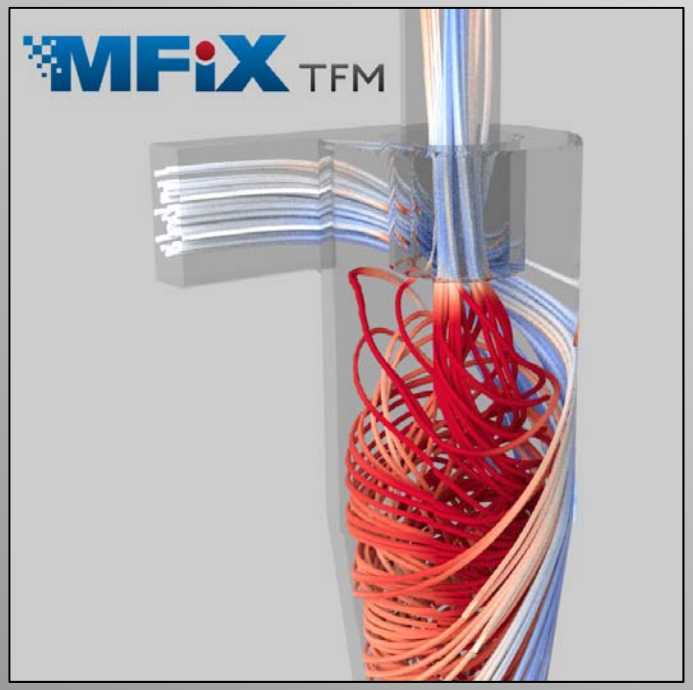


Recent Advances in MFiX

Mehrdad Shahnam

Research Engineer

Computational Science and Engineering Division

U.S. DEPARTMENT OF ENERGY | National Energy Technology Laboratory

2015 Crosscutting Technology Research Review Meeting, ***April 27-30, 2015***

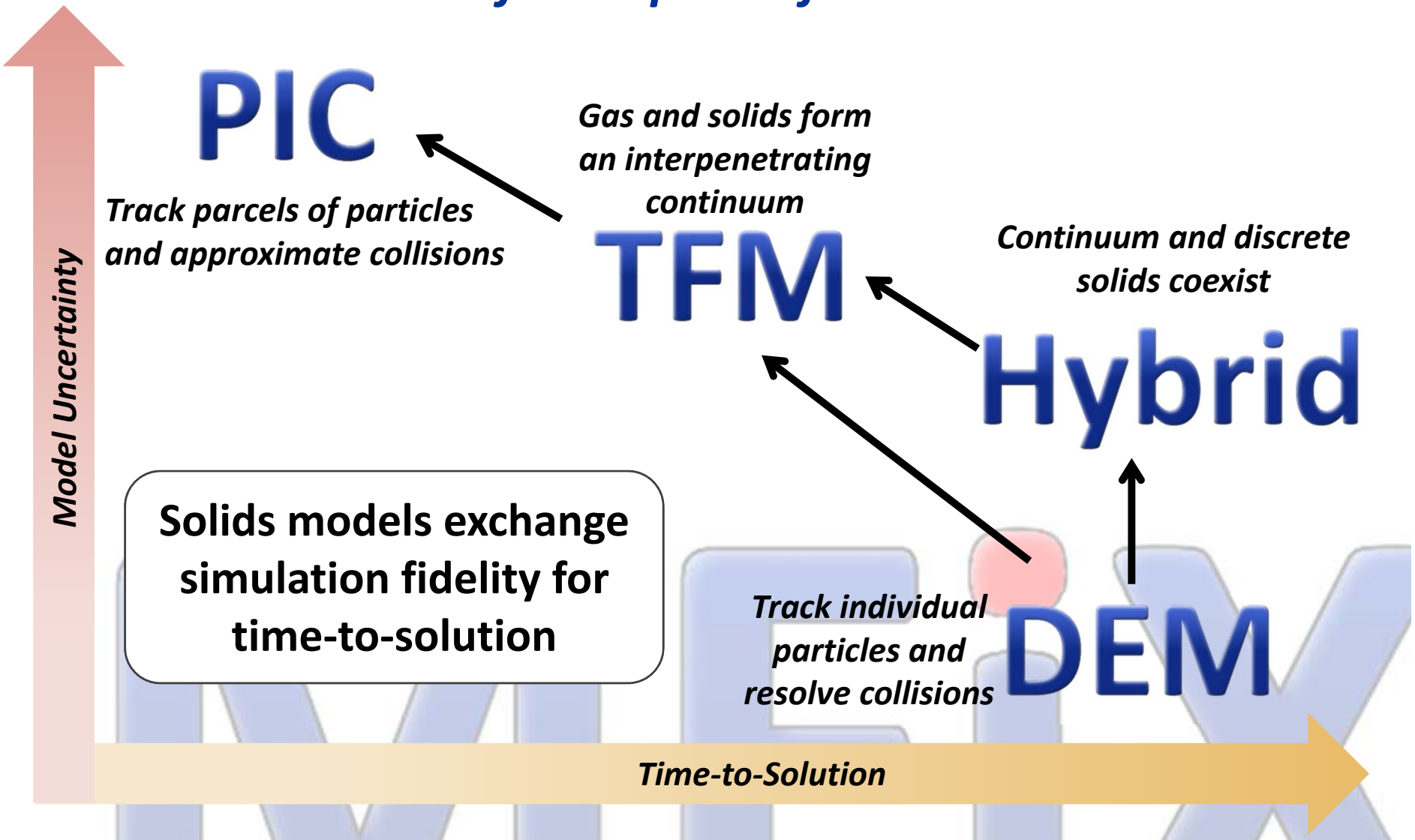
Sheraton Station Square Hotel, **Pittsburgh, PA**

MFiX Team

- Jordan Musser, DOE-ORD
- Janine Carney, DOE-ORD
- Sofiane Benheya, DOE-ORD
- Mark Meredith, Aeolus
- Jeff Dietiker, WVURC
- Tingwen Li, USR
- Rahul Garg, USR
- Aytekin Gel, Alpemi
- Aniruddha Choudhary, ORISE
- Surya Deb, ORISE
- Vikrant Verma, ORISE

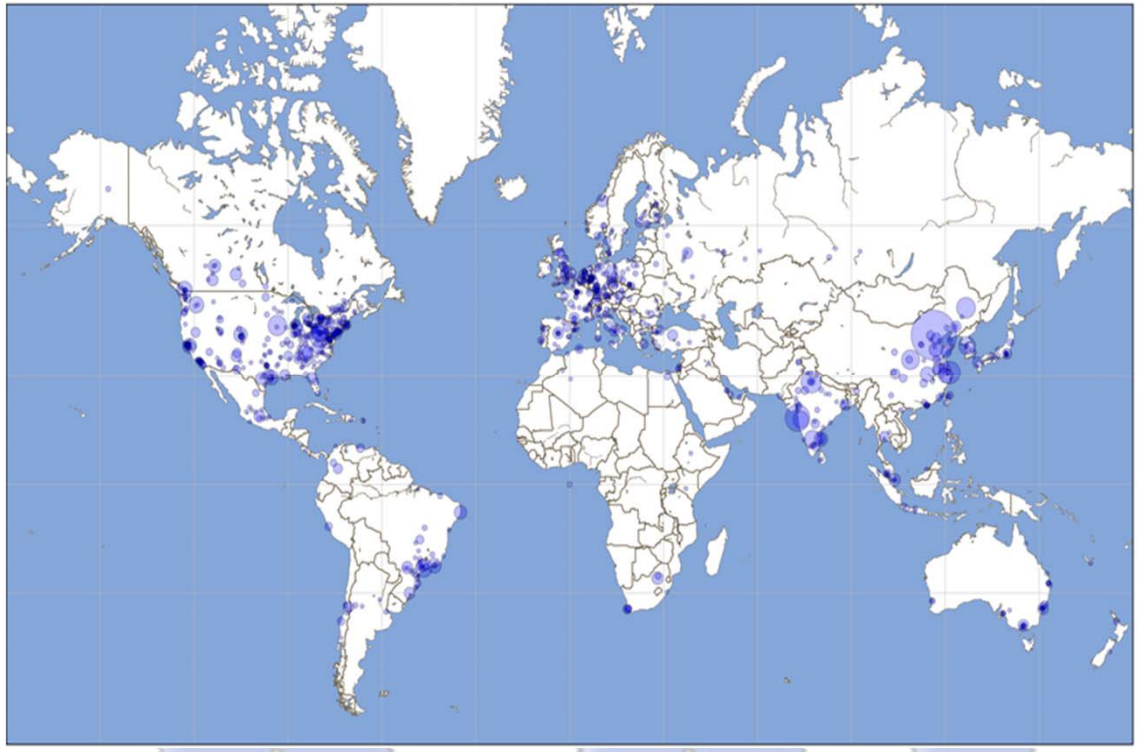
MFIX Overview

A suite of multiphase flow models



MFIX User Community

MFIX Registrations by Metropolitan Areas



3513 Registered Users from 73 Countries!

Community Demographics

Top Registrant Countries:
74 countries, Top 5:

