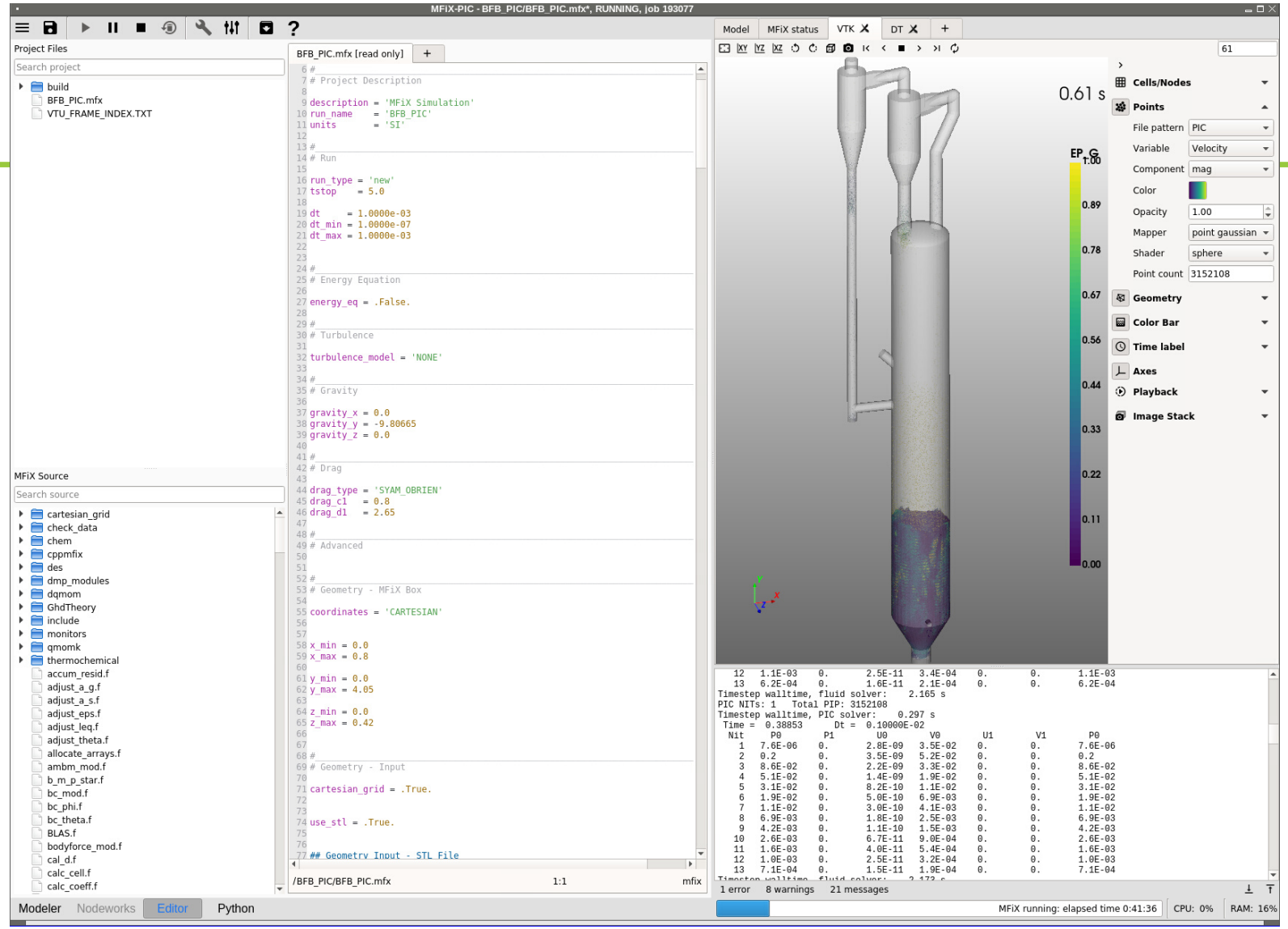
MFiX Suite Development Update



Jeff Dietiker

Multiphase Flow Science Group

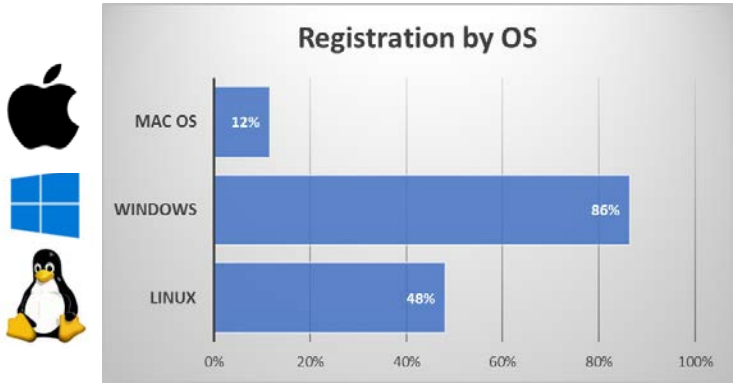
August 8, 2019

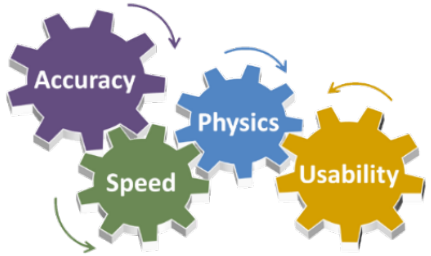
MFiX Development Activities

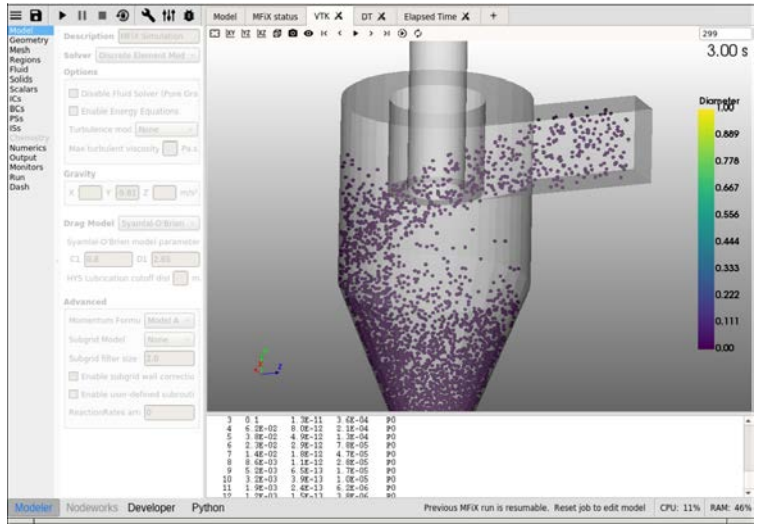
- **2018-2019 development**
  - **Graphical User Interphase** (GUI) redesigned in 2017
  - Flow solver (TFM, DEM, **PIC**)
  - Website
  - Quality Assurance (next talk)

- Future development

- Short GUI demo







MFiX Development Activities

MFiX 19.1 Release (April 2019):

- **New implementation of the Particle in Cell (PIC) model:**
  - Hydrodynamics
  - Heat transfer
  - Chemistry
  - Serial and parallel run
- Ability to view STL normals and flip normal from the GUI
- Ability to save image stack for animations
- Quickly parse through the solver output to view Error/Warning/Info messages
- PGI compiler support (non interactive solver)
- Gridengine job submission script
- Bug report (zip file) can be saved from GUI
- Ability to read several non-overlapping STL files to generate the geometry.
- Addition of implicit function buttons to the modeler toolbar
- Log files: Ability to save Solid inventory, solver output, DT and NIT to files
- Ability to plot Cp vs. Temperature for each species
- Mass inflow BCs can overlap
- User guide in PDF format
- Updated documentation
- Additional PIC tutorials
- Various other bug fixes

- Bug fixes
- Improvement
- New
- No longer supported
- Workflow
- Cosmetic
- Documentation

MFiX GUI

Special thanks to GUI team:
Justin Weber
Mark Meredith
Charles Waldman
Jordan Musser

MFiX Development Activities

MFiX 19.2 Release (July 2019):

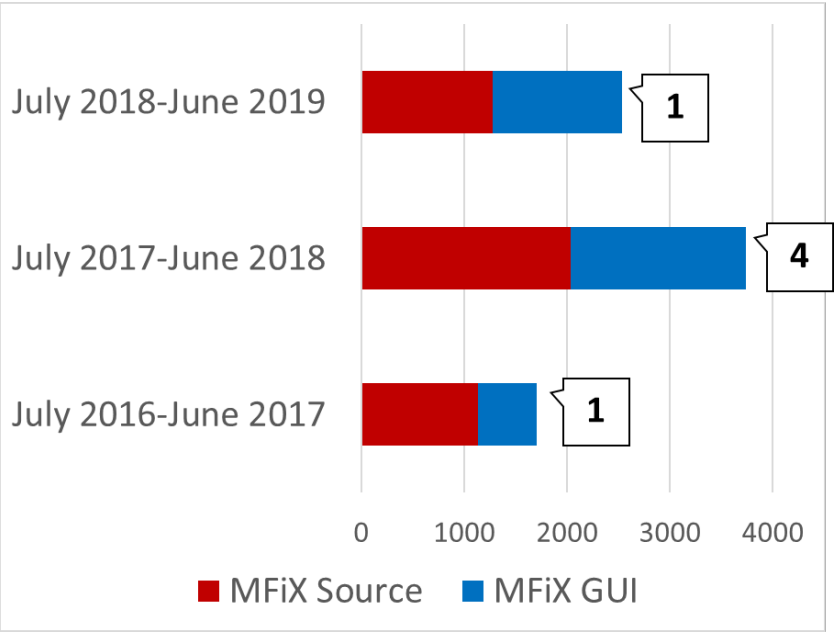
- Text Editor and File Browser:
  - Open/edit files from the project directory or the MFiX source tree.
  - The text editor allows users to edit UDFs or other files (particle_input.dat, gridmap.dat etc.) directly from the GUI.
  - Syntax highlight, find/replace, go to line features.
  - Source code files are automatically copied to project directory for easy build.
- MFiX Keyword browser:
  - Users can search for a known keyword to get documentation.
  - Keywords can be located in the GUI by automatically moving to the widget controlling the keyword, and briefly highlighting the keyword.
- Advanced pane:
  Users can now add/edit keywords that don't have a widget in the GUI. This includes regular keywords, and user-defined keywords.
- Material Database
  Solids phase diameter and density can be imported from a database of common NETL materials.
- Updated documentation
- Updated tutorial
- Various other bug fixes

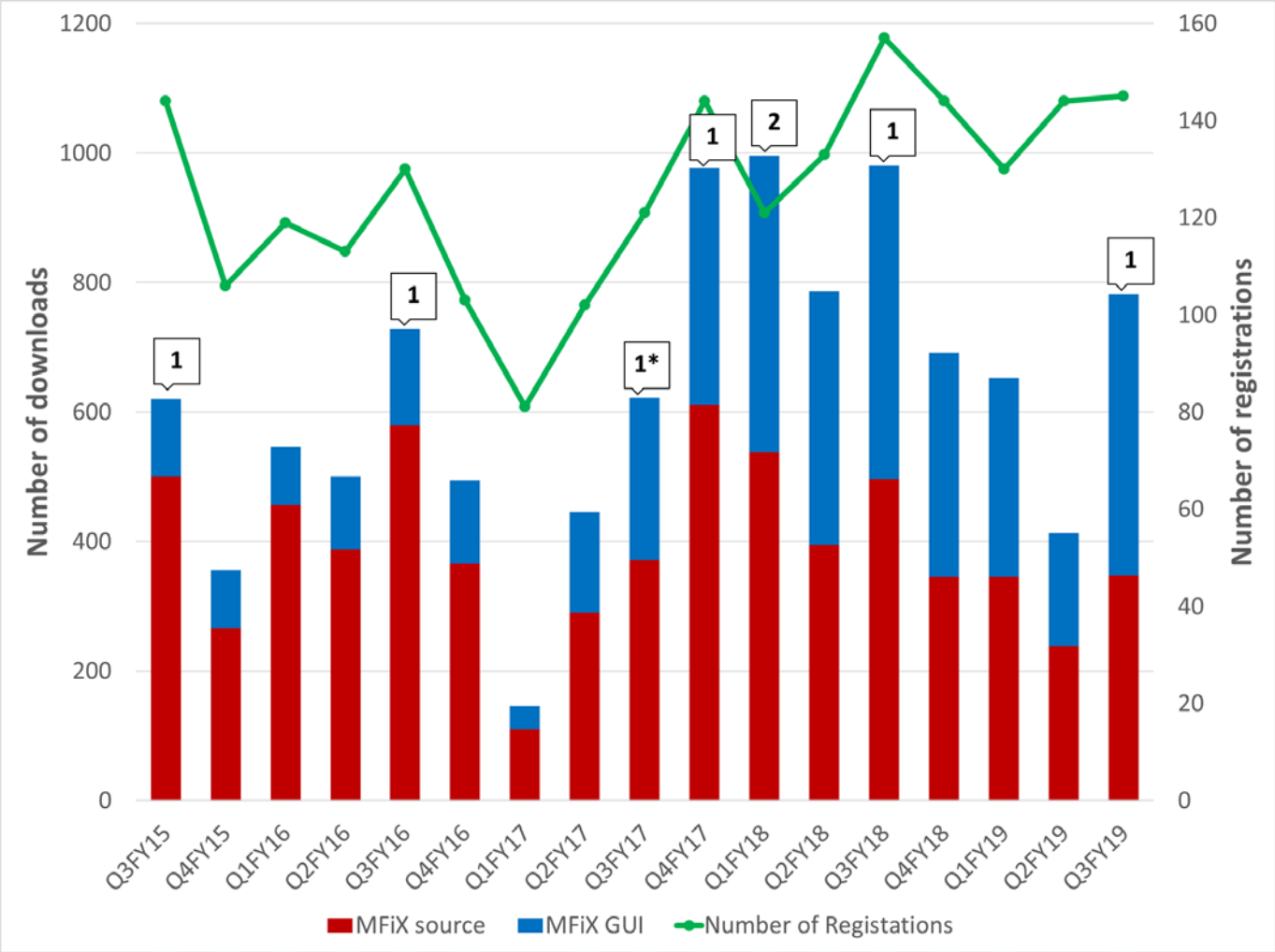
- Bug fixes
- Improvement
- New
- No longer supported
- Workflow
- Cosmetic
- Documentation

