Advanced Post-Processing Workshop

Barracuda Virtual Reactor Users' Conference

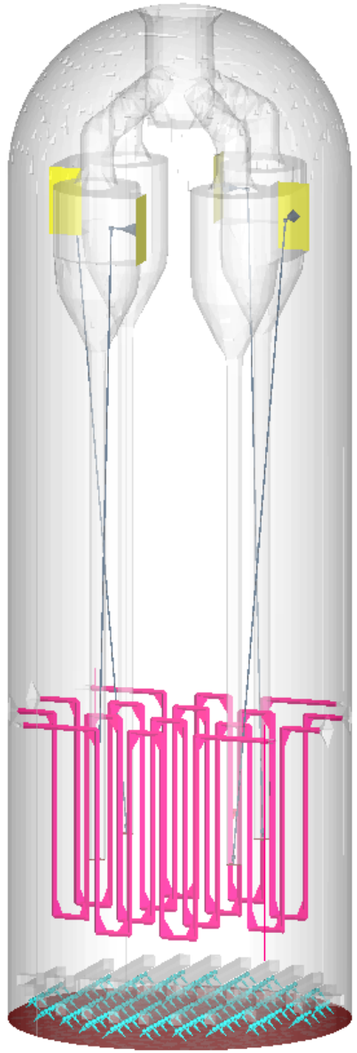
October 1, 2015

Santa Ana Pueblo, New Mexico

Outline

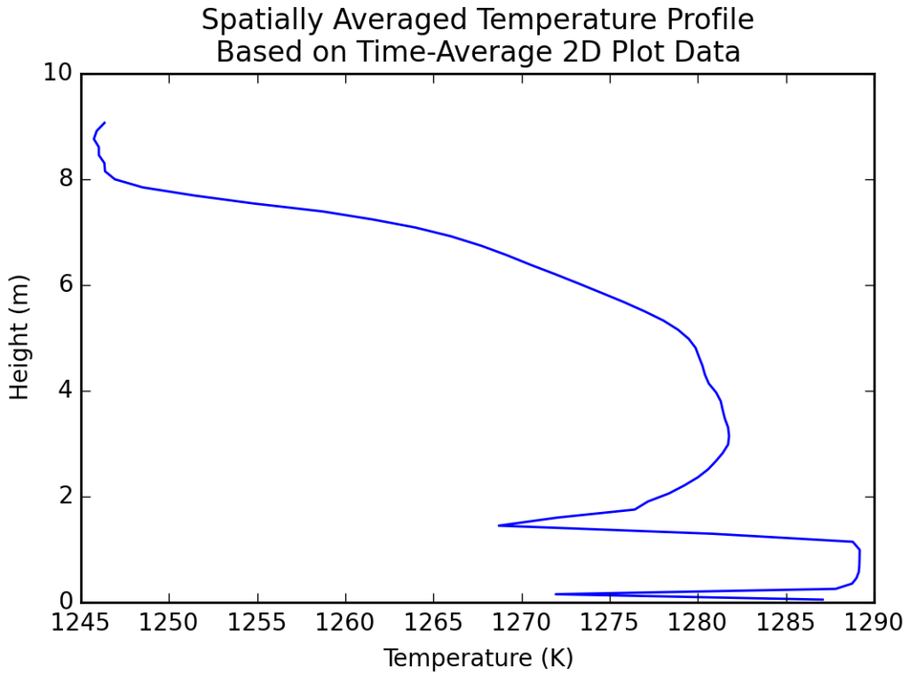
Introduction to Example Simulation: Wednesday Gasifier

- From Barracuda VR Training Course
  - Coal gasification example
  - Chemistry: 9 volume-average chemical reactions from open literature
  - Thermal: flow streams at various temperatures, and heating coils within fluidized bed
  - Multiple multi-material particle species
    - Initial char bed
    - Fresh coal feed



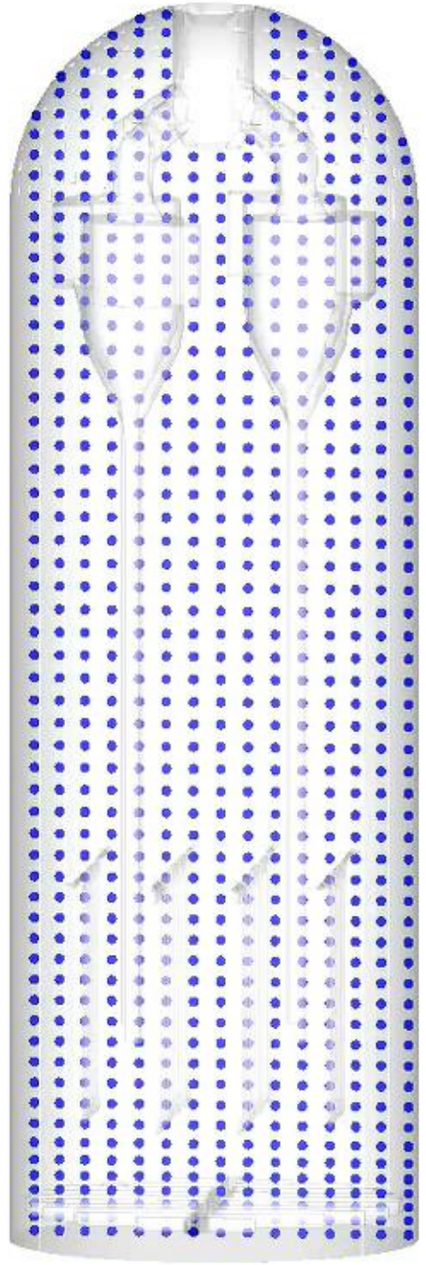
Goal 1: Plot Profile of Temperature vs Height

- Achieving Goal 1: Using 2D Plot Data
  - Introduction to 2D Plot Data
  - Creating a basic 2D data plot using Plot Manager
  - Calculating a spatially-averaged temperature profile using Python

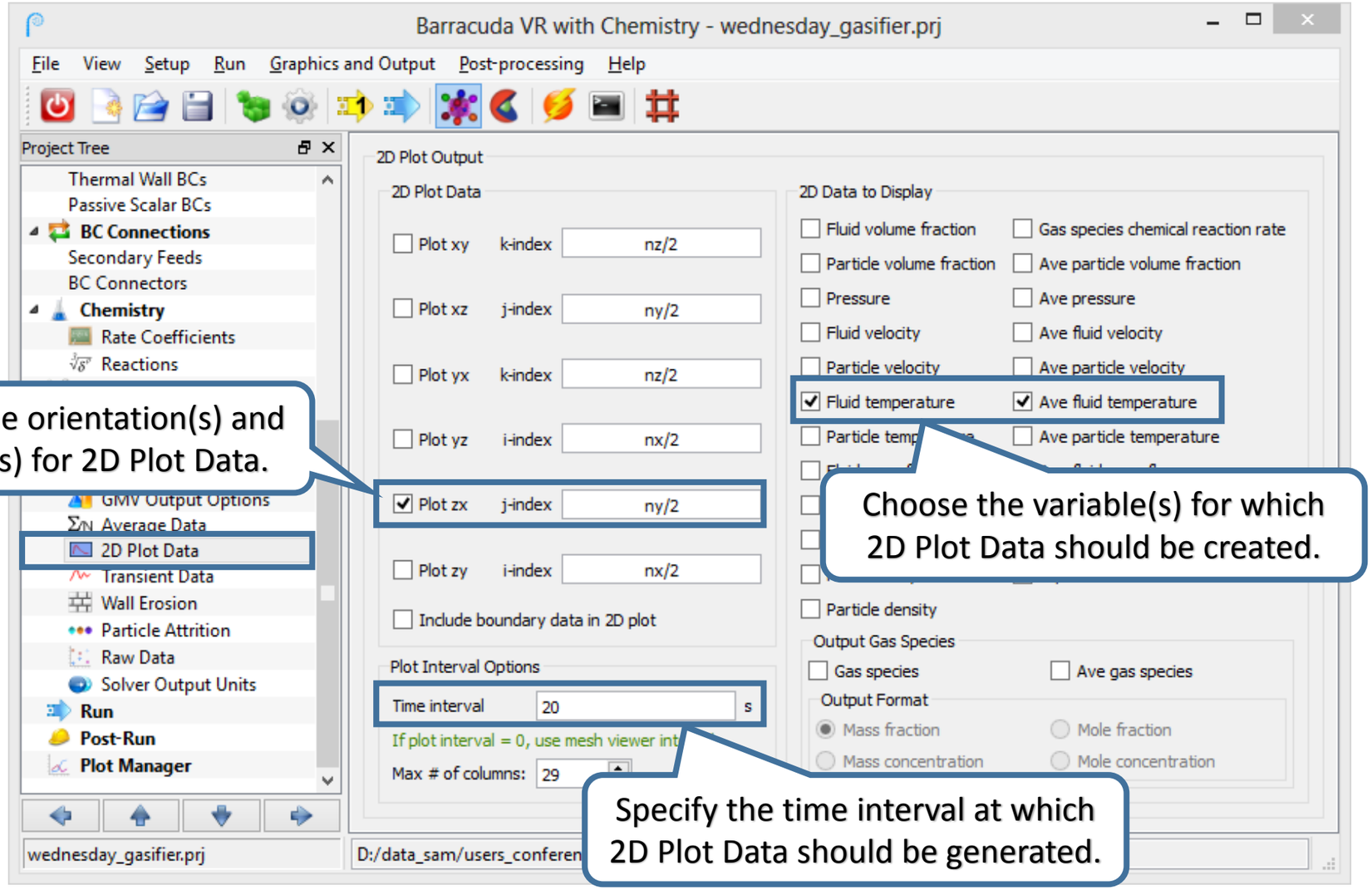


What is 2D Plot Data?

- 2D Plot Data gives you information about a selected variable over an entire plane within the simulation domain.
- 2D Plot Data is available for many variables, including instantaneous and time-average:
  - Particle volume fraction
  - Pressure
  - Fluid velocity
  - Fluid temperature
  - Many more…
- 2D Plot Data is output at a user-specified time interval during a simulation.

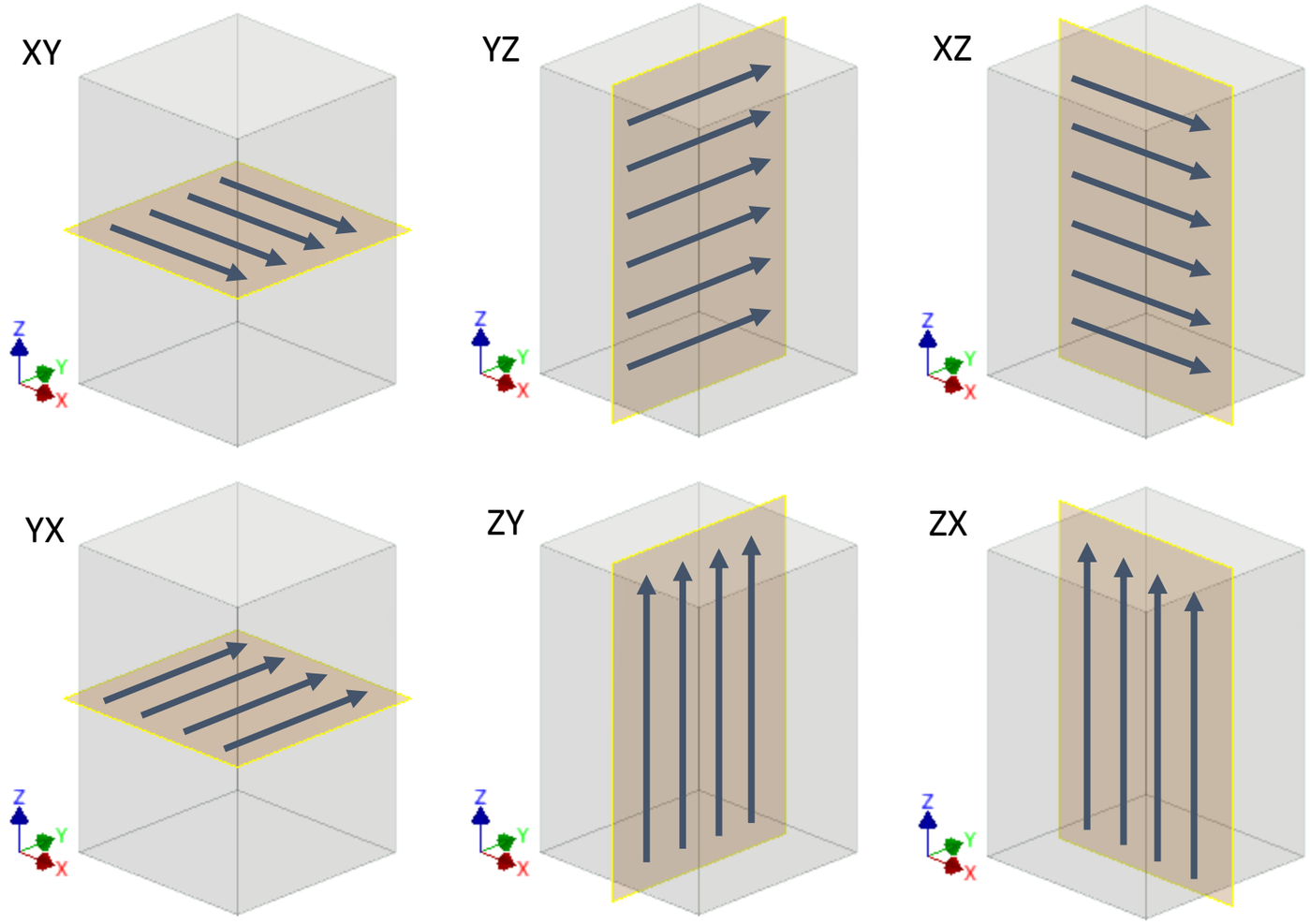


How to Enable Output of 2D Plot Data



Choosing the 2D Plot Data Orientation

- 2D Plot Data can be output in any combination of the 6 orientations shown at right.
- Choosing the correct orientation can make data processing much easier.
- The arrows indicate the arrangement of data columns in output files.



