Development Update: What's New and What's Coming

James Parker

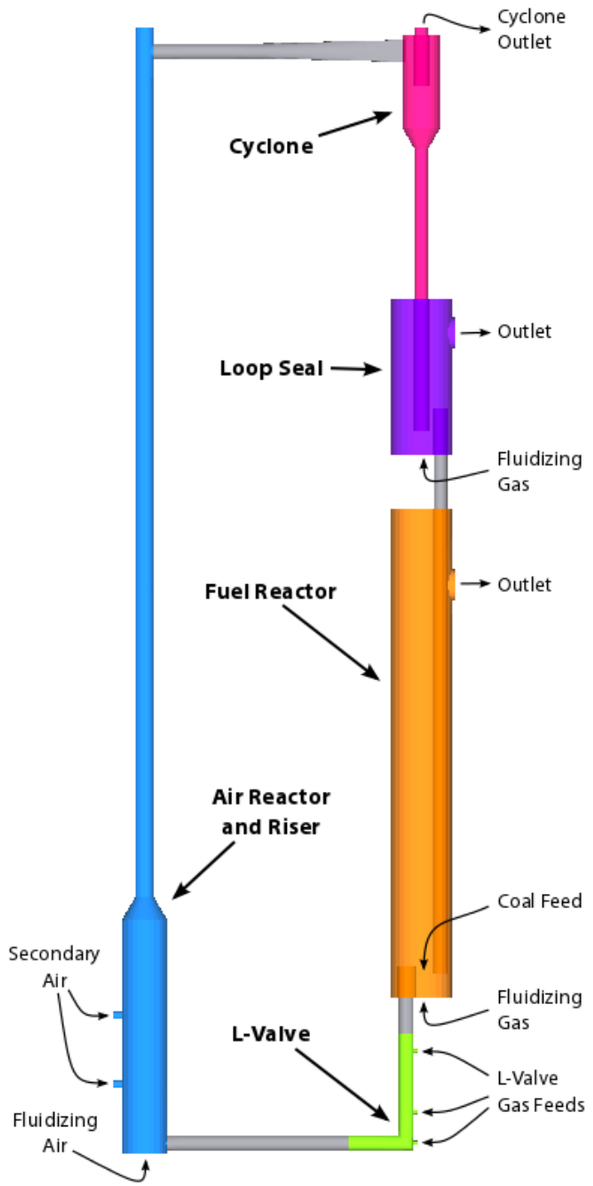
Barracuda Virtual Reactor Users Conference

June 27 – 28, 2019

Chemical Looping Reactor (CLR) Model

- Work performed with NETL in 2011-2012
- Full loop consisting of *reactor/riser, cyclone, loop seal, fuel reactor, L-valve*
- Ilmenite carrier
- Methane and coal as fuel source
- Reaction chemistry
  - Oxidation/reduction of ilmenite
  - Coal chemistry: drying, devolatilization, oxidation, water-gas shift, gasification

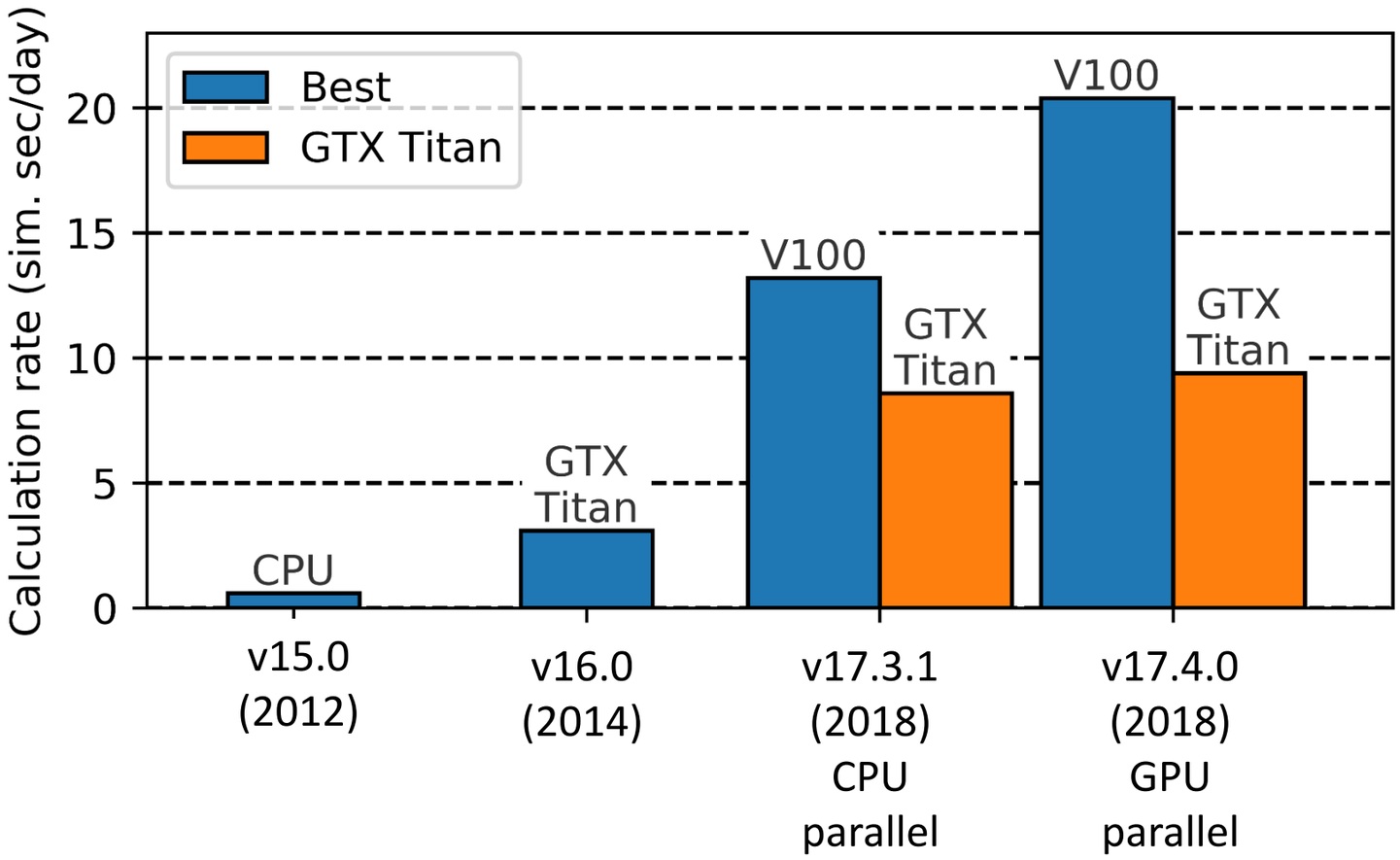
Parker, J. (2014) Powder Technology 265, 47-53



