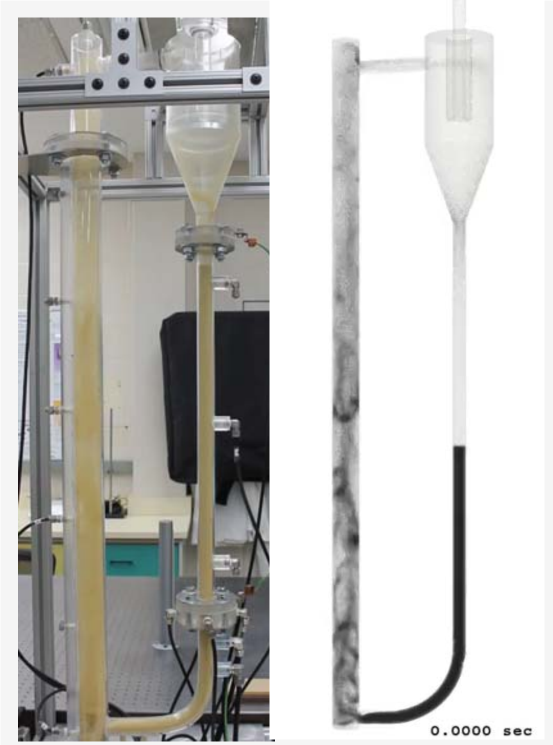
Verification and Validation

Model Development

Experimentation

Application

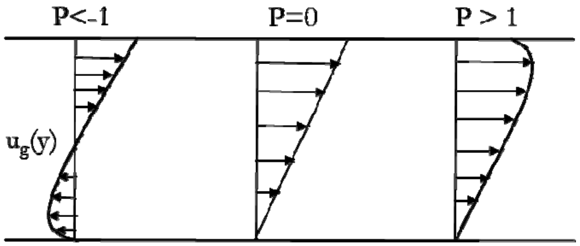
Multiphase Flow Analysis Lab



Small-scale CFB

CFD Verification and Validation

- **FLD05: Couette flow with zero, favorable and adverse pressure gradients**

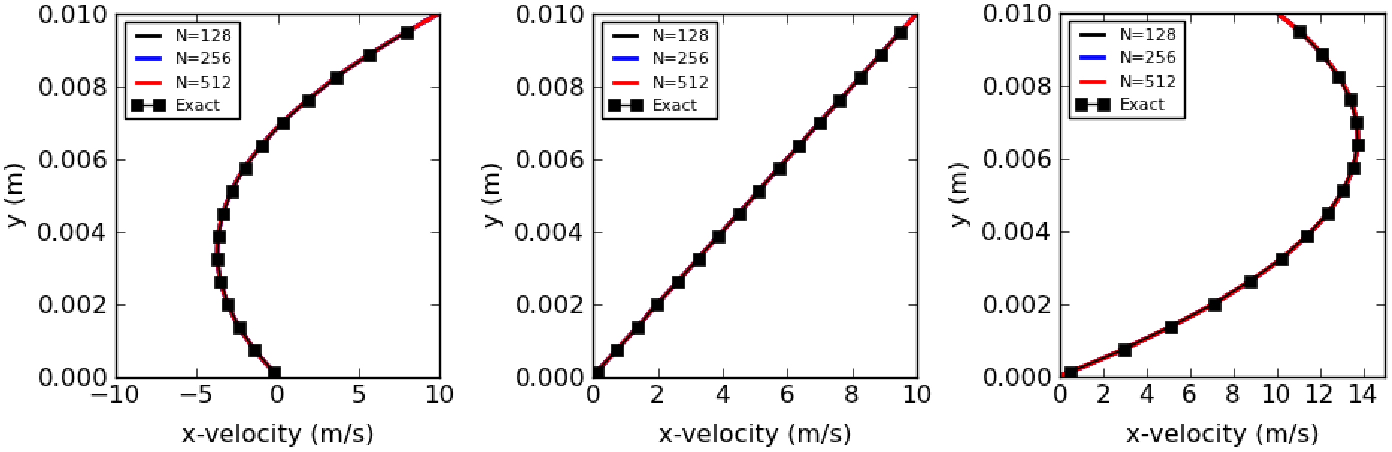


$$P = -\frac{H^2}{2\mu_g}\frac{dP_g}{dx}$$

- **Exact solution**

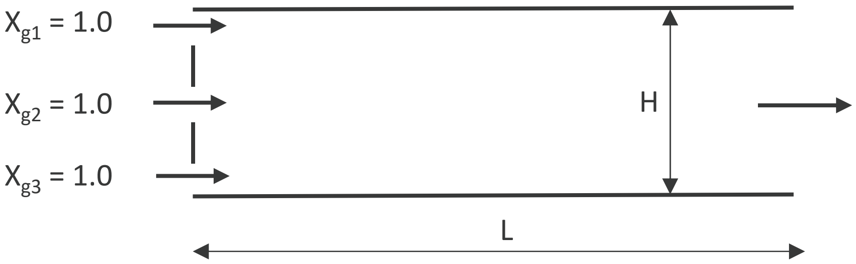
$$\boxed{u_g(y) = \frac{1}{2\mu}\frac{dp}{dx}(y^2 - yH) + U\frac{y}{H}}$$

- **MFIX**