Output Format of 2D Plot Data

- Each 2D Plot Data file contains text data in space-separated columns

This example is a "zx" 2D Plot Data file. It covers a y-plane.

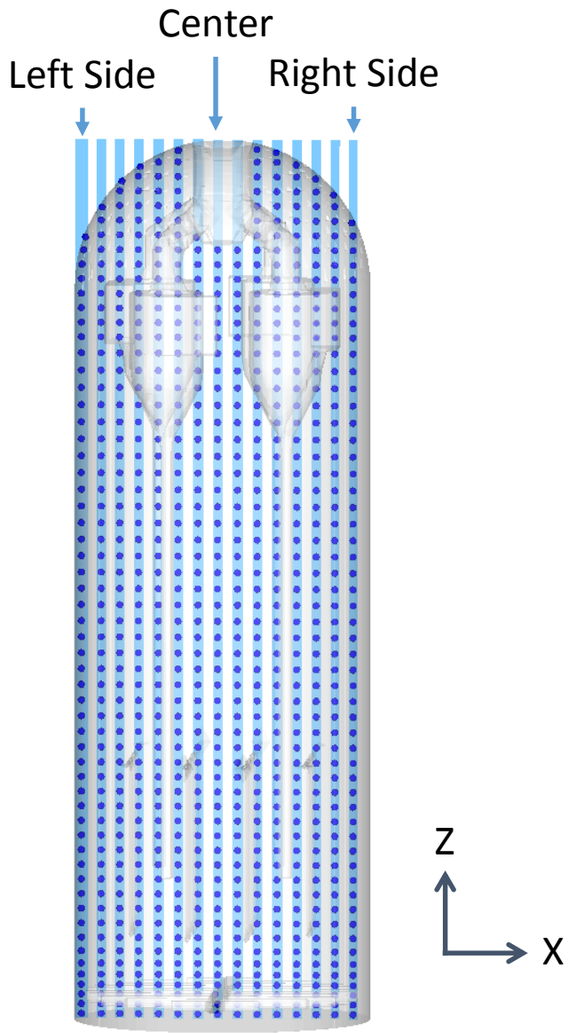
The data is fluid temperature.

"zx" means the first data column has z-values, and subsequent columns hold data at evenly-spaced x-positions.

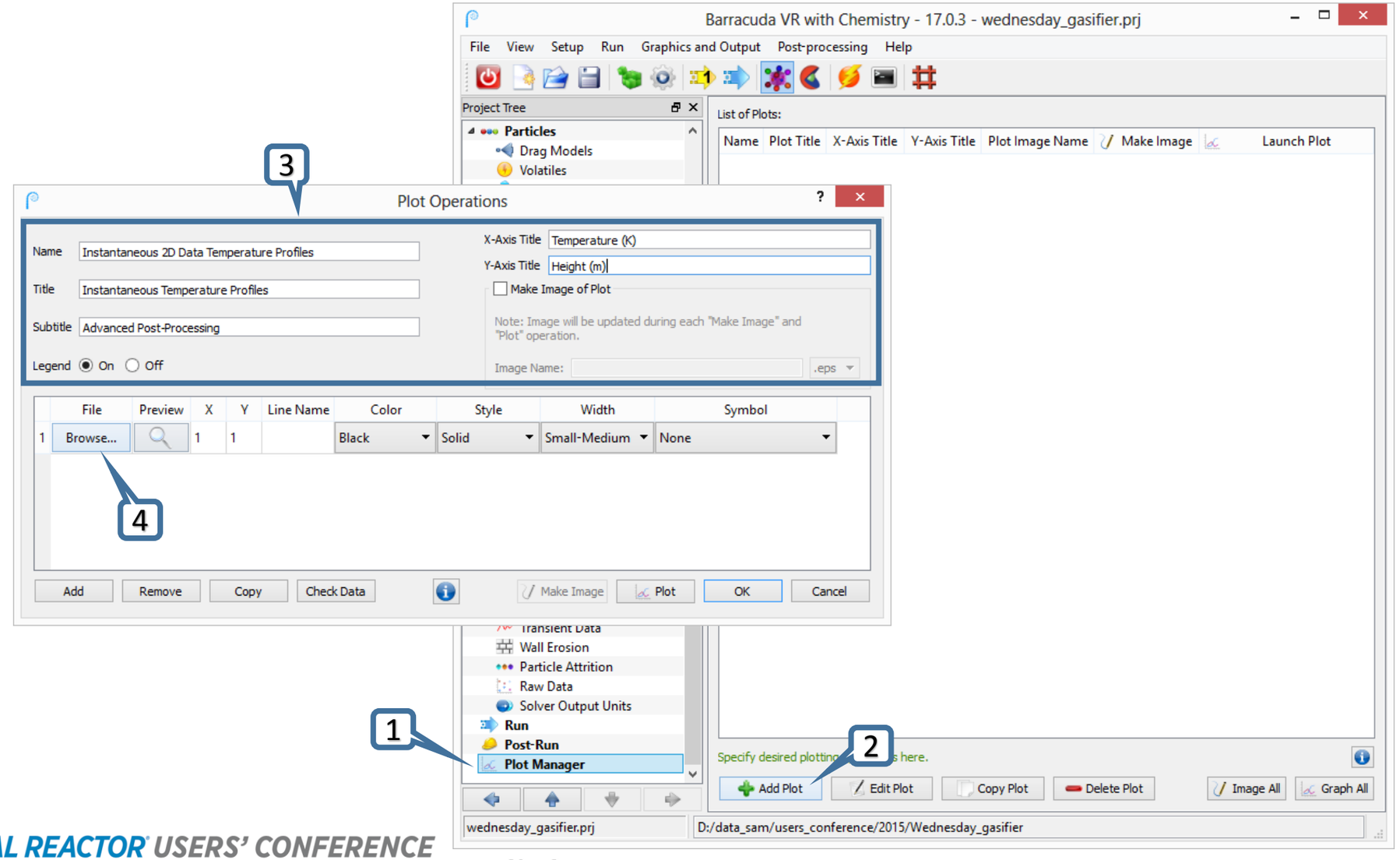
```
# Time =  2.00015e+01 (s)
# y = -1.52578e-03 (m) (j=17)
# First column z-distance (m). Following columns are temperature (K) at x-locations
#  1 z
#  2 x=-1.45617e+00m (i= 1)
#  3 x=-1.25138e+00m (i= 3)
#  4 x=-1.06082e+00m (i= 5)
#  5 x=-8.66964e-01m (i= 7)
#  ... more column headers ...
5.109293e-02 1.300826e+03 1.303385e+03 1.303440e+03 ... more columns of data ...
1.532788e-01 1.299528e+03 1.301458e+03 1.300700e+03 ... more columns of data ...
2.543134e-01 1.299502e+03 1.301873e+03 1.301868e+03 ... more columns of data ...
3.544176e-01 1.298454e+03 1.301121e+03 1.301696e+03 ... more columns of data ...
4.597586e-01 1.297426e+03 1.294514e+03 1.301106e+03 ... more columns of data ...
5.756338e-01 1.296742e+03 1.294430e+03 1.299496e+03 ... more columns of data ...
7.030965e-01 1.296732e+03 1.296648e+03 1.298808e+03 ... more columns of data ...
8.433054e-01 1.296276e+03 1.300004e+03 1.297590e+03 ... more columns of data ...
... more rows of data ...
```

Plot Temperature Profiles at Left Side, Center, and Right Side

- Using 2D Plot Data output files, we will plot instantaneous and time-average temperature profile curves.
- We will plot data at **t = 100 s**.
- To visualize the temperature variation across the reactor, we will plot profiles at the **Left Side**, **Center**, and **Right Side** of the vessel.