CLR model schematic

Improvements in calculation rate over time

- In 2012 (v15.0, CPU), **82 days**
- In 2014 (v16.0, GPU), **16 days**
- In 2018 (v17.3.1), less than **4 days** required with V100 card (13.2 sec/day)
- With 17.4.0, less than **2.5 days** (20.4 sec/day)



Development Goal

<u>Increase the value of a simulation solution and reduce the time and effort required to obtain that solution</u>

- Reduce user time and effort to set up, modify, and analyze a simulation: *physical models, UI features*
- Reducing total computer time to achieve a result: *GPU parallelization, license flexibility, number of simulations in project*
- Maintaining version-to-version consistency

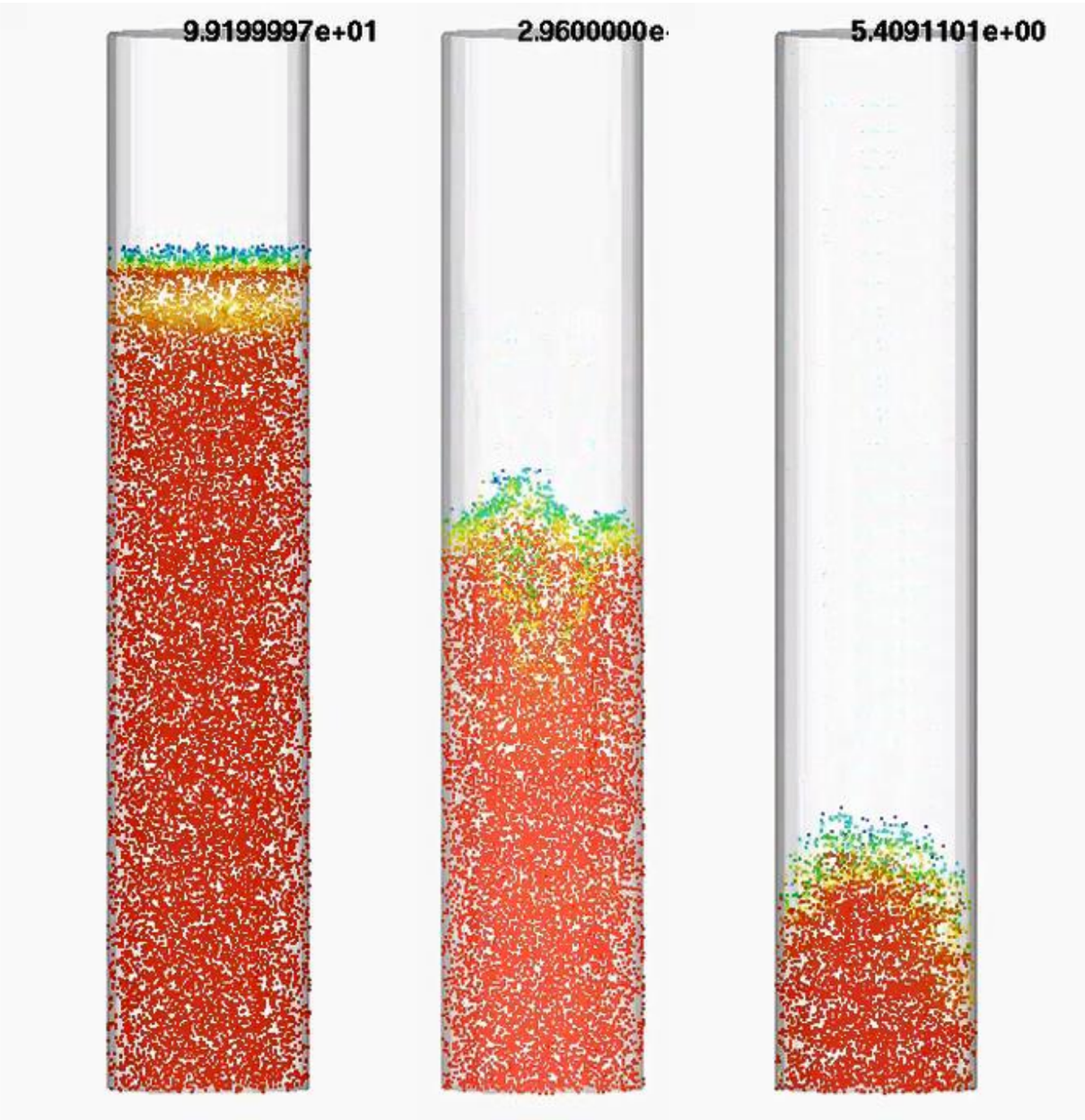
Development process for maintaining quality

1. Design / development / review of new features. Creation of new tests
2. Assembly of new features and fixes into version of Barracuda – some as beta features
3. Development testing
4. Internal use of software on projects and validation
5. Sharing as “preview” with interested users and distributors
6. Final release to users

What has been released?