CFD Verification and Validation

- **FLD06: Chemical species transport**
- **Assumptions: Ideal gas law, incompressible, complete mixing**



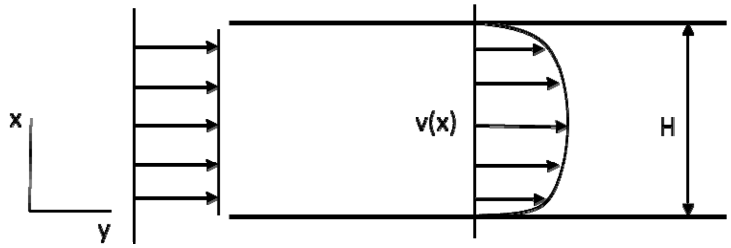
- **Exact solution:** $$X_{gi} = \frac{M_{gi}}{\sum_k M_{gk}}$$

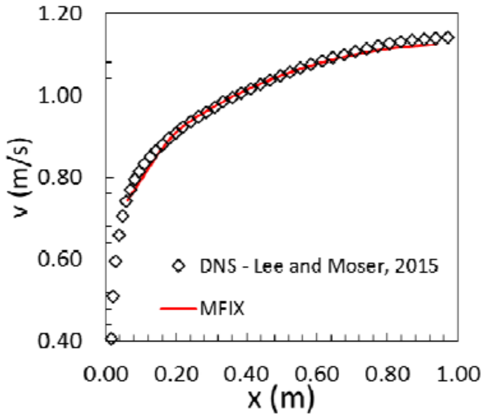
- **Results:**

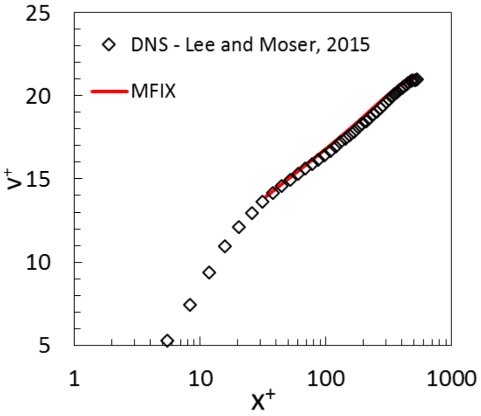
Species	MW (kg/kmol)	MFIX-X_{gi}	L_2 error
1	1	0.027778	5.86e-7
2	10	0.277776	2.07e-6
3	25	0.694446	1.48e-6

CFD Verification and Validation

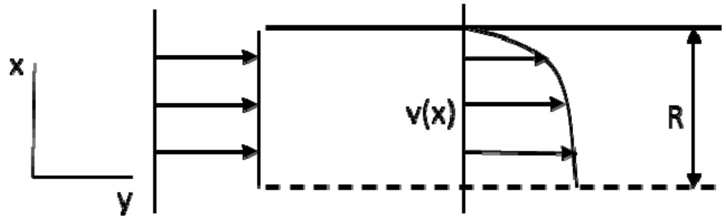
- **FLD07: Turbulent flow in a channel, Lee and Moser (2015)**