MFiX Impact

July 2018-June 2019 Stats:

- **Registrations = 563**
- **MFiX GUI = 1,264 downloads**
- **MFiX source code = 1,275 downloads**





1 Number of major releases

July 2018-June 2019 Stats

- MFiX registrations = **563**
  - University = 420
  - Industry = 61
  - National Labs = 25
  - Other = 57

- **Top 5 countries:**

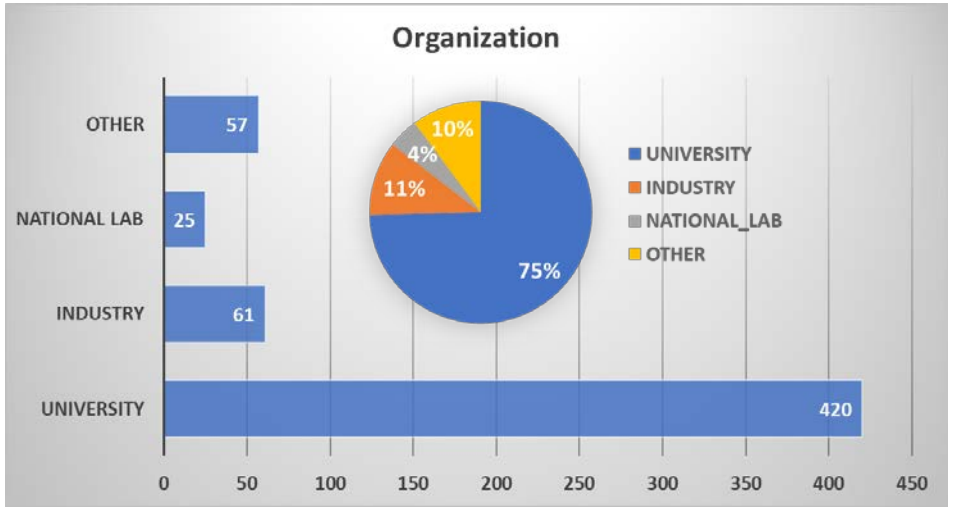
USA : 171

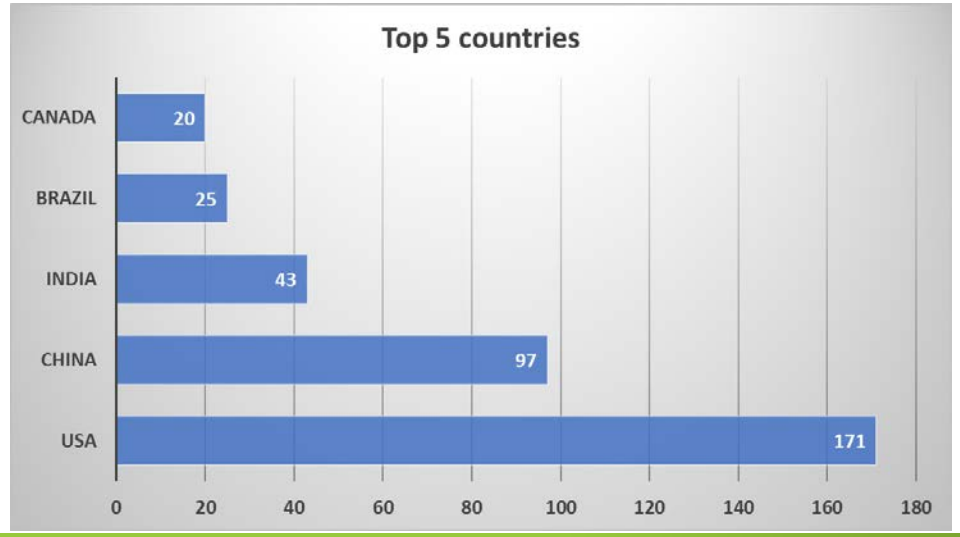
China : 97

India : 43

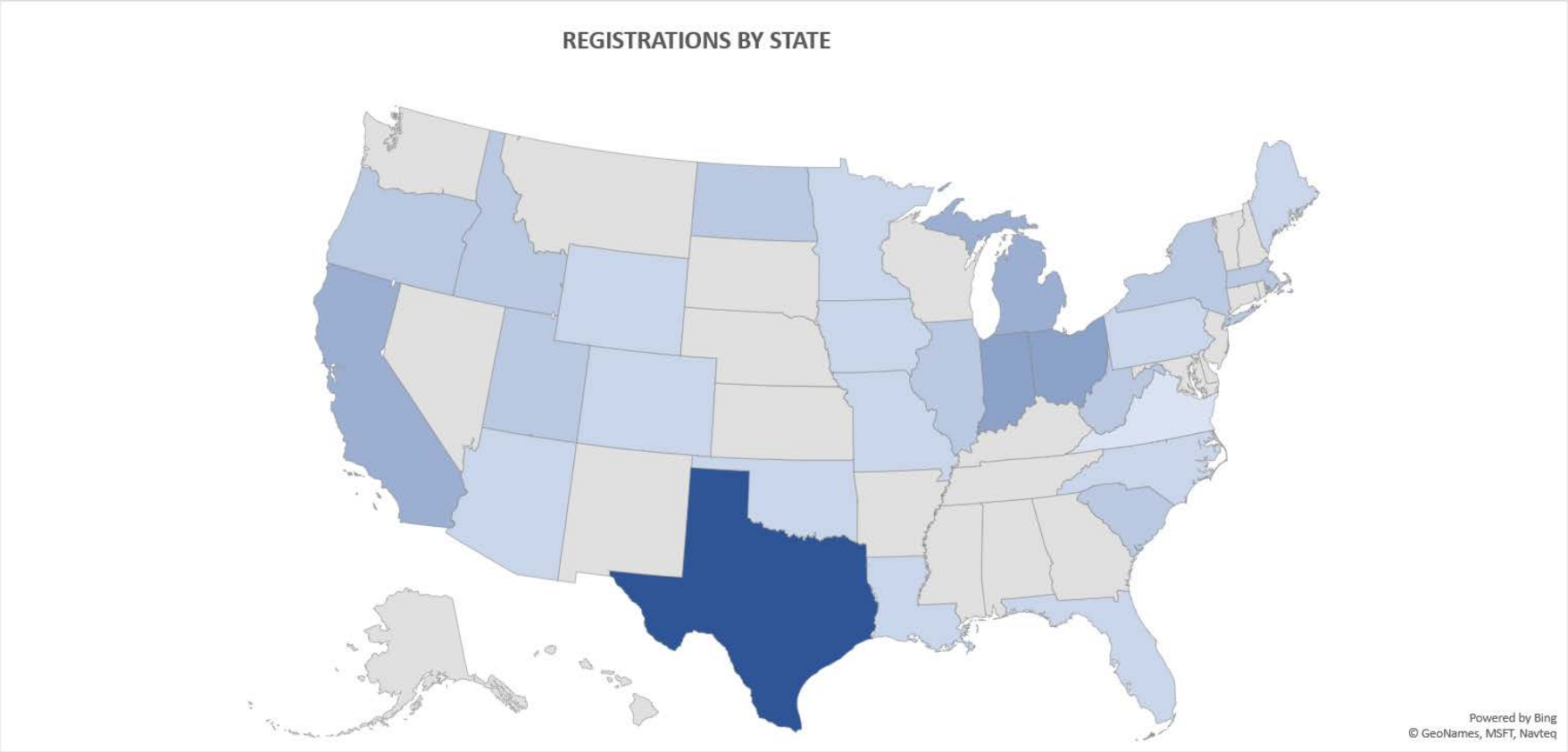
Brazil : 25

Canada : 20

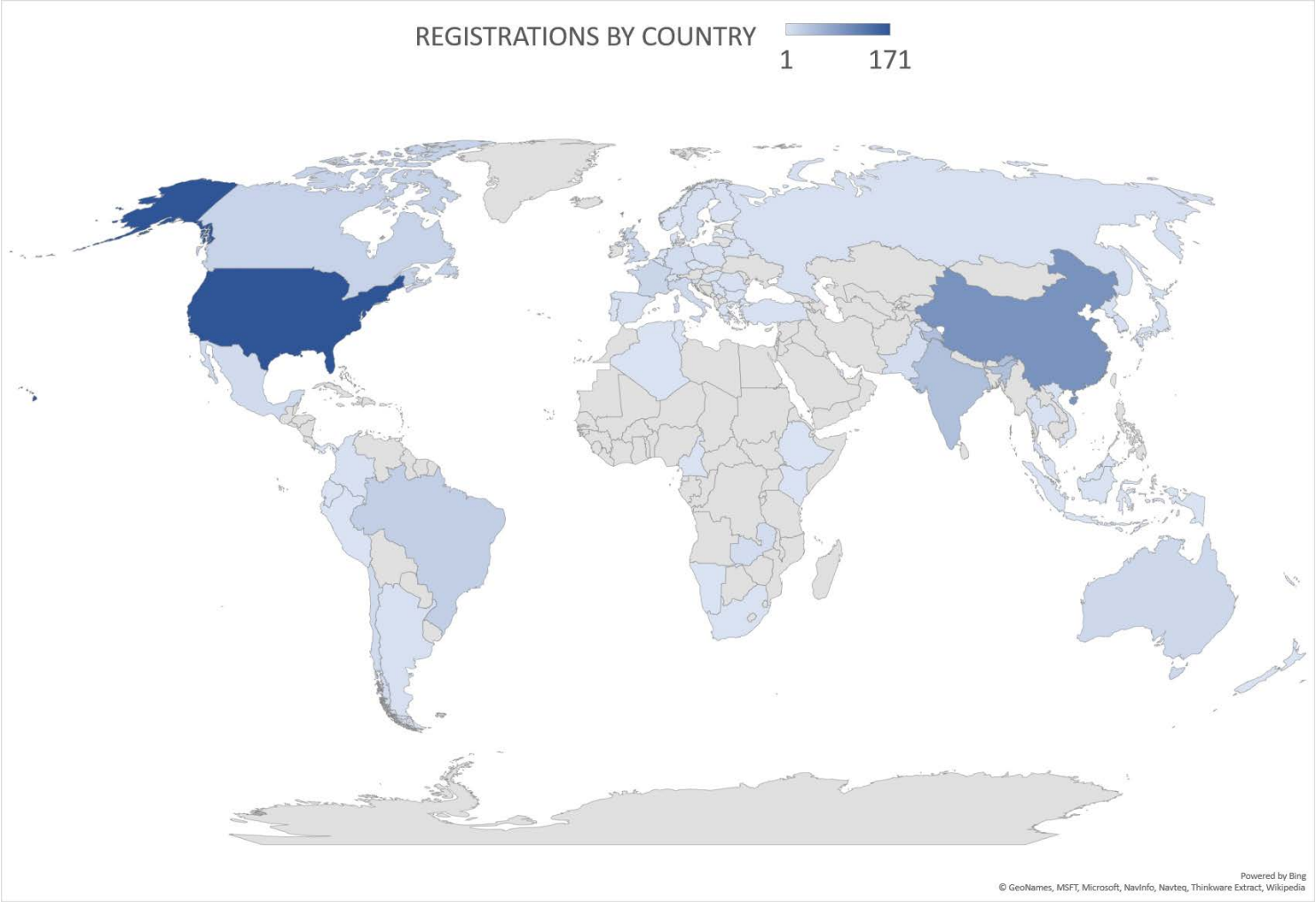




July 2018- June 2019 registrations USA map



July 2018- June 2019 registrations World map



All-time MFiX Stats (as of June 2019)

- All-time MFiX registrations = **5,583**
  - University = 4,020
  - Industry = 824
  - National Labs = 274
  - Other = 465