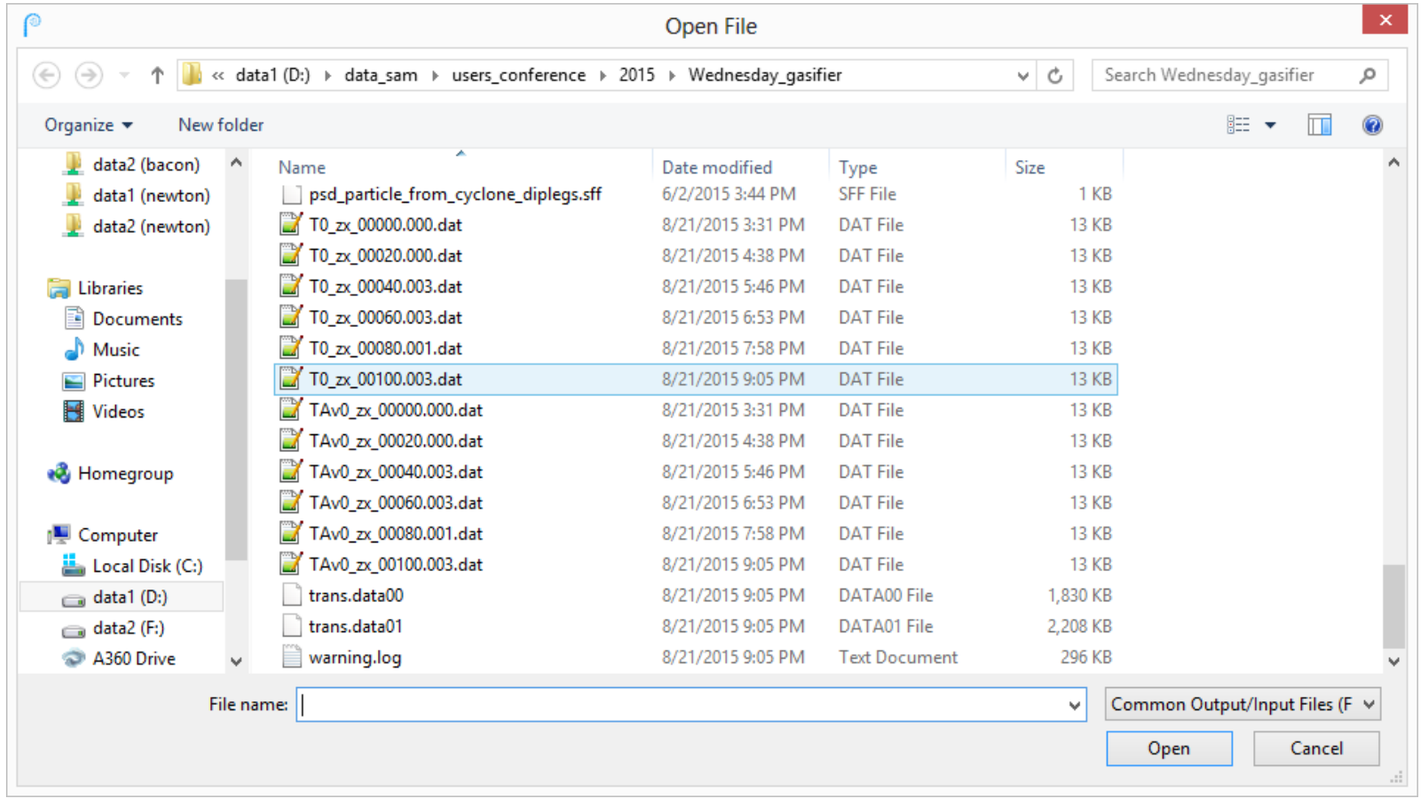


Use Plot Manager in the Barracuda VR GUI



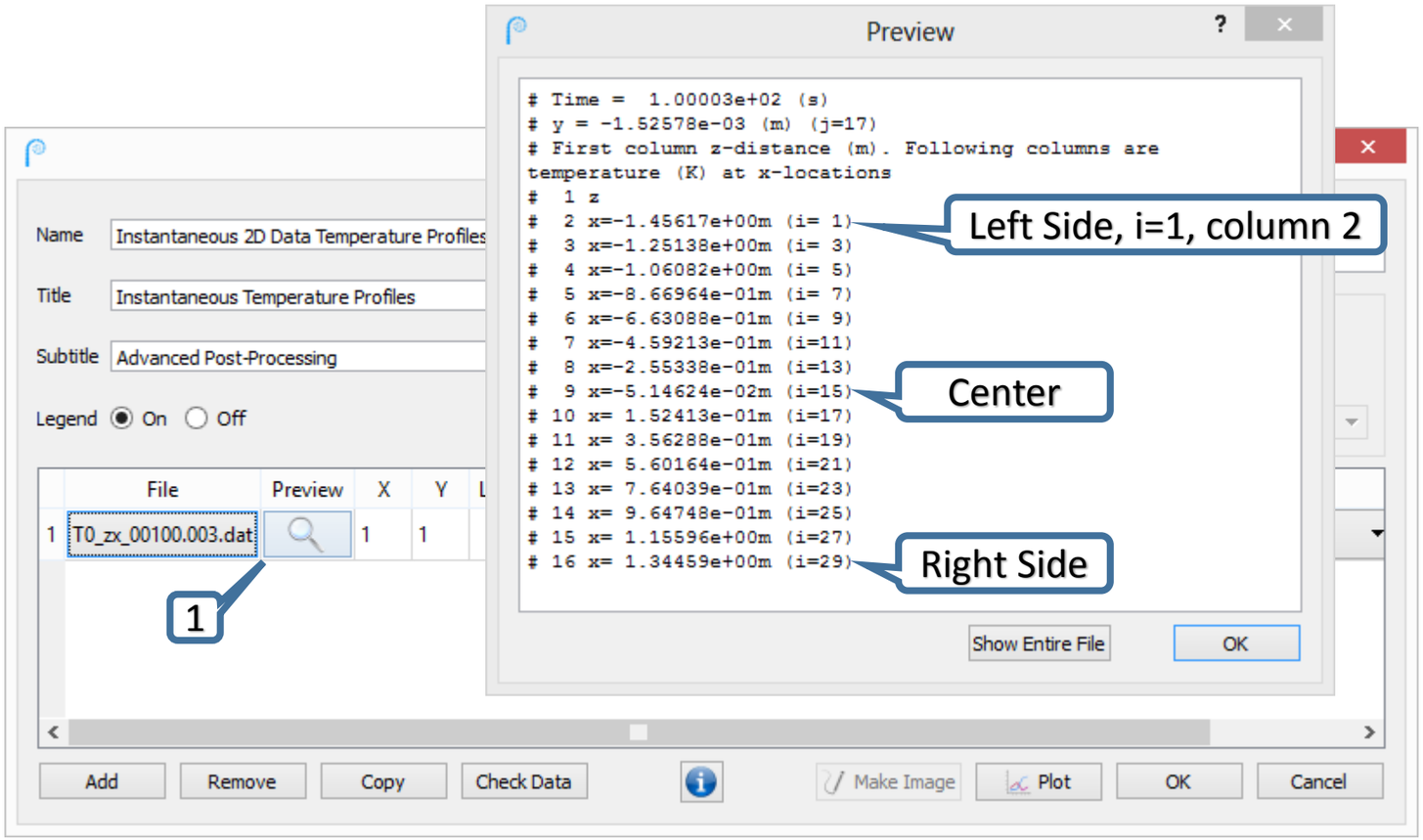
Select the Instantaneous Fluid Temperature File at t=100 s

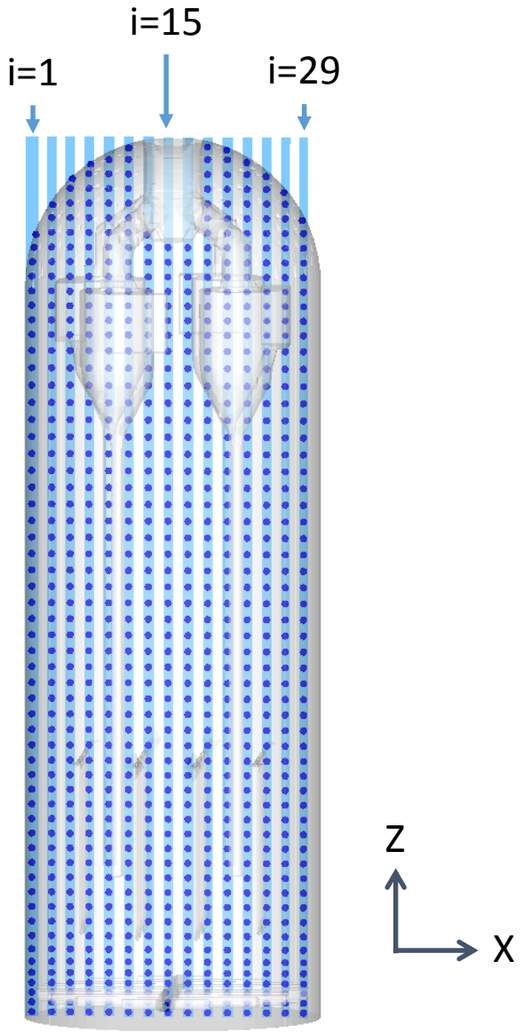
- Note the file naming convention:
  - **T0** indicates instantaneous fluid temperature data.
  - The simulation time, t = **100.003** s, is embedded in the file name.
- A table listing all 2D Plot Data output file names is available in the Barracuda User's Manual



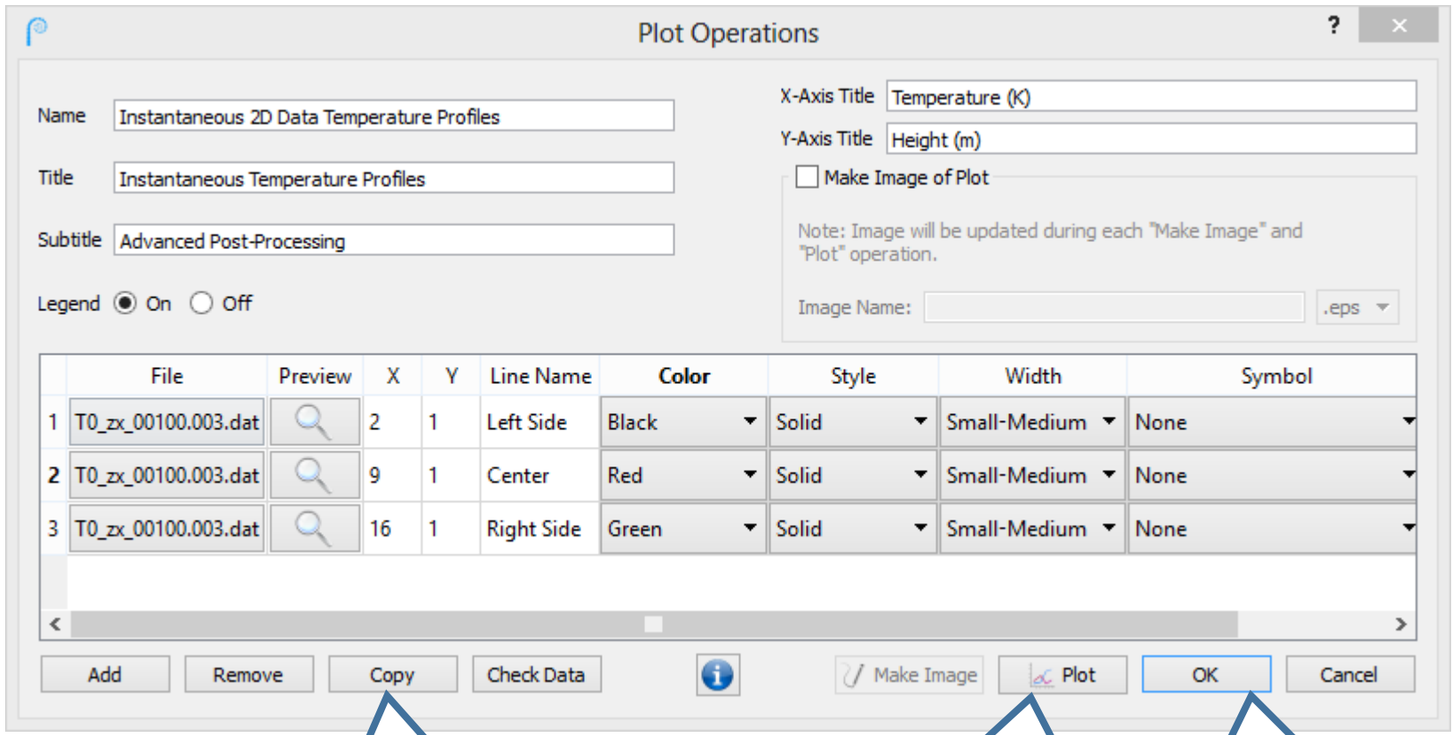
Use Preview to Choose Data Columns for Plotting

- The **Preview** button quickly displays the header section of a data file.





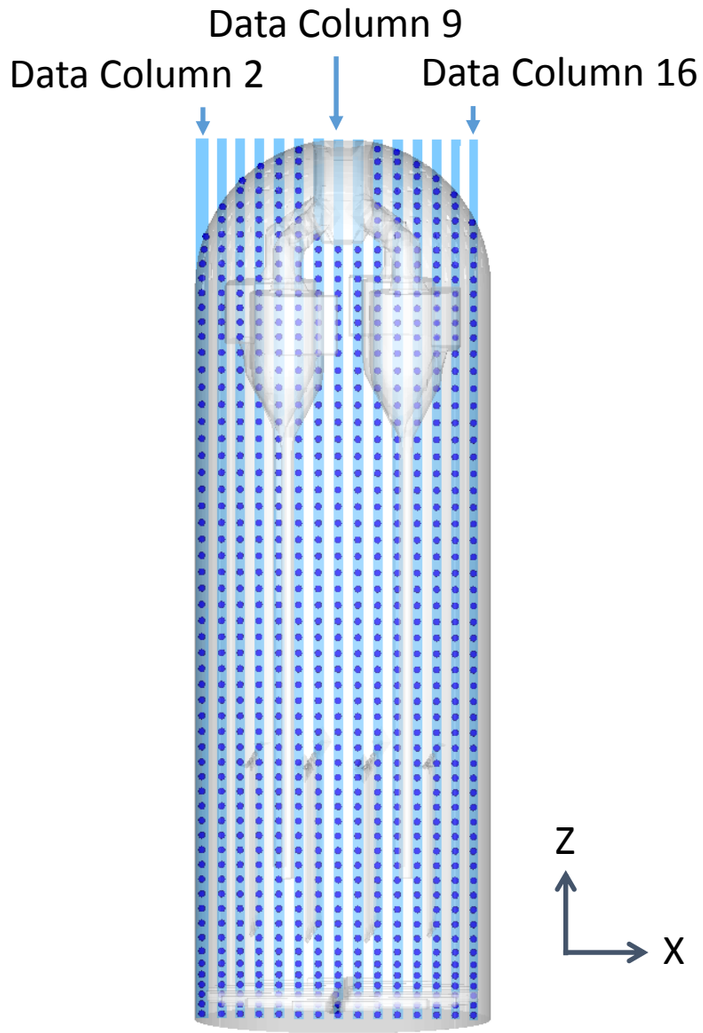
Define the X and Y Columns for Plotting



Use the **Copy** button to create rows 2 and 3

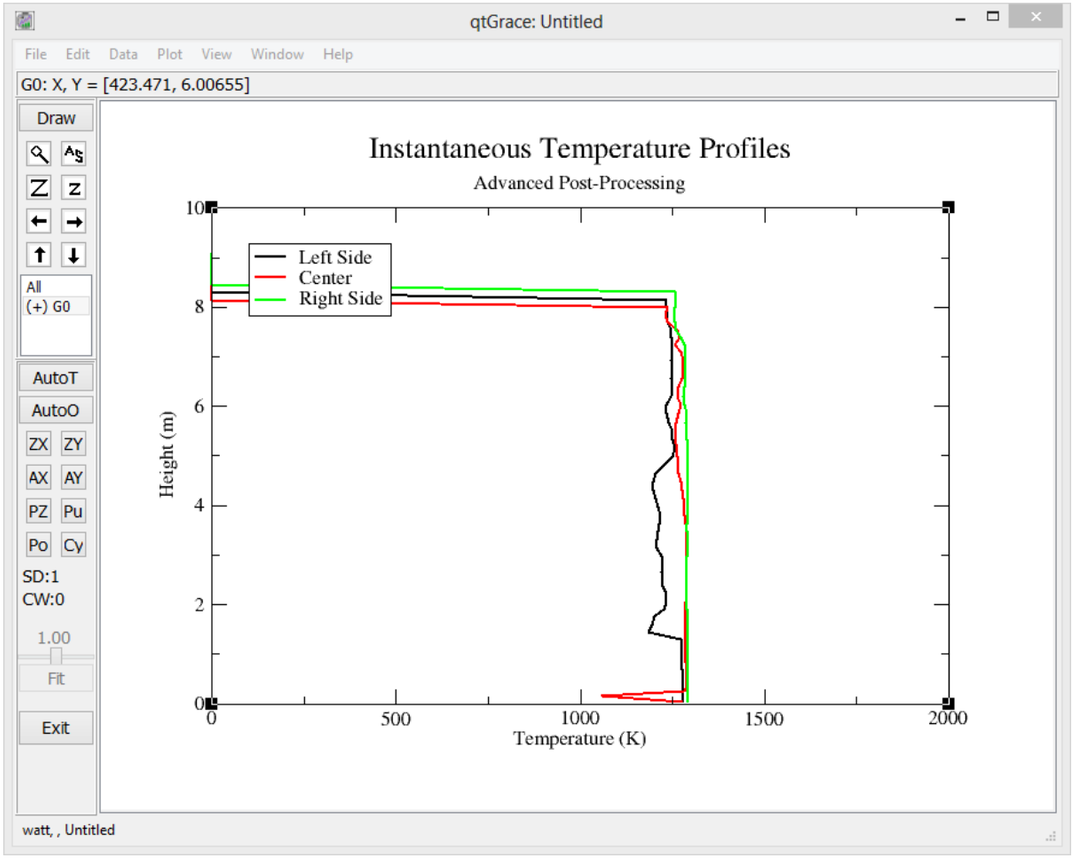
Click **Plot** to launch the plotting utility (Xmgr / qtGrace)