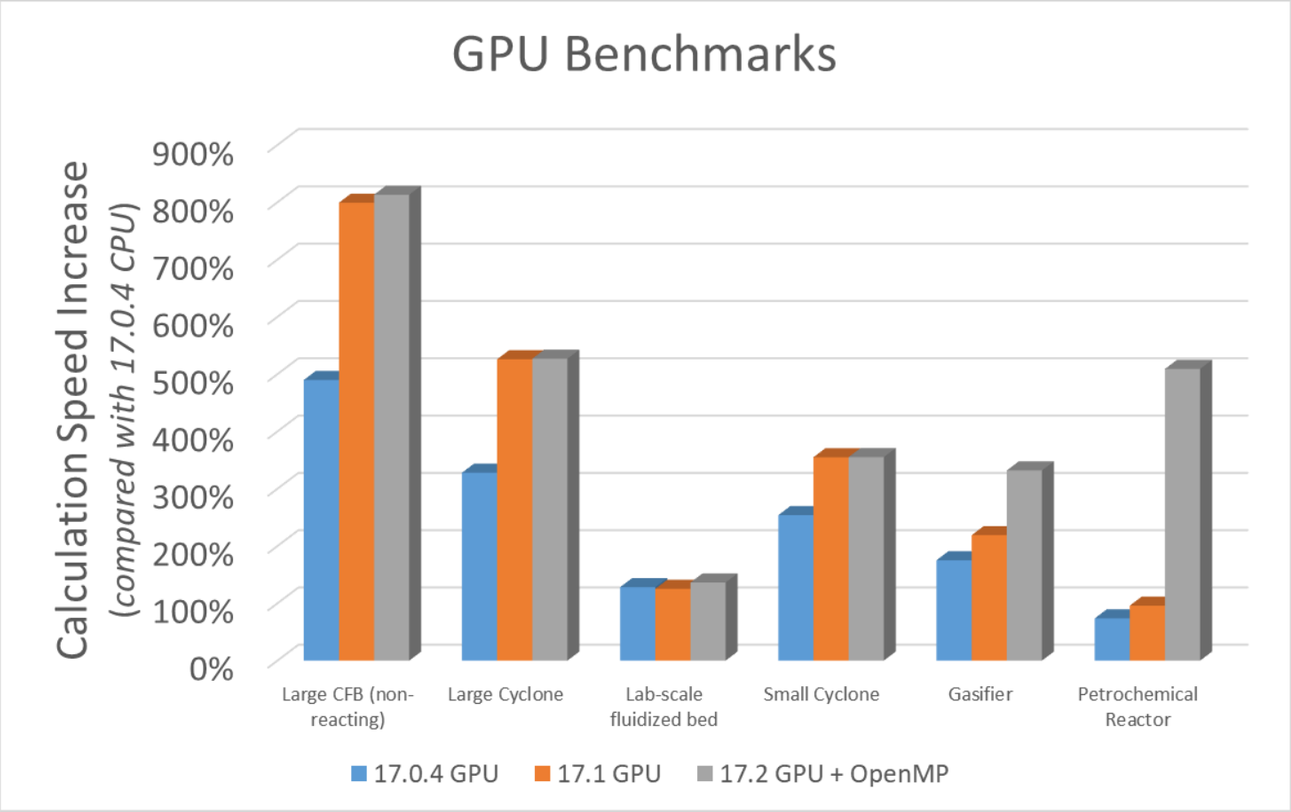
Version 17.1 *(Dec 2016)*

- Particle exit boundary
- Adjustable particle feed rates at boundaries
- GPU parallelization of fluid solvers
- Direct links between GUI and user manual