- **81 countries, Top 5:**

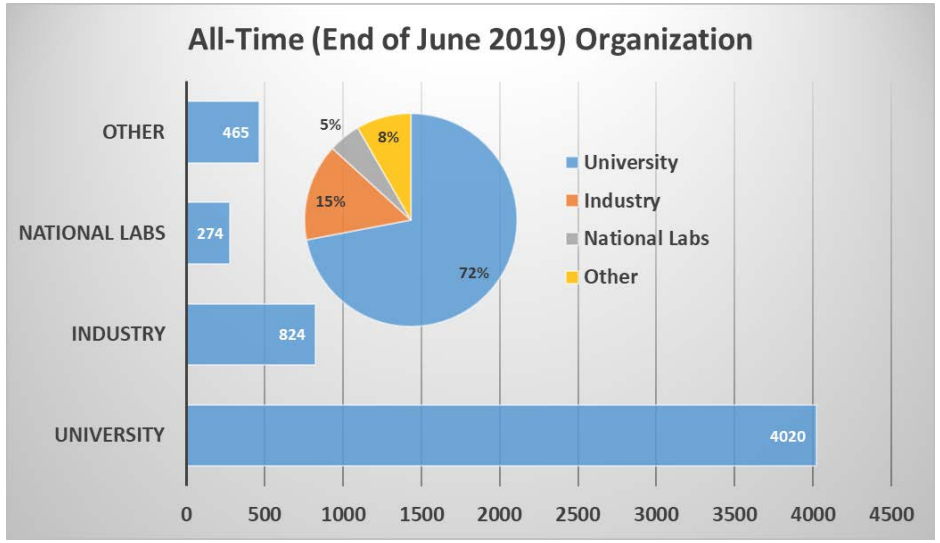
USA : 1,632

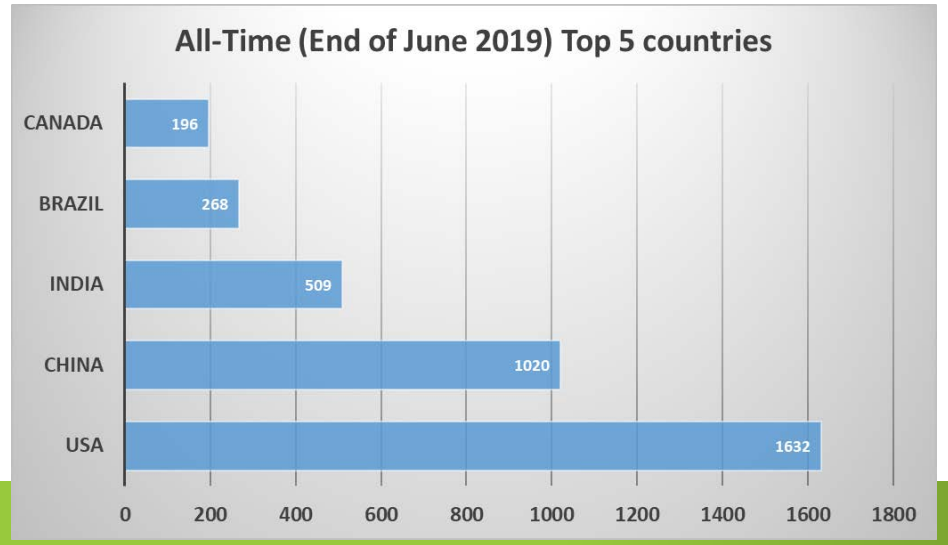
China : 1,020

India : 509

Brazil : 268

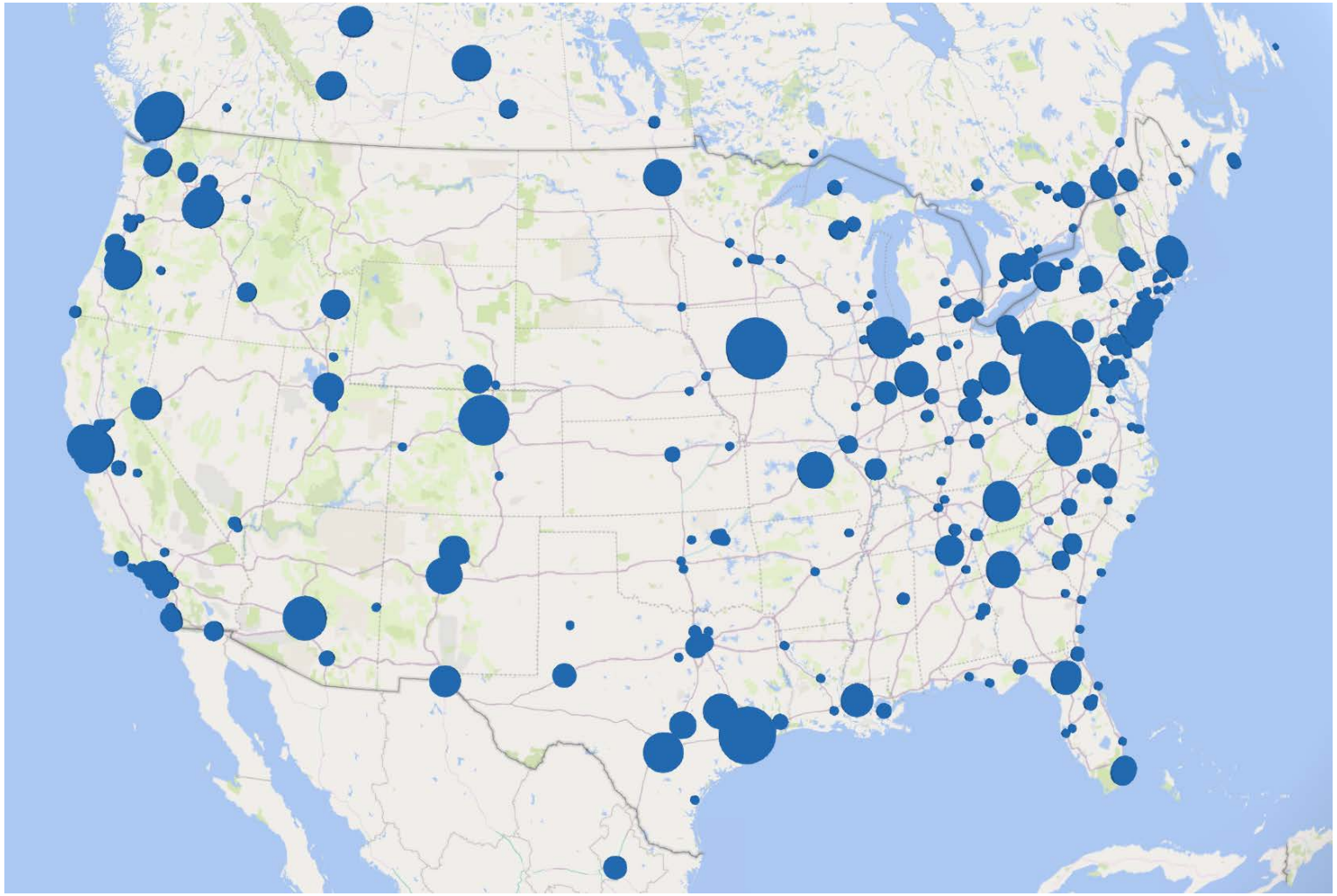
Canada : 196

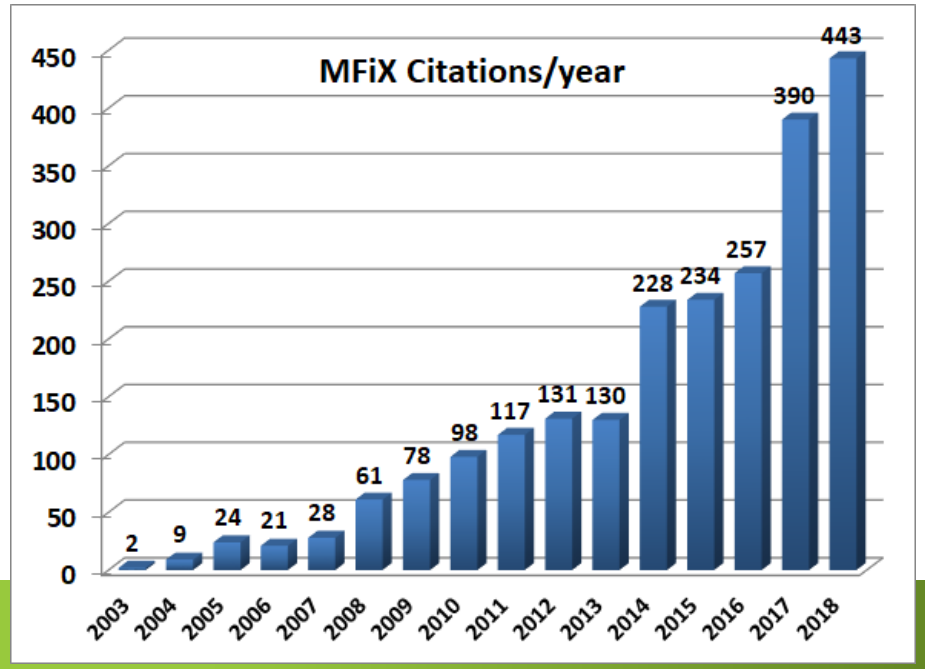




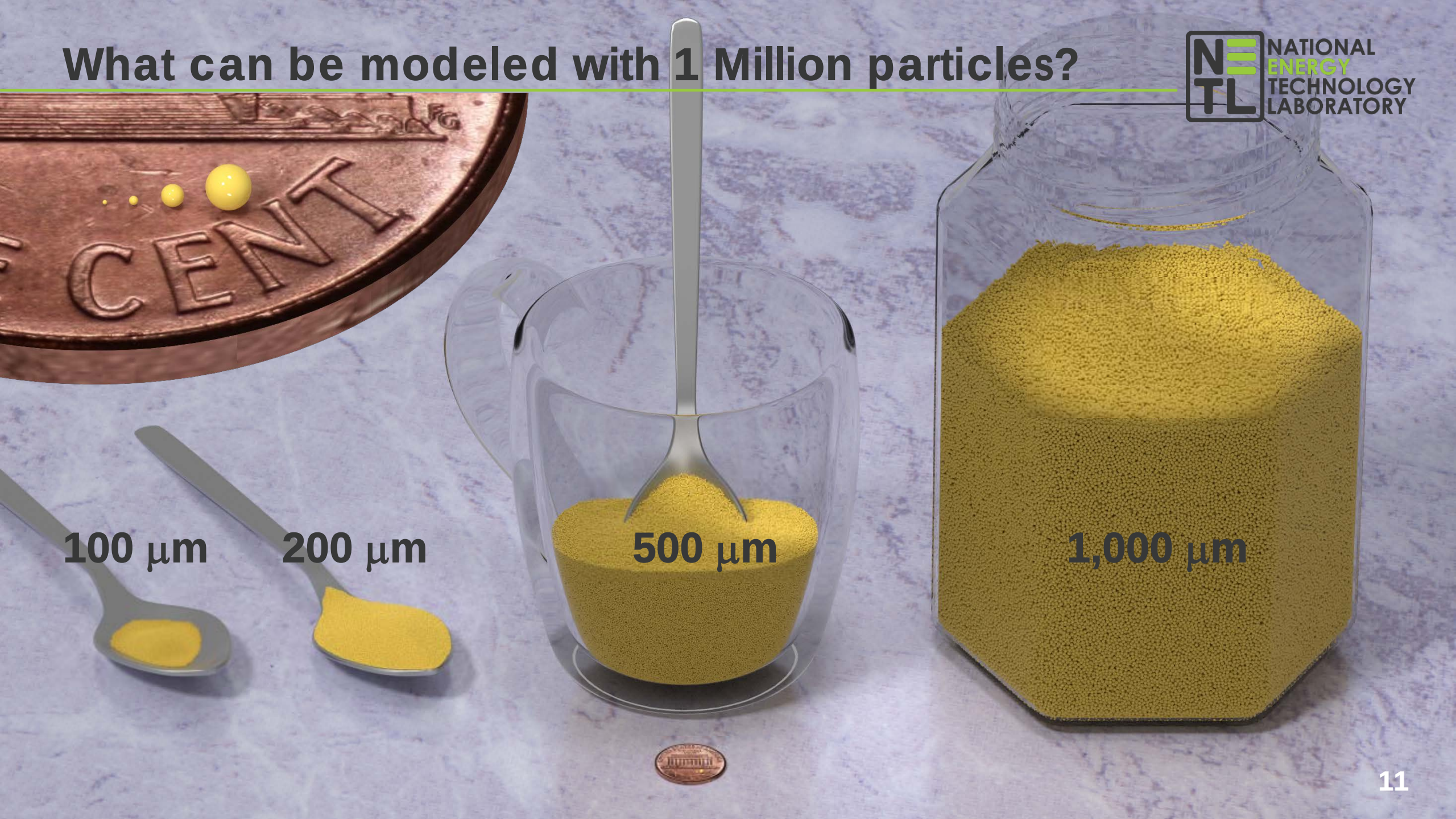
MFIX User Community Statistics

5,500+ all-time MFIX registrations





What can be modeled with 1 Million particles?



MFiX DEM

DEM example

Height = 0.68 m

Particle diameter = 800 microns

Particle count = 500,000 particles

MFiX – Moving to large scale simulations

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

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

Multiphase Particle In Cell (MP-PIC)

Use MP-PIC for computational speed and averaged accuracy

REDUCED ACCURACY

SOLIDS REPRESENTATION

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

INCREASED COMPUTATIONAL SPEED

GENERALIZED IDEA FOR PARTICLE INTERACTIONS

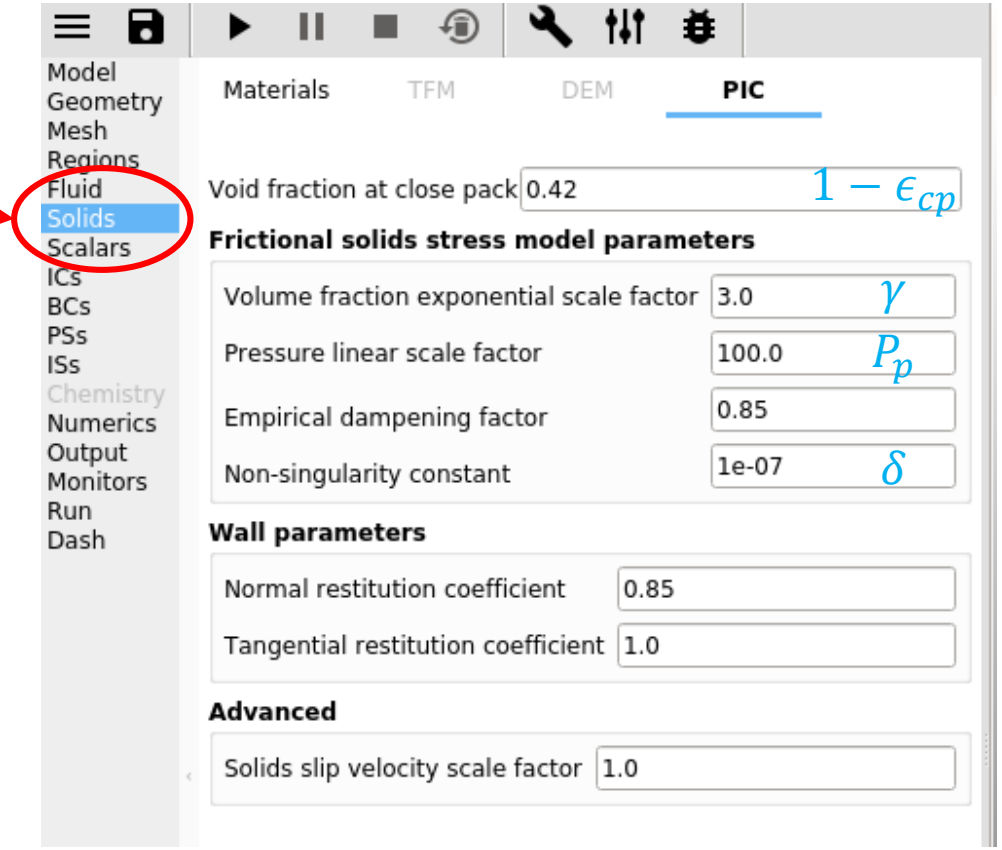
MP-PIC can significantly reduce computational effort, and in the right type of application, maintain accuracy.