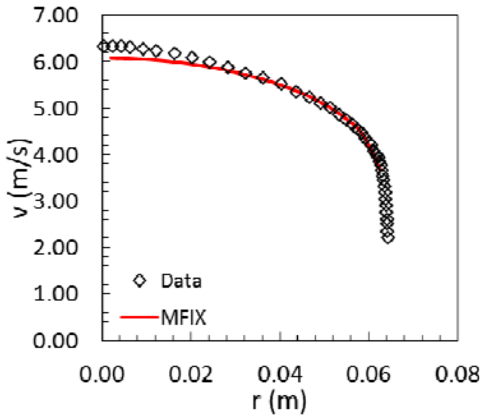


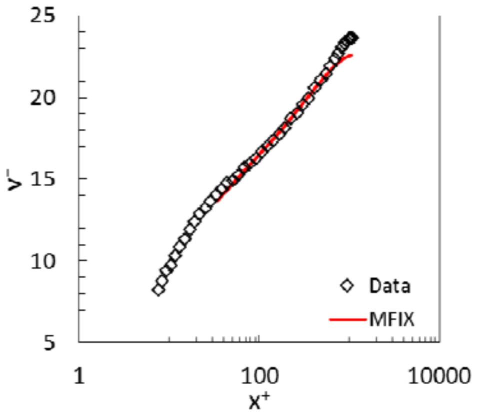




- **FLD08: Turbulent flow in a pipe, “Princeton superpipe”**

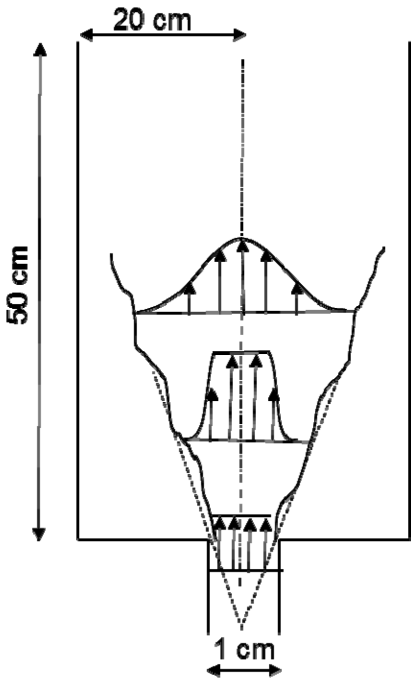


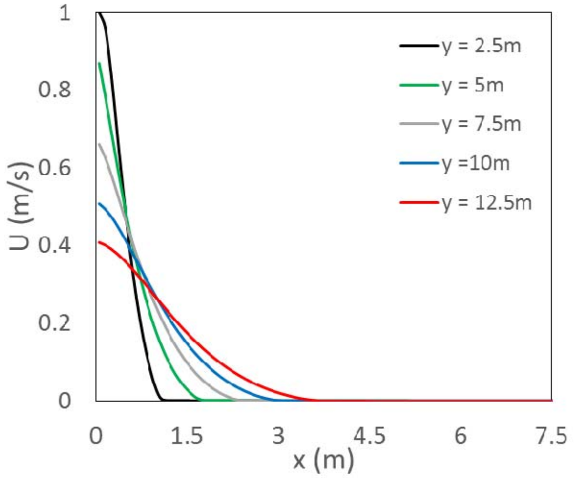


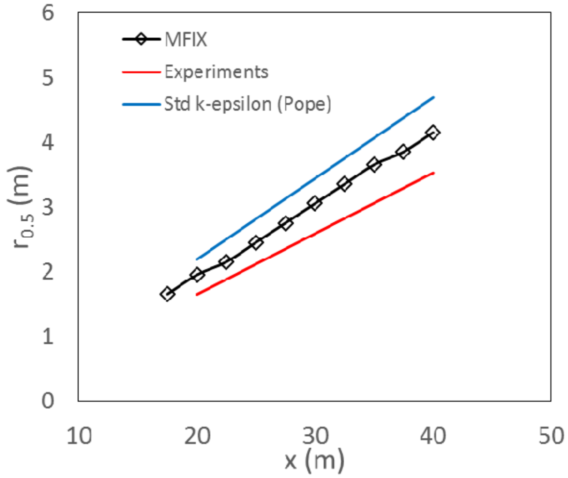


CFD Verification and Validation

- **FLD09: Turbulent round jet**





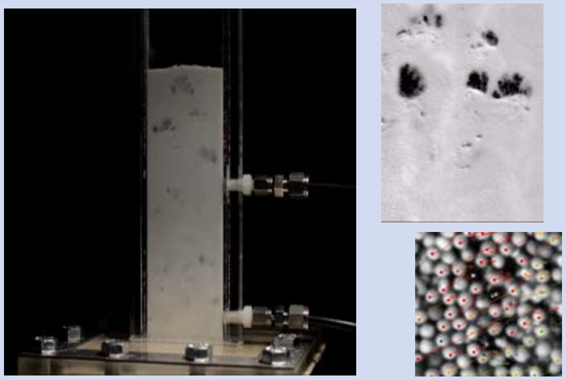


Source	Spreading rate
Experiments	0.094
MFIX - std. k-ε	0.122
Pope (1978) - std. k-ε	0.125