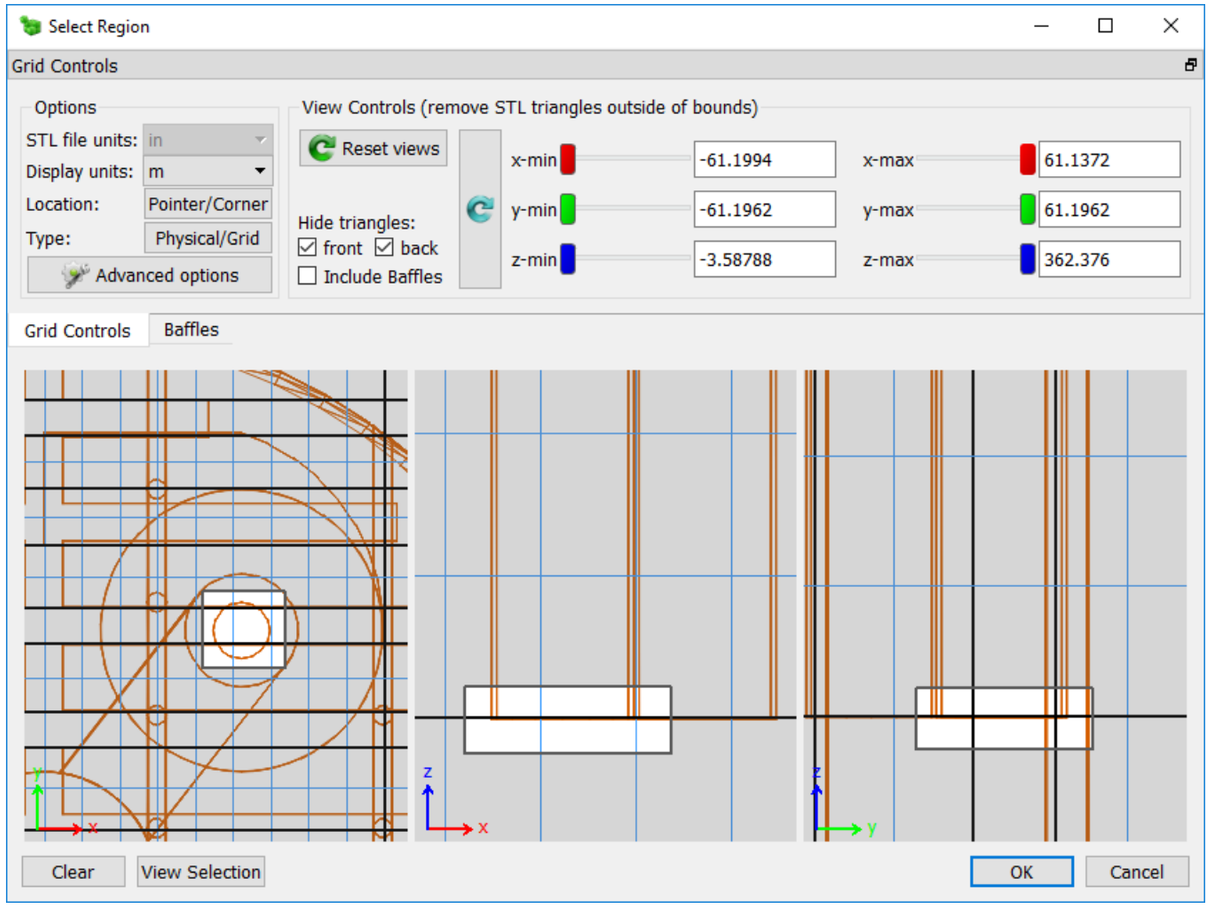
Version 17.2 *(June 2017)*

- Chemistry parallelization on CPU
- Heating / cooling loads on BC connectors
- Particle filters on BC connectors
- Secondary BC connector exits
- Particle feed algorithm improvements
- Additional 3D output variables
- License usage tracking



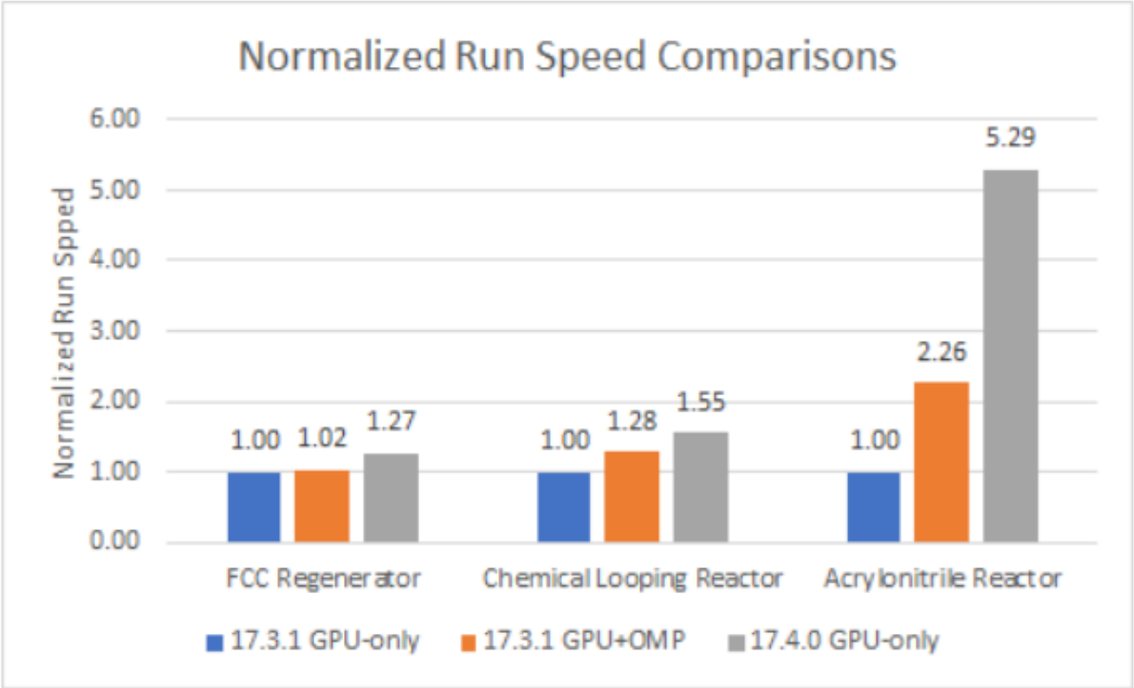
Version 17.3 *(March 2018)*

- Graphically select BCs and ICs in physical coordinates (grid independent)
- Initialize new simulations from the IC file of a previous simulation
- Specify particle initial conditions by mass
- Material property bounds and look up table
- Particle feed warnings