Particle Flow in Cyclone

MFiX-PIC

Basic Set-Up Information

The PIC model parameters are clustered under the Solids tab.



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

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

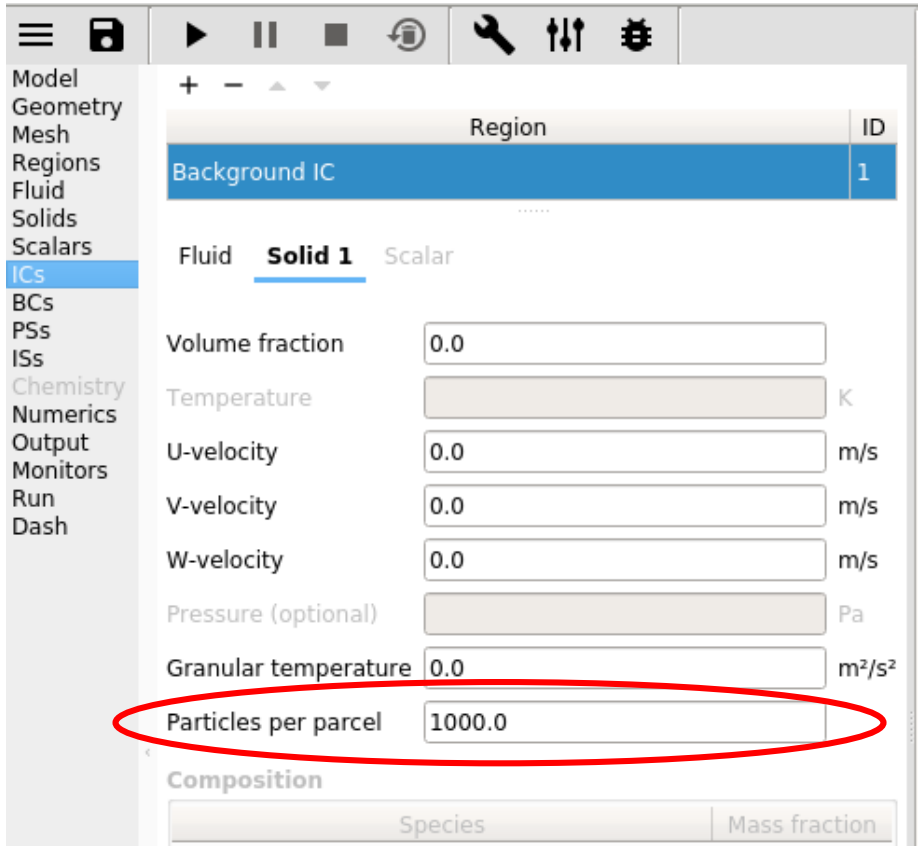
$$\frac{d\vec{V_p}}{dt} = \beta\left(\vec{U_g} - \vec{V_p}\right) - \frac{1}{\rho_p}\nabla p - \frac{1}{\epsilon_p \rho_p}\nabla \tau_p + \vec{g}$$

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

MFiX-PIC

Basic Set-Up information

Hardest thing to do in PIC is to define a reasonable value for particles per parcel.



PIC was originally designed for simulations that have so many particles that models like DEM are no longer practical.

For PIC to work at its best, you need to create a simulation where a gradient of solids fraction values drives solids motion (lots of parcels), while still progressing as quickly as possible (more coarse mesh).

So, create a balance of good enough mesh for the fluid solver, and ample parcels to form gradients of solids fraction.

MFiX-PIC

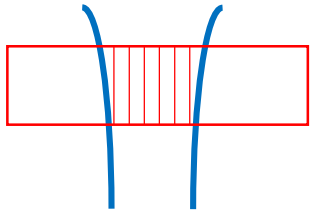
Basic Set-Up Information, Rules of thumb for mesh and particles/parcel

Create your geometry, and select a grid that will give you good fluid hydrodynamics.

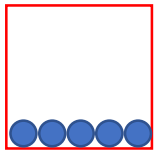
THEN:

1. Be careful to use a minimum of 3 (preferably 5) cells through constricted areas. PIC needs a minimum of 3 for interpolation methodology to work.
2. Full cells should accommodate (roughly) 3 to 5 parcel diameter widths (min).
3. Watch timing information and keep solids wall-time to (roughly) 1/10th fluid computational wall-time, or less.
4. Note that very small cut cells may be problematic if parcels are larger than available volume.

1.



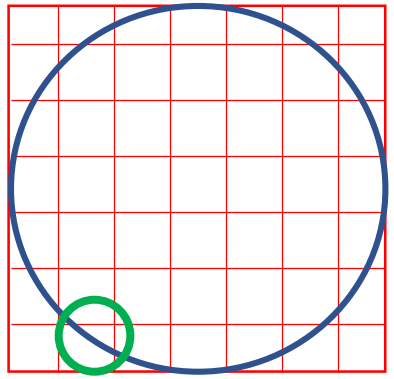
2.



Key: PIC is driven by volume fraction fields.

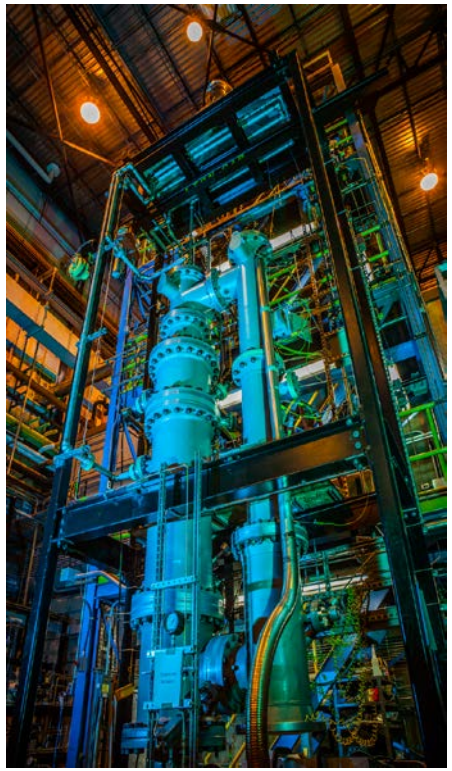
3. Timestep walltime, fluid solver: 0.812 s
PIC NITs: 1 Total PIP: 3808
Timestep walltime, PIC solver: 0.014 s

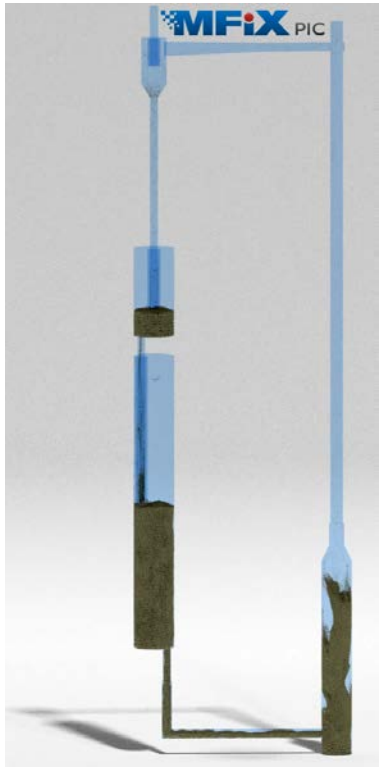
4.

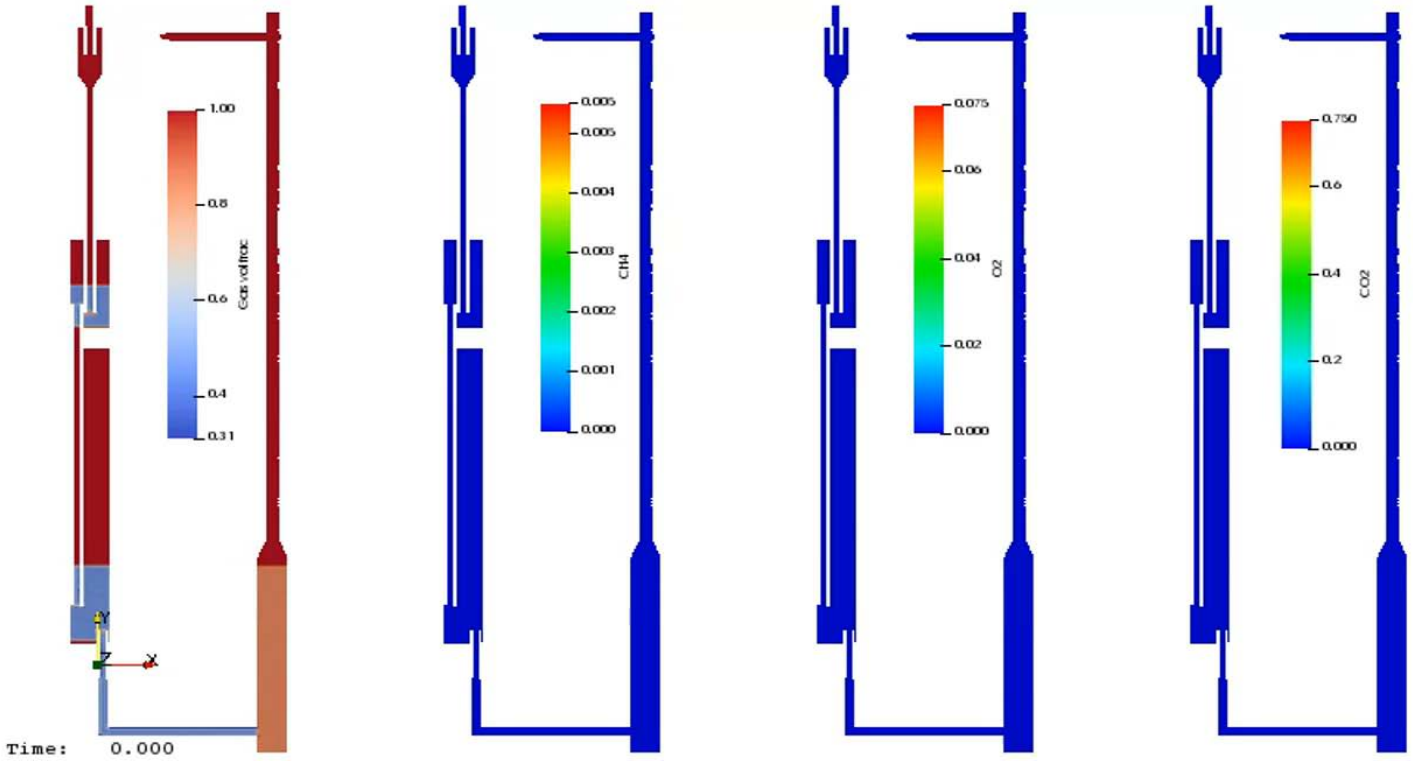


Note: PIC is only 3D.