Click OK to exit the **Plot Operations** dialog



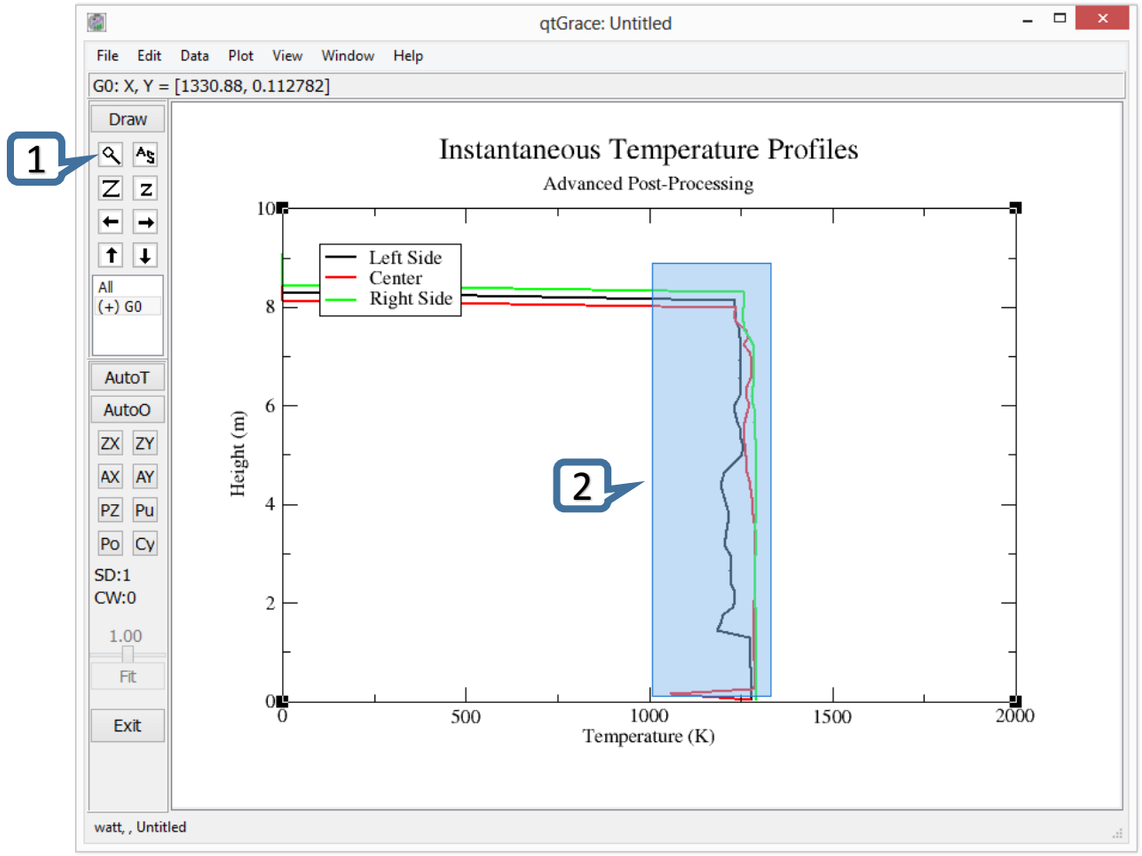
Interpreting the 2D Plot Data Instantaneous Temperature Profile

- Three curves are plotted, as defined in the **Plot Operations** dialog.
- Values of **0** or **-1** are reported for null cells.
- A low-temperature spike is seen in the **Center** profile, corresponding to the steam sparger Injection BC.



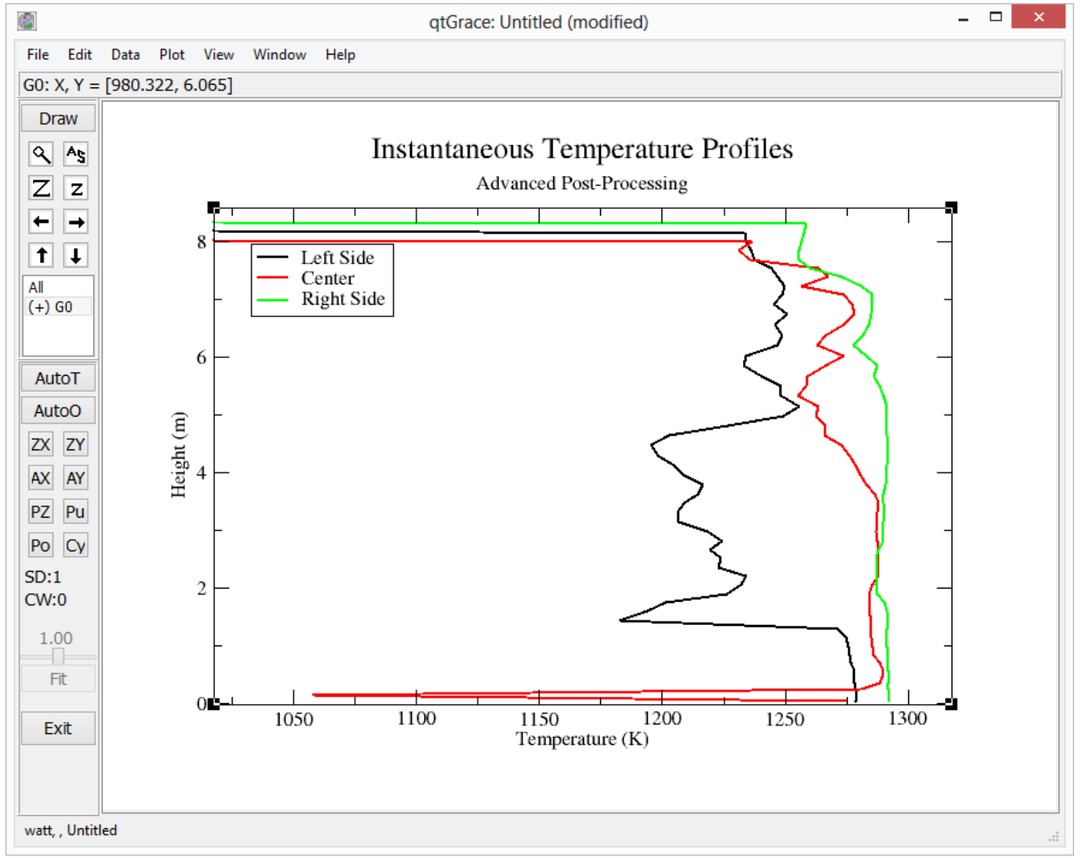
Use the Zoom Tool to Select a Smaller Region for Plotting

- The 0 and -1 values are not valid temperature data. We want to focus on the temperature region above T = 1000 K.
- Click the **Zoom** tool (magnifying glass)
- Draw a rectangle around the region of interest.
- You can specify exact x- and y-ranges using "World Scaling"
  - On Windows: Plot → Graph Appearance → Viewport
  - On Linux: Plot → World scaling



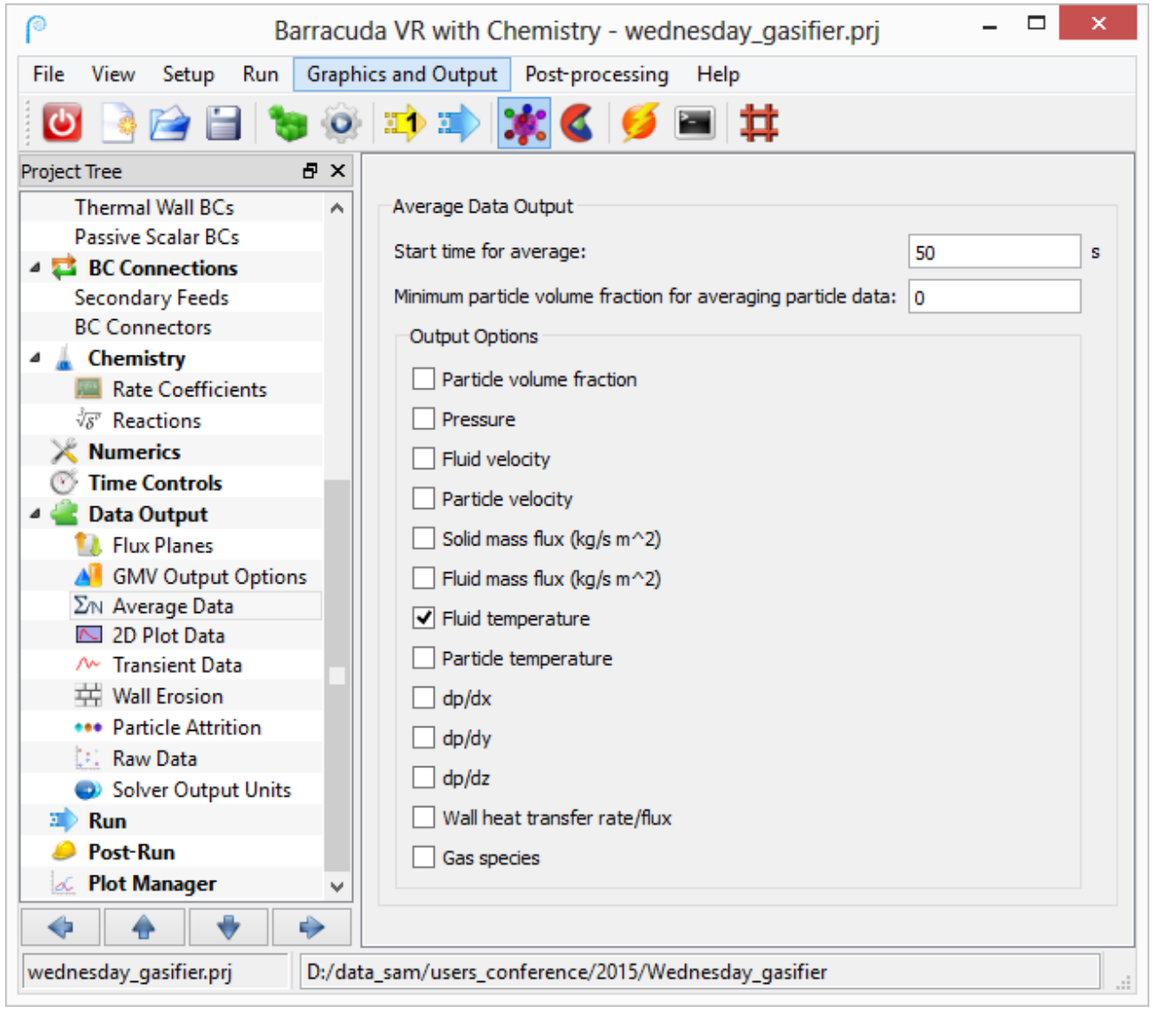
Final View of Instantaneous Fluid Temperature (2D Plot Data)

- The **Center** curve has a low-temperature spike at the location of the steam sparger.
- The **Left Side** is at the lowest temperature in the upper portion of the vessel.
  - Devolatilization of fresh coal feed (endothermic)
  - The Center and Right Side are hotter, and more uniform from top to bottom.