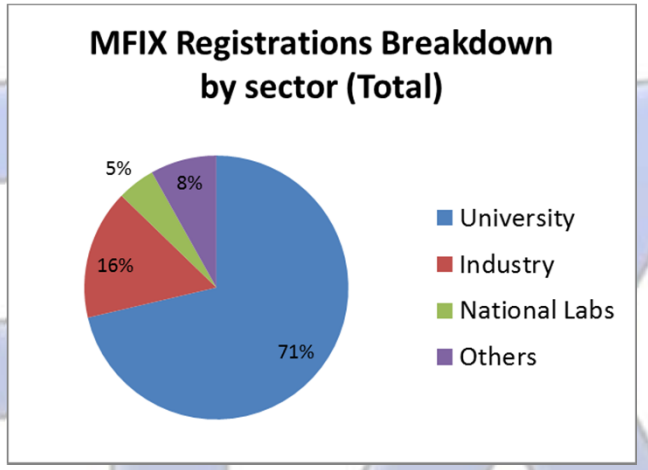

USA : 947


China : 618


India : 336


Brazil : 181

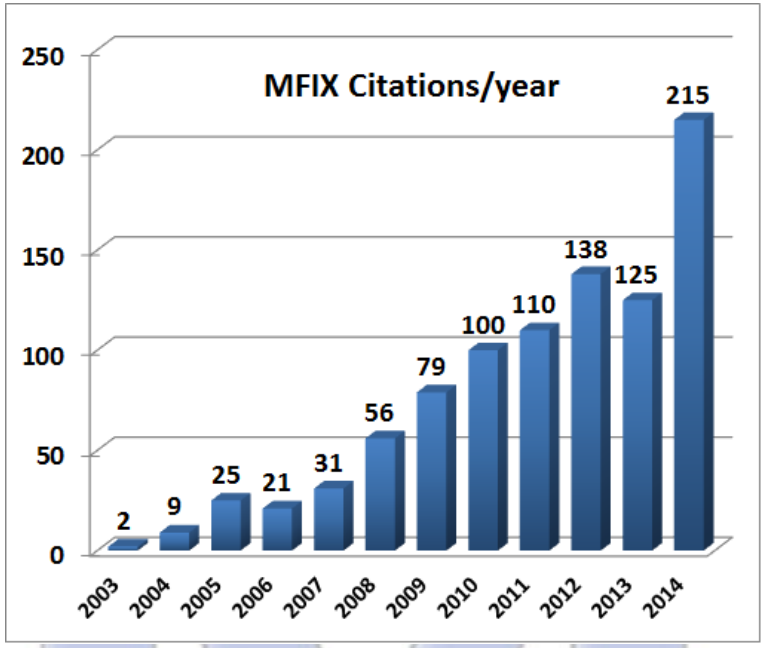

Germany : 149



MFIX Impact on Research

"The open-source MFIX code … is technically mature to predict well fluidization phenomena based on the Eulerian-Eulerian method."

Herzog et al. (2012) Computers & Chemical Engineering v39, p46



Statistics obtained from Web of Science citation report using a basic topic search for 'MFIX' or 'Multiphase flow with interphase exchange'. (7/29/2014) http://apps.webofknowledge.com

Recent Publications:

Galvin Janine E., Benyahia Sofiane. The Effect of Cohesive Forces on the Fluidization of Aeratable Powders. Aiche Journal. 2014 Feb;60(2):473-84.

Holloway William, Sundaresan Sankaran. Filtered models for bidisperse gas-particle flows. Chemical Engineering Science. 2014 Apr 28;108:67-86.

Mitrano P. P., Zenk J. R., Benyahia S., Galvin J. E., Dahl S. R., Hrenya C. M. Kinetic-theory predictions of clustering instabilities in granular flows: beyond the small-Knudsen-number regime. Journal of Fluid Mechanics. 2014 Jan;738.

Agrawal K., Holloway W., Milioli C. C., Milioli F. E., Sundaresan S. Filtered models for scalar transport in gas-particle flows. Chemical Engineering Science. 2013 May;95:291-300.

Bai Wei, Keller Norman K. G., Heindel Theodore J., Fox Rodney O. Numerical study of mixing and segregation in a biomass fluidized bed. Powder Technology. 2013 3//;237(0):355-66.

Choudhuri A. Tehnical Report on Investigation of Gas Solid Fluidized Bed Dynamics with Non-Spherical Particles. 2013. National Energy Technology Laboratory (NETL) Morgantown, WV, USA, University Of Texas El Paso, Texas, USA. p. 106.

Estep Joe, Dufek Josef. Discrete element simulations of bed force anomalies due to force chains in dense granular flows. Journal of Volcanology and Geothermal Research. 2013 3/15/;254(0):108-17.

Gel A., Garg R., Tong C., Shahnam M., Guenther C. Applying uncertainty quantification to multiphase flow computational fluid dynamics. Powder Technology. 2013 Jul;242:27-39.

Gopalakrishnan Pradeep, Tafti Danesh. Development of parallel DEM for the open source code MFIX. Powder Technology. 2013 Feb;235:33-41.

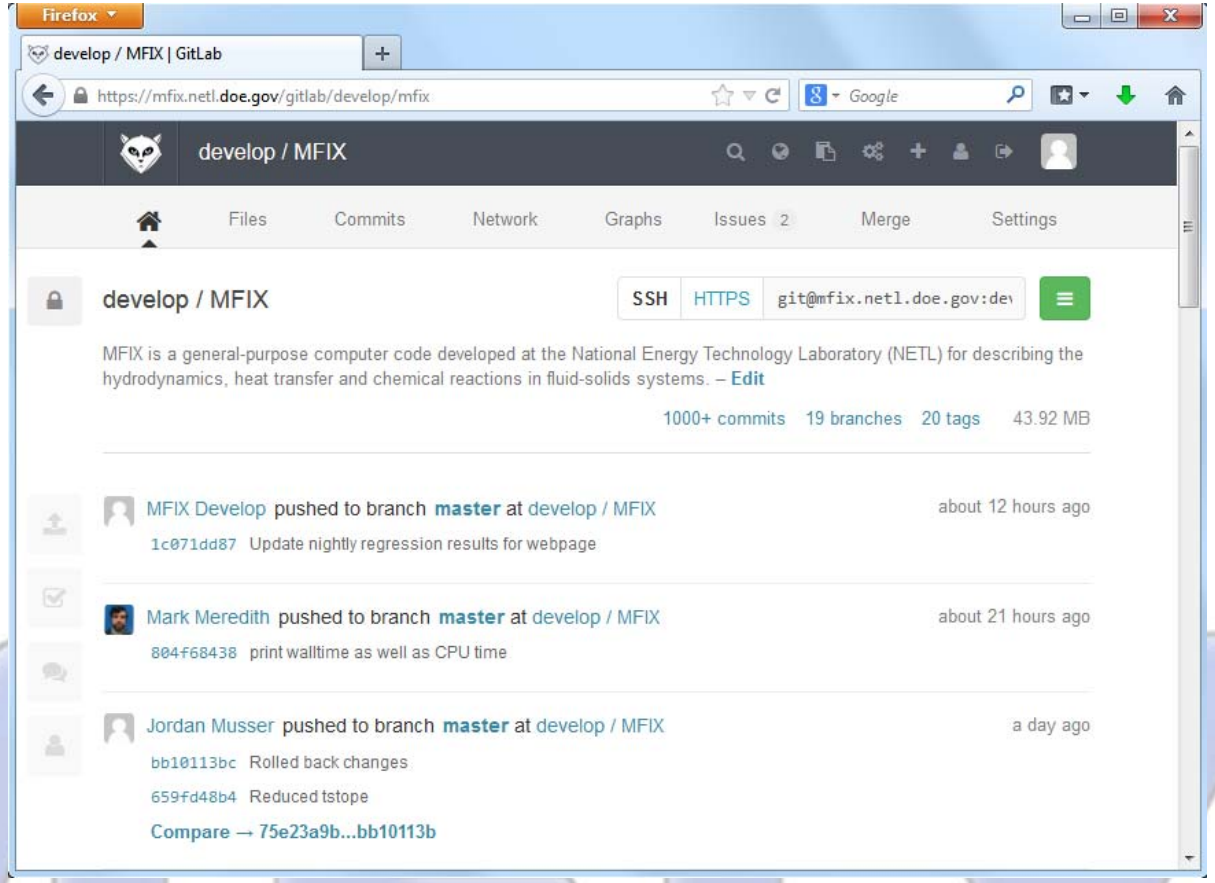
Hernandez-Jimenez F., Sanchez-Prieto J., Soria-Verdugo A., Acosta-Iborra A. Experimental quantification of the particle-wall frictional forces in pseudo-2D gas fluidised beds. Chemical Engineering Science. 2013 10/11/;102(0):257-67.