MFiX-PIC released in MFIX 19.1







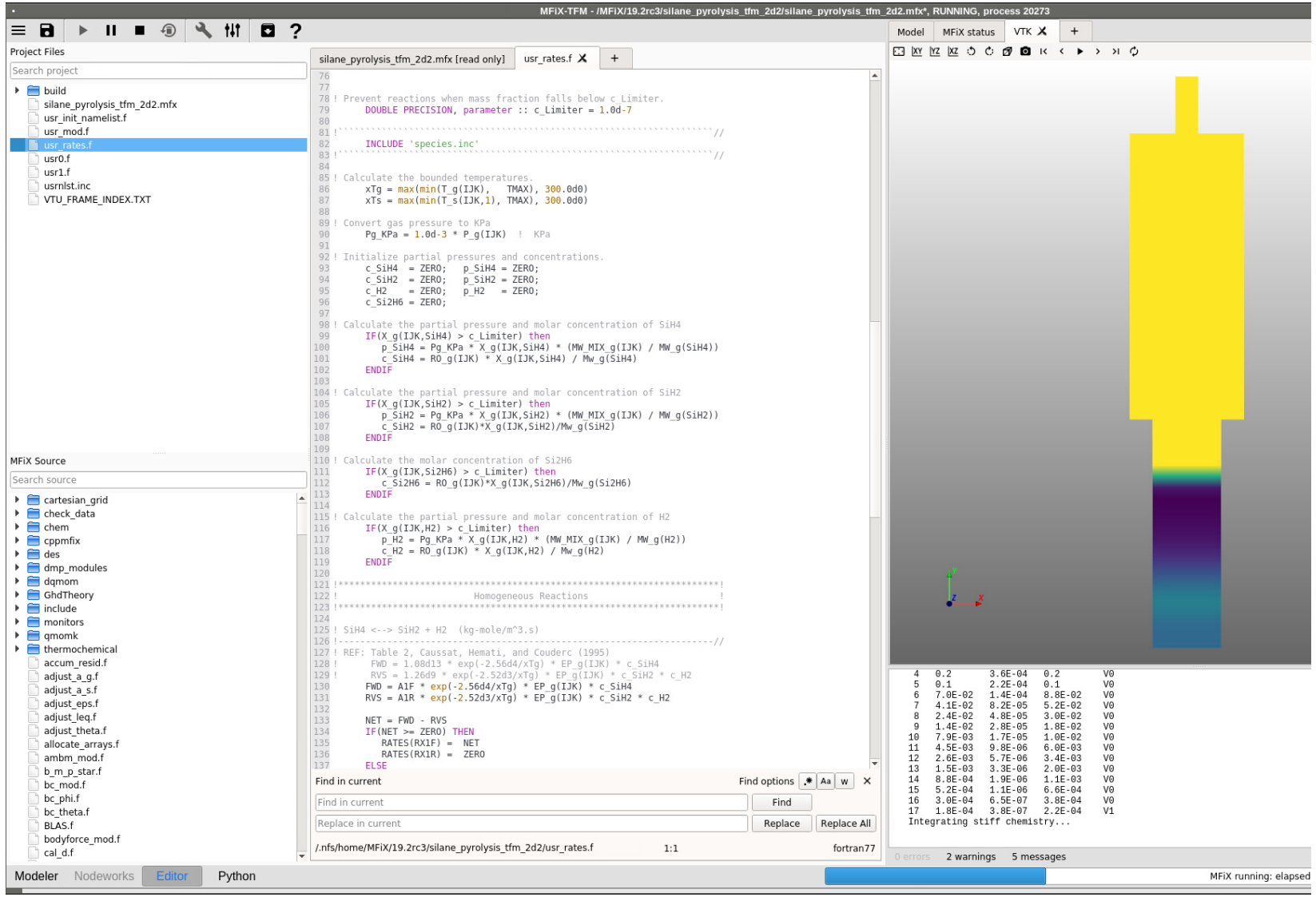
Simulation of industrial scale multi-phase flow devices is within MFiX's grasp!

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

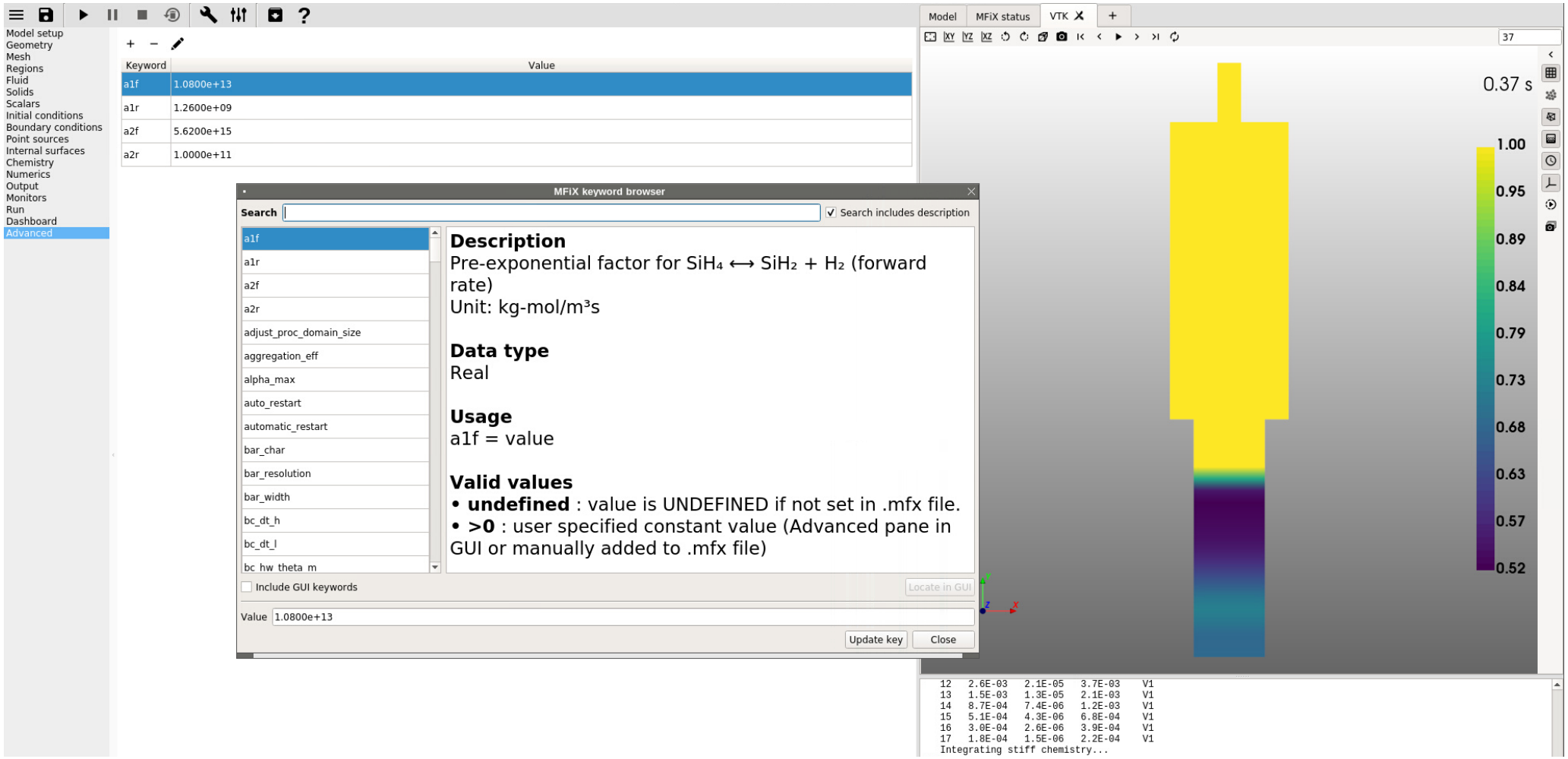
Excellent matching to pressure drop, temperature profiles and chemical species production at industrial scale.

Tractable time to solution.

