Barracuda Virtual Reactor Users' Conference 2024
Advanced Training Workshop

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June 21, 2024

Outline

Cloud-based Linux VMs provided by rescale

Example Case Overview

Barracuda Virtual Reactor Feature Highlights

10:20 – 10:40 am: Break

Basic Post-Processing

Advanced Post-Processing by Scott Fowler from tecplot

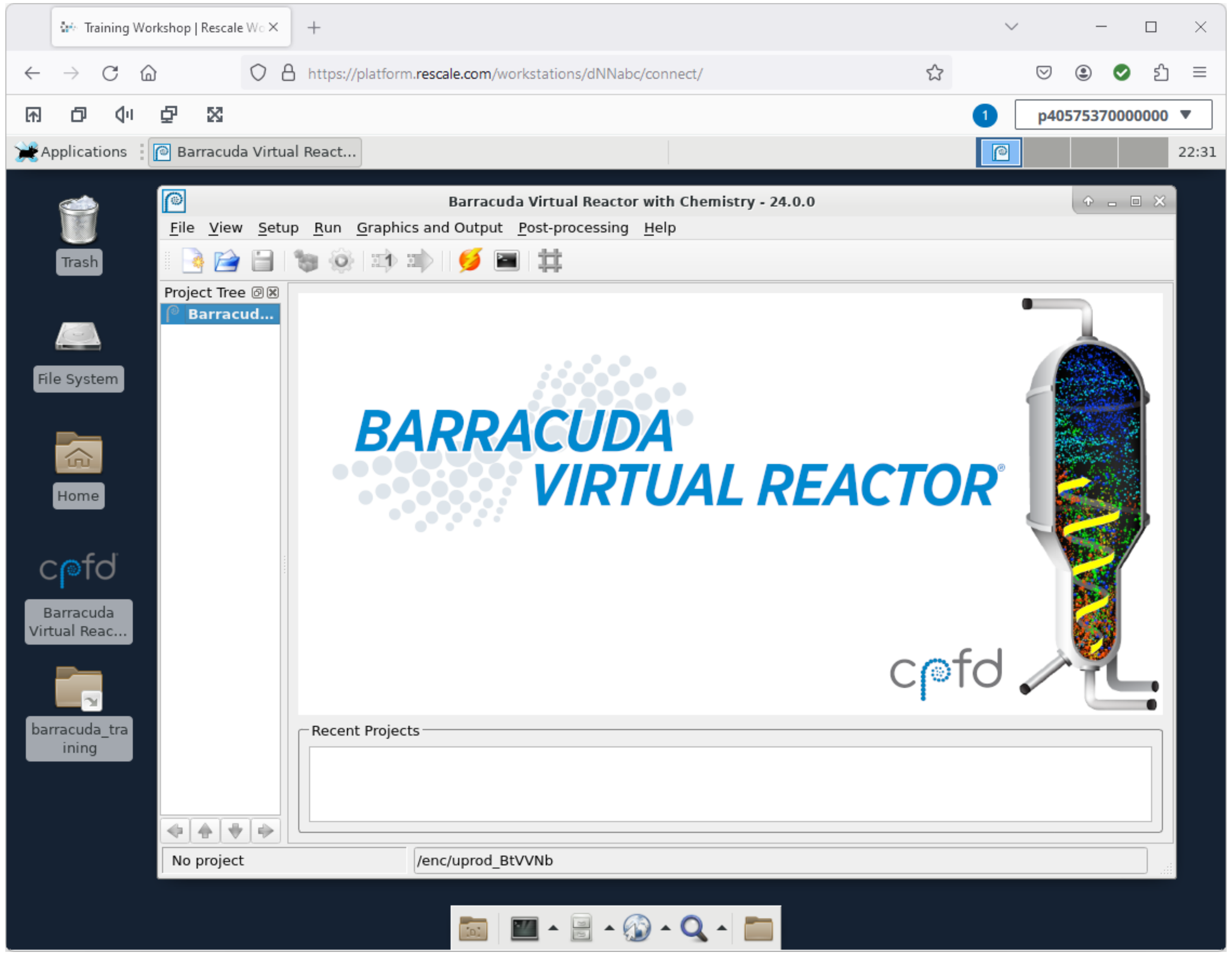
Q&A

Cloud-based Linux VMs Provided by rescale

CPFD thanks Rescale for sponsoring cloud-based Linux VMs for training attendees to use

Log in based on instructions provided during the training workshop

NVIDIA GPU cards are available on the VMs, make sure to take advantage of them when running the training example!



Example Case Overview

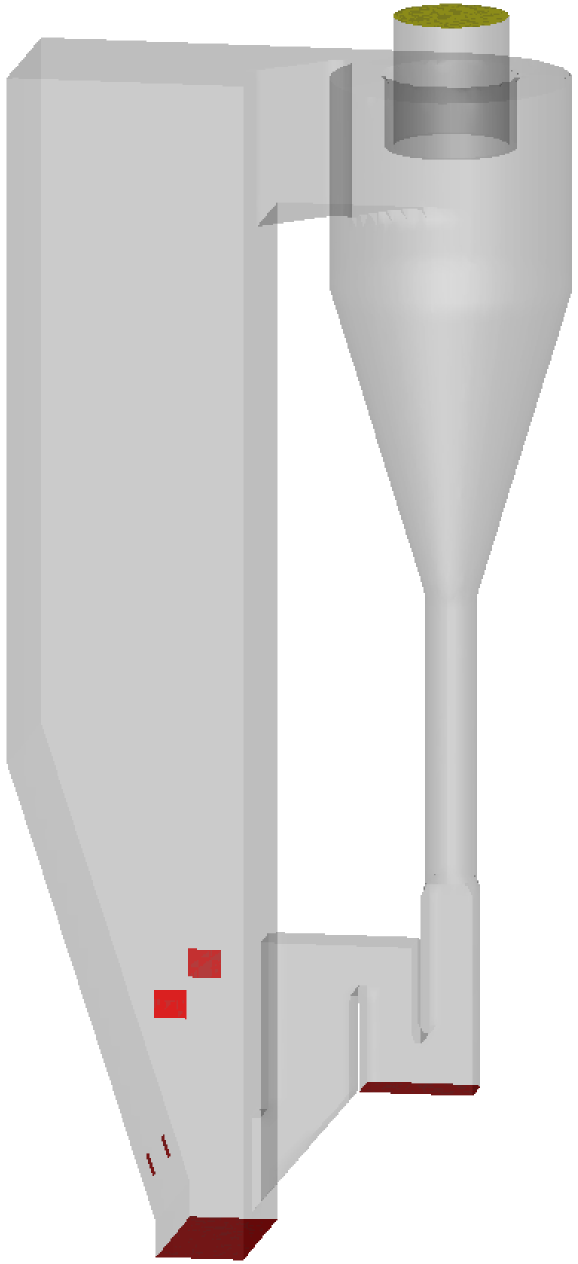
[Supplemental Training: CFB Erosion](#) was used as a starting point

Modifications made for this training workshop:

- Thermal calculations were enabled
- Additional base materials were added
- Chemical reactions were added

Open the Barracuda project and we will walk through the setup as a group during the in-person training session

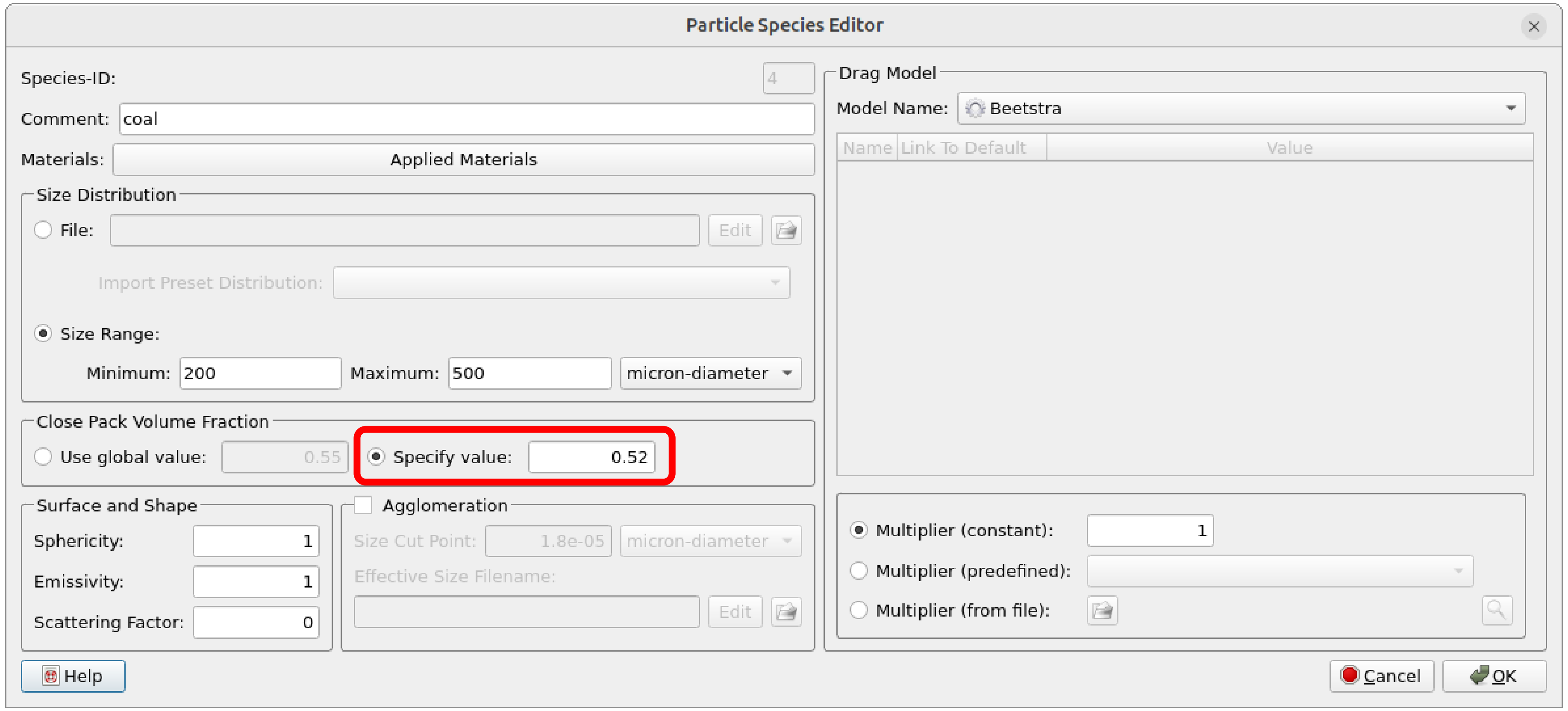
- Significant new features are highlighted in the following slides