MFIX Source Code Management

Self-Hosted GitLab Repository

- 20 Project Members
- Over 3400 commits
- 1364 master files
- Nearly 15 years

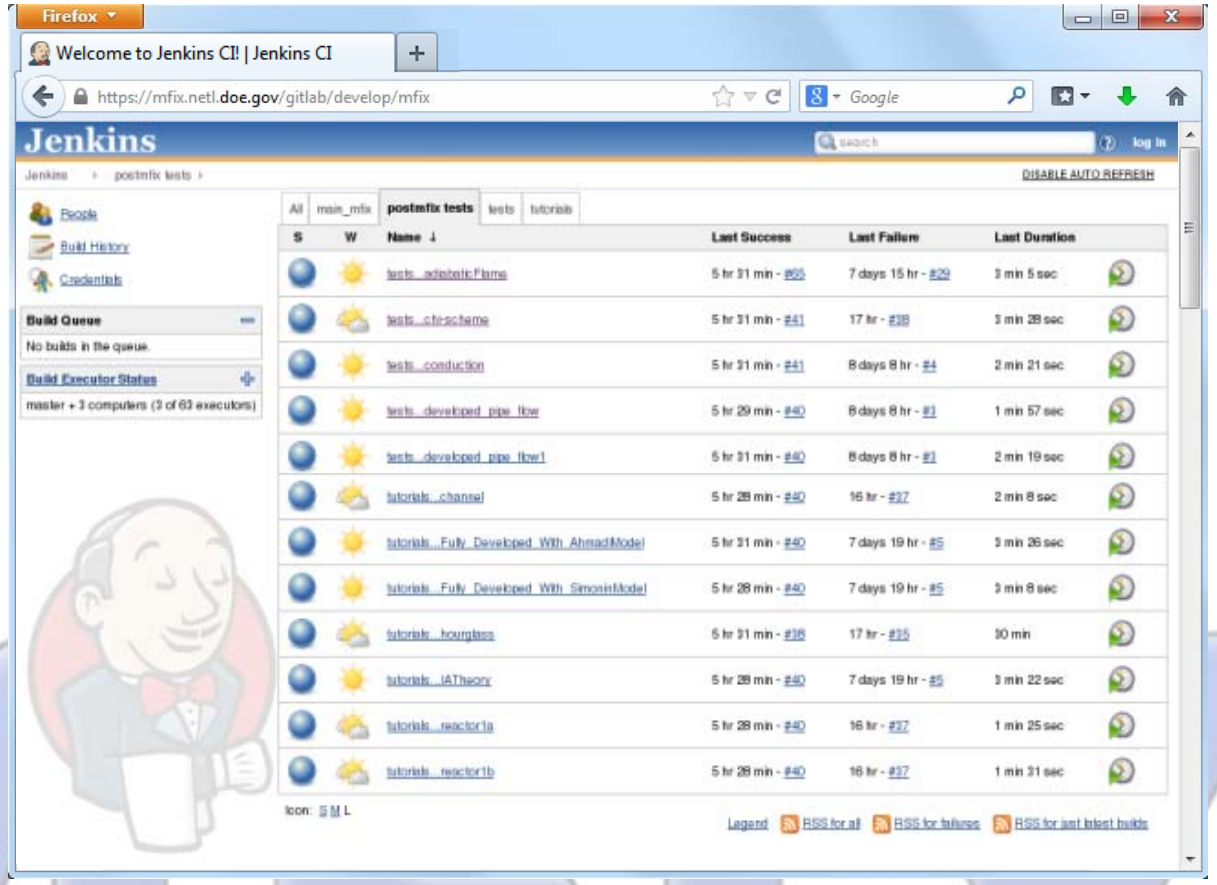
Access to non-NETL personnel is available upon request!



MFIX Source Code Management

Continuous Regression Testing

- Verifies that MIFX builds in serial, DMP, SPM and hybrid modes with Intel and GNU.
- Runs over 140 cases
- Covers nearly 70% of the MFIX source code
  (reported by Intel codecov tool)
- Email notifications of recent test failures.
- Archives results nightly and updates website information



MFIX and HPC

MFIX has been ported and run on a diverse set of clusters and HPC systems.

- Cray: XT4, XT5, XE6
- IBM: BlueGene/P and /Q
- SGI

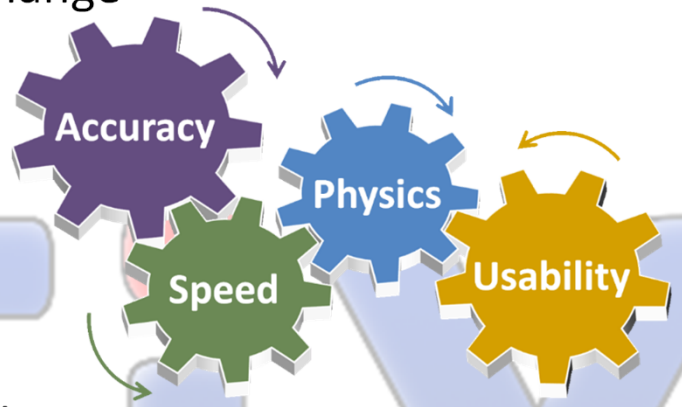
- 2014 ALCC Award Allocation; 37.5Million core hours (NERSC)
- 2008-10 INCITE Award Allocation; 22Million core hours (OLCF)

National Energy Research Scientific Computing Center

Leadership Computing Facility

The Four Guiding Principals of MFiX Development

- **Develop physics with respect to the targeted application**
  - Physical model development is guided by targeted validation experiments
  - What does the model need to capture observed physical behavior?
- **Ensure the results of the code are accurate**
  - Verification cases identify weaknesses
  - Continuous integration; retest with every change
- **Increase speed to reduce time-to-solution**
  - Identify problematic algorithms
  - Optimize for modern computing platforms
- **Increase usability by reducing complexity**
  - Simplify user interaction with the code
  - Better, clearer, more complete documentation



MFIX Release 2014-1

- New Features
- Feature Improvements
- External contributions
- Bug fixes

Improved Usability

- **Improved build utility: further automates compilation of MFiX**
- **Input simplification and better error management**
- **Parallel build support**

Variable Solids Density

Example Variable Solids Density input:
tutorials/variable_density/mfix.dat

```
! Initial Mass Fractions
  X_s0(1,1) = 0.95
  X_s0(1,2) = 0.00
  X_s0(1,3) = 0.00
  X_s0(1,4) = 0.05

! Material Densities
  RO_Xs0(1,1) = 0.5944
  RO_Xs0(1,2) = 0.6490
  RO_Xs0(1,3) = 0.4500
  RO_Xs0(1,4) = 0.4500

  INERT_SPECIES(1) = 4
```