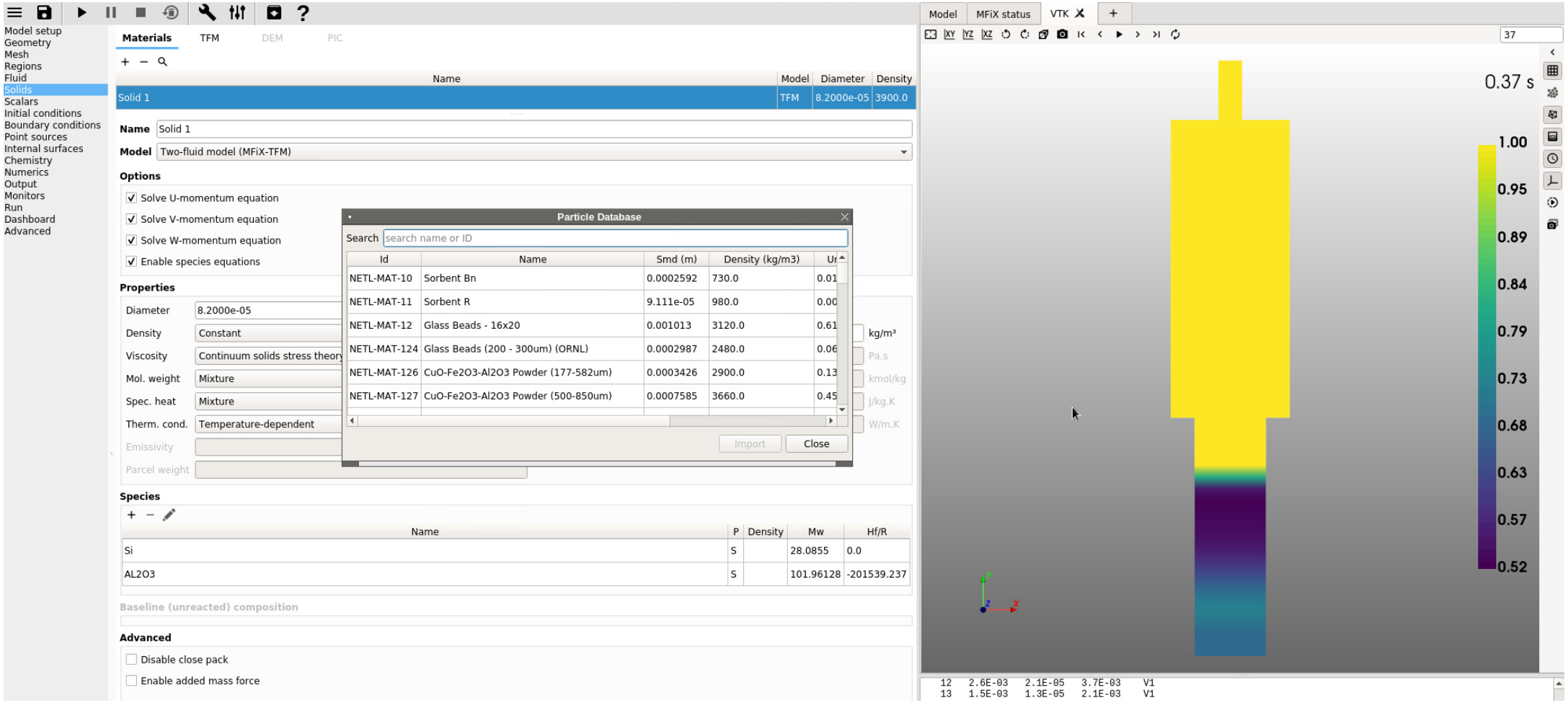
MFiX GUI 19.2 – Text editor



MFiX GUI 19.2 – Advanced pane

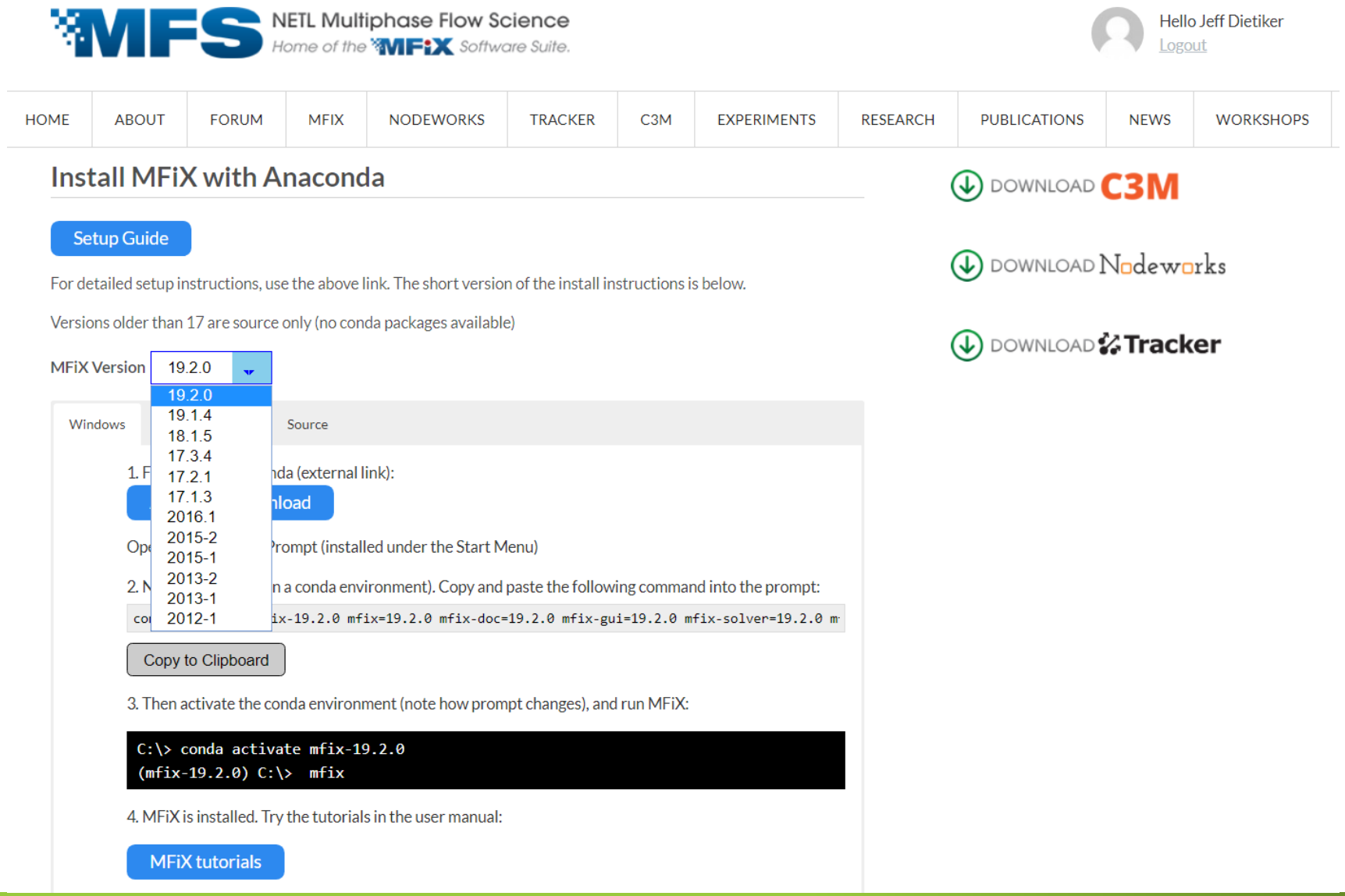


MFiX GUI 19.2 – Material Database



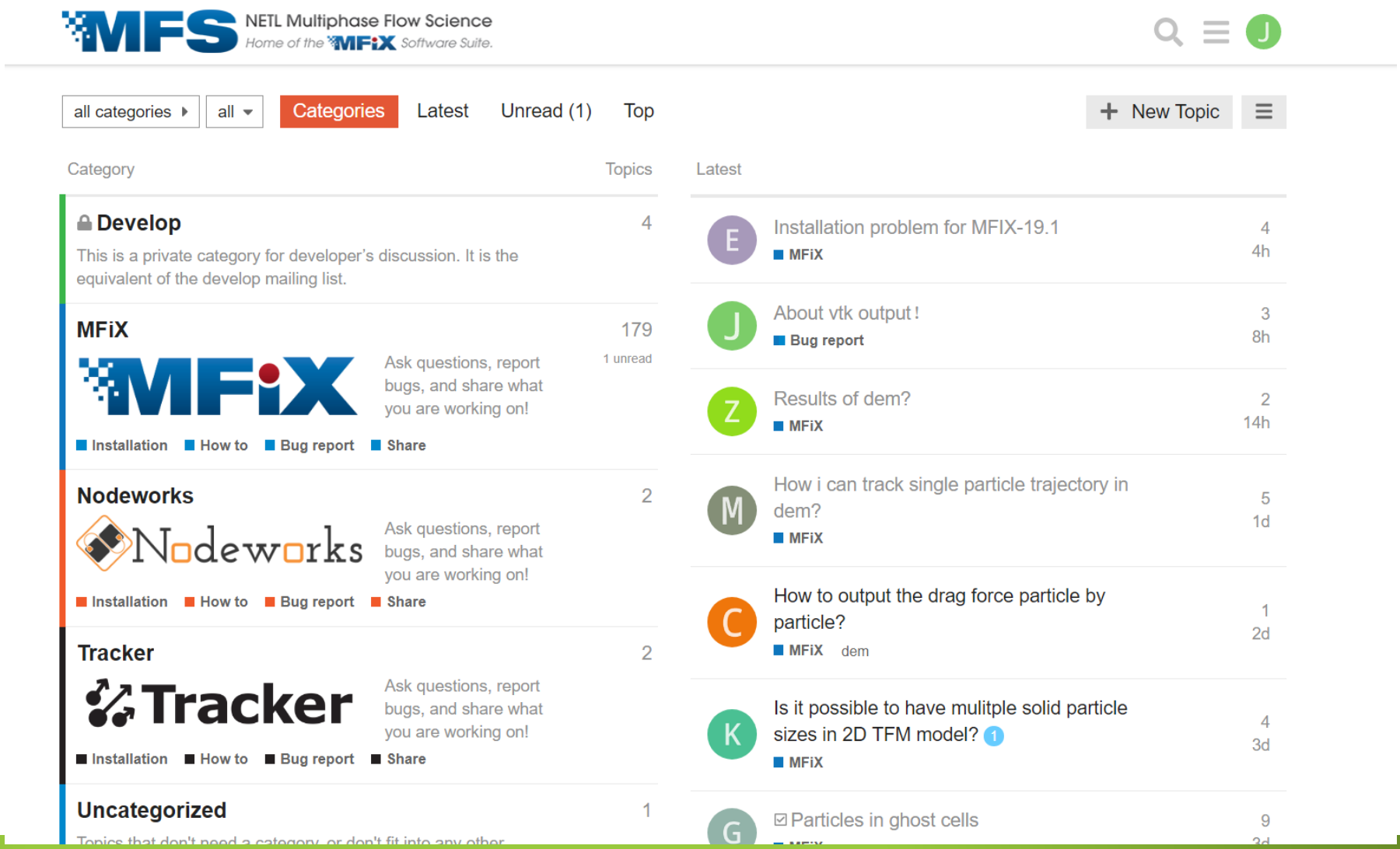
MFiX Website – New download page

- Simpler installation
- Access to all MFiX versions
- GUI and source tarballs

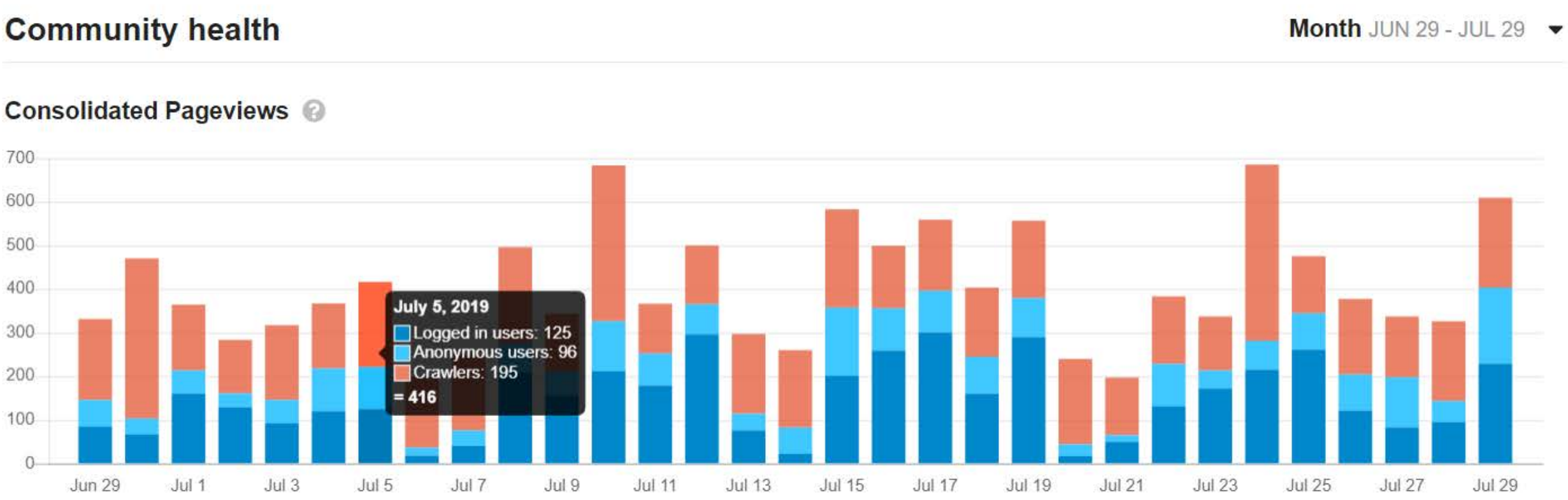


MFiX Website –Forum

- User support
- Categories, topics
- File attachment
- Searchable

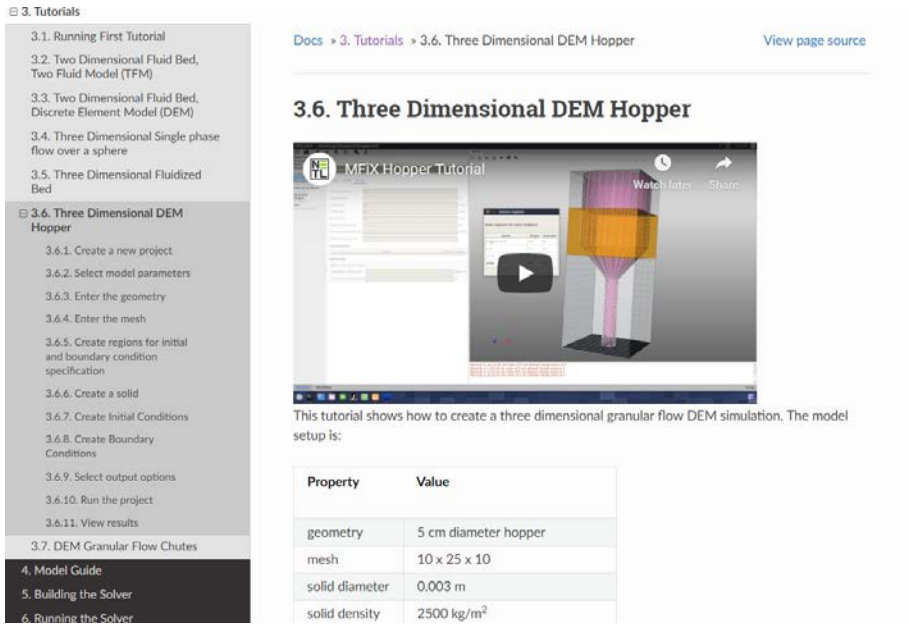


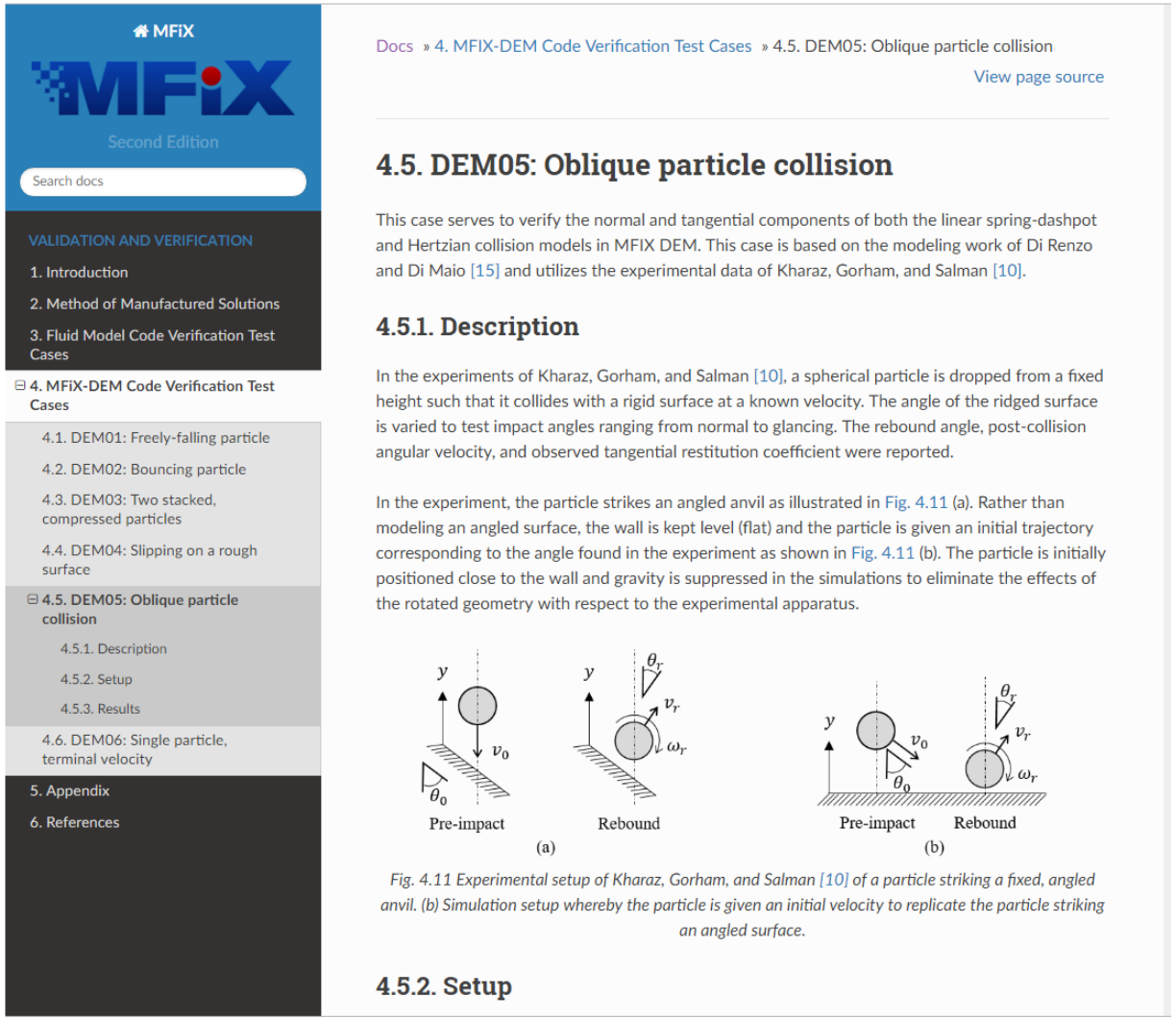
MFiX website – Forum



MFiX website – Online documentation

- User manual
- V&V manual
- Html and pdf
- Text and video tutorials

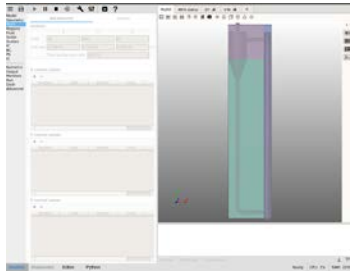




MFiX – Future development

Current Workflow

GUI



.mfx

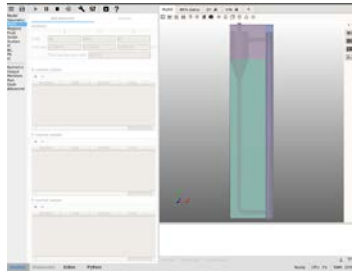