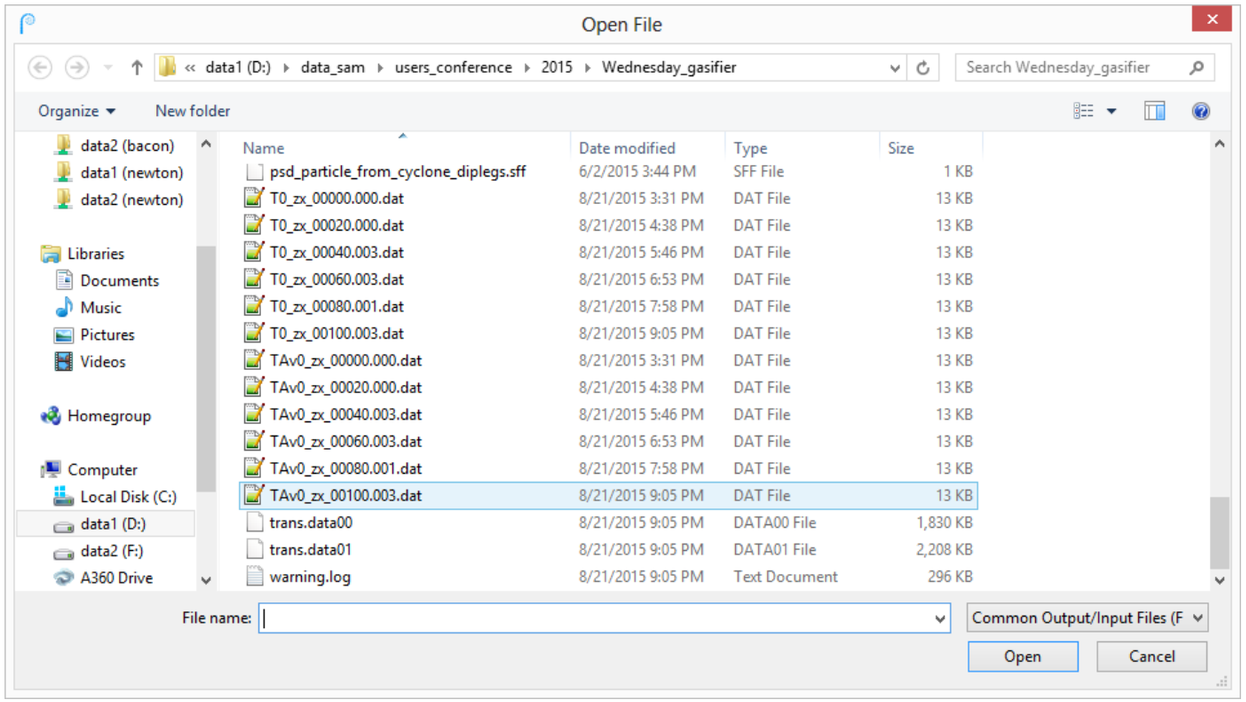
Time-Averaged Temperature Profiles from 2D Plot Data

- Previous plot was **instantaneous** data at **t = 100 s**.
- In this simulation, **time averaging** was started at **t = 50 s**.
- Time-average data is often very useful in Barracuda VR simulations, because it can better represent “steady state” behavior.



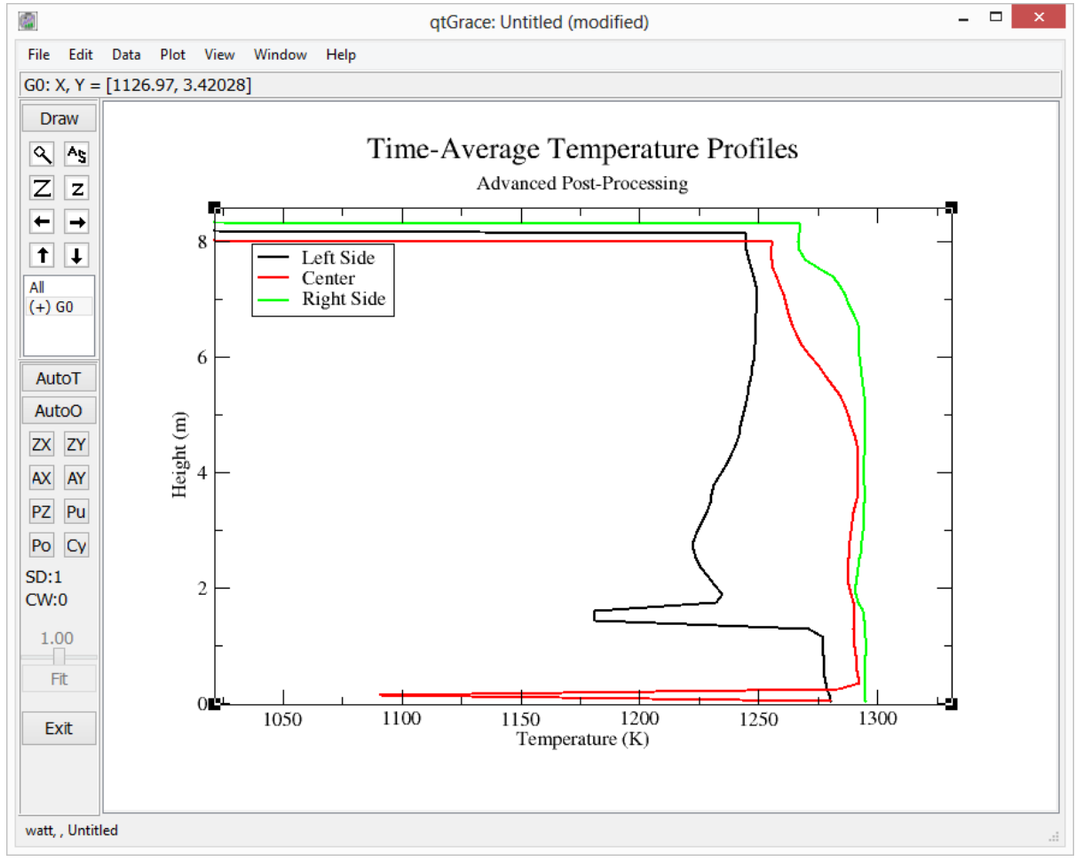
Select the Time-Average Fluid Temperature File at t=100 s

- Use the **Plot Manager** procedure from previous slides and choose **time-average file** instead of **instantaneous file**
- Note the file naming convention:
  - **TAv0** indicates time-average fluid temperature data.
  - The simulation time, t = **100.003** s, is embedded in the file name.
- Use the **Copy** feature in **Plot Manager**, since this plot is very similar to the previous one.



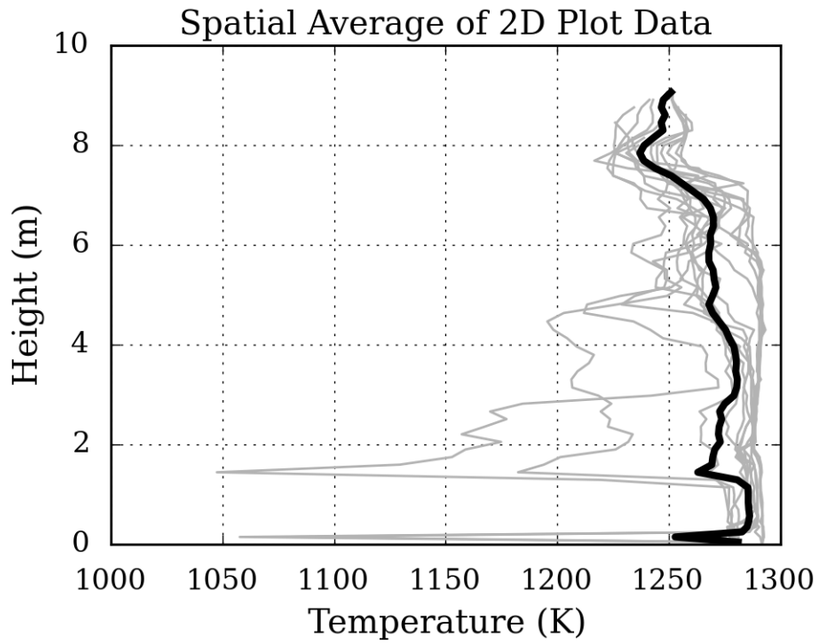
Final View of Time-Average Fluid Temperature (2D Plot Data)

- Lines are more smooth than instantaneous data (as expected).
- **Left Side** is still showing a lower temperature than **Center** and **Right Side**.
- When plotting 2D Data:
  - Values of 0 and -1 are reported for null cells.
  - Use the Zoom feature (magnifying glass) to select the region of interest.



When **Plot Manager** is not enough

- More complex data analysis may require using a different tool
- Spatial averaging of multiple columns of 2D Plot Data is not supported in **Plot Manager**
- There are many options for approaching this task, including:
  - Excel
  - Matlab
  - Mathematica
  - Ensight
  - Python

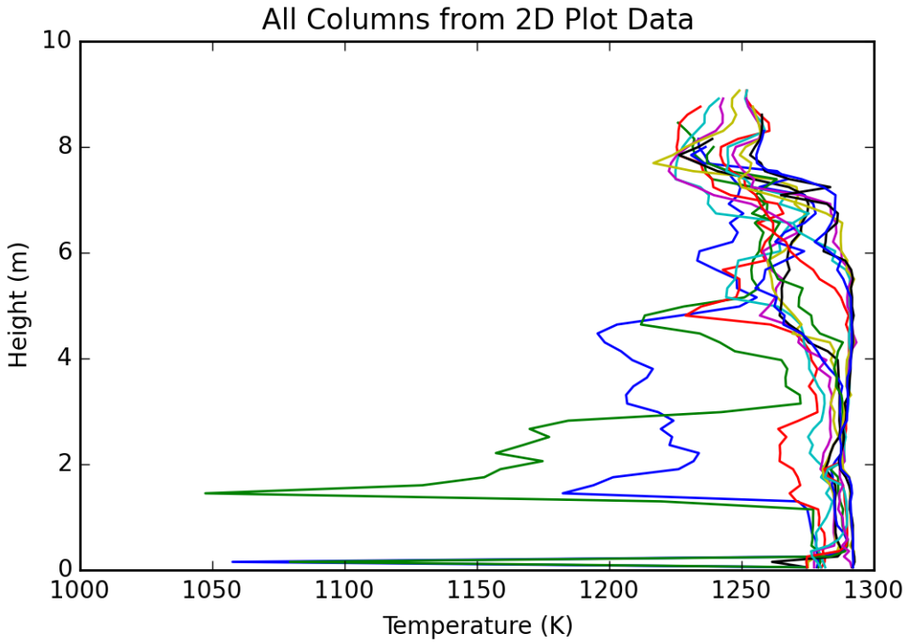


About Python

- Python is a programming language that is popular among engineers and scientists due to its numerical analysis capabilities.
- Python can be freely downloaded. The distribution we recommend is from http://continuum.io/downloads
- A great deal of information about Python is available online and in print
  - https://docs.python.org/3/
  - https://wiki.python.org/moin/PythonBooks

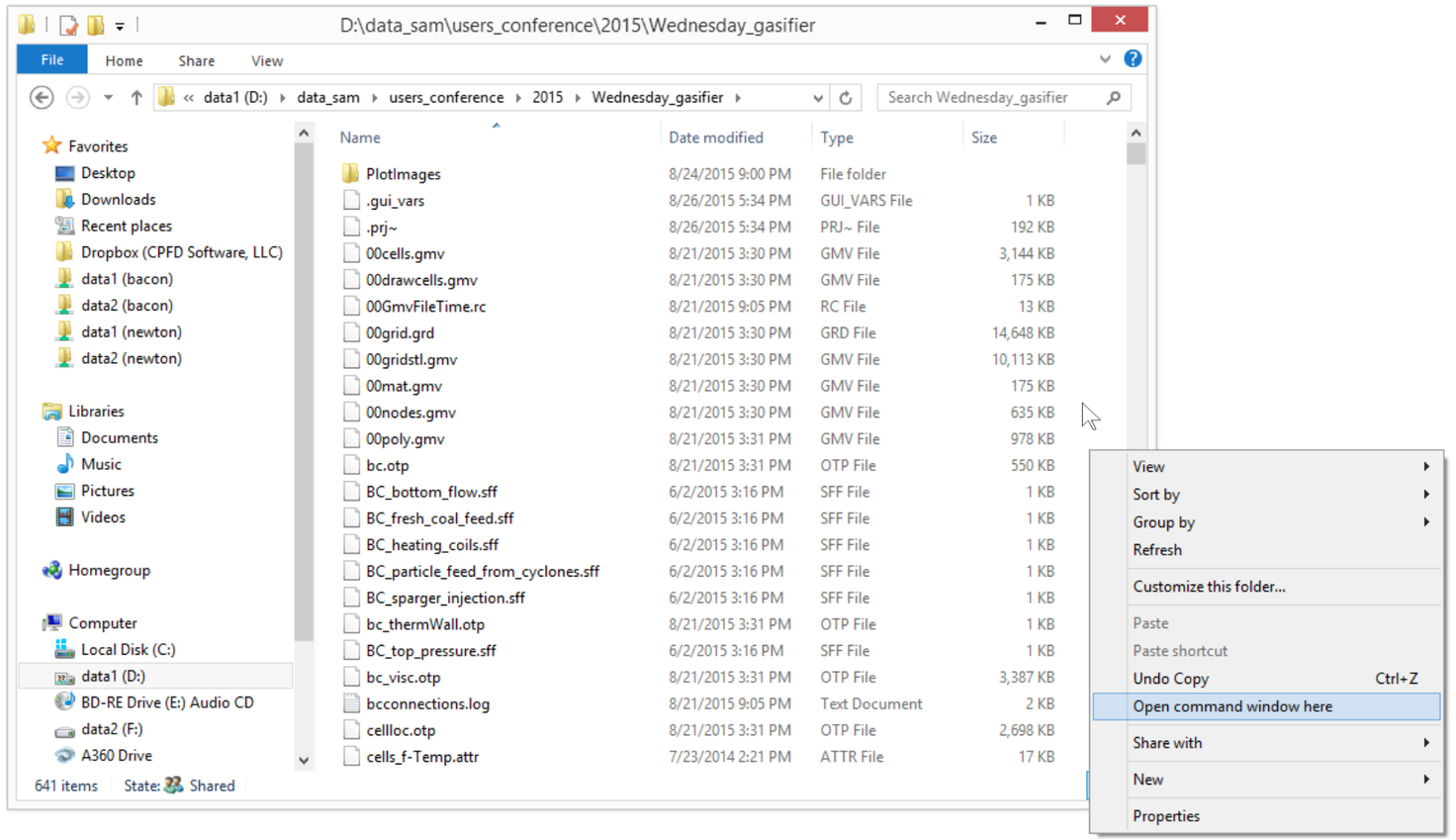
Calculating Spatial Averages from 2D Plot Data

- Previous plots were for specific x-locations.
- Sometimes it is desirable to calculate a single **spatially-averaged** profile based on all x-locations from the 2D Plot Data output file.
- The 2D Plot Data output file contains 15 columns of data at different x-positions.
- We will calculate a “simple-minded” average of the values in the 2D data file. No weighting based on cell volumes.