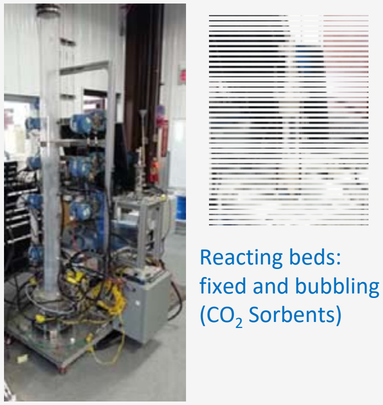
Multiphase Flow Analysis Laboratory

- New Lab supporting model development and validation

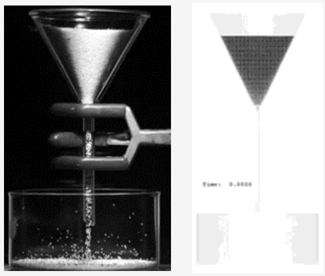
Small-scale CFB



Small bubbling beds with image analysis



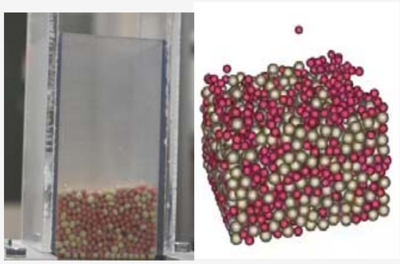
Reacting beds: fixed and bubbling (CO_2 Sorbents)



Granular hopper flow

- Particle size distribution
- Umf
- Sphericity
- Particle density, including skeletal and bulk
- Porosity
- Micrograph

Particle characterization

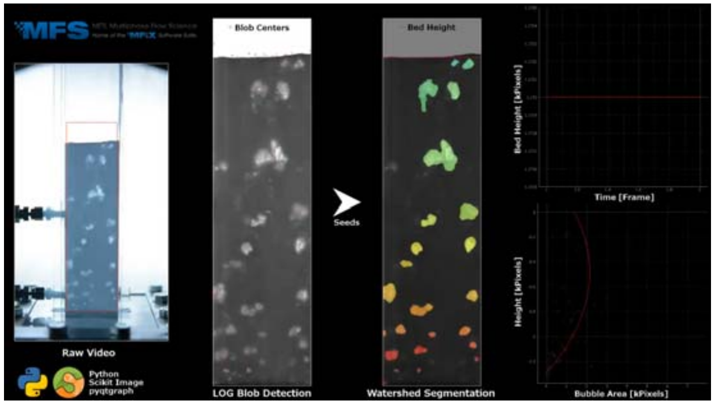


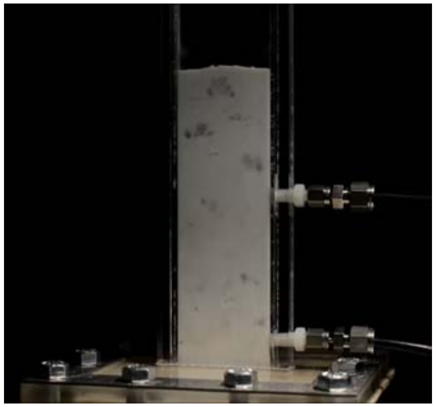
Particle separation and flow control

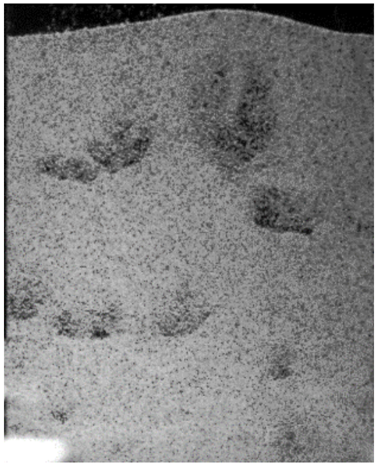
Multiphase Flow Analysis Laboratory

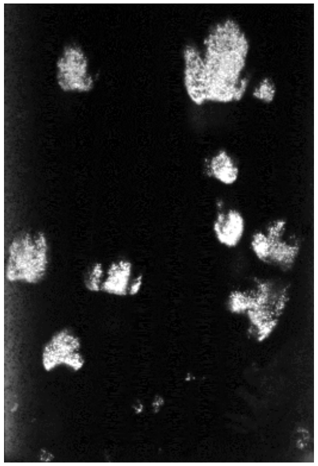
MFAL supporting model development and validation