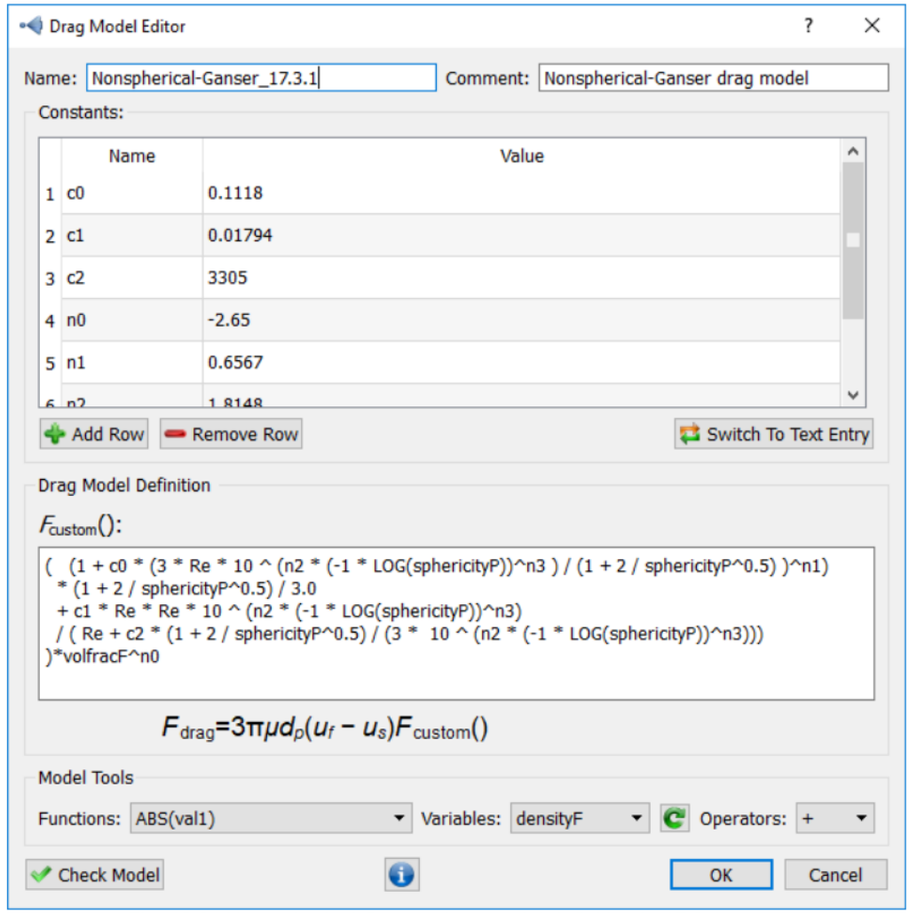


Version 17.4 *(March 2019)*

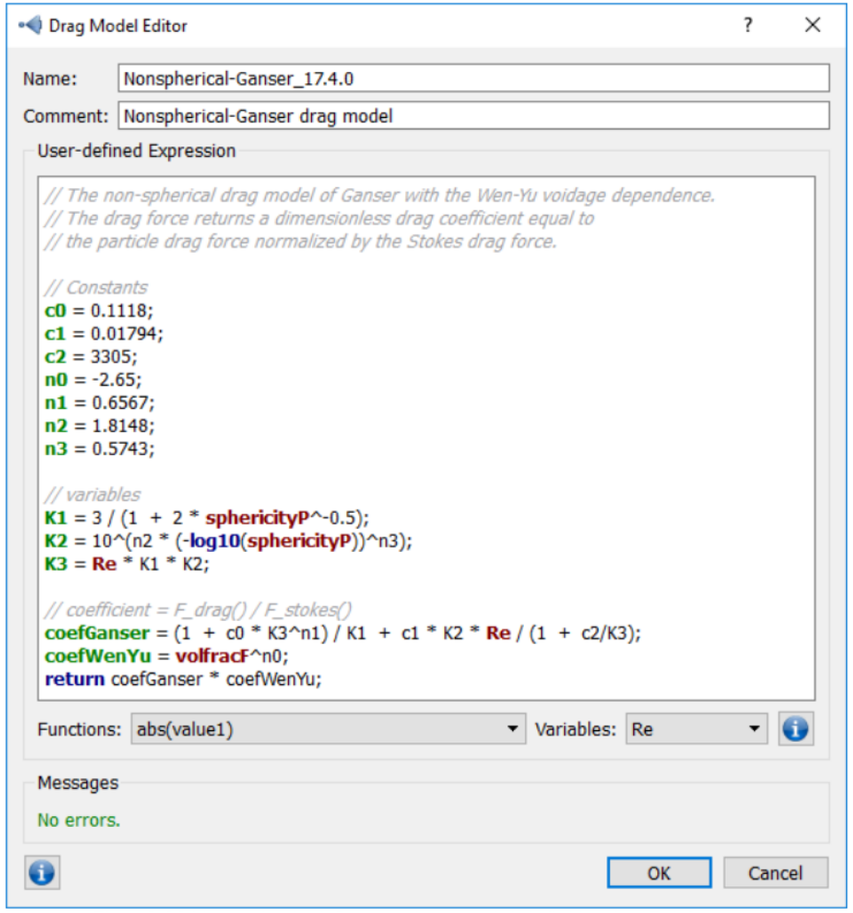
- GPU Parallelization of Volume Average Chemistry
- User-defined drag model improvements
- User-defined chemical rate coefficients - new variables