Per-Species Close Pack Volume Fraction

Different particle species can have different close pack volume fractions

- Added in Barracuda Virtual Reactor 23.1

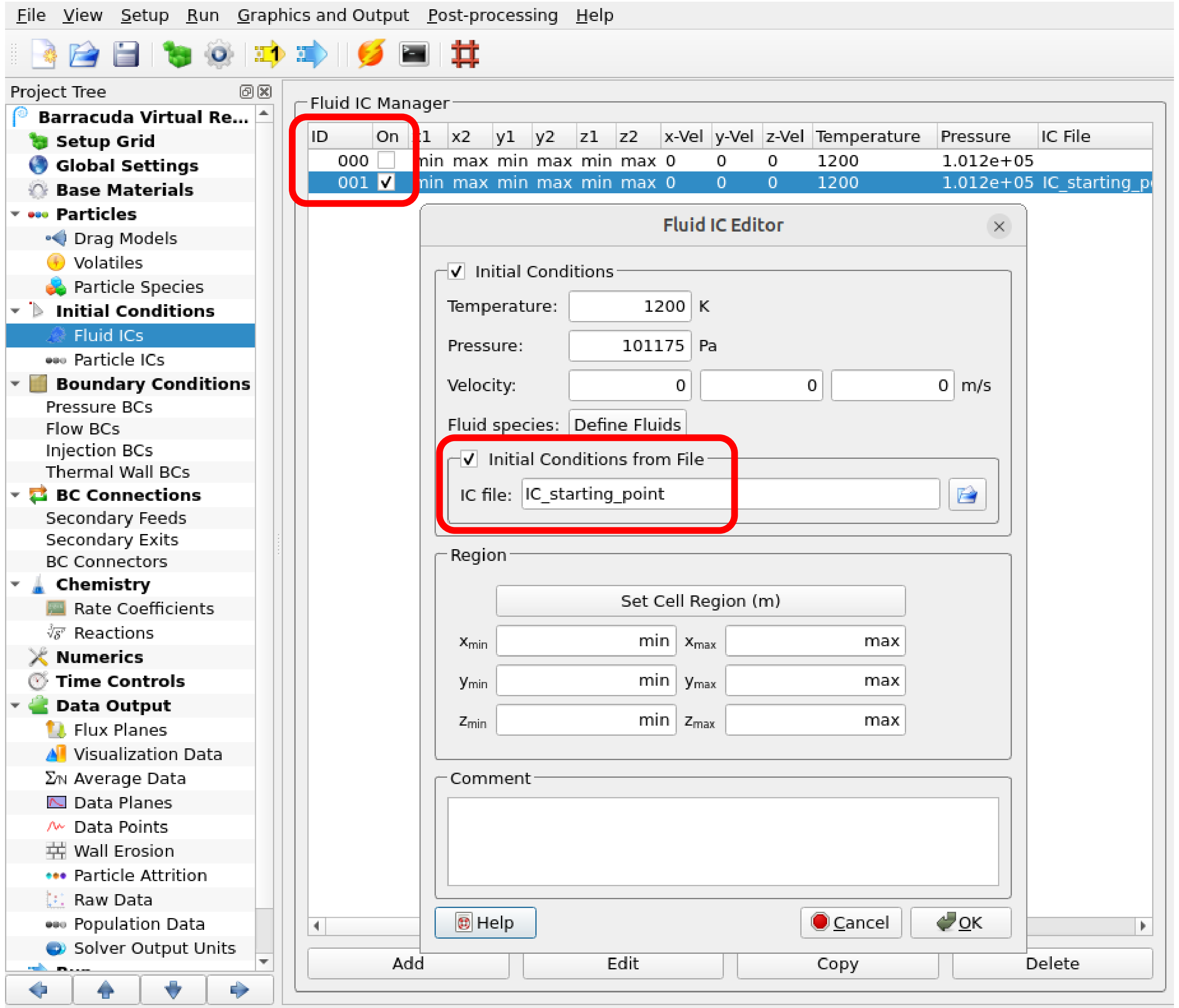


Fluid IC Definition

Disable the existing Fluid IC

Add new Fluid IC

Initialize the entire domain using the IC file: `IC_starting_point`

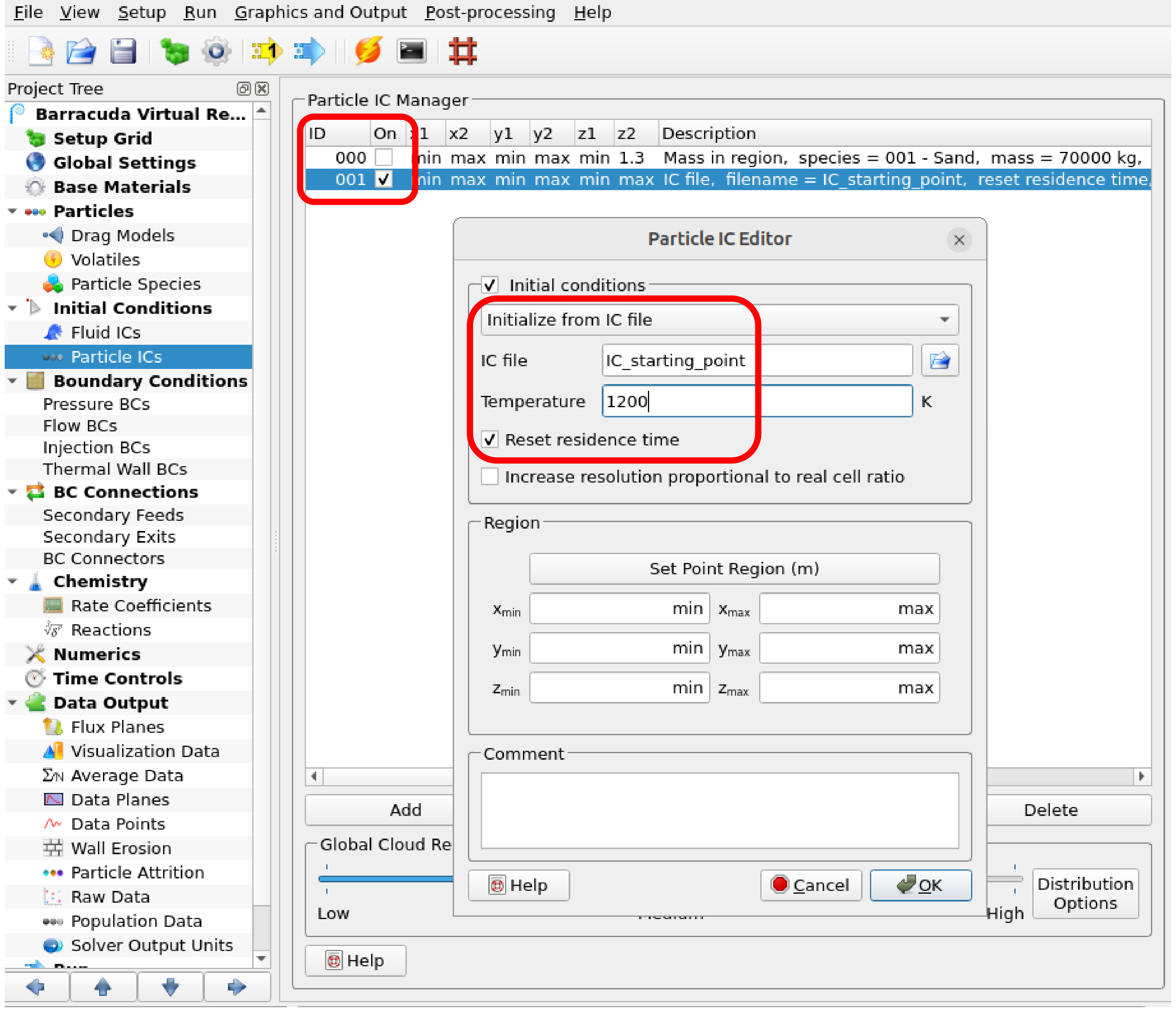


Particle IC Definition

Disable the existing Particle IC

Add new Particle IC

Initialize the entire domain using the IC file: `IC_starting_point`



Output Tracer Data at Pressure BC Flux Plane

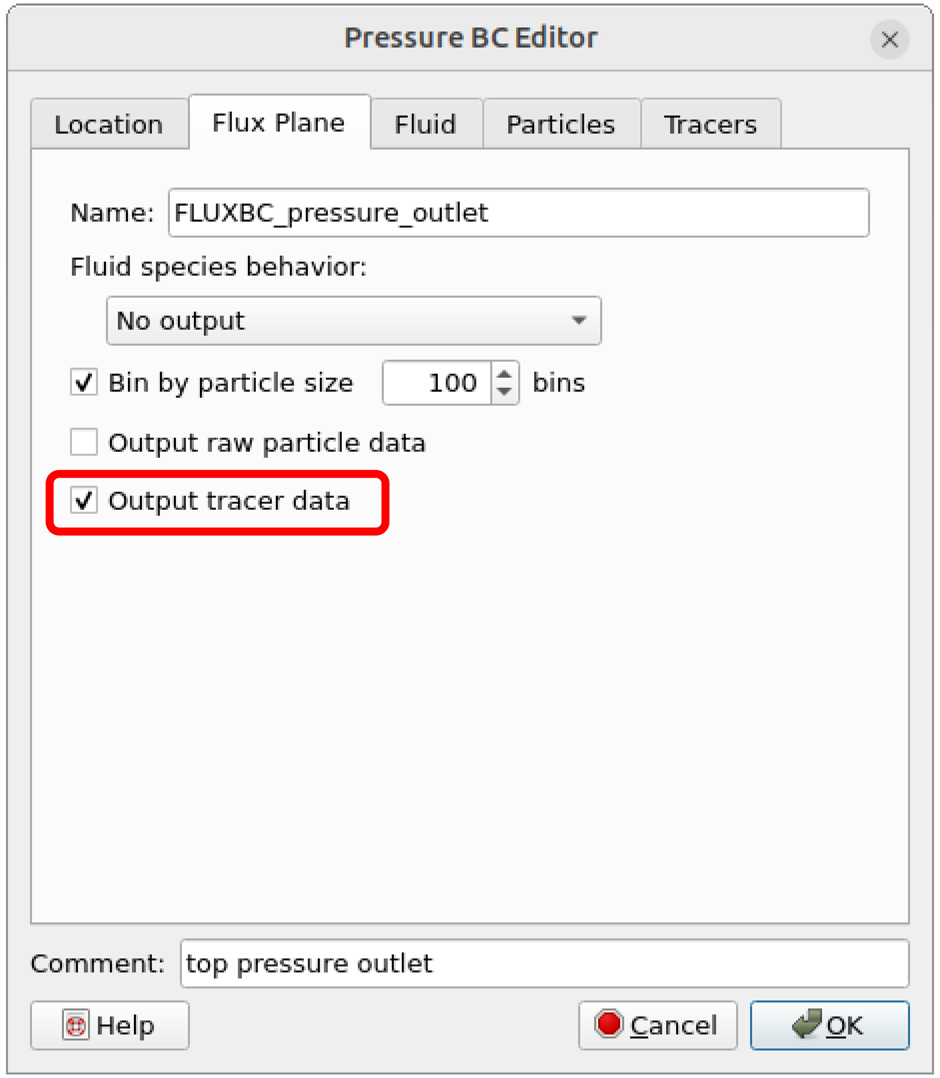
Tracers are Lagrangian entities that can be injected at BCs for tracking fluid flow and calculating fluid residence time

- Substantial updates to Tracers capabilities were made in Barracuda Virtual Reactor 22.1

Edit the Pressure BC

In the "Flux Plane" tab, enable: Output tracer data

This will allow us to analyze fluid residence time at the Pressure BC flux plane



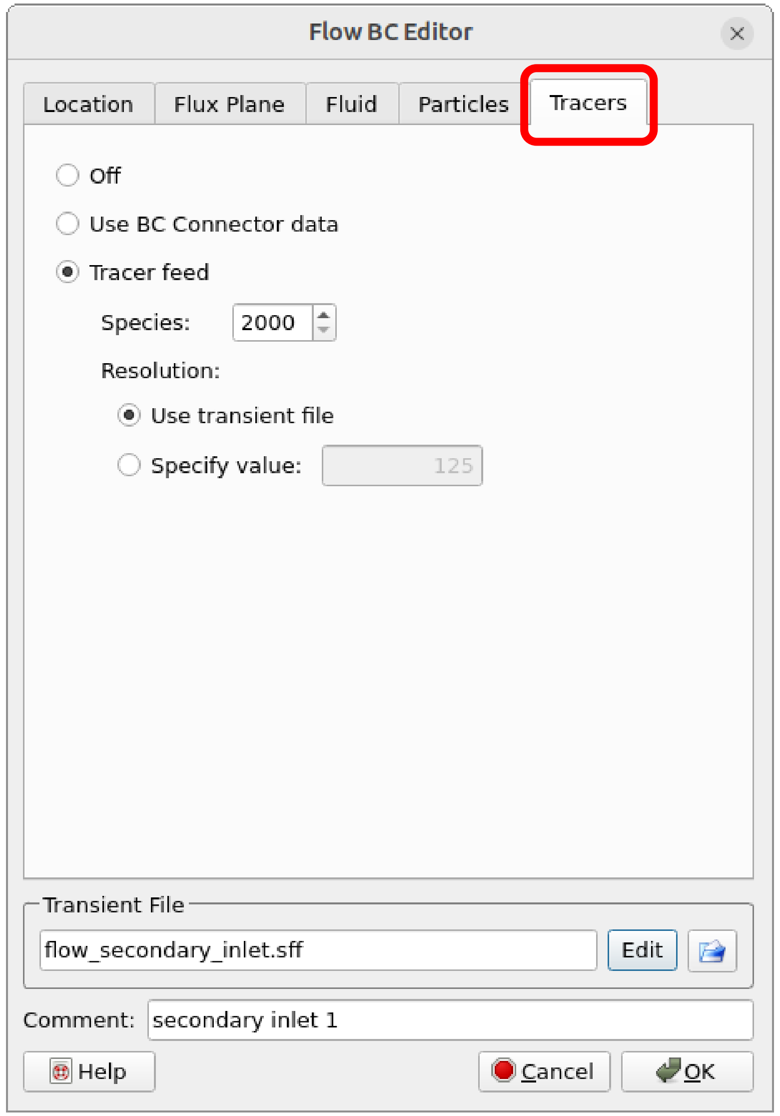
Feed Tracers at a Flow BC (Secondary Inlet 1)

Tracers can be fed from Pressure, Flow, or Injection BCs

Edit Flow BC 001, which is Secondary Inlet 1

Go to the "Tracers" tab, and enable tracer feed as shown in the screenshot

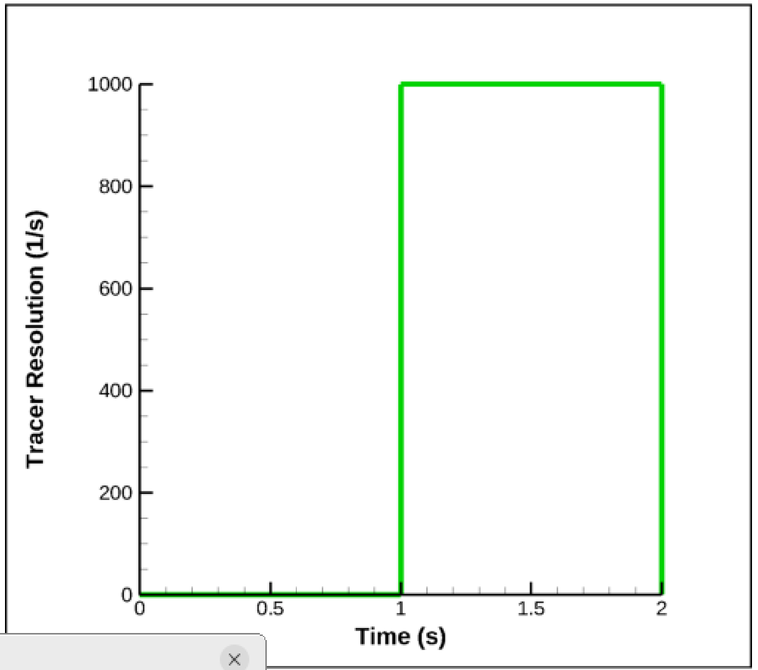
- Species numbers for tracers begin at 2000, and can be adjusted by the user
- Time-varying tracer feed can be specified by using a transient file (next slide)