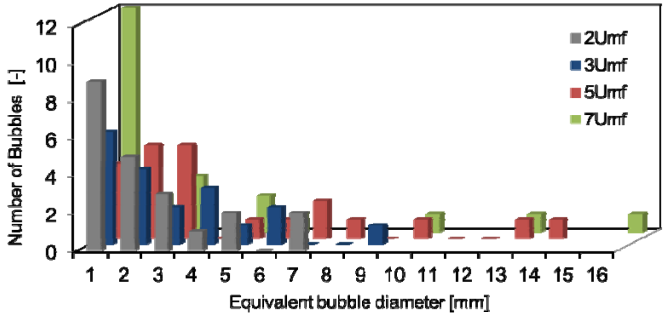
- **2-D bed for detailed measurements for validation data**







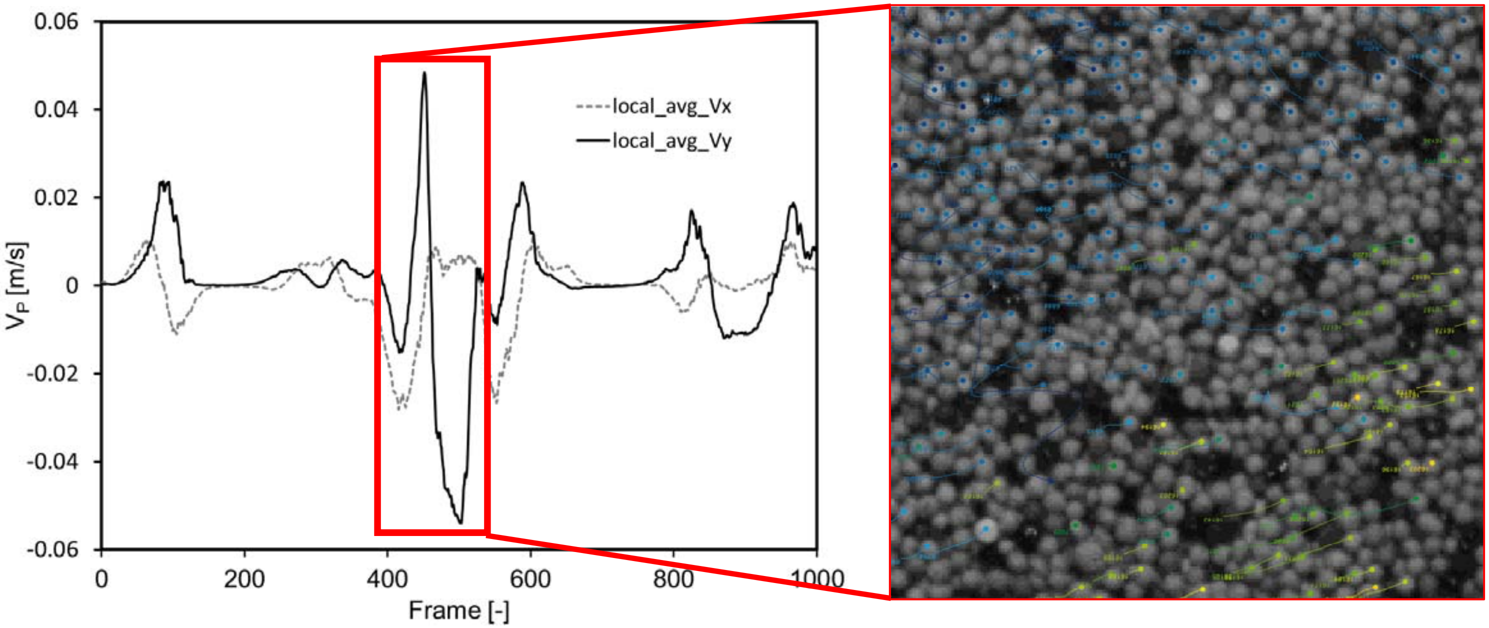




Multiphase Flow Analysis Laboratory

MFAL supporting model development and validation

- **High Speed PIV for local particle velocity, solids concentration**



FCC at U = 2Umf

Frame = 400-600

Multiphase Flow Analysis Laboratory

MFAL supporting model development and validation

3-D printing of prototypes – quick and accurate