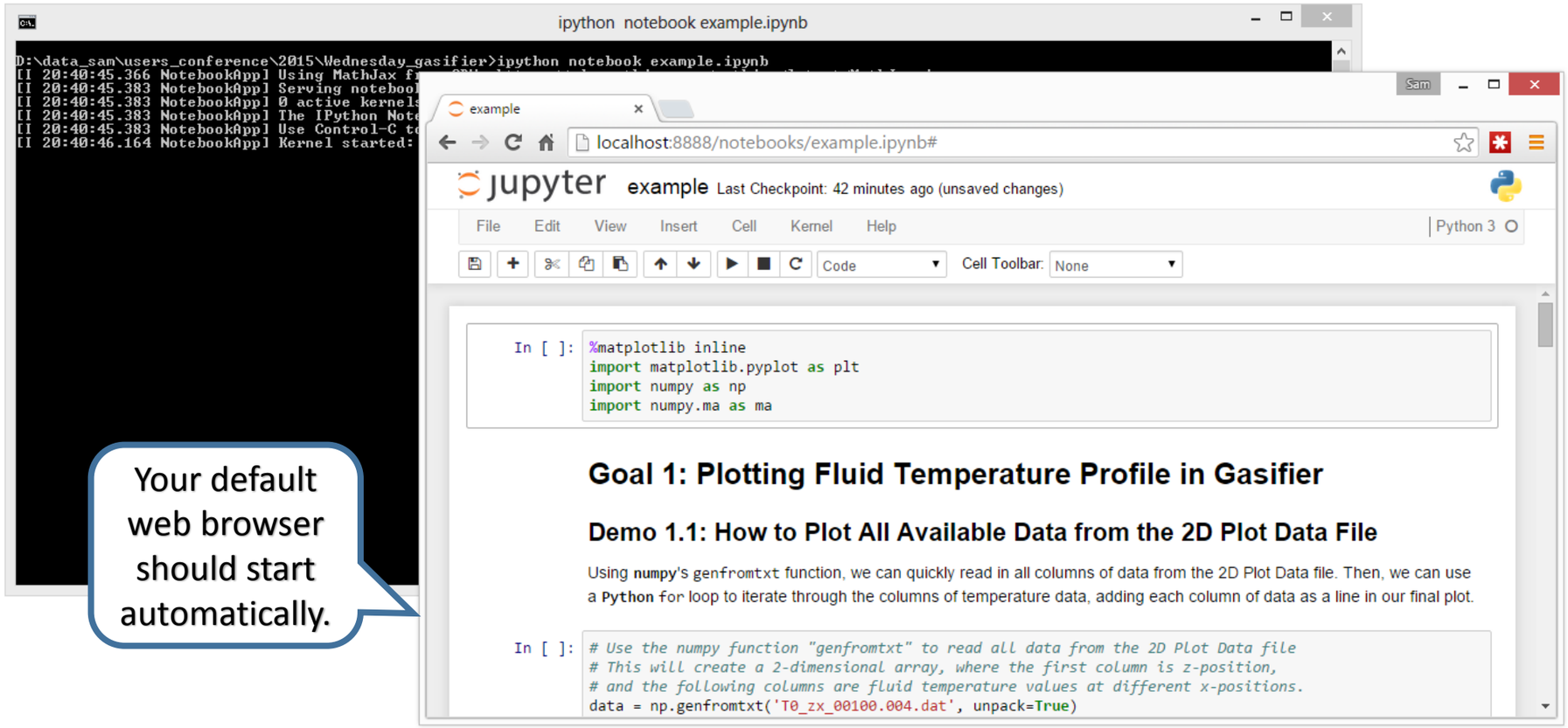
Open a Command Window in the Current Directory

- On Windows: Shift + Right-click → Open command window here
- On Linux: open a terminal in the normal way



Start the iPython Notebook Server

- In the command window, type:
  `ipython notebook example.ipynb`



Example iPython Notebook Overview

- The first cell has several import commands to bring in the functions we'll be using for reading data, creating plots, etc.

```
In [ ]: %matplotlib inline
        import matplotlib.pyplot as plt
        import numpy as np
        import numpy.ma as ma
```

Instead of remembering the exact syntax of the import commands, it is recommended that you keep a template somewhere on your system as a starting point for new iPython notebooks.

- Any additional Python modules you need can be imported similarly, and by convention should be imported at the top of the notebook.

Demo 1.1: Plotting All Data from a 2D Plot Data File

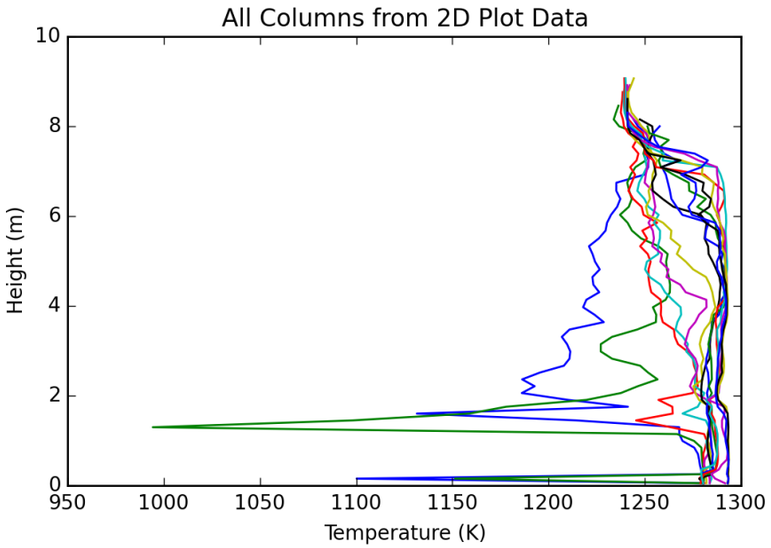
- The next cell shows how to plot all of the available data from the instantaneous 2D Plot Data file.

In [ ]:

```
# Use the numpy function "genfromtxt" to read all data from the 2D Plot Data file
# This will create a 2-dimensional array, where the first column is z-position,
# and the following columns are fluid temperature values at different x-positions.
data = np.genfromtxt('T0_zx_00100.004.dat', unpack=True)
numColumns = data.shape[0]

fig, ax = plt.subplots()
ax.set_title('All Columns from 2D Plot Data')
ax.set_xlabel('Temperature (K)')
ax.set_ylabel('Height (m)')

for i in range(1, numColumns):
    x = data[i]
    y = data[0]
    validData = (x > 0)
    ax.plot(x[validData], y[validData])

p = "all_data_columns_from_instantaneous_2d_plot_data"
fig.savefig(p + '.png', format='png', dpi=200)
```

Use this syntax whenever you want to start a new plot.

Add lines to the plot by using the ax.plot( ) command.

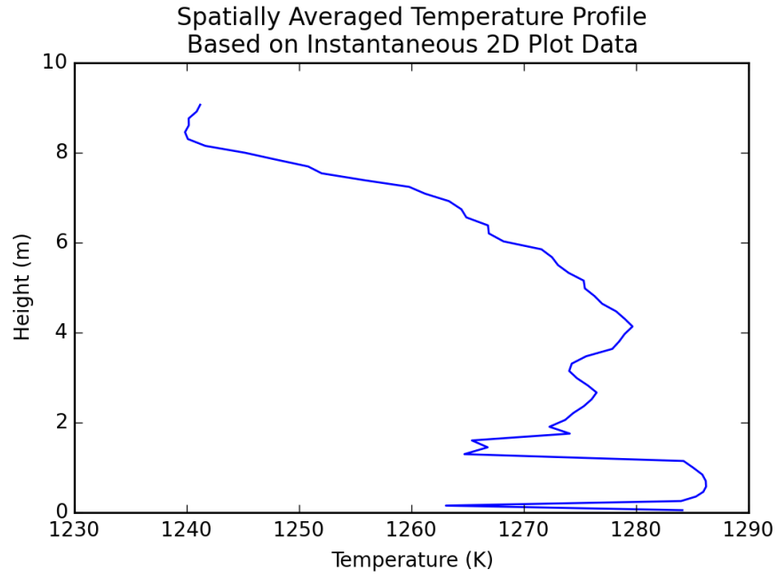


Demo 1.2: Calculating a Spatial Average of 2D Plot Data

- The next cell shows how to use a special feature of `numpy` called "masked arrays" to calculate a spatial average of the **instantaneous** 2D Plot Data for fluid temperature.

In [ ]:
```
# The vessel height is the first column of the 2-dimensional "data" array.
height = data[0]

# We can use numpy's *masked array* feature to calculate a spatial average
# and intentionally ignore values of 0 and -1 reported at null cells in
# Barracuda's 2D Plot Data output files.
x = ma.masked_less_equal(data[1:], 0)
averageTemperature = ma.average(x, axis=0)

fig, ax = plt.subplots()
ax.set_title('Spatially Averaged Temperature Profile\nBased on Instantaneous 2D Plot Data')
ax.set_xlabel('Temperature (K)')
ax.set_ylabel('Height (m)')
ax.plot(averageTemperature, height)

p = "spatial_average_of_instantaneous_2d_plot_data"
fig.savefig(p + '.png', format='png', dpi=200)
```

These two lines calculate the spatial average, ignoring values ≤ 0.

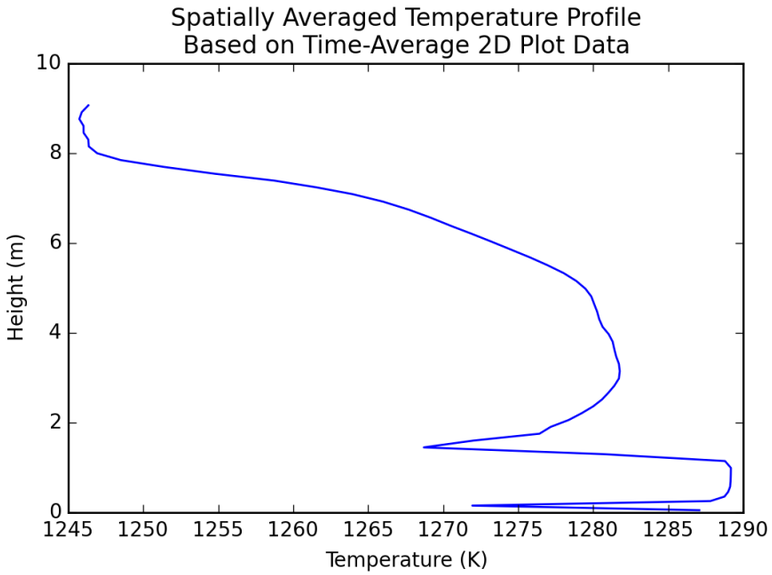


Demo 1.3: Spatial Average of Time-Average 2D Plot Data

- The next cell is very similar, but in this case we use the **time-average** 2D Plot Data file.