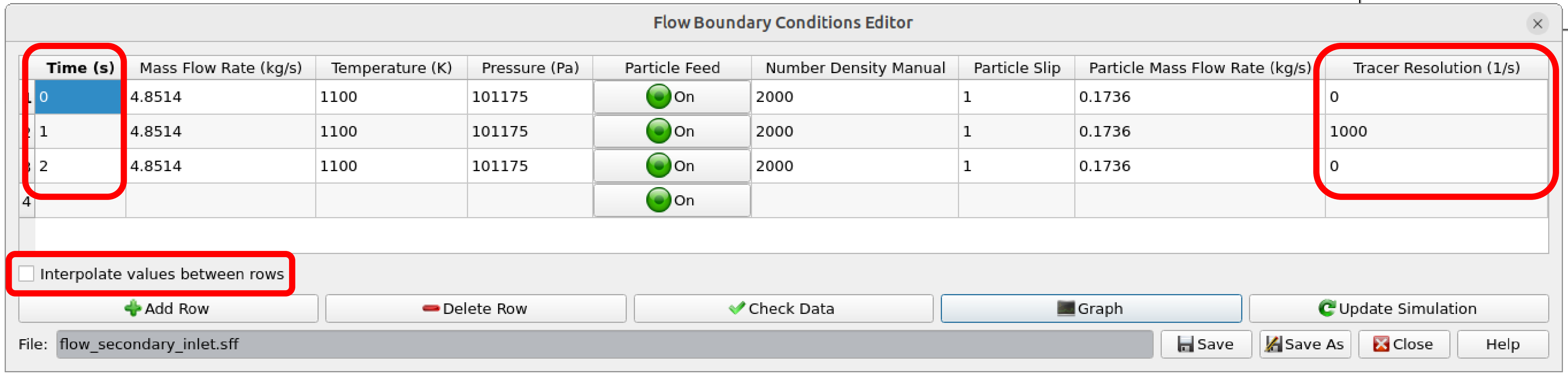


SFF File Option: Interpolate values between rows

Configure the tracers to be introduced as a 1-second "square pulse" using an SFF file

- New feature added in 24.0
- Uncheck the "Interpolate values between rows" option
- Click "Graph" button to see signal shape





	Time (s)	Mass Flow Rate (kg/s)	Temperature (K)	Pressure (Pa)	Particle Feed	Number Density Manual	Particle Slip	Particle Mass Flow Rate (kg/s)	Tracer Resolution (1/s)
1	0	4.8514	1100	101175	On	2000	1	0.1736	0
2	1	4.8514	1100	101175	On	2000	1	0.1736	1000
3	2	4.8514	1100	101175	On	2000	1	0.1736	0
4					On				

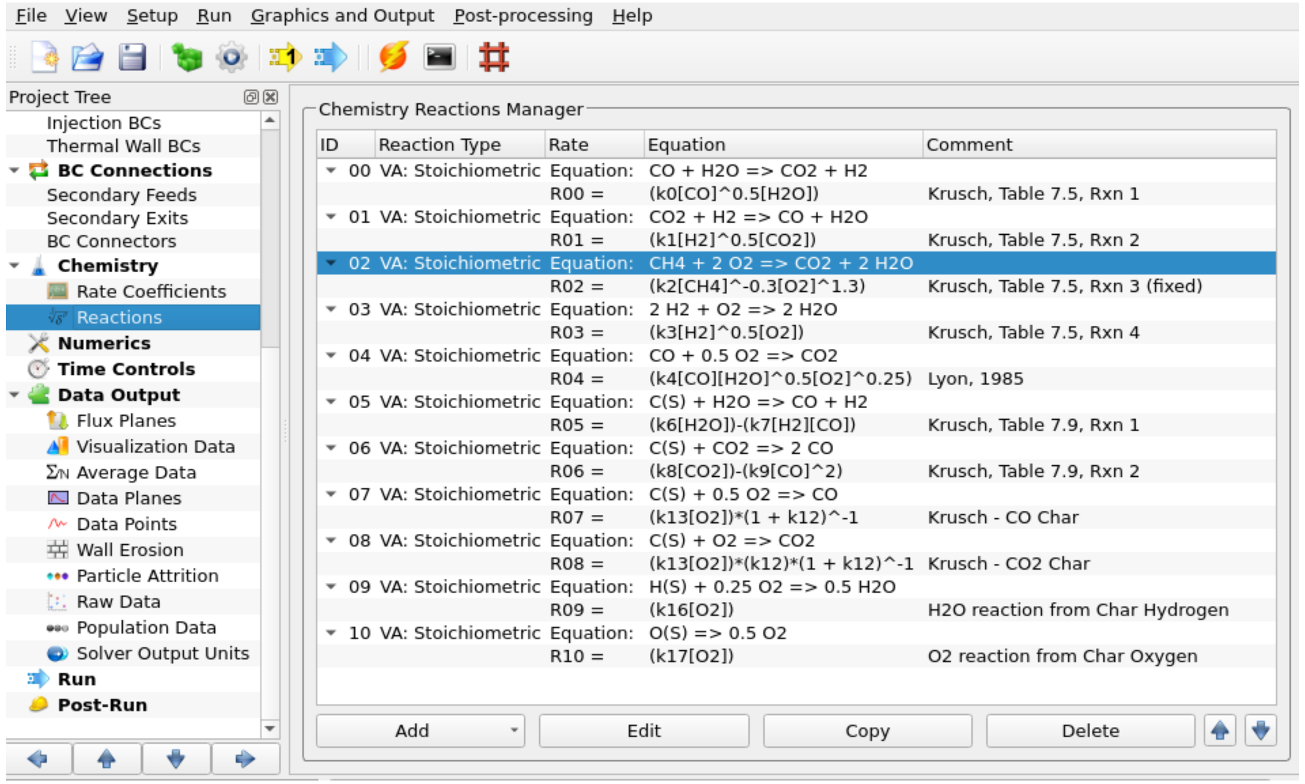
Chemical Reactions Used in this Example

Reactions included in this example were primarily derived from:

- Krusch, S., Scherer, V. and Scala, F. (2018) *Experimental examination and simulation of a pilot-scale circulating fluidized bed reactor.* Universitätsbibliothek, Ruhr-Universität Bochum. https://doi.org/10.13154/294-6389 / https://bibliographie.ub.rub.de/work/20164
- Lyon, R. K., Hardy, J., and Von Holt, W. (1985) Oxidation kinetics of wet CO in trace concentrations, Combustion and Flame, Volume 61, Issue 1, Pages 79-86. https://doi.org/10.1016/0010-2180(85)90074-4

The set of reactions in this example is not comprehensive. Reactions neglected in this example include:

- Calcination
- Sulfation
- NOx formation



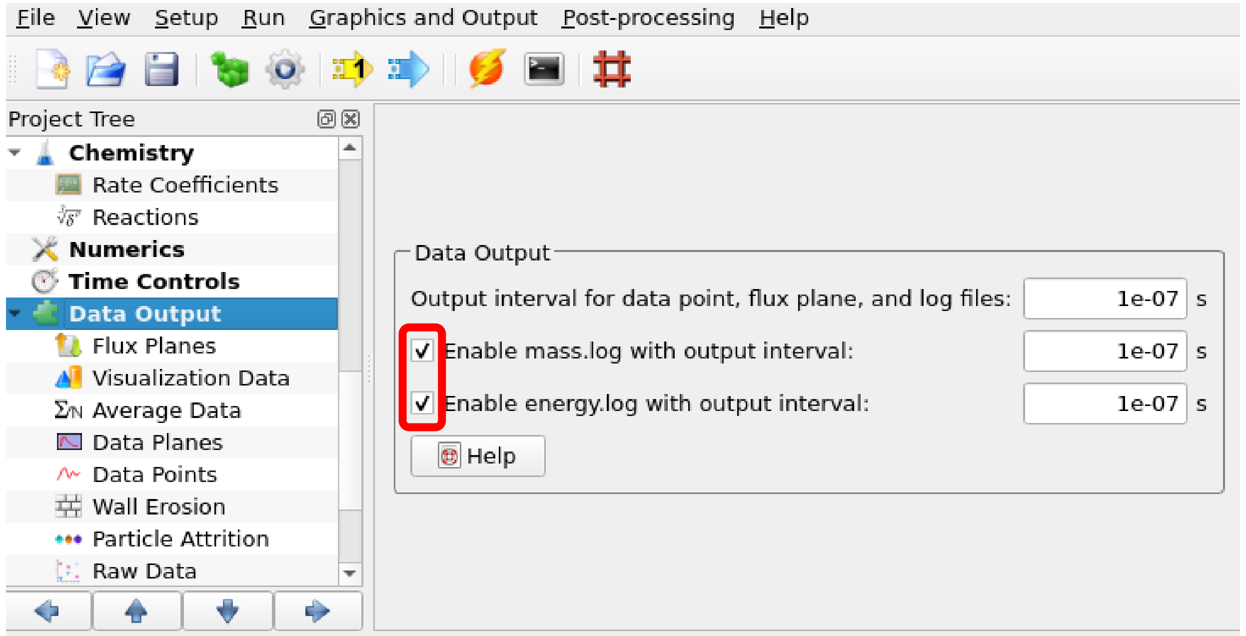
Enable Output Files mass.log and energy.log

Go to the "Data Output" page to enable mass.log and energy.log

- Added in Barracuda Virtual Reactor 23.1

These log files are useful for:

- Monitoring total mass and energy of fluids, particles, and bubbles
- Performing system mass and energy balances
- Determining whether steady state has been reached



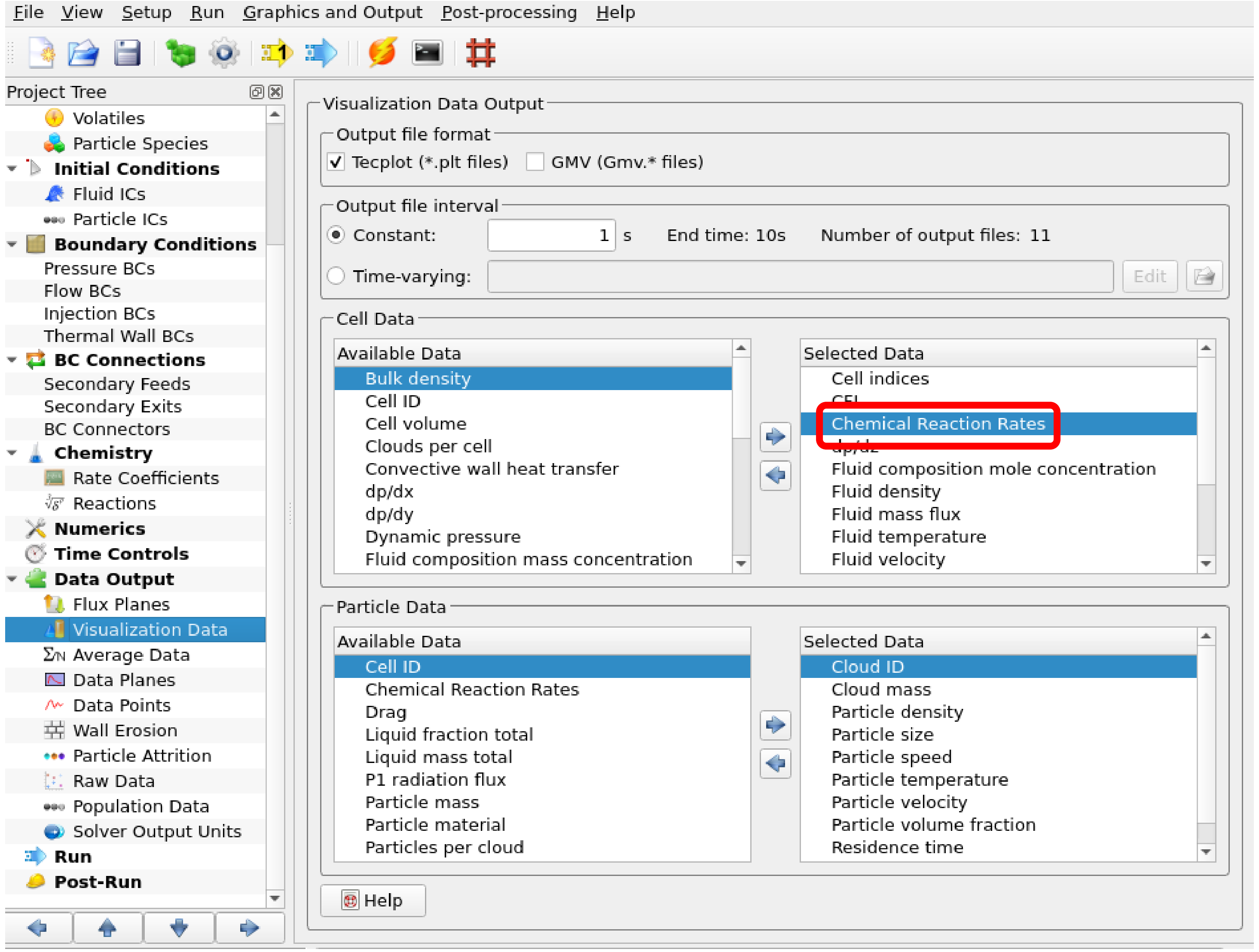
Chemical Reaction Rate Data Output

Chemical reaction rates are available in all data output locations

- Added / expanded in Barracuda Virtual Reactor 23.1

Go to "Visualization Data" and select "Chemical Reaction Rates" for output to Tecplot's Cell Data