Initial (baseline) Solids density

$$\frac{1}{\rho_m^0} = \sum_n \frac{X_{m,n}^0}{\rho_{m,n}^0}$$

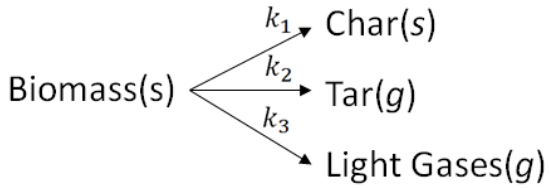
Instantaneous Solids density

$$\rho_m = \rho_m^0 \frac{X_{m,I}^0}{X_{m,I}}$$

MFIX 2014-1 Release

Variable Solids Density

Competitive Reaction Scheme



Materials:

Sand: 0.052 cm, 2.6 g/cm^3

Biomass: 0.050 cm

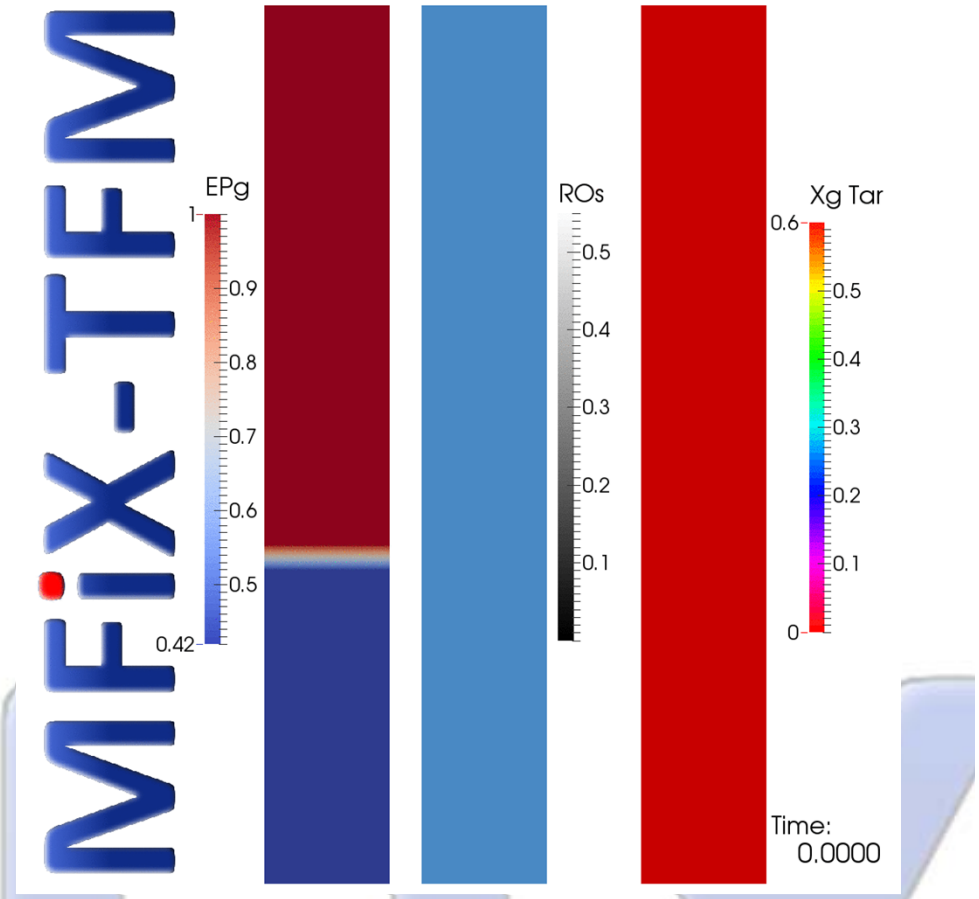
Inlets:

Bottom - Air, 23.7 cm/sec

Side - Air (0.993022), 12.375 cm/sec

Biomass, 12.375 cm/sec

** Gasification and combustion reactions are not included.*

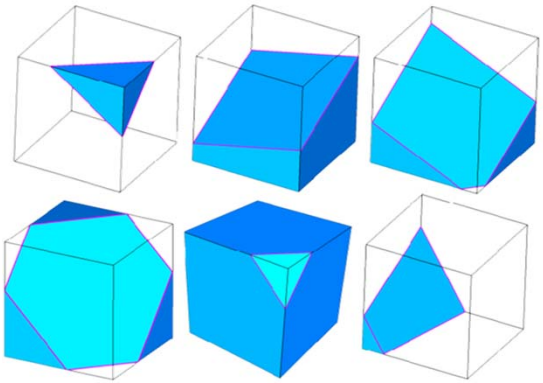


Xue and Fox, "Multi-fluid CFD modeling of biomass gasification in polydisperse fluidized-bed gasifiers." Powder Technology, Vol 254, pp.187-198, 2014.

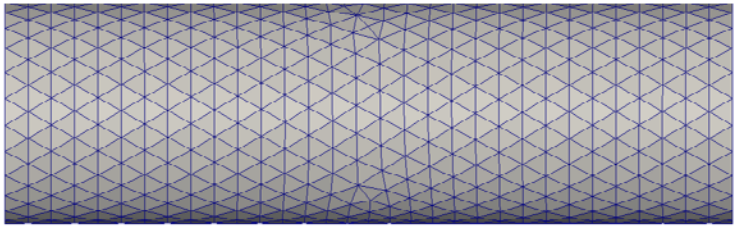
Complex Boundary Support

- **Overcome Cartesian cut-cell derived wall limitations**
  - Not “water tight” allowing particles to “leak”
  - Limited domain complexity
  - Dependent on mesh quality
- **STL provide better framework**
  - Mesh independent walls
  - ‘Water tightness’ is offloaded onto quality of STL geometry
  - Leverage gaming industry collision algorithms

Types of Cut cells

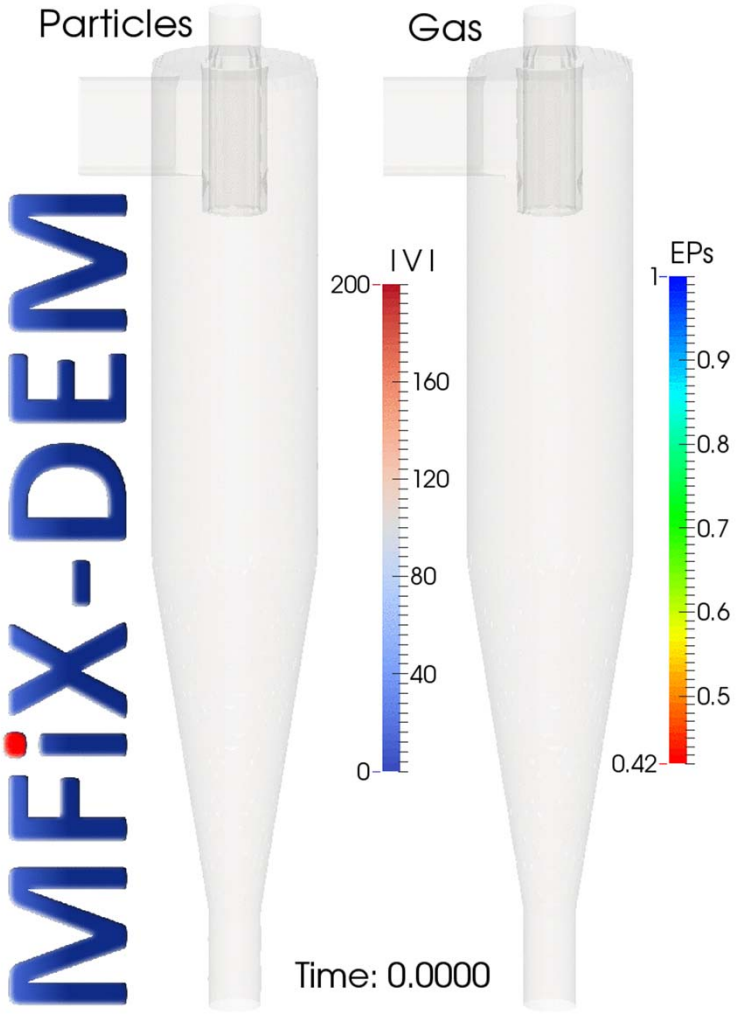


STL based walls



MFIX 2014-1 Release

DEM Wall Boundaries via STL



Materials:
DEM Particles: 0.04 cm, 2.0 g/cm^3
Gas phase: Air (*compressible*)