MFiX solver

mesh

results

Future workflow

GUI



mesh

.mfx

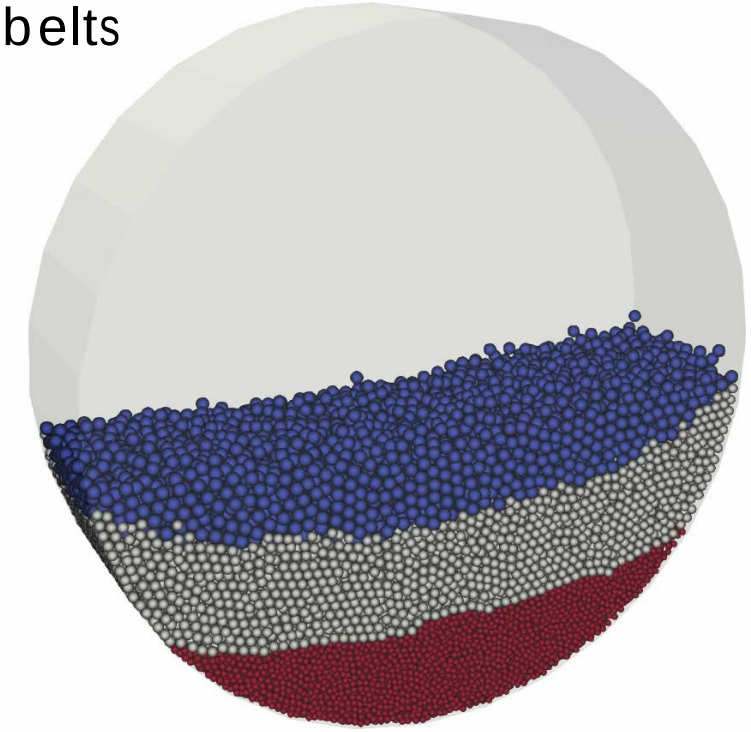
MFiX solver

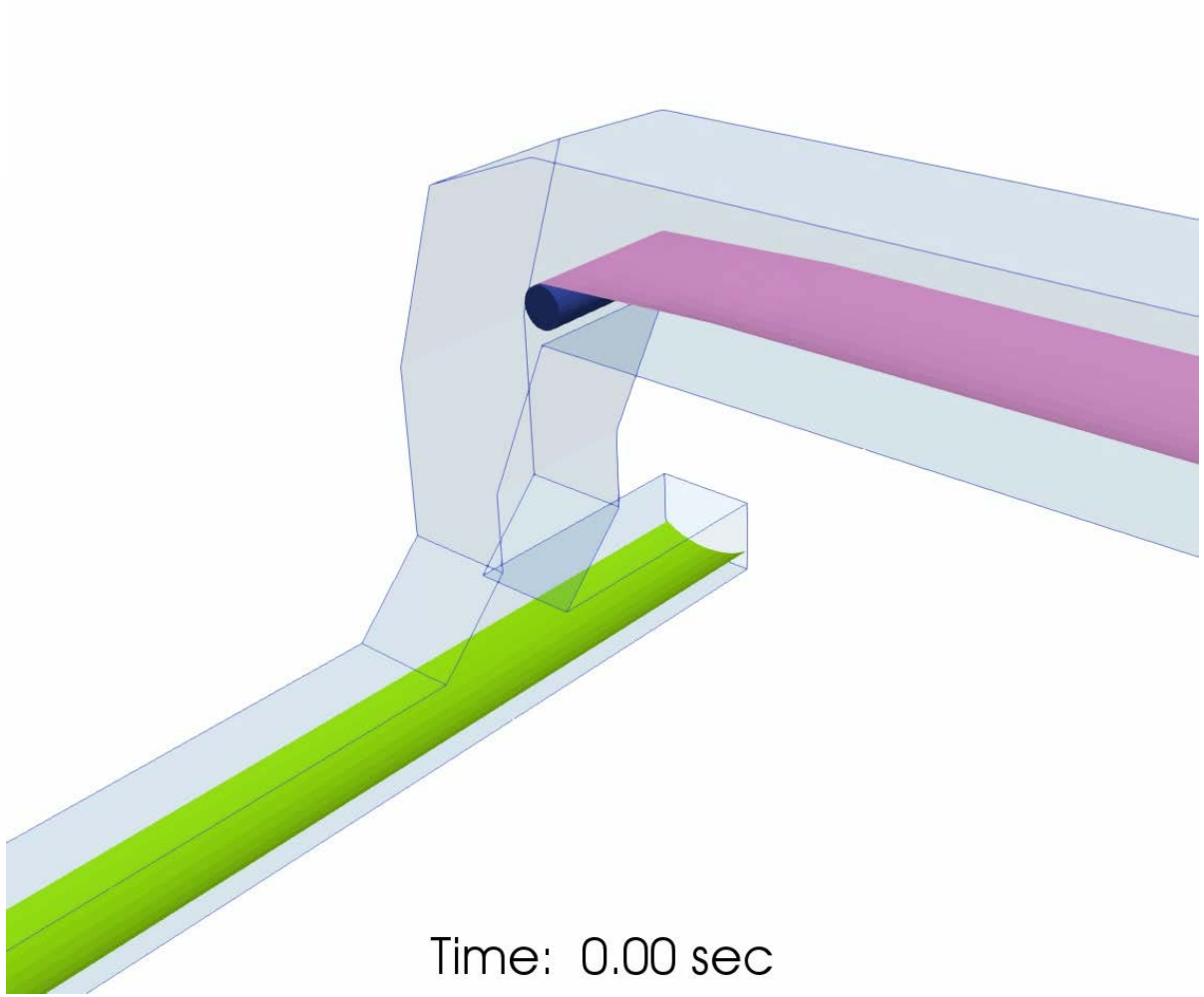
results

MFiX – Future development: Moving walls

Moving STL walls through tangential velocity

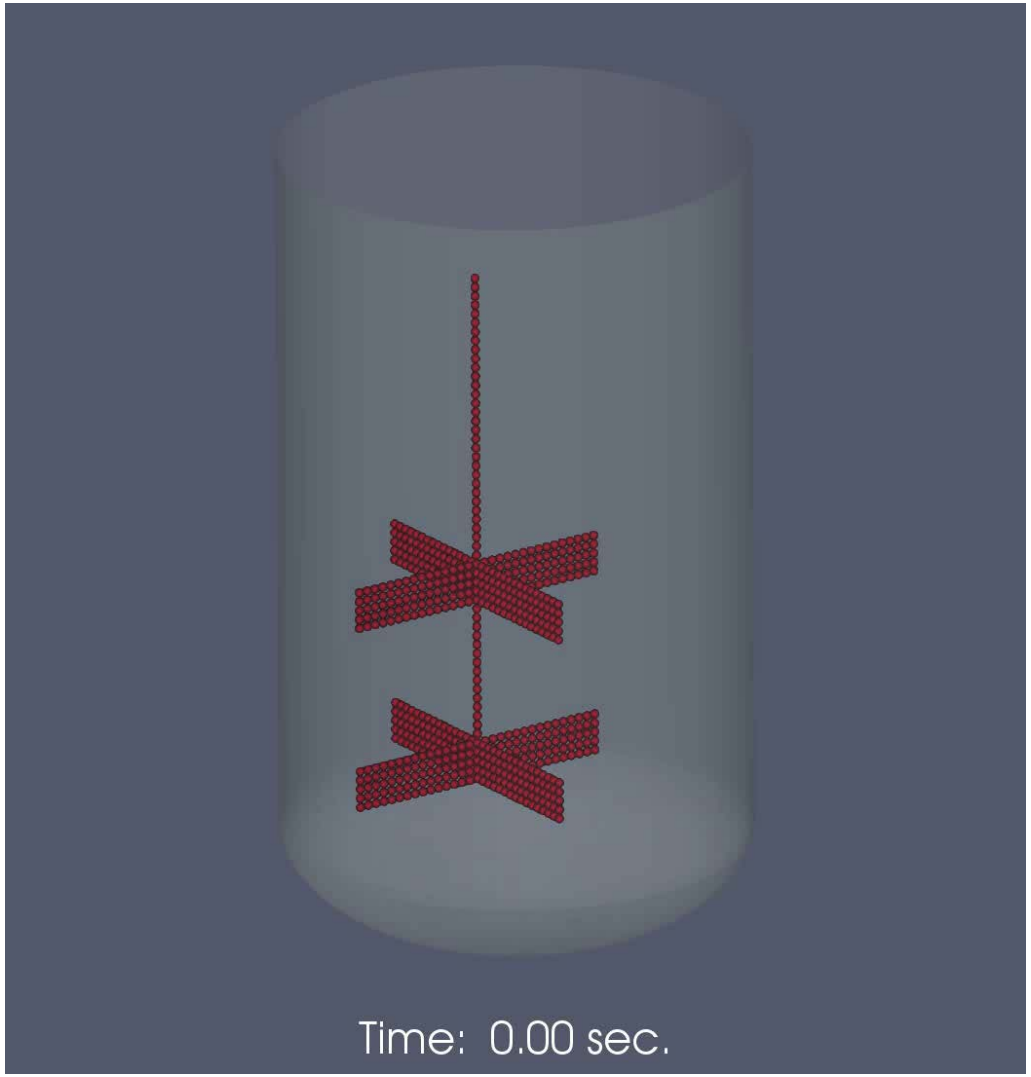
- Add Collection of UDFs and tutorials
- Rotating drum
- Conveyor belts





MFiX – Future development: Moving walls

Freeze or set particle velocity



MFiX – Future development: Non-spherical particles

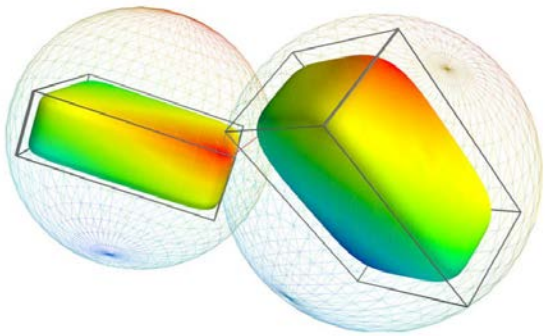
- Superquadrics are a family of geometric shapes defined as

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

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

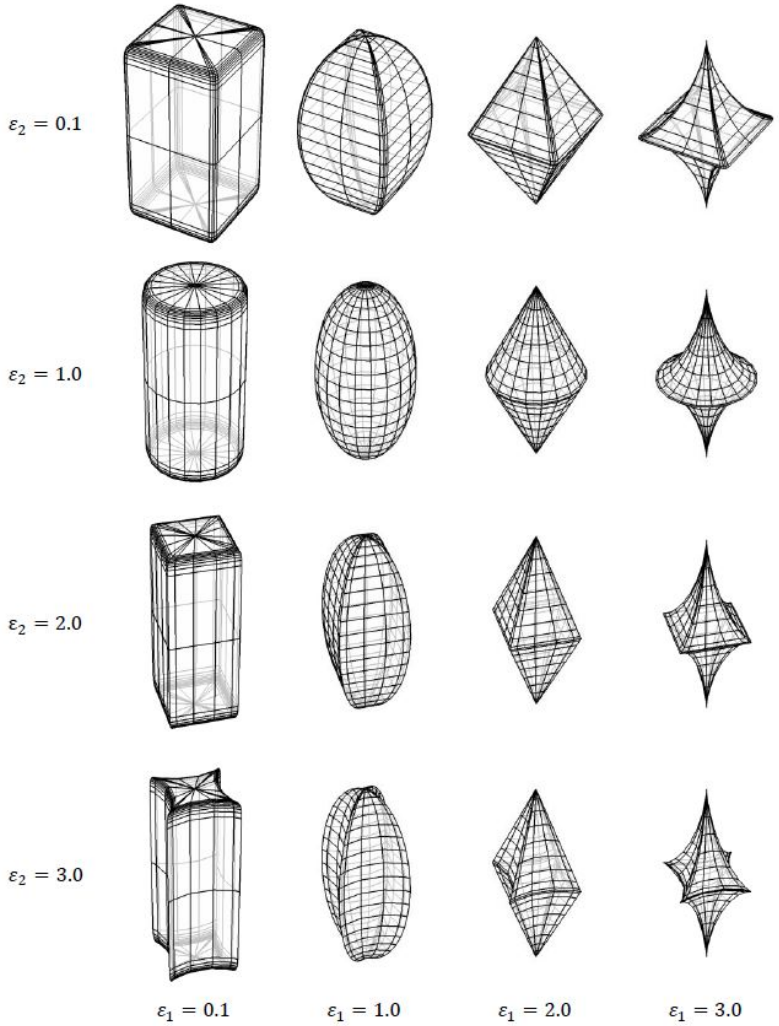
$$[a_1, a_2, a_3, \varepsilon_1, \varepsilon_2]^T$$