- Reaction rate information for all reactions in the project (both volume-average and discrete) will be output to Visualization Data

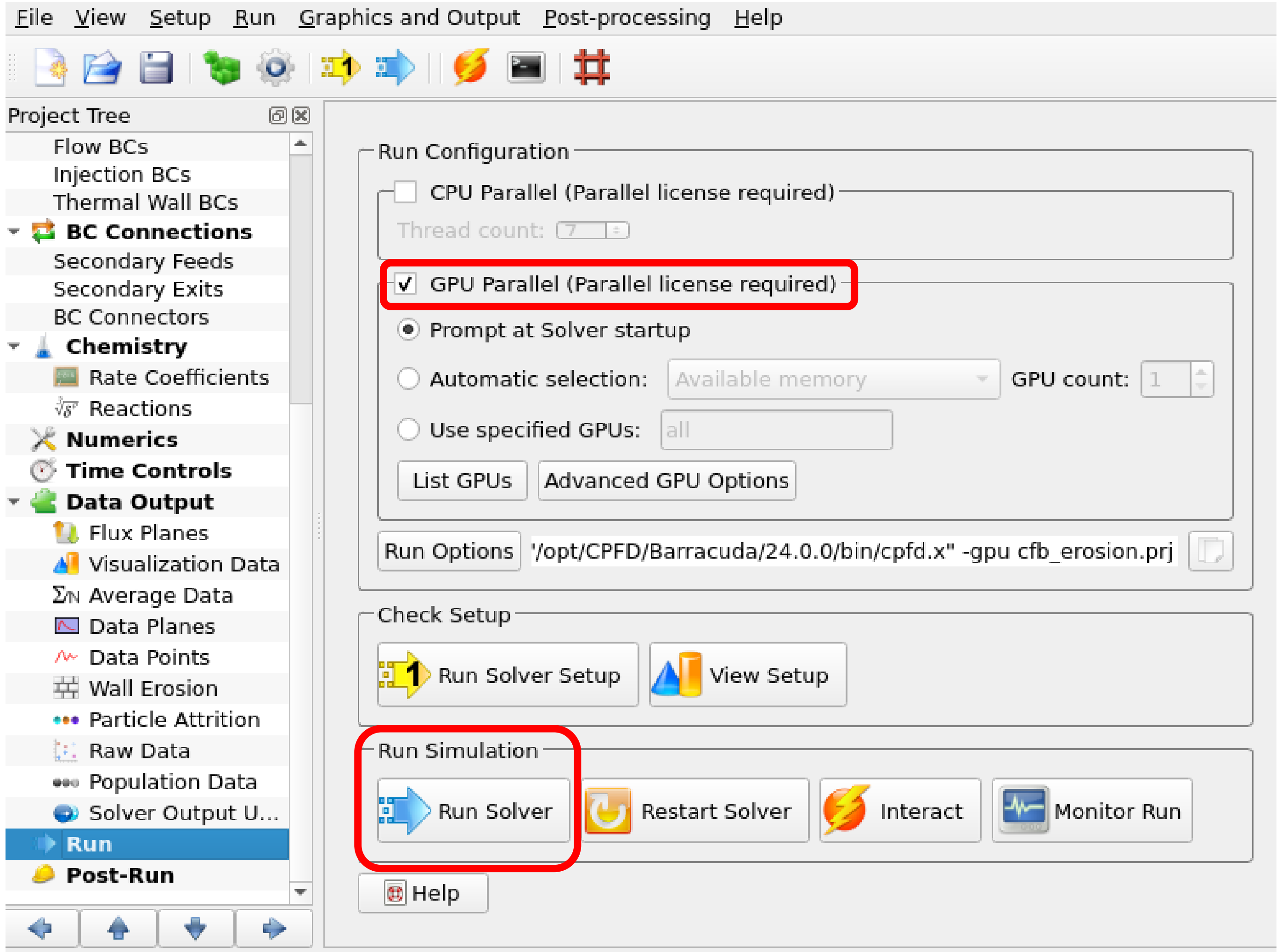


Run the Simulation

On the Run page:

- Make sure to enable GPU Parallel
- Click Run Solver

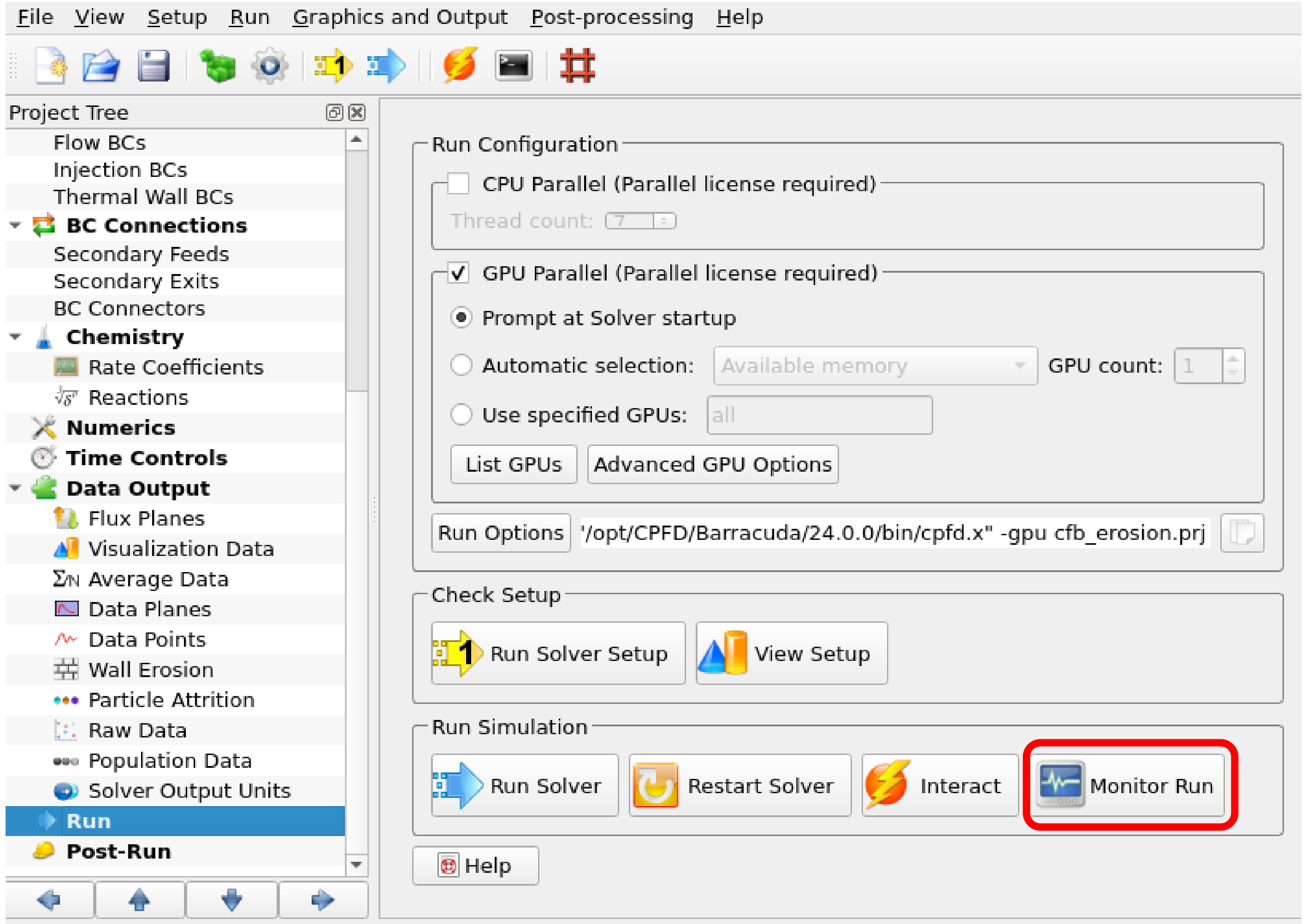
The simulation should take about 45 minutes to reach an end-time of 10 seconds on the Rescale VM



Monitor Run

Once the simulation is running, click the "Monitor Run" button

- Files must contain at least a few rows of data. If you get blank plots, close the Tecplot window and click Monitor Run again
- This feature can also be used after a simulation is completed, as long as the necessary output files are still present in the directory



Monitor Run Views in Tecplot

Plots use Tecplot's "Pages" feature

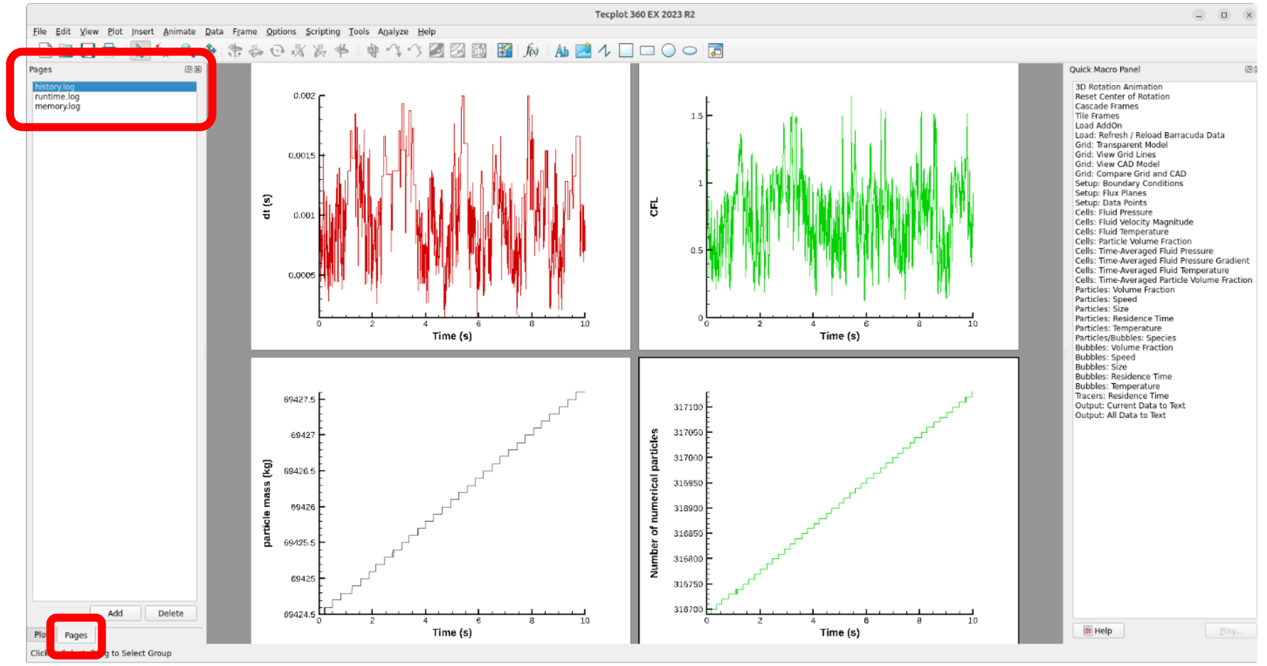
- View → Pages sidebar

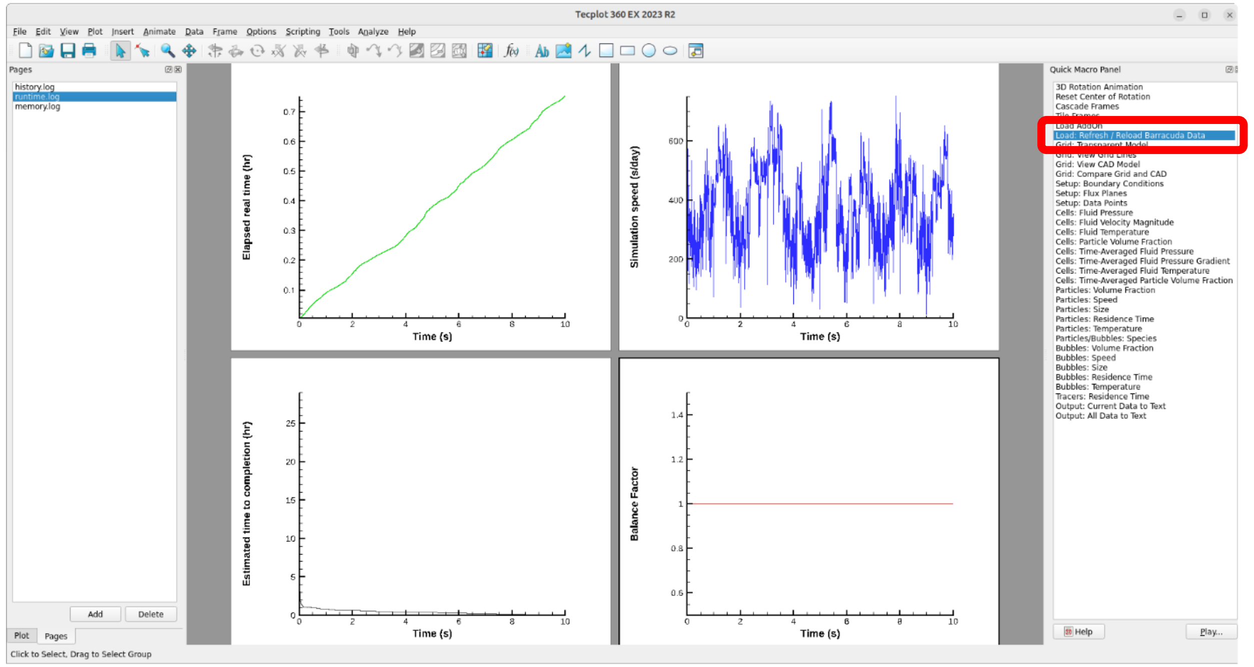
Files plotted automatically:

- history.log
- runtime.log
- memory.log

Use Quick Macro Panel to refresh data as the simulation progresses

- Load: Refresh / Reload Barracuda Data





Visualizing Tracers in Tecplot for Barracuda

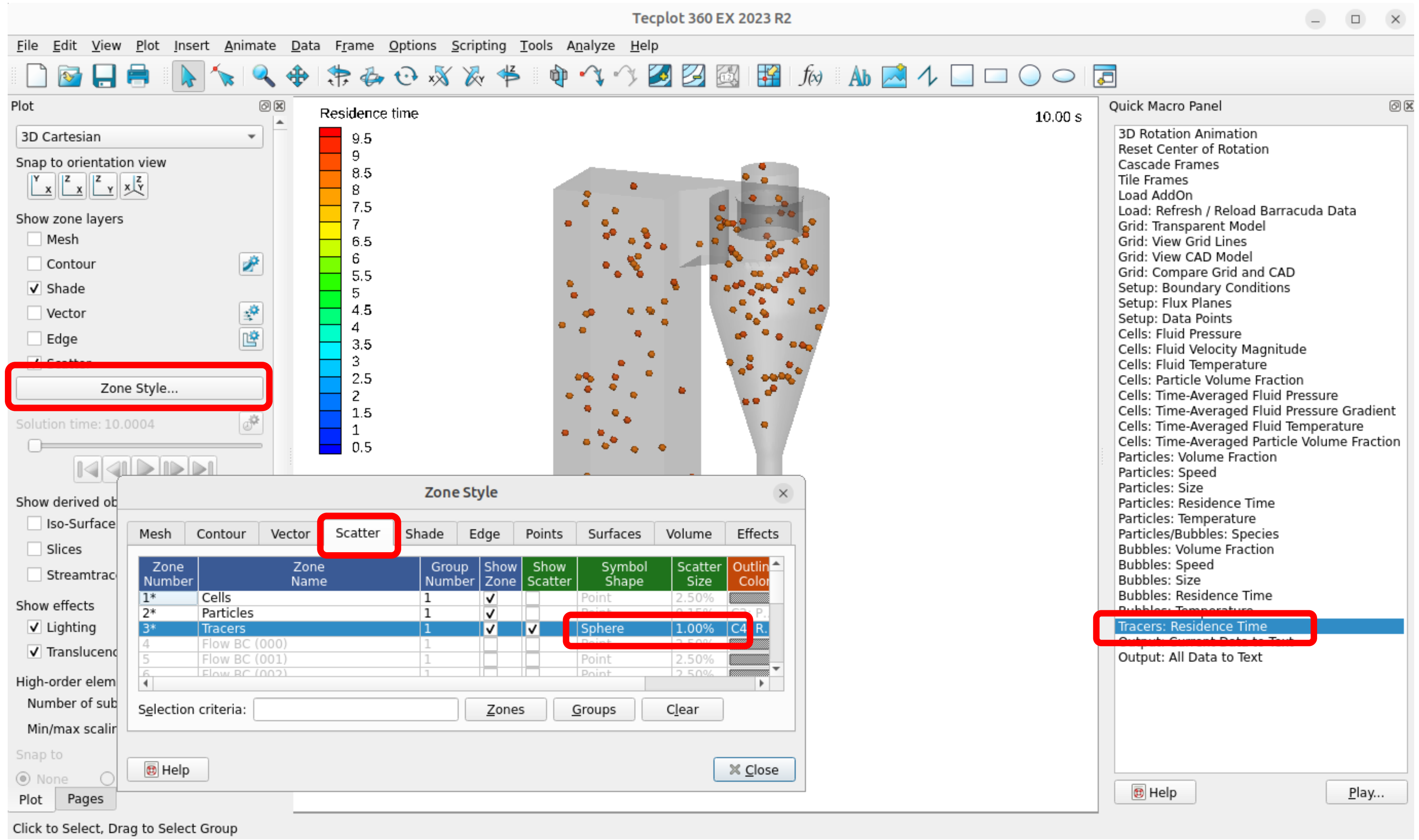
Post-Run → View Results

Use Quick Macro Panel:

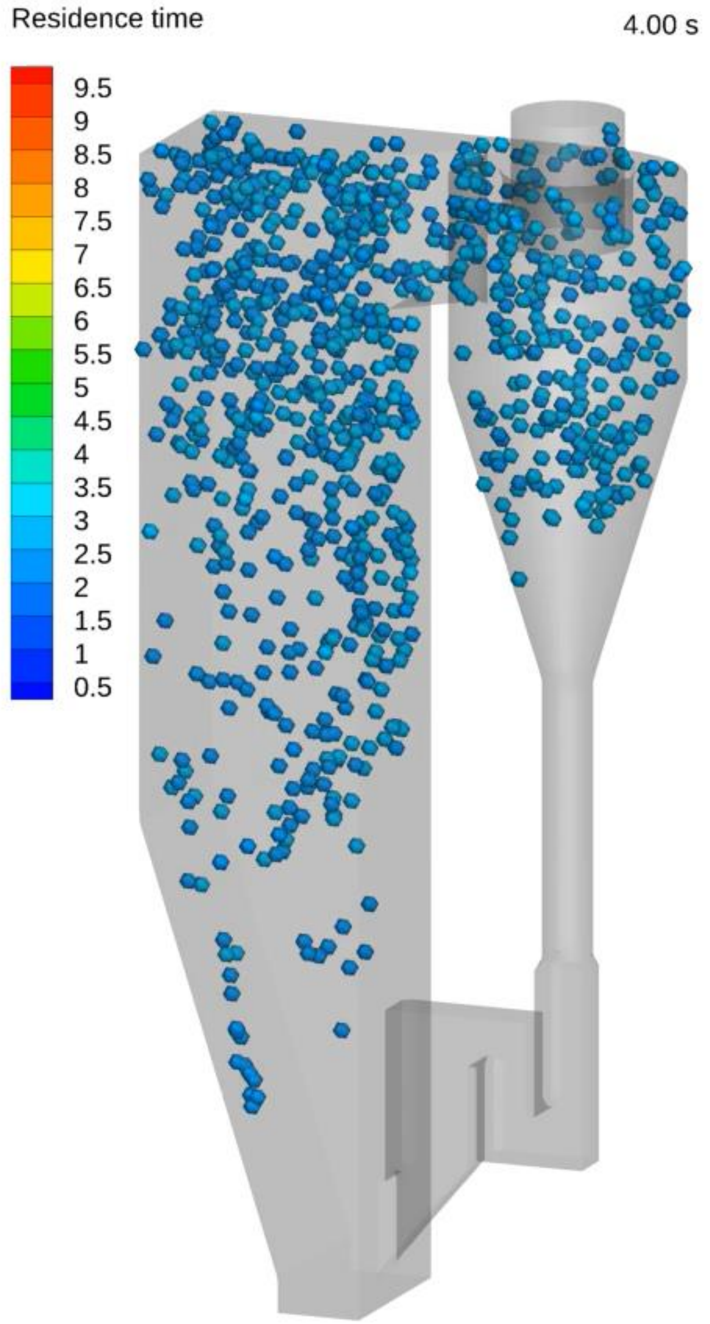
- Tracers: Residence Time

Zone Style… → Scatter tab

- Symbol Shape: Sphere
- Scatter Size: 0.5



Creating an Animation of Tracer Flow



Load all solution times

- File → Load Barracuda Data
- Tecplot Files to Load: All
- Refresh / Reload

Click "Play" on the solution time slider to visualize the tracer flow

Analyzing Residence Time of Tracers

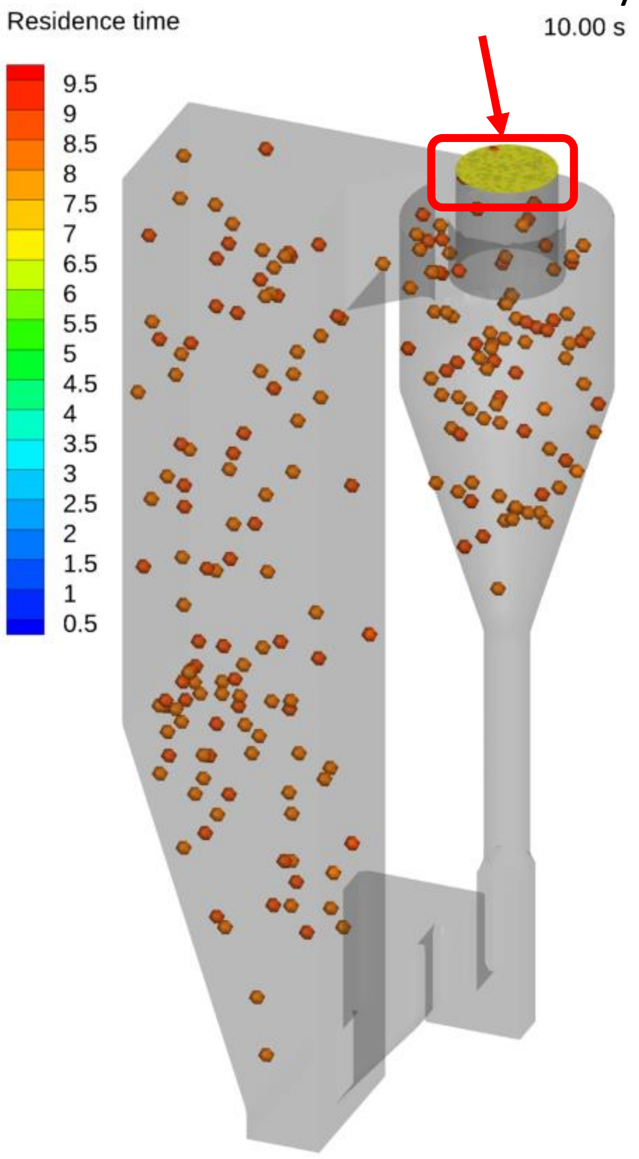
Tracer residence time distributions (RTDs) are usually plotted as histograms

We will use a Jupyter Notebook to create a plot

CPFD Support Site posts related to this exercise (for future reference):

- Using Jupyter Notebooks to Analyze Virtual Reactor Results
- Using Tracers in a Barracuda Virtual Reactor Model

The `_raw_tracer` file from the Pressure BC flux plane records the residence time of every tracer that exits the system



The _raw_tracer Flux Plane File Format

Open a terminal from the Barracuda GUI, and run this command to see the first 20 lines from the file:

```
head -n 20 FLUXBC_pressure_outlet_raw_tracer
```

```
# top pressure outlet
#
#@   1  "Time"                                                          "s"
#@   2  "Unique tracer ID"                                              ""
#@   3  "Species"                                                       ""
#@   4  "Residence time"                                                "s"
#@   5  "x"                                                             "m"
#@   6  "y"                                                             "m"
#@   7  "z"                                                             "m"
#@   8  "x-velocity"                                                    "m/s"
#@   9  "y-velocity"                                                    "m/s"
#@  10  "z-velocity"                                                    "m/s"
#@  11  "Speed"                                                         "m/s"
 2.364960e+00   319407  2000  2.212769e+00  4.752035e-01  6.039956e-01  2.351394e+01  1.214128e+01 -5.651420e+00 -2.738963e+01  3.048838e+01
 2.406046e+00   319397  2000  2.325361e+00 -4.917556e-01 -9.936733e-01  2.349287e+01 -1.696444e+01  7.327595e+00 -2.747476e+01  3.311115e+01
 2.427583e+00   319429  2000  2.155551e+00  7.273328e-01 -6.798310e-01  2.347497e+01 -8.855214e+00 -1.400932e+01 -3.137292e+01  3.548148e+01
 2.487058e+00   319387  2000  2.470055e+00 -1.022772e+00 -6.357252e-01  2.351106e+01 -8.039836e+00  1.296738e+01 -2.524422e+01  2.949682e+01
 2.487058e+00   319401  2000  2.374681e+00  6.116487e-01  5.049670e-01  2.348655e+01  1.105051e+01 -8.558693e+00 -2.952998e+01  3.267085e+01
 2.490040e+00   319395  2000  2.417787e+00  7.981942e-01  2.072166e-01  2.349024e+01  7.071736e+00 -1.285507e+01 -3.037791e+01  3.373544e+01
 2.590982e+00   319434  2000  2.286828e+00  9.906930e-01  7.058860e-02  2.350330e+01  3.679012e+00 -1.287379e+01 -2.528076e+01  2.860746e+01
```