17.4 – Updated Parser & Rate Expressions

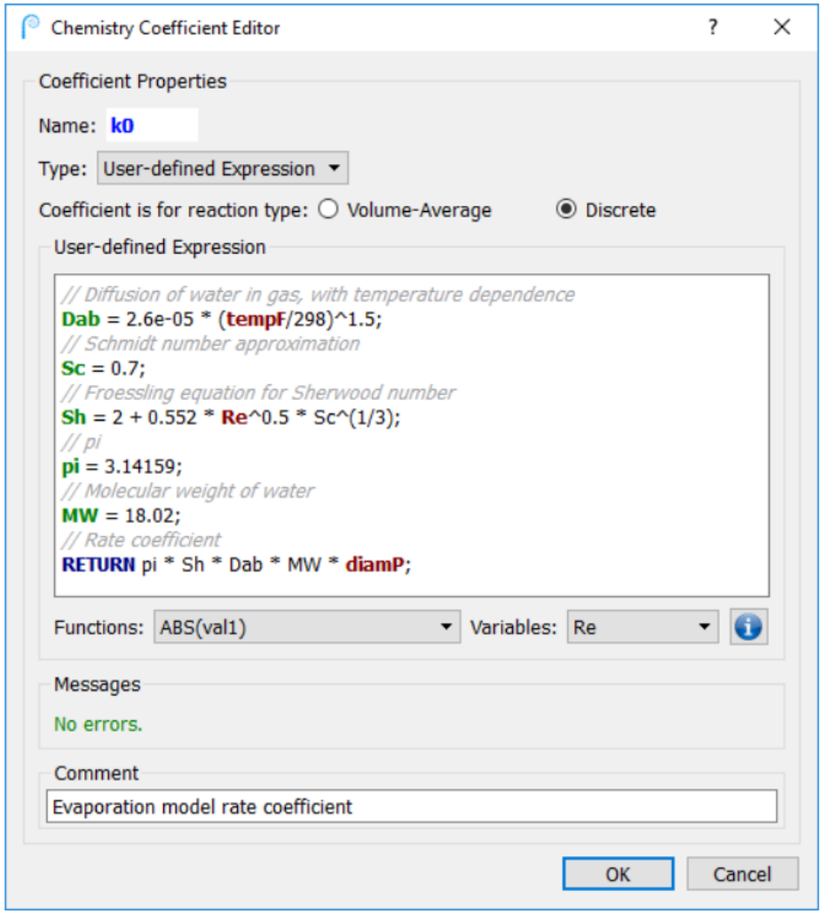


Old Drag Parser



New Drag Parser

17.4 – Updated Parser & Rate Expressions



User-Defined Chemistry Coefficients

New Variables

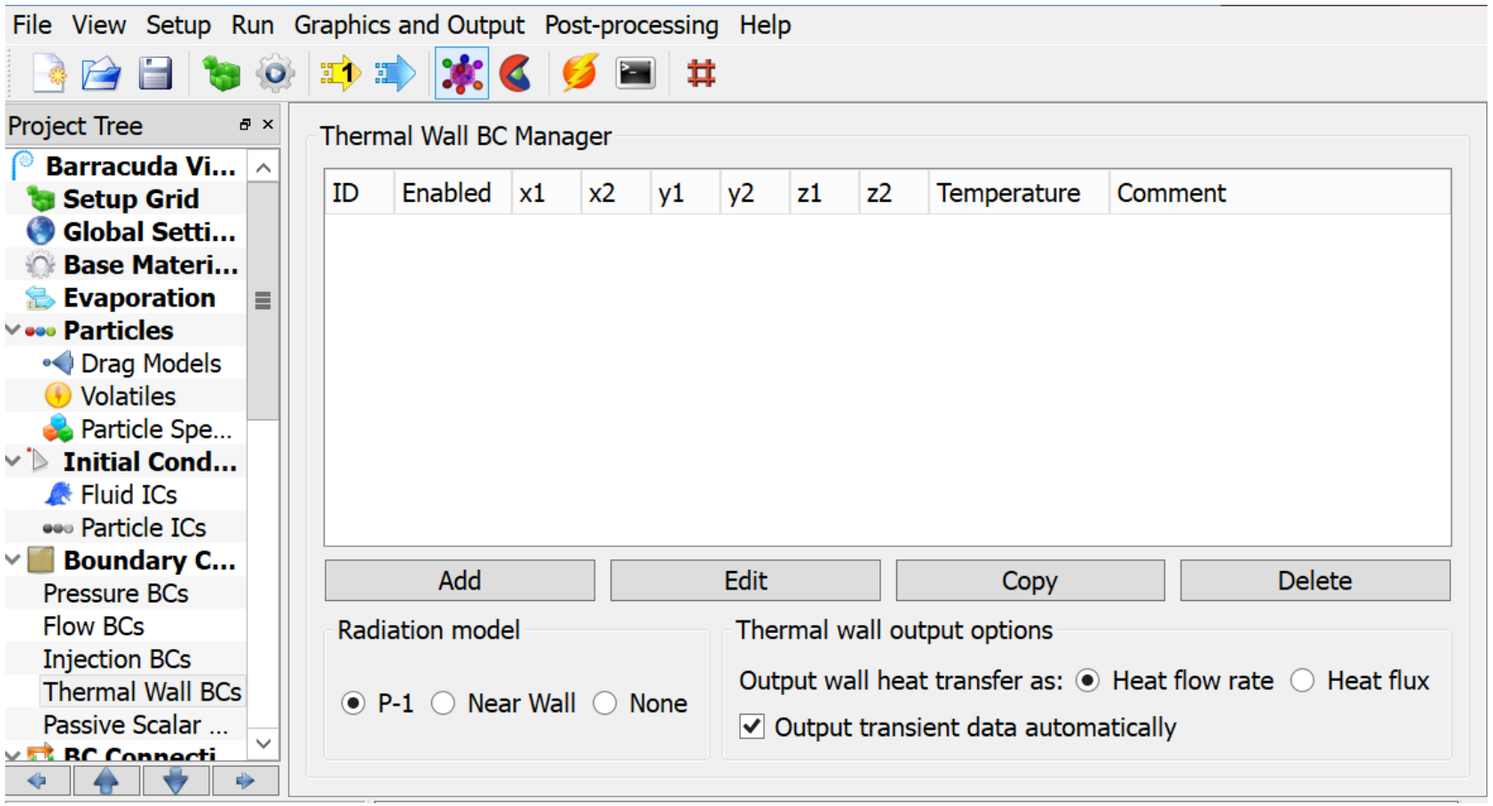
- `Re` - Reynolds number
- `thetaCP` - close-pack particle volume fraction
- `diamSauterP` - Sauter mean diameter within a computational cell in units of microns
- `sphericityP` - particle sphericity
- `viscF` - fluid viscosity in units of $\mathrm{Pa} \cdot \mathrm{s}$
- `dVelPF` - the difference between particle velocity and fluid velocity in units of $\mathrm{m/s}$
- `residenceTime` - the residence time of a particle in units of s
- `time` - simulation time in units of s
- `X` - x-position in the domain in units of m
- `Y` - y-position in the domain in units of m
- `Z` - z-position in the domain in units of m

What are we working on now?

What are we working on now?