Domain: STL Defined (*4cm x 15cm x 4cm*)
120K background mesh
~28.5K active cells (>25%)

Gas pressure outlet at top
Solids outlet at bottom

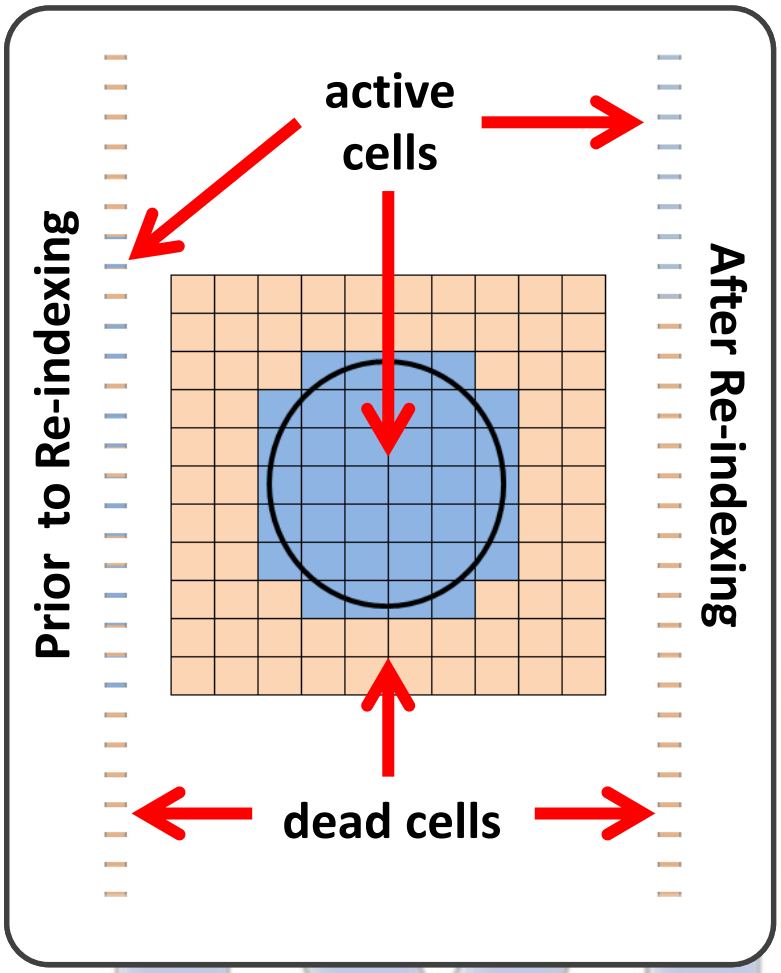
Inlet: 100 cm/sec
0.99 Air, 0.1 Solids
(~17.5K particles/second)

Steady-state inventory ~12K particles

Chu, Wang, Xu, and Chen, "CFD-DEM simulation of the gas-solid flow in a cyclone separator." Chemical Engineering Science, Vol 66, pp. 834-847, 2011.

MFIX 2014-1 Release

Cut-Cell Array Re-Indexing

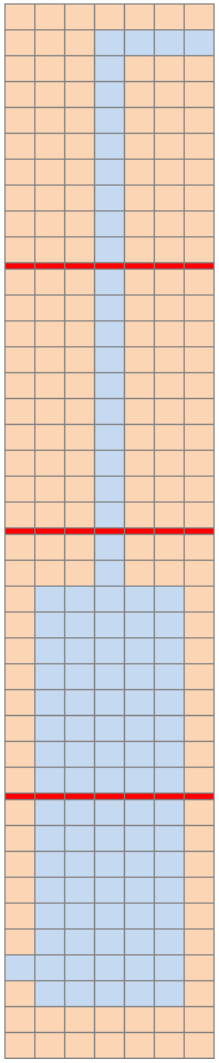


- **Cartesian cut-cell technique**
  - More realistic geometries without unstructured mesh
  - Inactive computational cells persist to fill the 'dead' space
- **Re-Indexing minimizes waste by sorting arrays so that loops only "see" active cells**
  - Mostly hidden from users
  - Adds some overhead as some calculated indices are changed to array accesses

MFIX 2014-1 Release

Cut-Cell Load Balancing

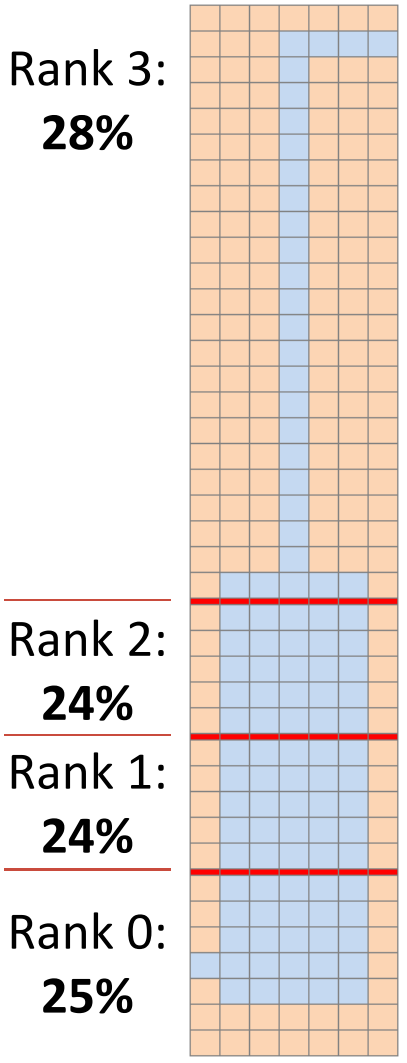
Even Mesh Distribution



MFIX attempts to setup MPI partitions by evenly distributing the mesh leading to large load imbalances.

After re-indexing, MFIX minimizes the load imbalance by trying to assign a uniform number of active cells.

Even Load Distribution



MFIX 2014-1 Release

Cut-Cell Array Re-Indexing

Chemical Looping Reactor

- 64 core, 60 second simulation
- 2.7M cells (background mesh)
- 315K re-indexed cells

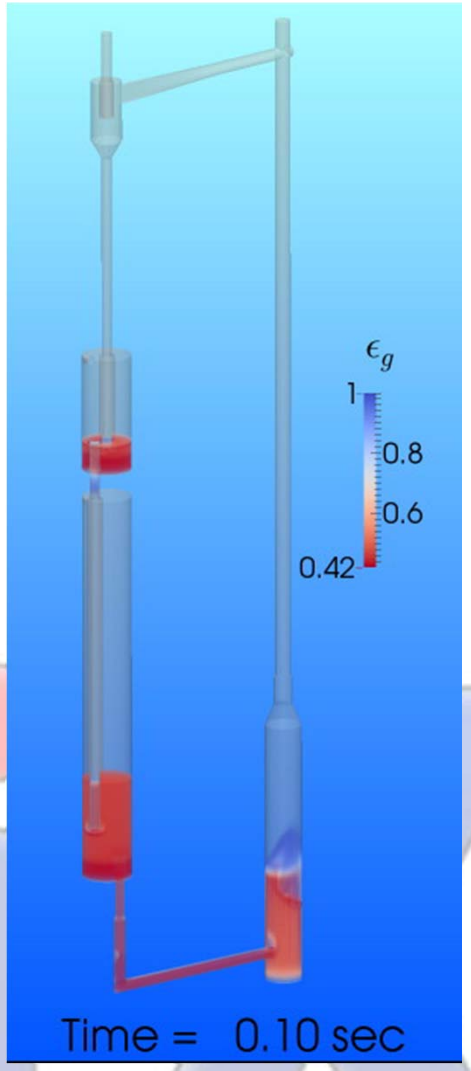
No re-indexing: 7.7 days

Re-indexing: 4.9 days (1.6x speedup)

Re-indexing w/optimized MPI layers:

1.7 days (4.5x speedup)

Right image courtesy of Jeff Dietiker, NETL/WVURC
Left image courtesy of Justin Weber, NETL/DOE