Header section has lines that start with # symbol, and records meaning of each column of data in the file

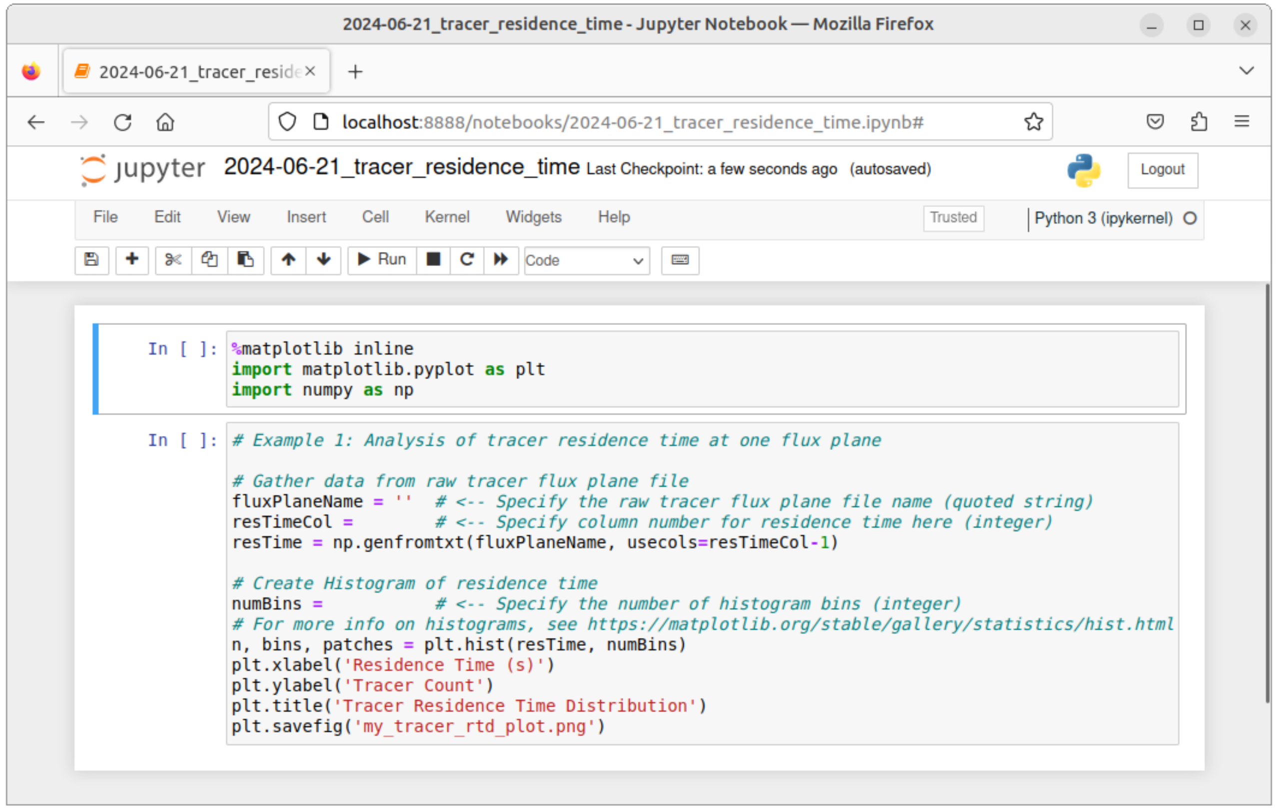
One row of data per tracer that crosses flux plane

Open Example Jupyter Notebook

In the terminal opened from the Barracuda GUI, enter the command:

```
jupyter-notebook 2024-06-21_tracer_residence_time.ipynb
```

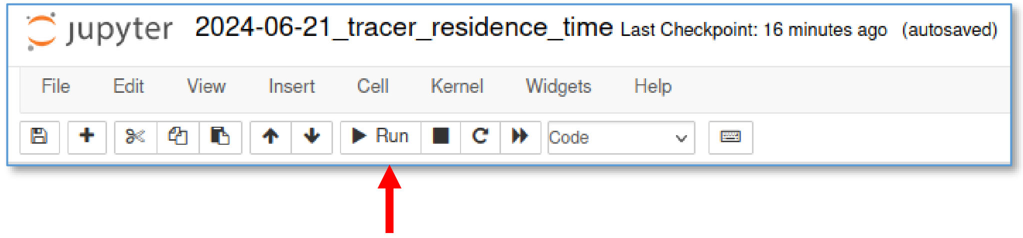
A web browser will open with the specified file, which has some code already entered as a starting point for today's training workshop



Use Jupyter Notebook to Create RTD Histogram Plot

Specify the information indicated by # <-- comments

- fluxPlaneName
- resTimeCol
- numBins



Run the notebook

- Click in the top cell and press the “Run” button
- As long as no errors occur, focus will move to the next cell
- Click the “Run” button again
- As long as no errors occur, you should see an RTD plot similar to the one shown here

Explore the Data and Close the Jupyter Notebook

What happens if you use higher or lower values for numBins?

- If you change any content in a cell, rerun the cell to update the plot

How many tracers have passed through the Pressure BC flux plane?

- Python's `len()` function will show you how many values are in an array
- Is this a high enough number to be statistically significant?

Close the Jupyter notebook when you're finished with the histogram

- Save the Jupyter notebook file and close the web browser window
- In the terminal used to start the notebook, press `Ctrl+C` twice to shut down the Jupyter notebook server

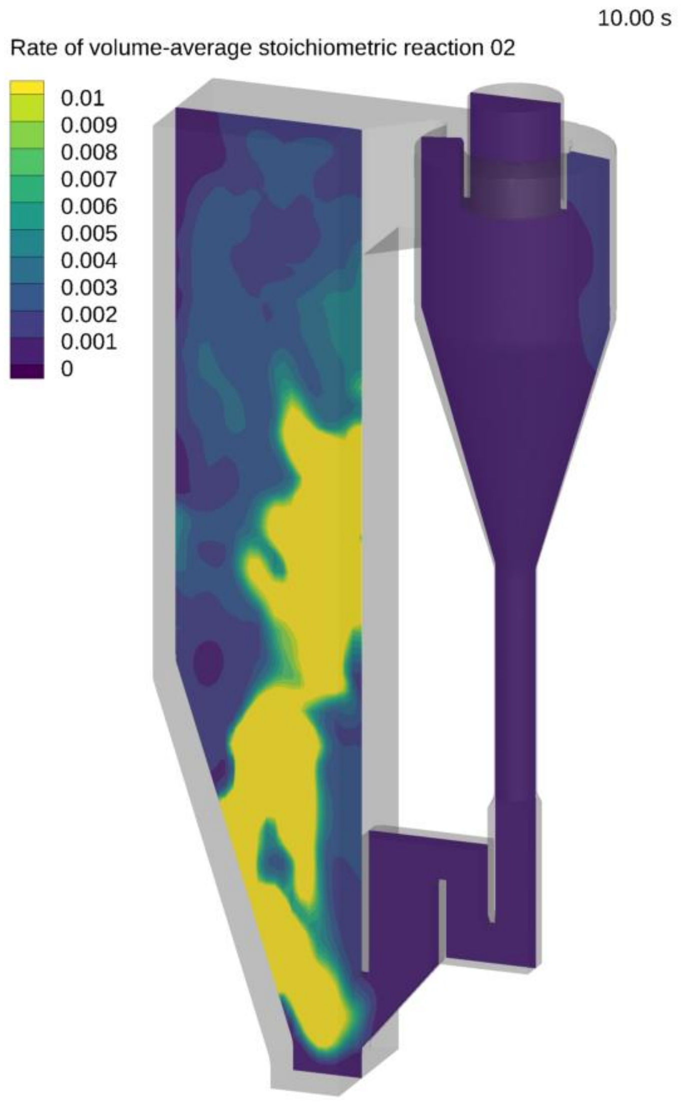
Viewing Chemical Reaction Rates in Tecplot

Since all reactions in this example are volume-average, we will visualize reaction rates as cell data

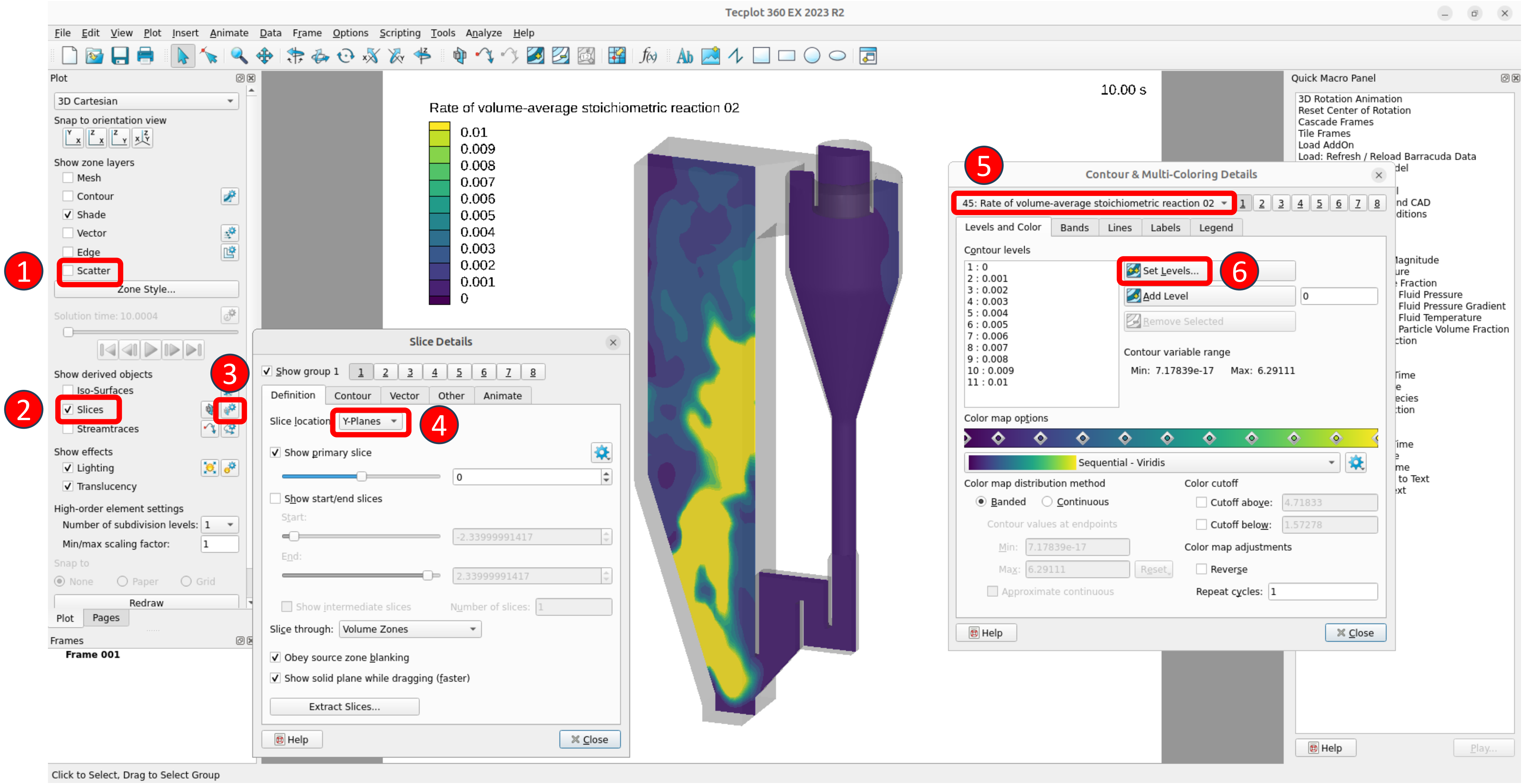
- For simulations with discrete particle chemistry, you can also display reaction rate information on the particles

Create a slice to show chemical reaction rate R02

- Use "Particles: Volume Fraction" to get a transparent vessel
- Un-check the "Scatter" layer to turn off particles
- Click the "Slices" checkbox, then the gear for slice settings
- Slice location → Y-Planes
- Color by **Rate of volume-average stoichiometric reaction 02**
- See next slide for details