Expanding applications and physical modeling

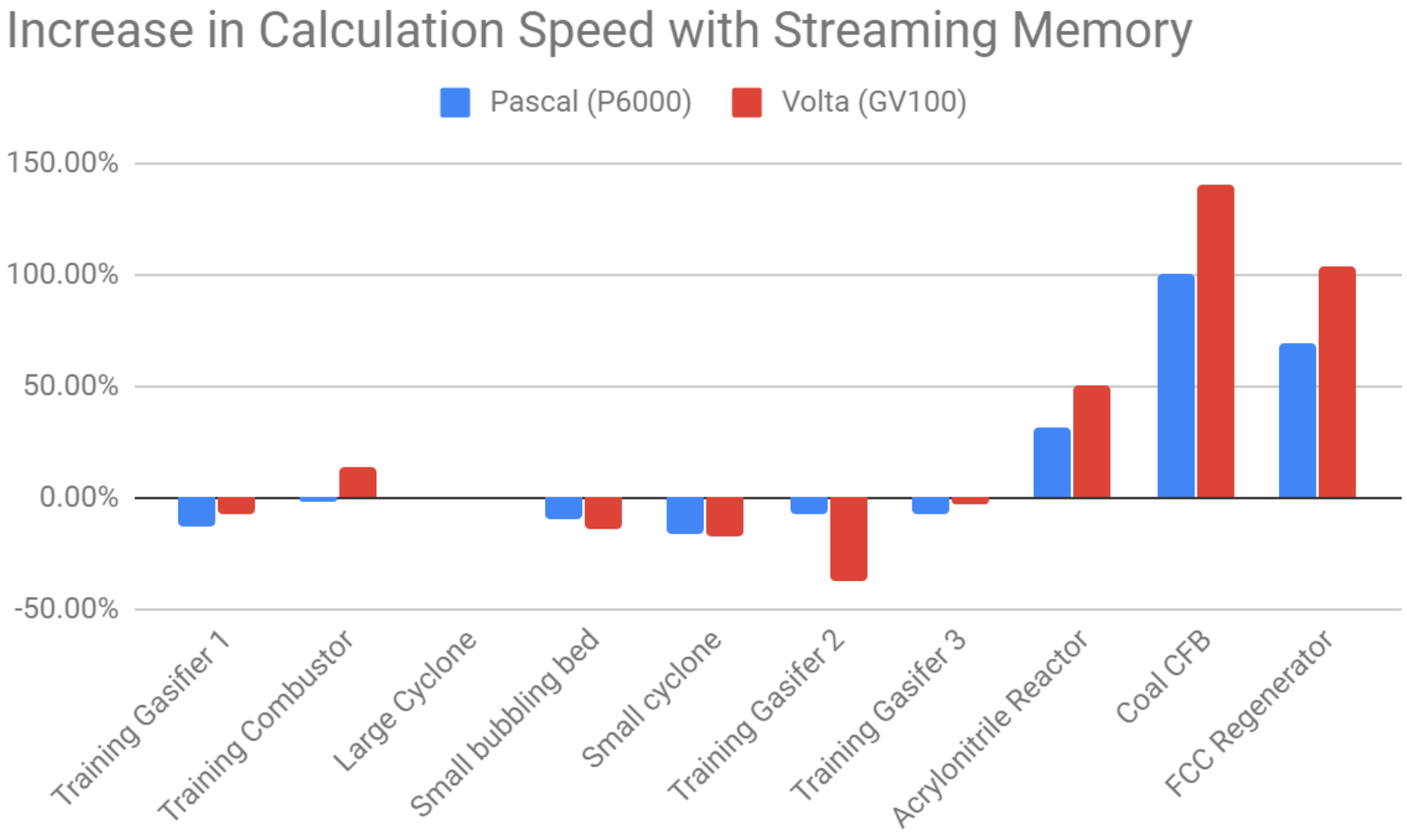
- P-1 Radiation model (beta in 17.4.0)
- Multi- liquids solver



What are we working on now?