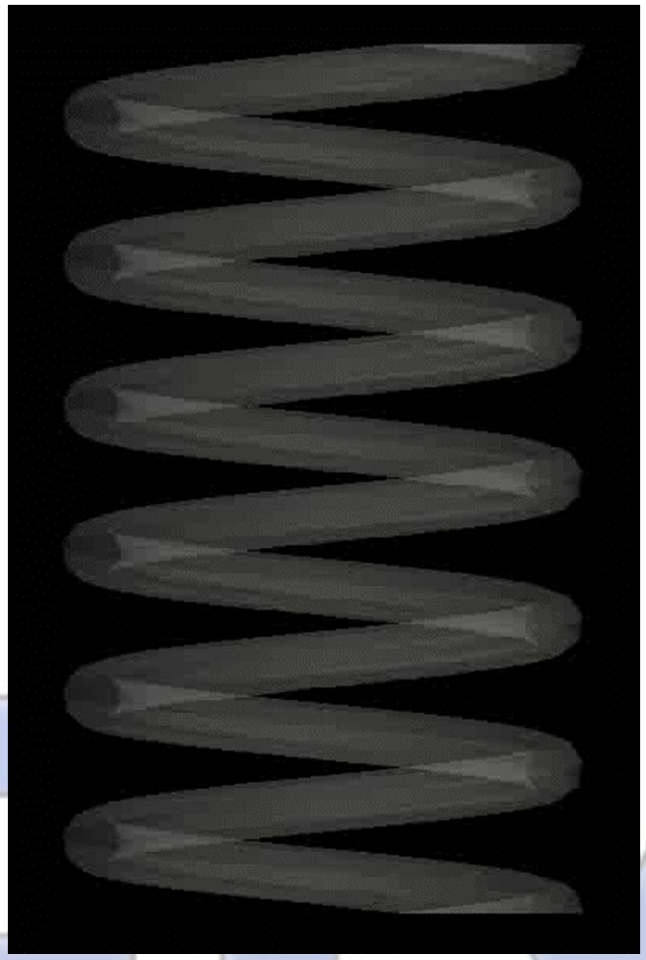
Application Driven Development of MFIX-DEM

- **Goal: Produce large-scale models employing chemical reactions and realistic geometries with particle counts appropriate to application**

- **Development Needs Overview**:
  - Improve boundary condition implementation
  - DEM thermochemical routine modifications
  - Incorporate into DEM-DMP modules
  - Extend thermochemical modules to PIC model
  - Reduce the time-to-solution

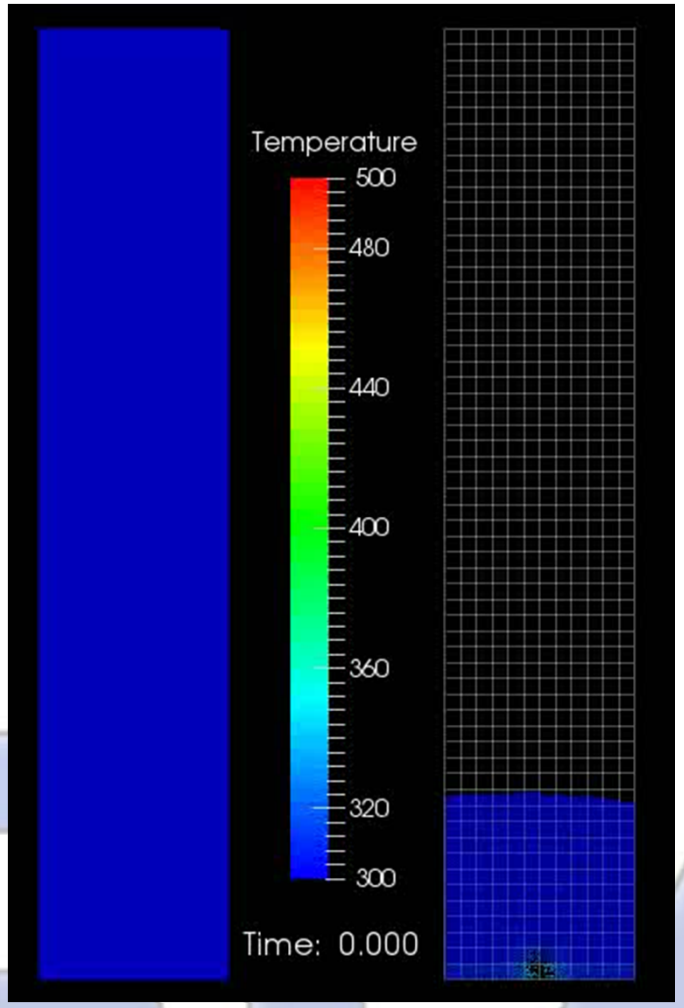
Geometric Flexibility with MFIX-DEM

- **Realistic geometry specification**
  - Faster particle-wall collision detection
    - Bounds checking to minimize more expensive calculations
    - Improved DEM STL preprocessing
  - New particle data mapping techniques
  - Efficient mapping between fluid grid and particles
    - Allows for grid independent DEM simulations for greater accuracy



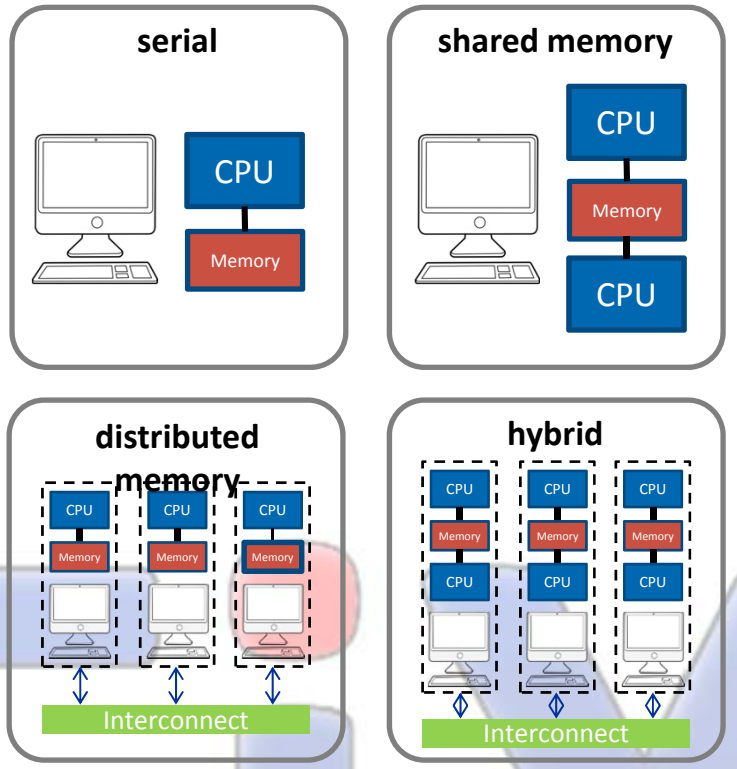
Heat Transfer Simulation with MFIX-DEM

- DEM routines were modified to included variables for modeling reacting flows and heat transfer.
- Refined DMP implementation to minimize future maintenance and development efforts
- Initial extension of PIC to DMP



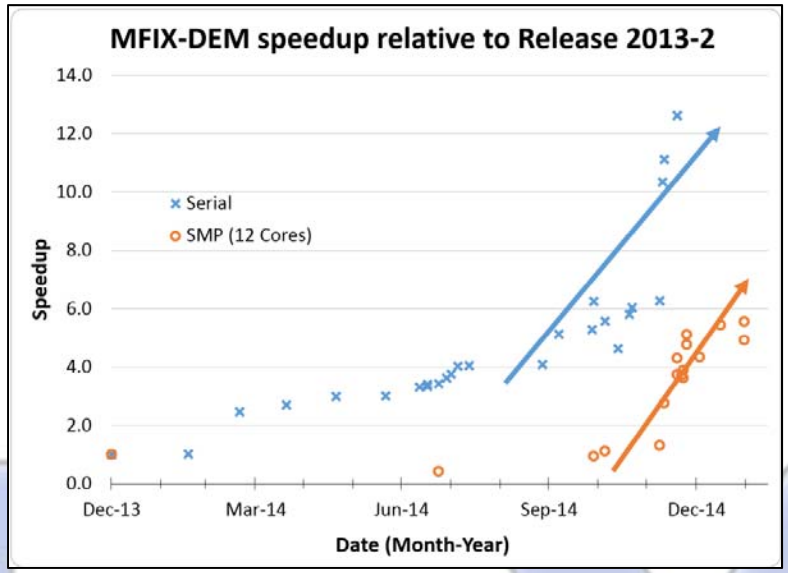
DEM Performance Enhancements

- Optimize serial execution
  - Profile runs to identify ‘hot spots’
  - Implement more efficient algorithms
  - Cache friendly data access patterns
- Incorporate OpenMP directives (SMP)
- Reduce DMP overhead (wait time)
  - Profile runs to identify ‘bottle necks’
  - Non-blocking MPI communications