Detailed Steps for Creating Slice

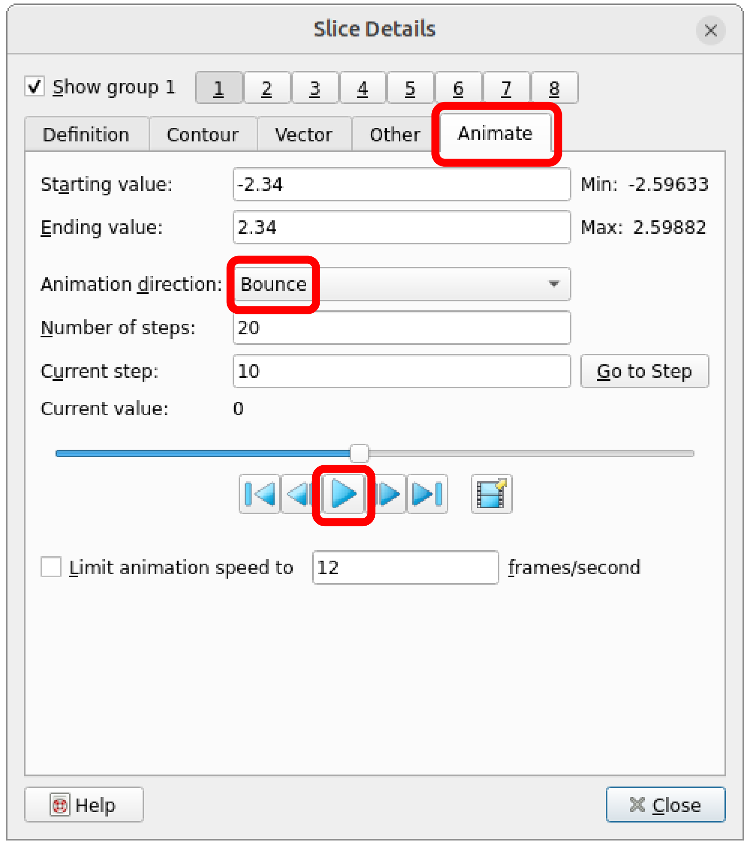


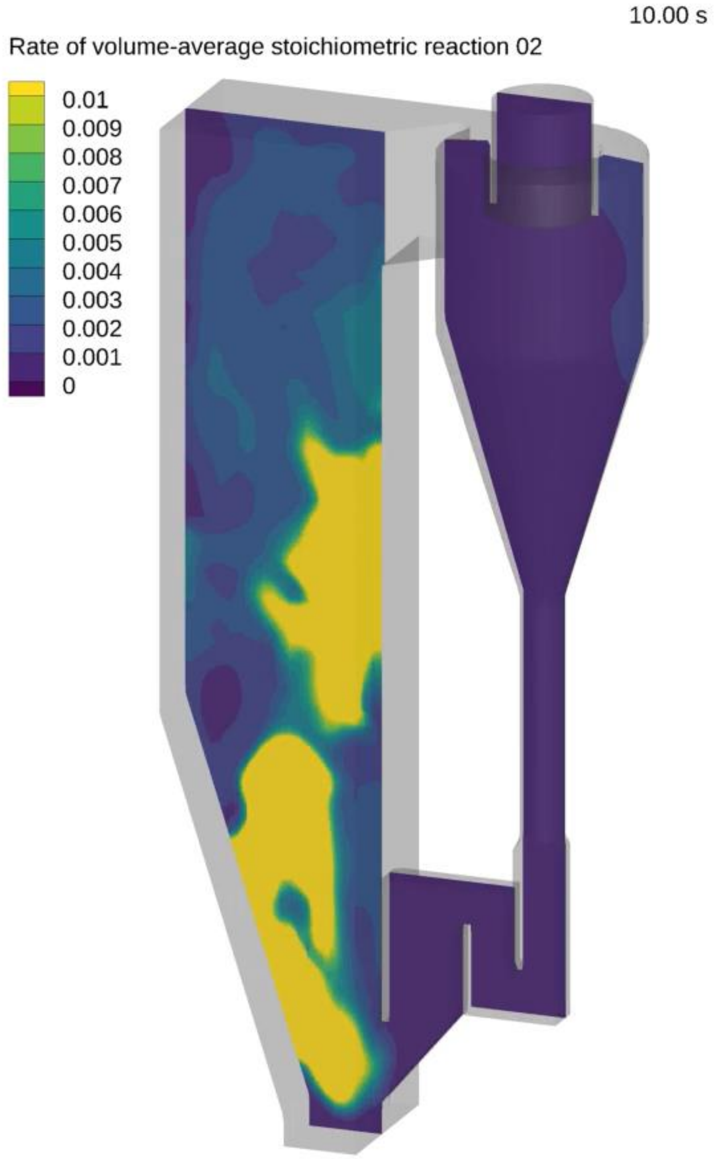
Animating a Slice to Gain More Insight

Using slice animation is helpful to get a 3-dimensional understanding of system behavior

In the Slice Details dialog:

- Go to the Animate tab
- Animation direction → Bounce
- Click Play



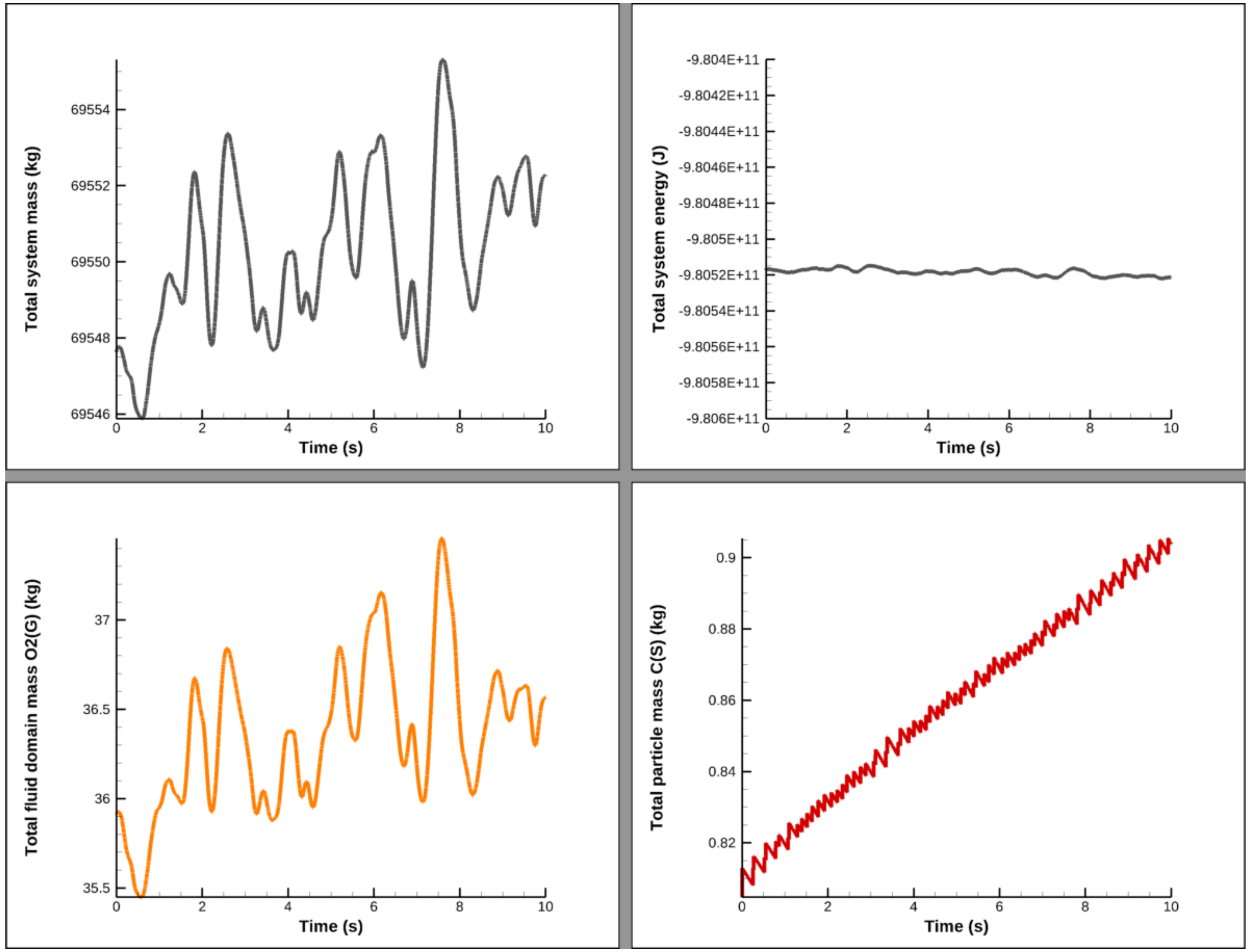


Using Data from mass.log and energy.log

Data in mass.log and energy.log is useful for determining things like:

- Are the total mass and energy in the system reaching steady state?
- What is the mass of a specific gas or solid material over time?

Detailed steps for creating a 4-frame plot view as shown here are covered on the next few slides



Detailed Steps for Creating Plot

Start a blank Tecplot for Barracuda window

- Run page → Launch Tecplot

Read the mass.log file first

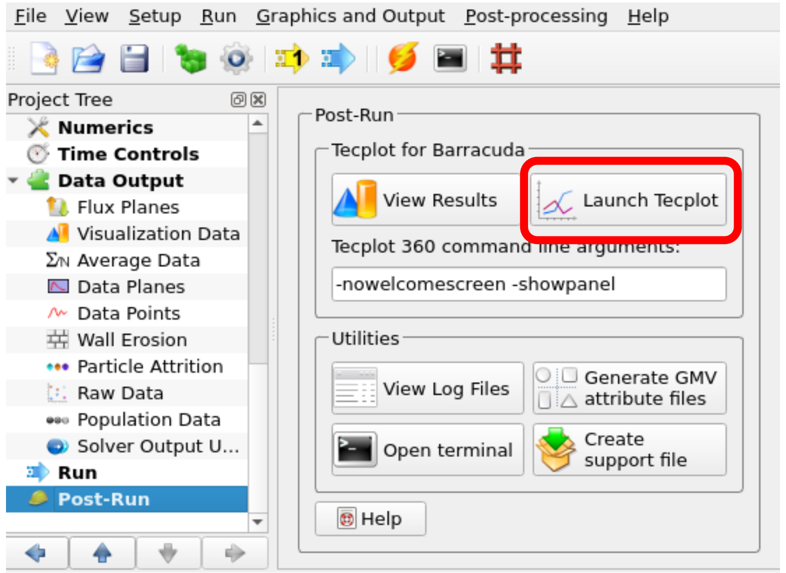
- File → Load Barracuda Data → Load Data Files → mass.log

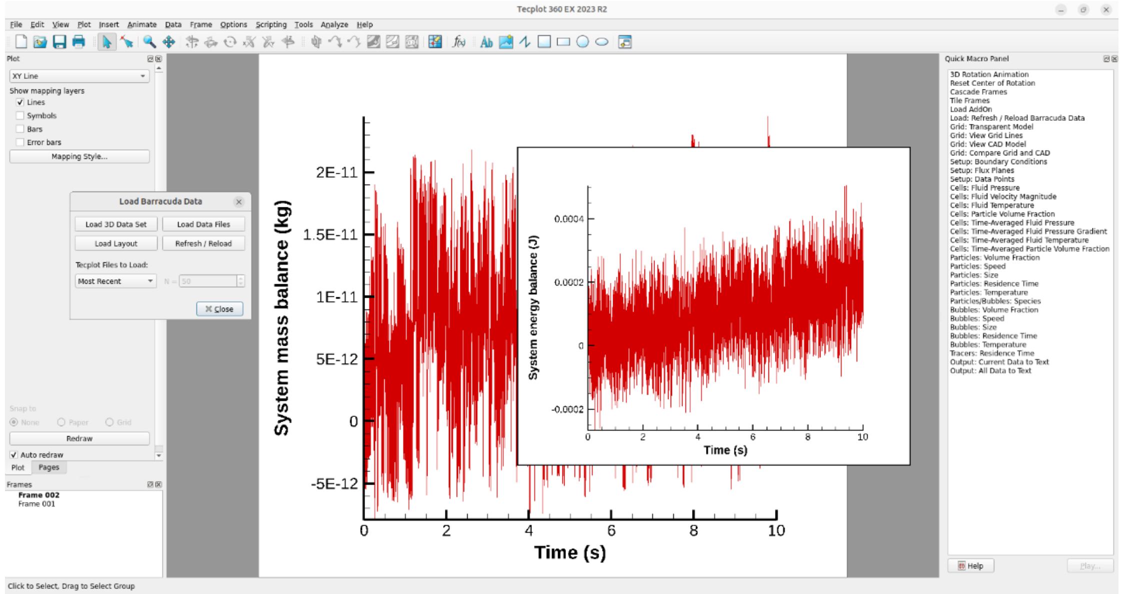
Create a new frame in Tecplot

- Frame → Create New Frame
- Click-and-drag to define a box for the new frame

Read energy.log into the new frame

- File → Load Barracuda Data → Load Data Files → energy.log





Detailed Steps for Creating Plot

Copy the mass.log frame and paste it twice

- Click the edge of the mass.log frame
- Copy using Ctrl+C
- Paste twice using Ctrl+V twice