Semi-axis roundness parameters



Bounding spheres and oriented bounding boxes

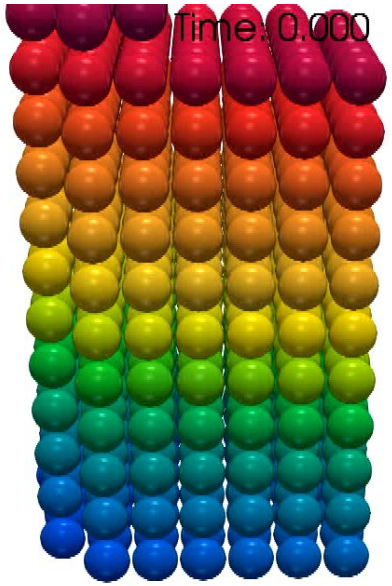
Superquadric particles

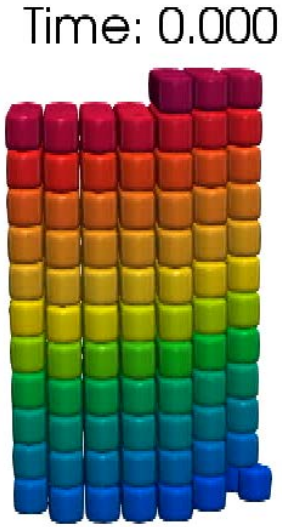


a1=2
a2=2
a3=4

MFiX – Future development: Non-spherical particles

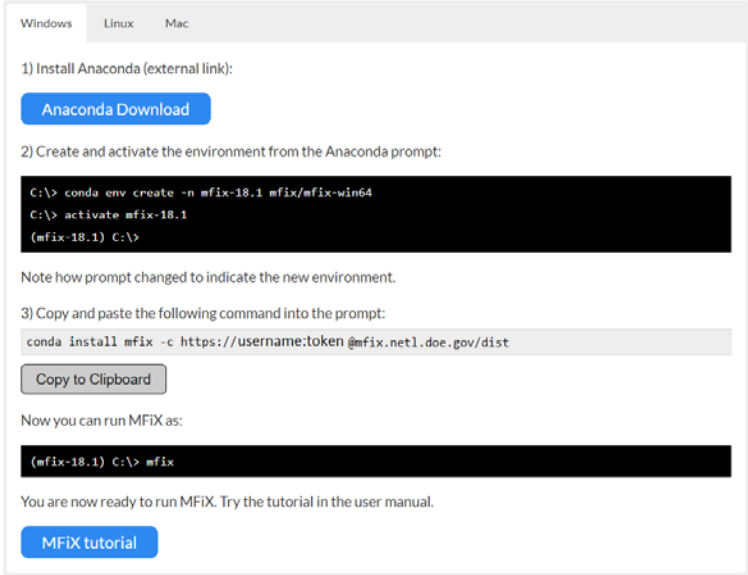
Proof of concept:**“M&M’s”, cylinders, cubes**





MFiX – How to get started

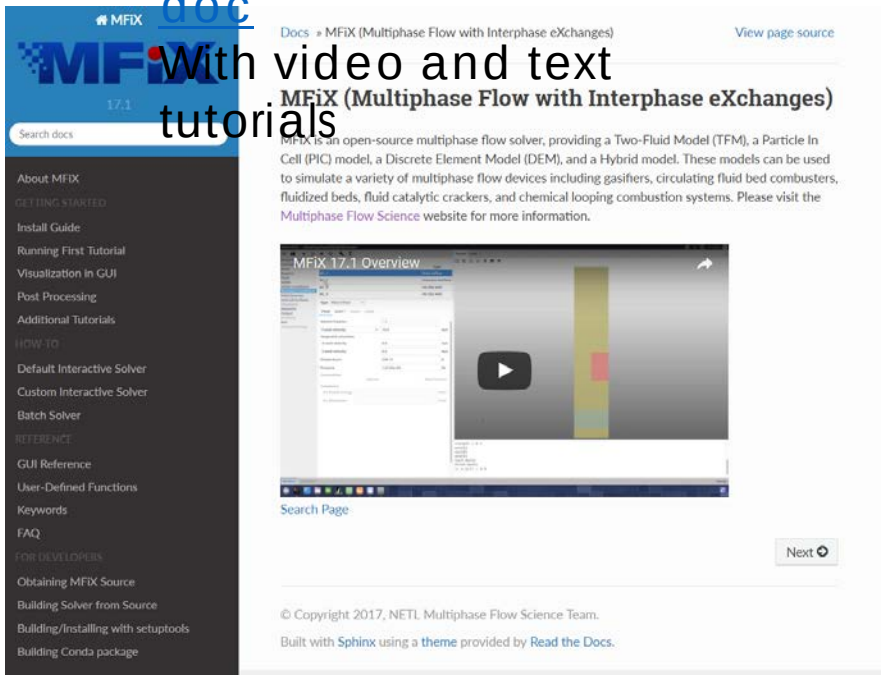
1. Register at https://mfix.netl.doe.gov (skip if MFiX member)
2. Install Anaconda on your platform (one-time installation)
3. Set and activate conda environment



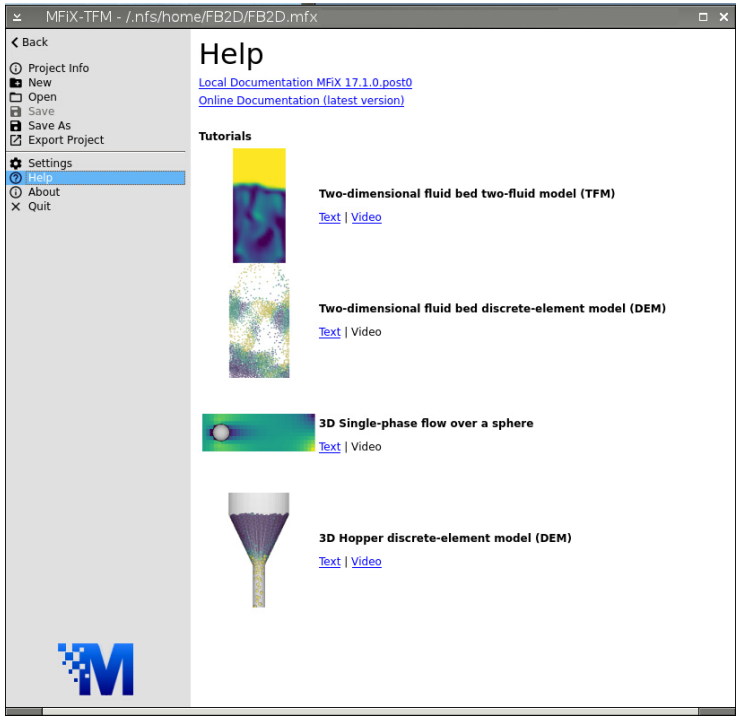
Online documentation:

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

- With video and text tutorials

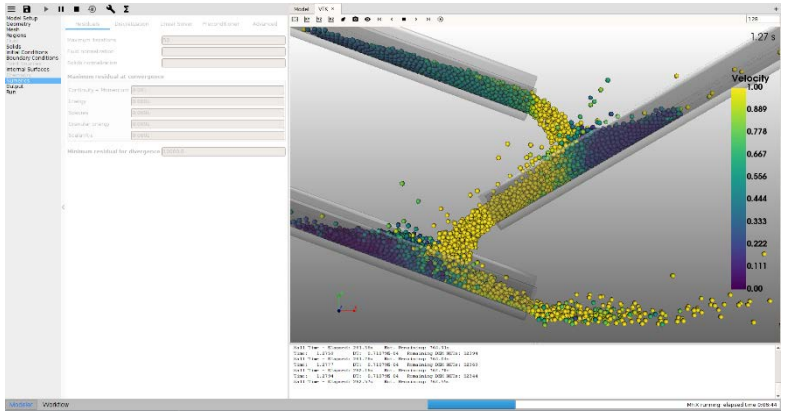


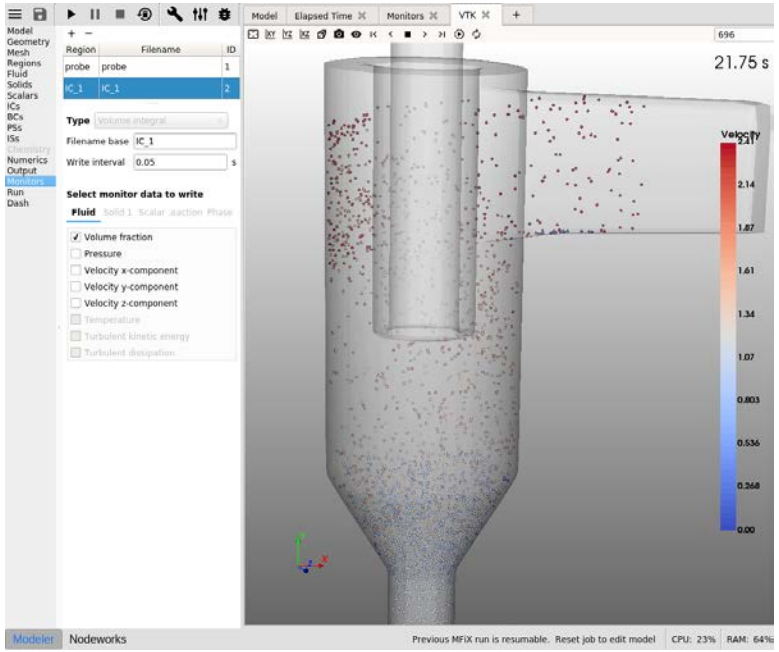
Access documentation from GUI

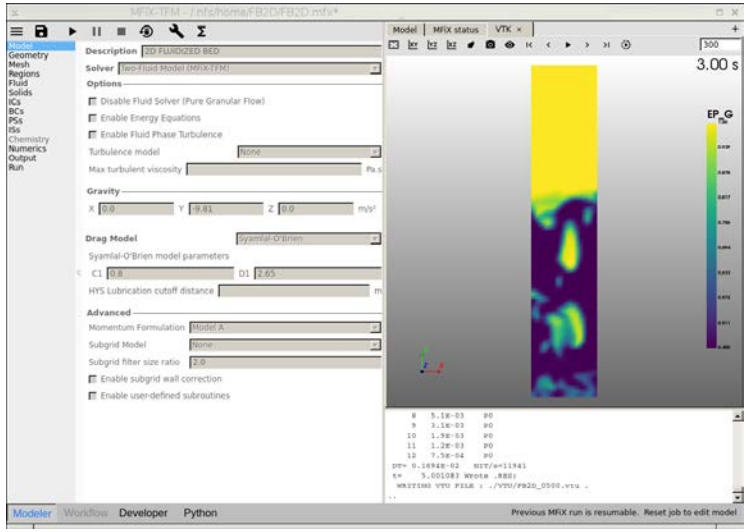


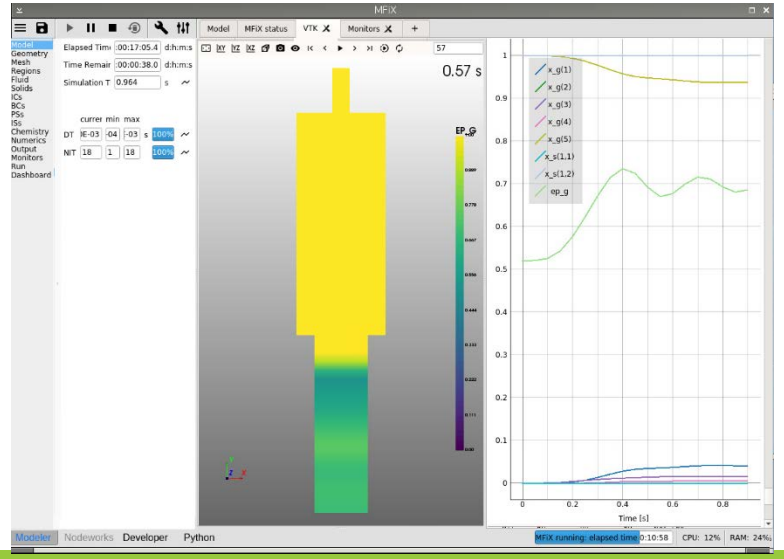
Happy Modeling with MFiX 19.2 !

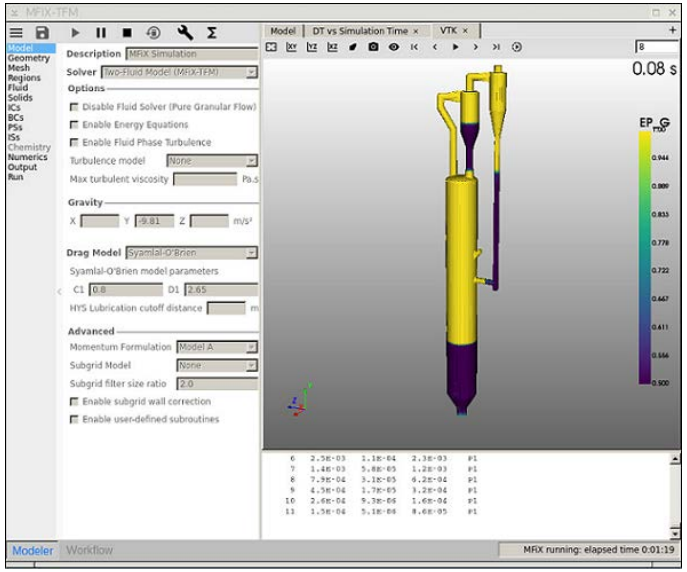
MFiX gallery

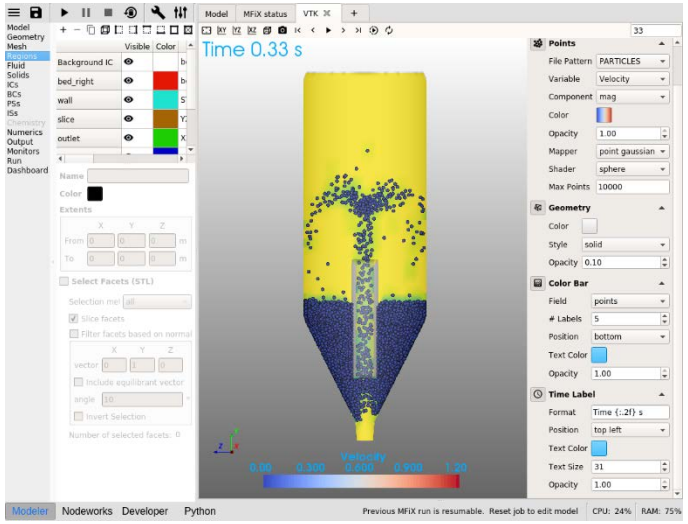












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