DEM Performance Enhancements

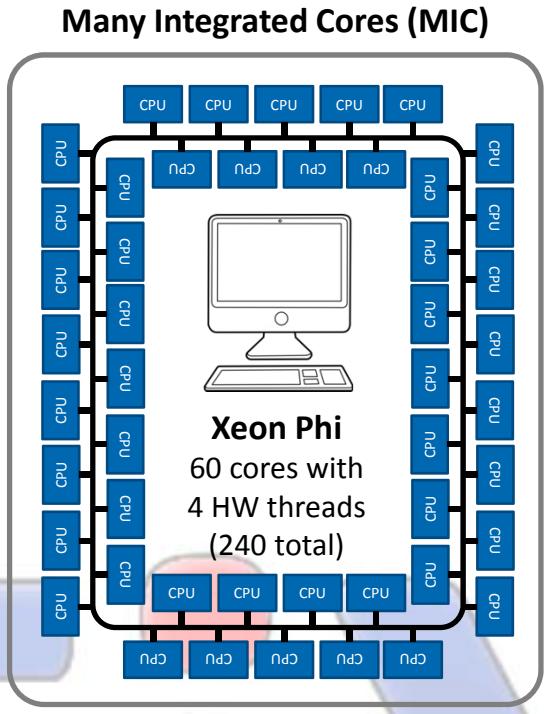
- Several algorithm and data structure changes were implemented in MFIX-DEM to reduce time-to-solution.
- Additional OpenMP directives (SMP)
- New explicit interphase coupling algorithm minimizes expensive calculations



DEM Performance Enhancements (porting to Intel® Xeon Phi architecture)

- Maximize SMP scalability
- Increase loop vectorization
- May need substantial modification to existing algorithms to achieve speedup

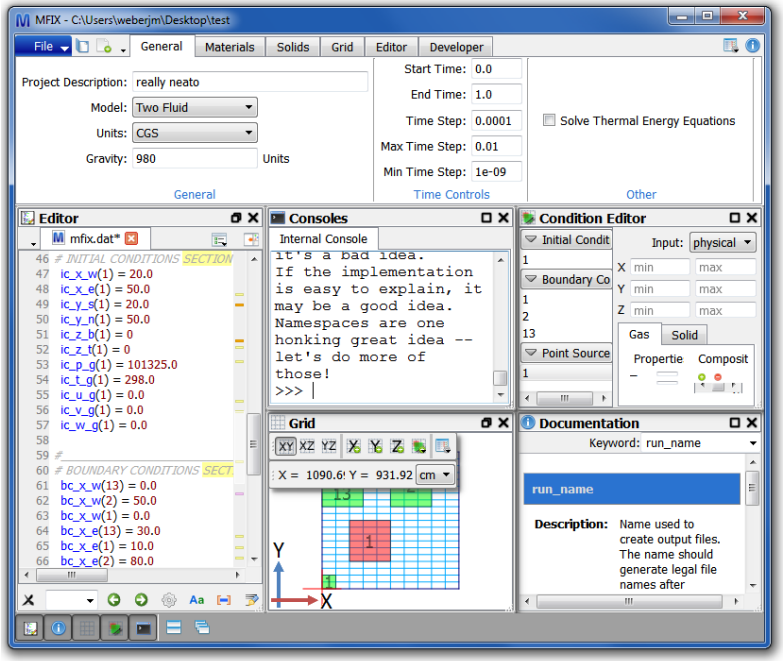
This is a difficult task, but any gains made also improve the overall speed of the code.

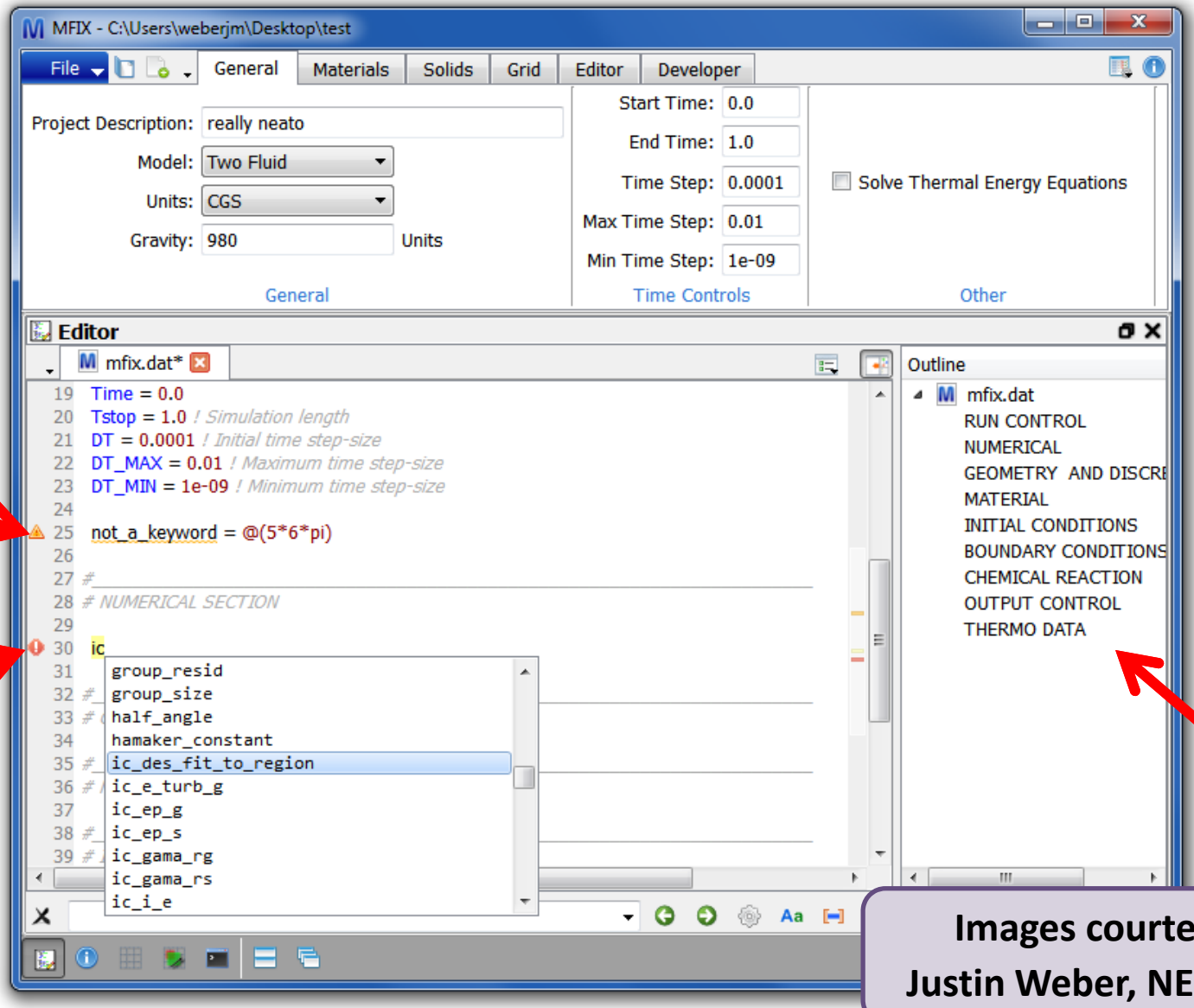


Beyond the 2014-1 Release

MFIX-GUI

- **Tool to guide a user through setting up mfix.dat**
- **Text editor**
  - Keyword documentation
  - Inline error checking
  - Tab completion
- **Grid editor**
- **Initial condition and boundary condition editor**
- **Cross platform**
- **Developed in Python**
- **Uses QT for GUI library**