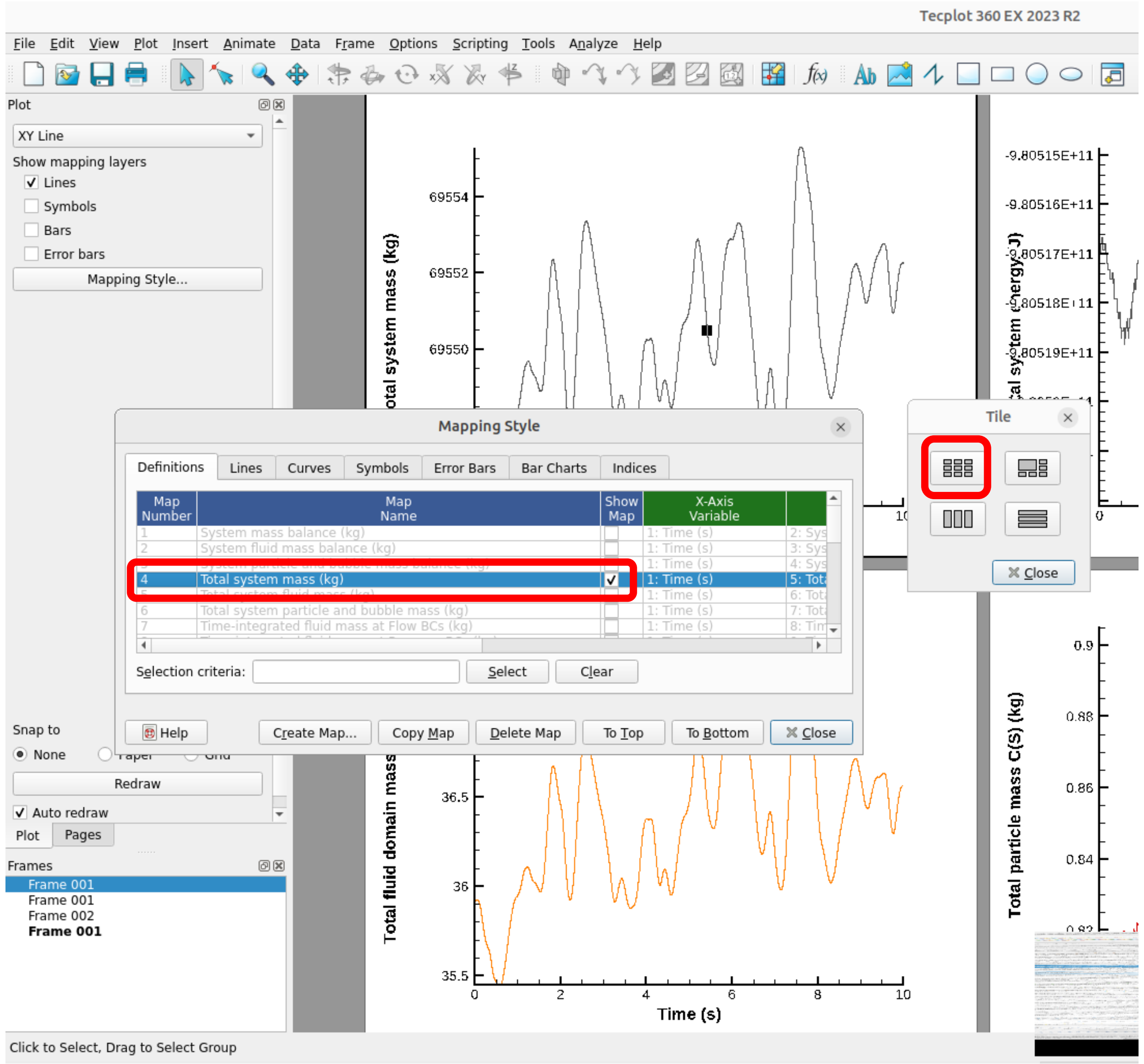
Tile the frames into a 2x2 grid

- Frame → Tile Frames → Tile for best square frames

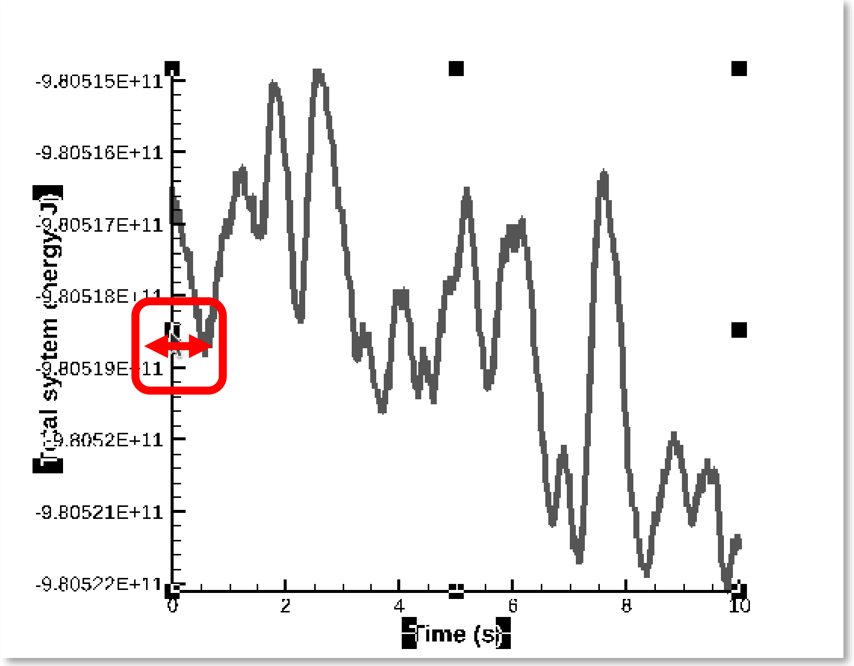
Select the desired data for each frame

- Mapping Style (or double-click the plotted data) → Select the desired map from the list

Auto-scale the view in each frame using Ctrl+F



Detailed Steps for Creating Plot

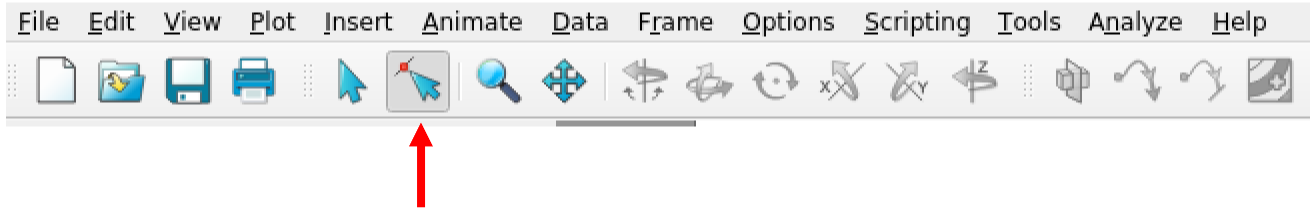


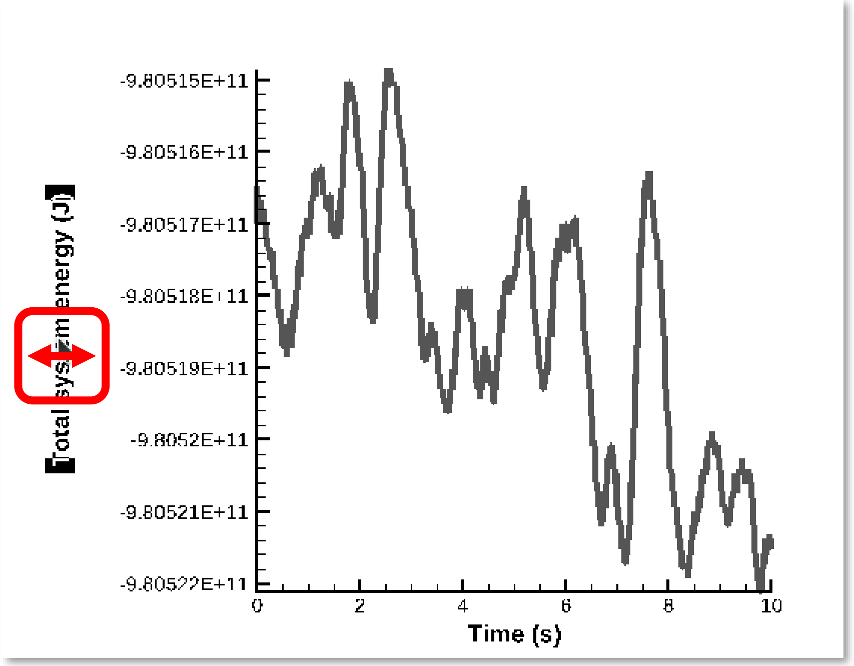
Increase line thicknesses if you'll be exporting an image with anti-aliasing

- Mapping Style → Lines → Line Thickness → 0.80%

Adjust the "Total System Energy" plot so that the y-axis title is not obscured

- Click and drag the y-axis to the right
- Use the "Adjust tool" to grab the y-axis title and drag it left

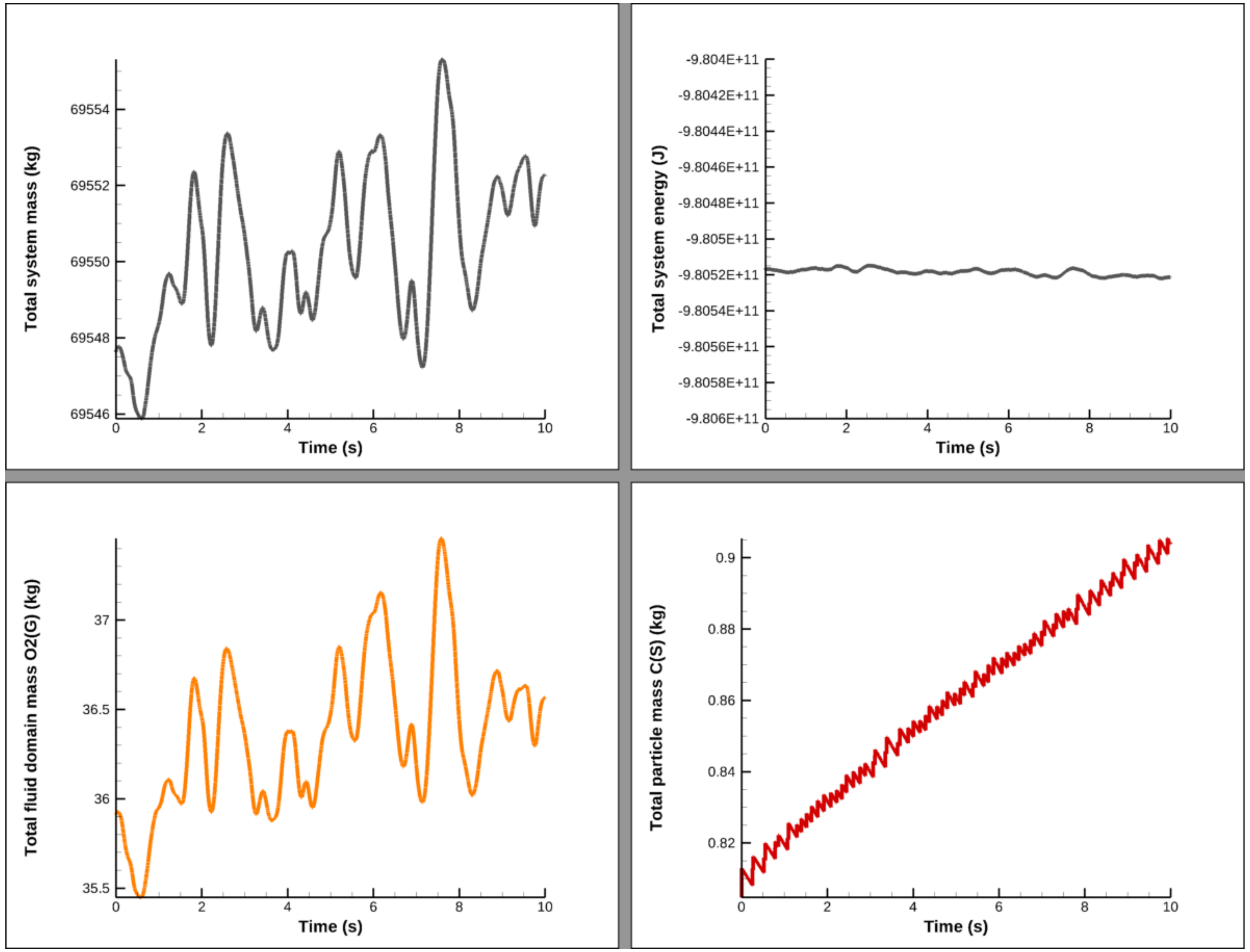




Final Plot of Data from mass.log and energy.log

Total system mass is relatively constant at about 69,550 kg

Total mass of O_2(G) in the fluid phase is about 36.5 kg



Total system energy is relatively constant at about -9.8e+11 J

Mass of C(S) is increasing over the simulation's 10 second run time

Advanced Post-Processing Topics

Presented by Scott Fowler, Tecplot, Inc.

tecplot® for BARRACUDA VIRTUAL REACTOR®

Q&A

We welcome your questions

For more information

- Visit our website: https://cpfd-software.com
- Follow CPFD on LinkedIn: https://www.linkedin.com/company/cpfd-software/
- Email: info@cpfd-software.com
- Phone: +1-713-429-1252