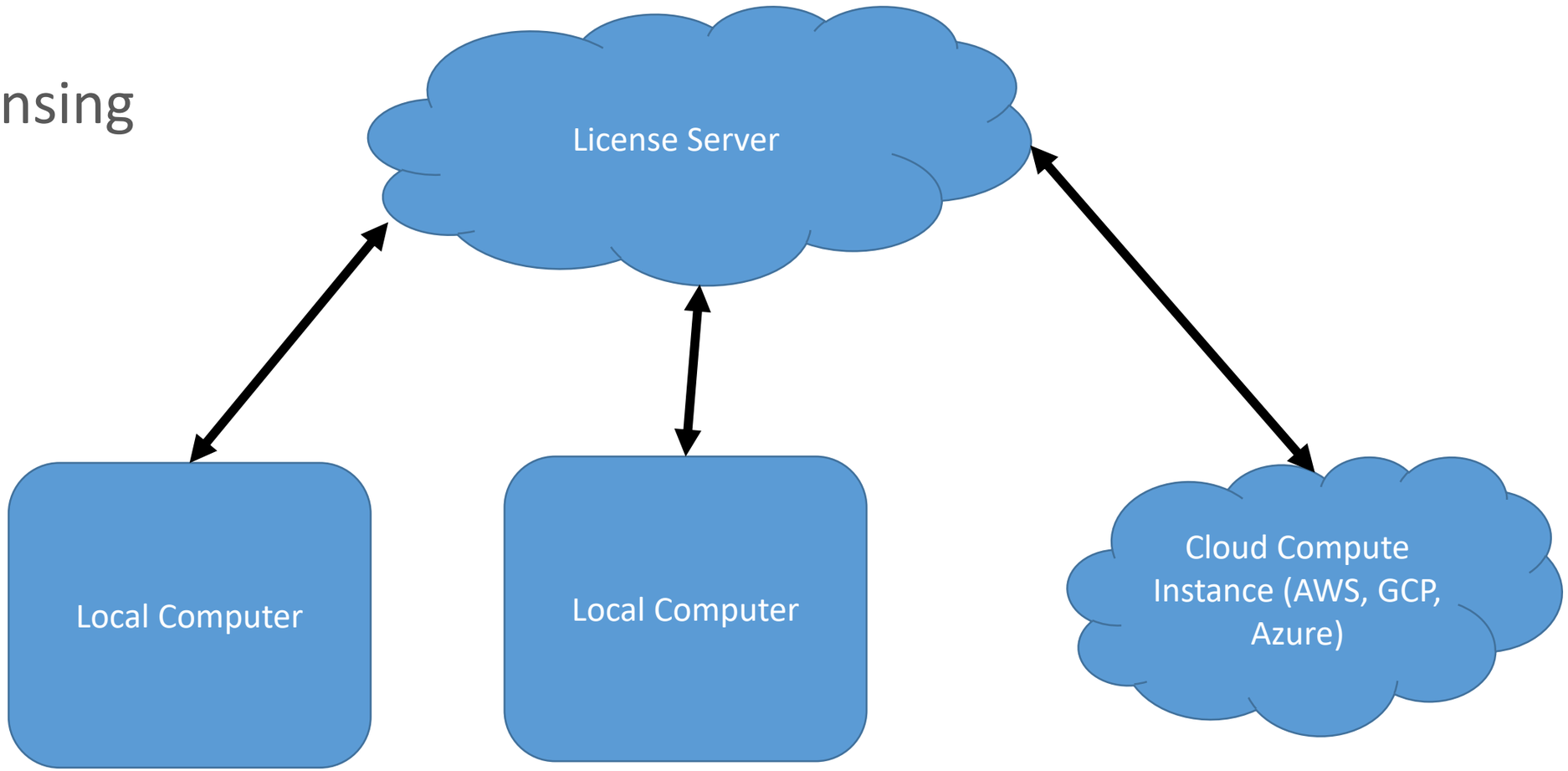
Larger, faster models

- Streaming memory
- Multiple GPUs



What are we working on now?

Flexible Licensing



What are we working on now?

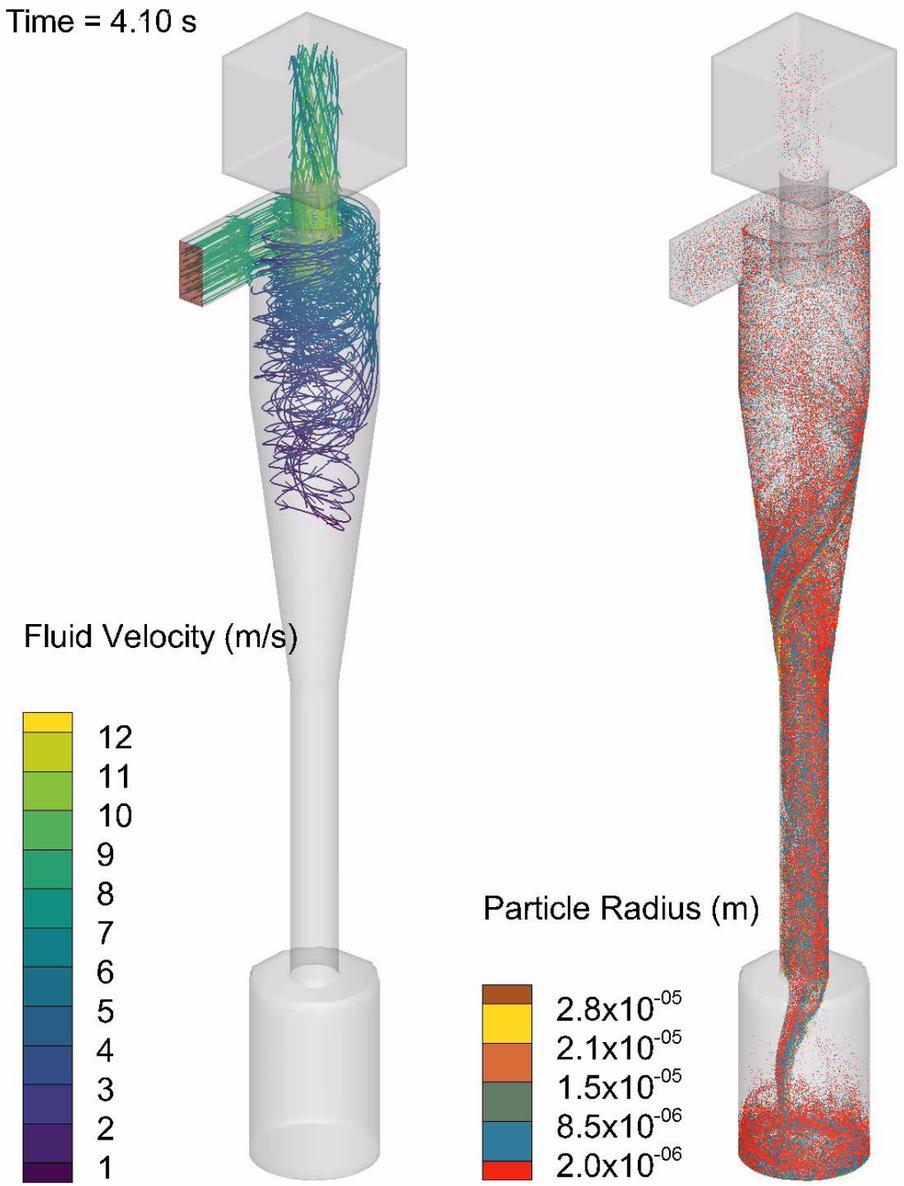
Improved data output and Post-Processing capability

- Revamp of Transient Data points interface
- Revamp of 2D data interface
- Replacement of GMV

Tecplot for Barracuda

- Tecplot for Barracuda, a special version of Tecplot 360, will replace GMV as the primary visualization tool

- Tecplot for Barracuda will be bundled and licensed with Barracuda Virtual Reactor



Tecplot for Barracuda

- Many of our users are already comfortable with Tecplot
- Powerful analysis of simulation results with less effort
- More precise display of boundary conditions
- Data display location – particles, cells, and walls
- Native Windows execution

Thank you!