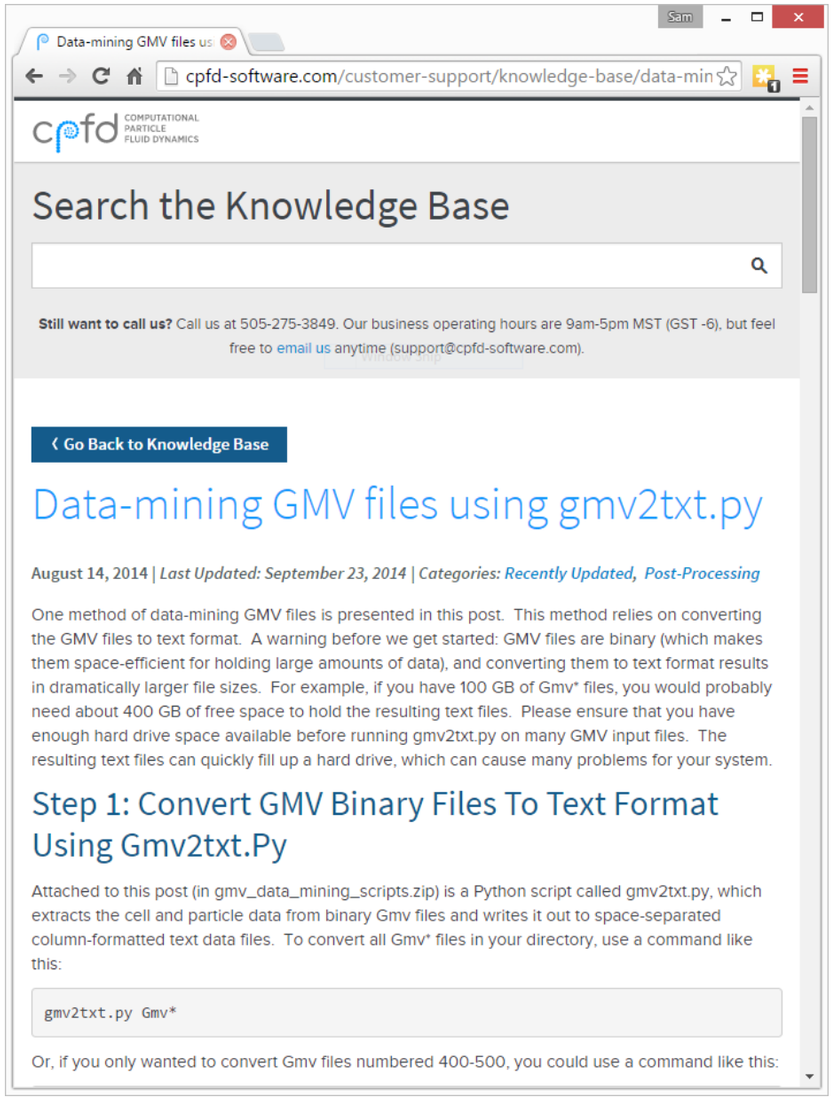
In [ ]:
```
# Following the principles above, we can calculate the spatial average
# for *time-average* temperature data.
data = np.genfromtxt('TAv0_zx_00100.004.dat', unpack=True)
height = data[0]
x = ma.masked_less_equal(data[1:], 0)
averageTemperature = ma.average(x, axis=0)

fig, ax = plt.subplots()
ax.set_title('Spatially Averaged Temperature Profile\nBased on Time-Average 2D Plot Data')
ax.set_xlabel('Temperature (K)')
ax.set_ylabel('Height (m)')
ax.plot(averageTemperature, height);

p = "spatial_average_of_time-average_2d_plot_data"
fig.savefig(p + '.png', format='png', dpi=200)
```

The file name passed to genfromtxt() is the only change.



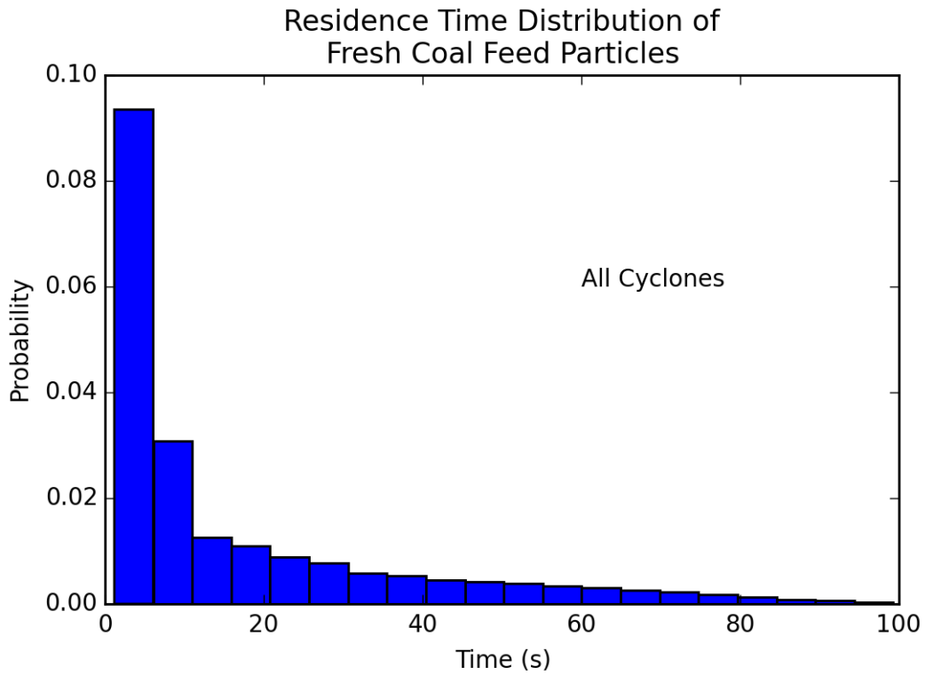
Further Reading for Better Spatial Averaging

- As stated previously, the spatial average calculated here using the 2D Plot Data is "simple-minded"
  - Numerical average of the data
  - No weighting based on cell size
  - Only uses data from one 2D plane
- More sophisticated methods are available for calculating spatial averages to address these shortcomings. One specific method is discussed in the CPFD Support Site post Data-Mining GMV Files Using gmv2txt.py. See this post for complete details.



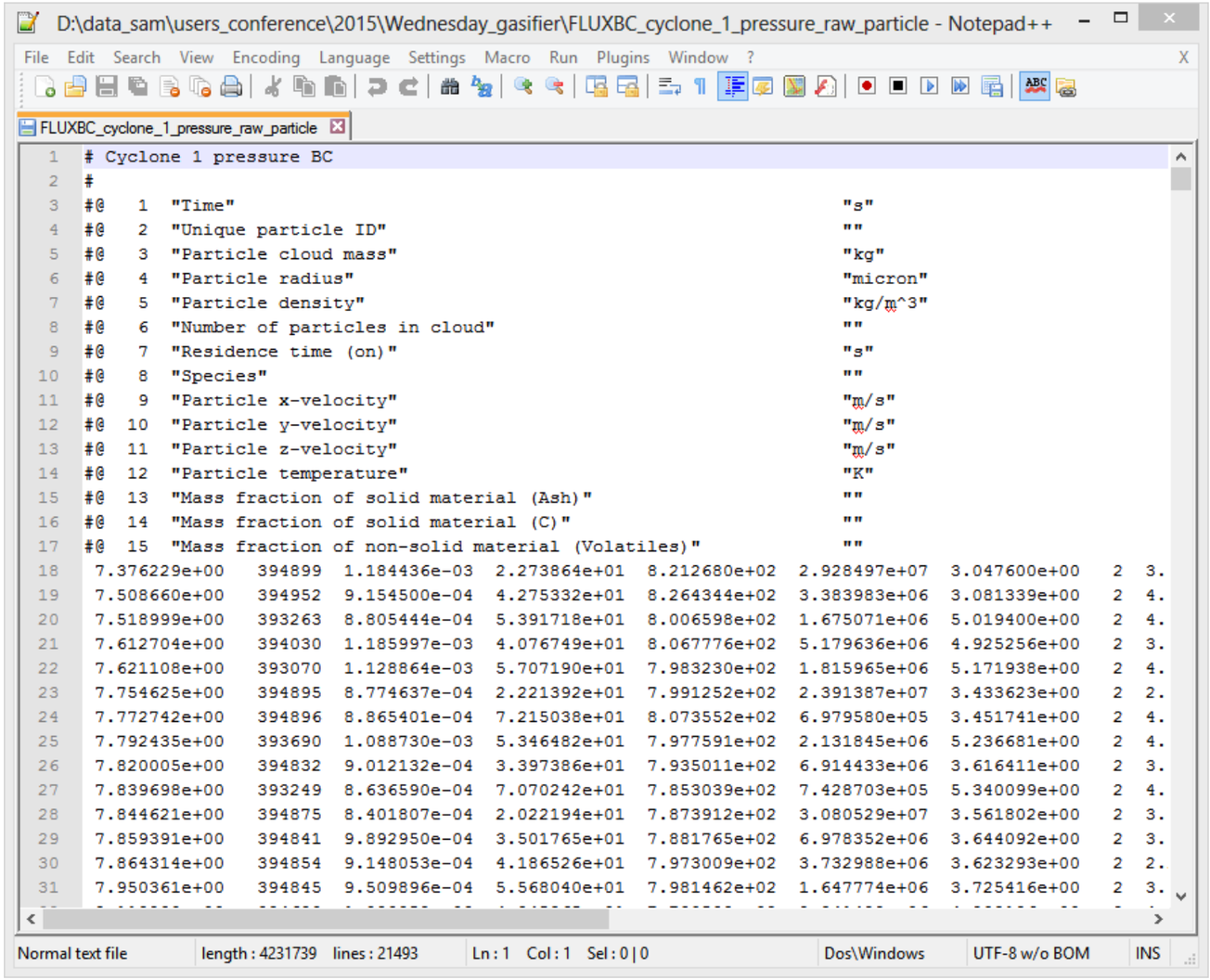
Goal 2: Residence Time Distribution (RTD) of Particles Exiting System

- Achieving Goal 2: Using **Raw Particle Data at Flux Planes**
  - Introduction to Raw Particle Data
    - What is it?
    - How to enable it?
  - Calculating and plotting RTD using Python



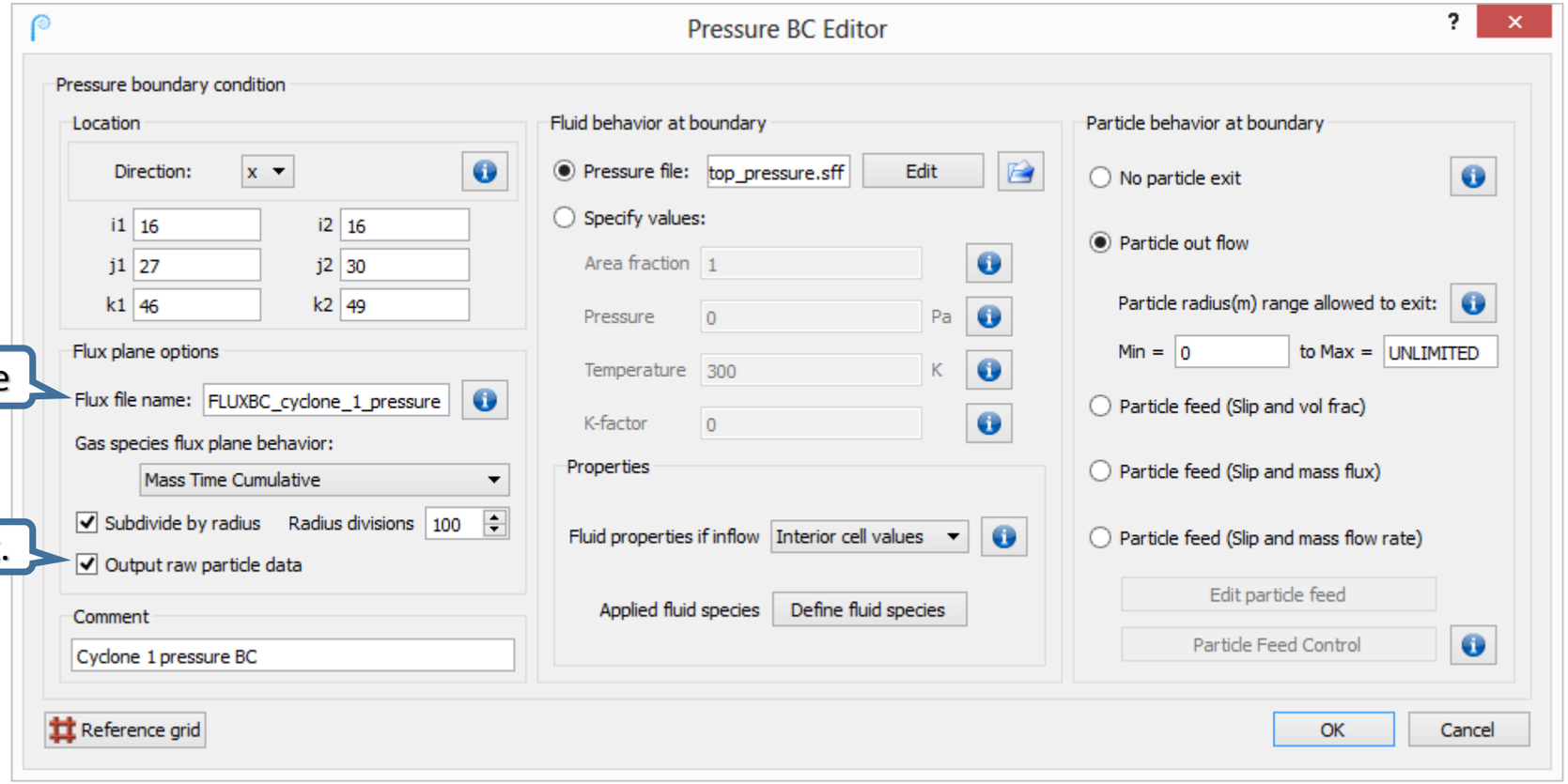
Raw Particle Data at Boundary Condition Flux Planes

- Detailed information is recorded for each computational particle that crosses the BC flux plane.
  - Time at which particle crossed plane
  - Unique particle ID
  - Cloud mass
  - Particle radius
  - Residence time
  - Species
  - Material composition



Enabling Raw Particle Data Output for BC Flux Planes

- Pressure, Flow, and Injection BCs support Raw Particle Data output.