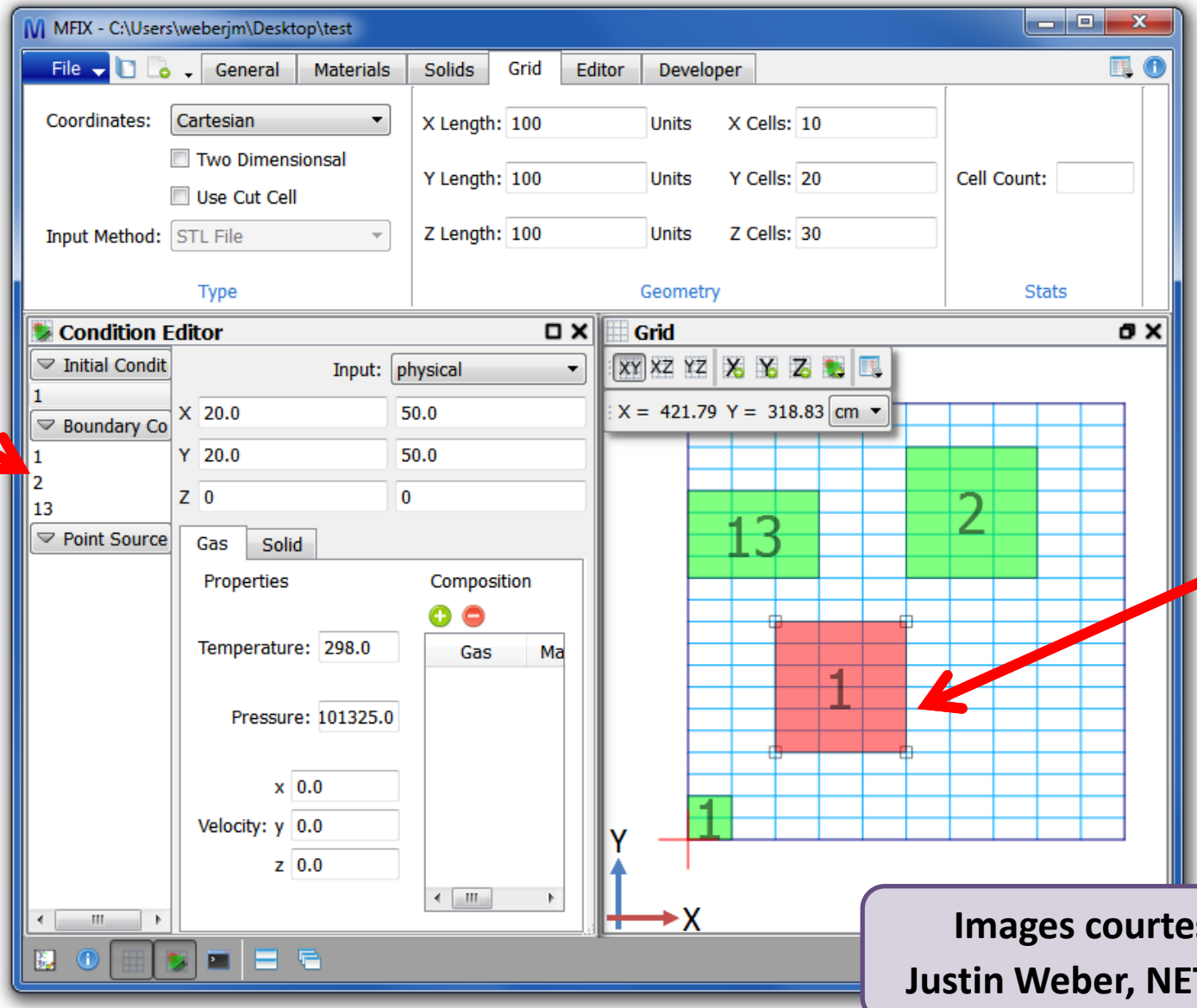
Error Checking

Tab Completion

Outline

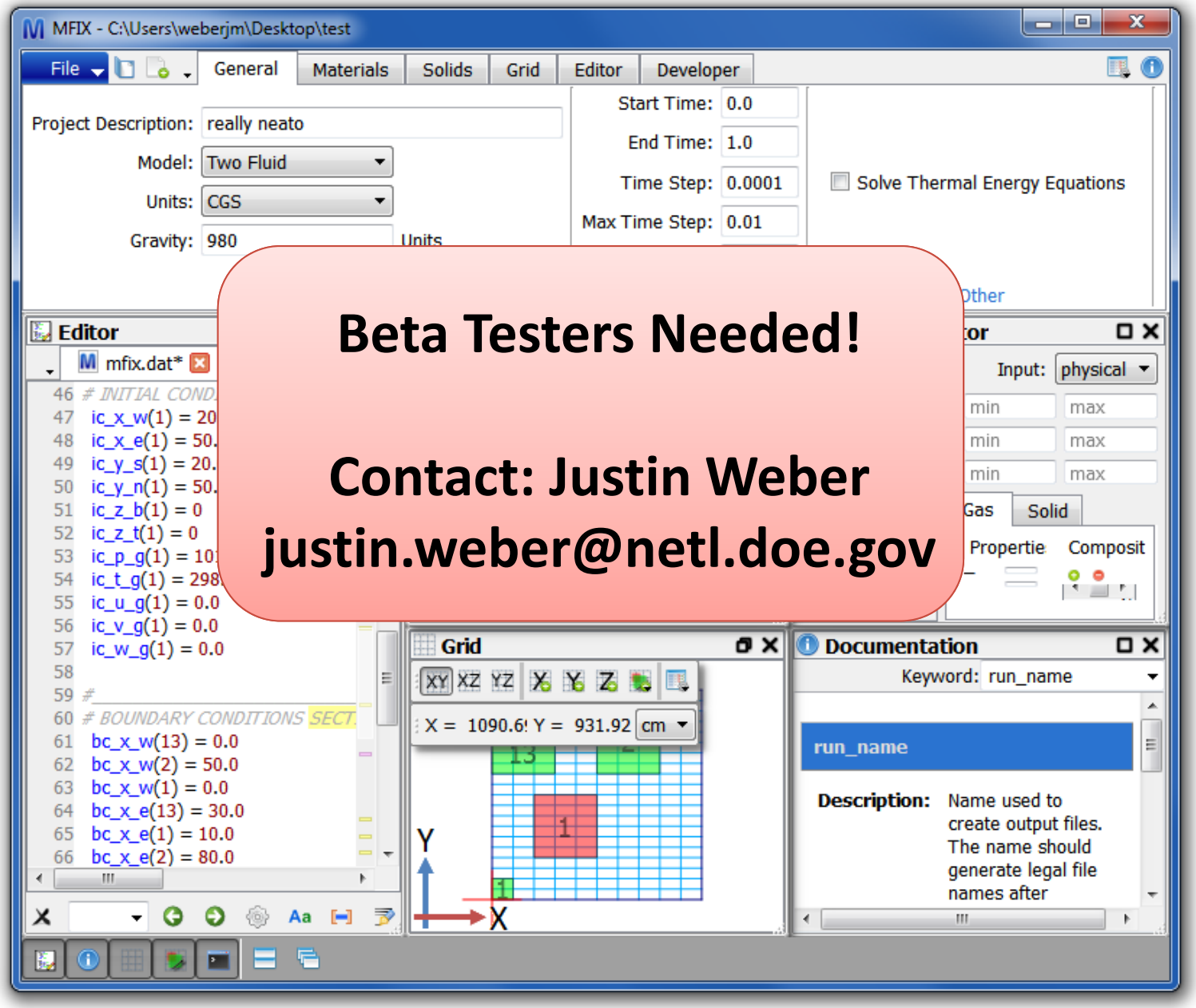
Images courtesy of Justin Weber, NETL/DOE

Condition Editor



Editable

Images courtesy of
Justin Weber, NETL/DOE



Beta Testers Needed!

Contact: Justin Weber
justin.weber@netl.doe.gov

MFIX-Hybrid :: Reacting!

Proof of concept

- Discrete particles heat, dry, and devolatilize
- Continuum solids, char and ash based, combust with incoming oxygen

- DEM particles shown at 10x of modeled size