Specify a Flux file name

Click the checkbox.

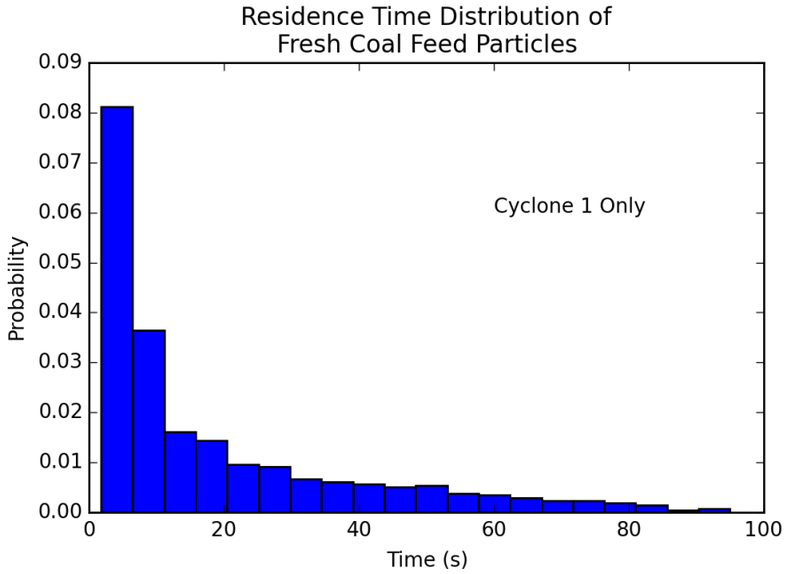
Demo 2.1: Plotting Residence Time Distribution (Single Cyclone)

- This cell demonstrates the basic procedure for plotting RTD as a histogram.

In [ ]:

```
# From the flux plane raw particle data, we only care about these columns:
#@   7  "Residence time (on)"                                    "s"
#@   8  "Species"                                                ""
# Note that genfromtxt's usecols function requires columns counted from 0,
# so subtract 1 from the Barracuda header numbers, which start at 1.
resTime, species = np.genfromtxt('FLUXBC_cyclone_1_pressure_raw_particle', usecols=(6,7), unpack=True)

# We only care about *Species 2* particles, Fresh Coal Feed
selectedSpecies = (species == 2)

print("Number of data points all species = ", len(resTime))
print("Number of data points (species 2) = ", len(resTime[selectedSpecies]))

fig, ax = plt.subplots()
ax.set_title('Residence Time Distribution of\nFresh Coal Feed Particles')
ax.set_xlabel('Time (s)')
ax.set_ylabel('Probability')
ax.annotate('Cyclone 1 Only', xy=(60,0.06))
ax.hist(resTime[selectedSpecies], bins=20, normed=True);

p = "pdf_rtd_of_fresh_coal_feed_particles_cyclone_1"
fig.savefig(p + '.png', format='png', dpi=200)
```

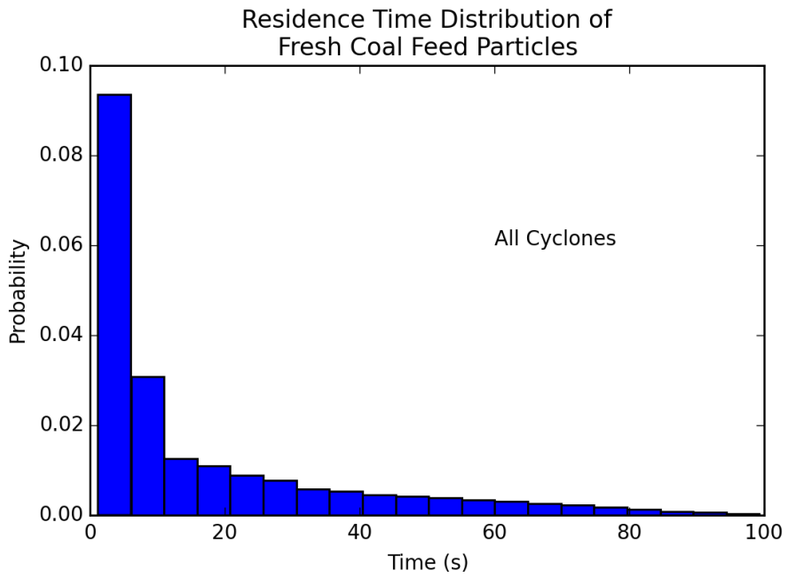
File naming convention.



Demo 2.2: Plotting RTD Based on Data from All Cyclones

- The next cell extends the plot to include data from all 4 cyclones.

In [ ]:
```
fList = ['FLUXBC_cyclone_1_pressure_raw_particle',
         'FLUXBC_cyclone_2_pressure_raw_particle',
         'FLUXBC_cyclone_3_pressure_raw_particle',
         'FLUXBC_cyclone_4_pressure_raw_particle']

resTime = []
species = []
for f in fList:
    resTime = np.concatenate((resTime, np.genfromtxt(f, usecols=(6))))
    species = np.concatenate((species, np.genfromtxt(f, usecols=(7))))

selectedSpecies = (species == 2)

print("Number of data points all species = ", len(resTime))
print("Number of data points (species 2) = ", len(resTime[selectedSpecies]))

fig, ax = plt.subplots()
ax.set_title('Residence Time Distribution of\nFresh Coal Feed Particles')
ax.set_xlabel('Time (s)')
ax.set_ylabel('Probability')
ax.annotate('All Cyclones', xy=(60,0.06))
ax.hist(resTime[selectedSpecies], bins=20, normed=True);

p = "pdf_rtd_of_fresh_coal_feed_particles_all_cyclones"
fig.savefig(p + '.png', format='png', dpi=200)
```

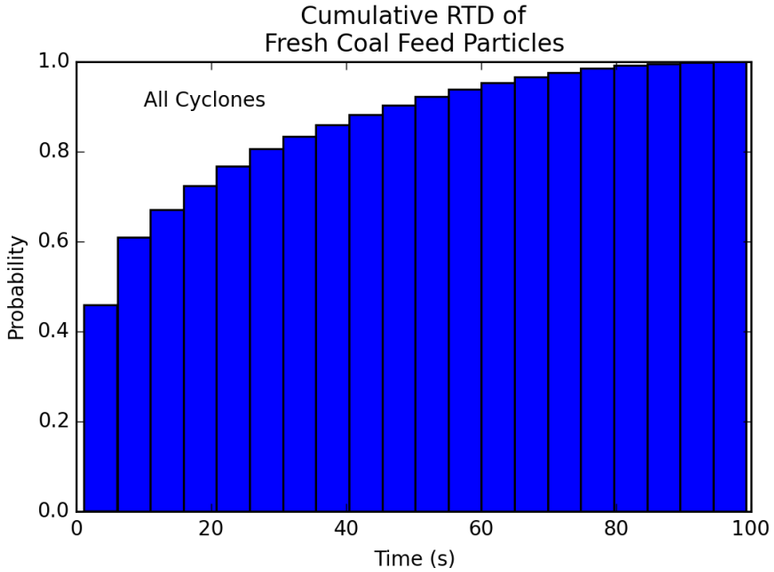


Demo 2.3: Plotting RTD as a Cumulative Distribution Function

- The final cell shows:
  - How to plot RTD as a cumulative distribution function
  - The concept of using data calculated in a previous iPython notebook cell

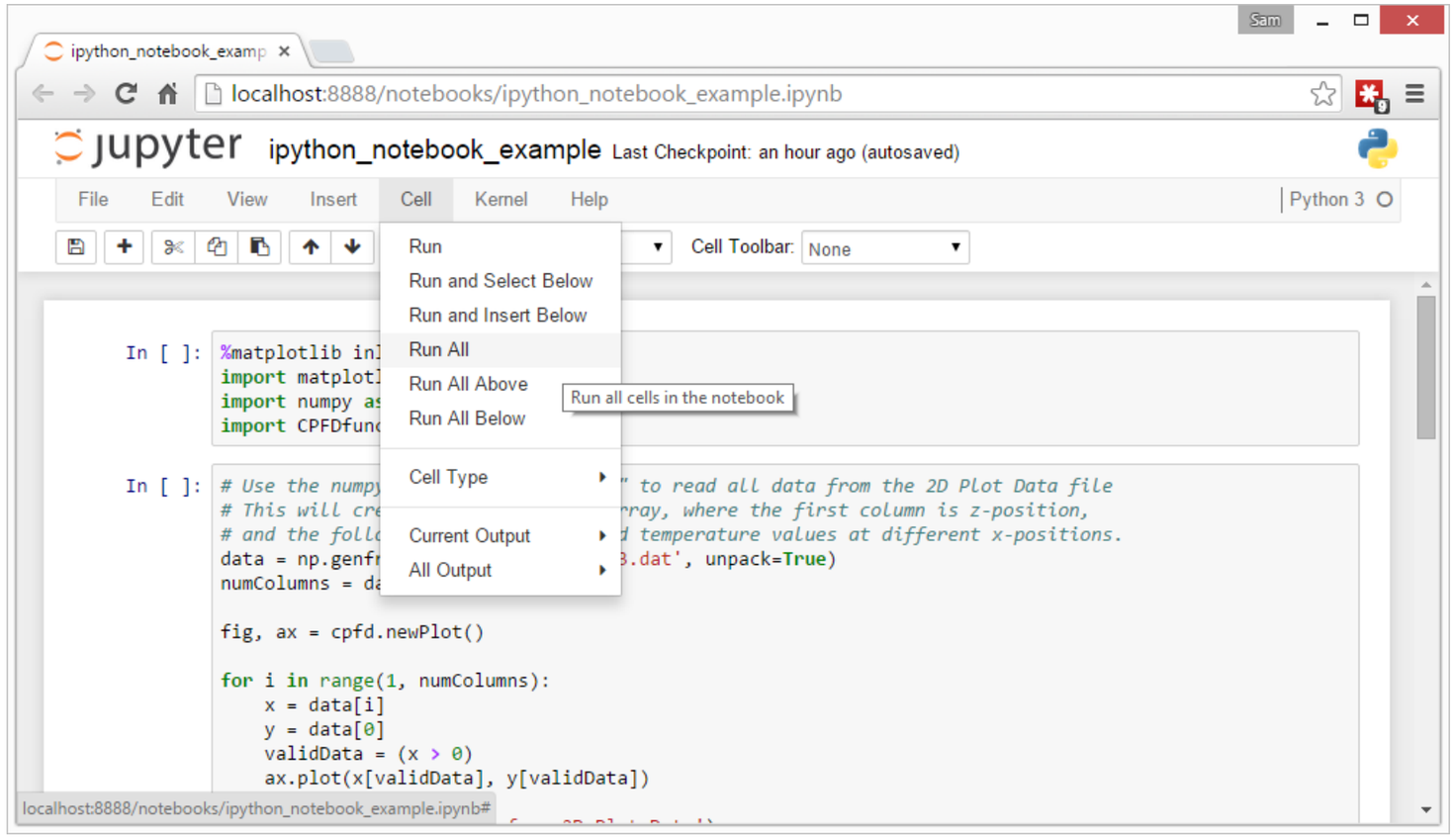
```
In [ ]: fig, ax = plt.subplots()
        ax.set_title('Cumulative RTD of\nFresh Coal Feed Particles')
        ax.set_xlabel('Time (s)')
        ax.set_ylabel('Probability')
        ax.annotate('All Cyclones', xy=(10,0.9))
        ax.hist(resTime[selectedSpecies], bins=20, normed=True, cumulative=True);

        p = "cdf_rtd_of_fresh_coal_feed_particles_all_cyclones"
        fig.savefig(p + '.png', format='png', dpi=200)
```

Using the cumulative option changes plot from probability to cumulative.



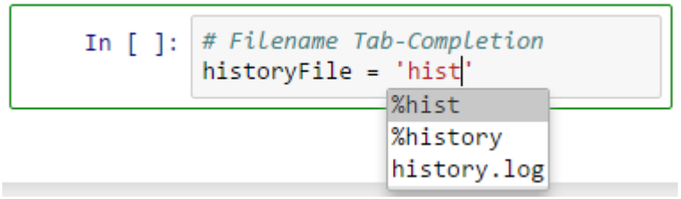
How to Run the Notebook

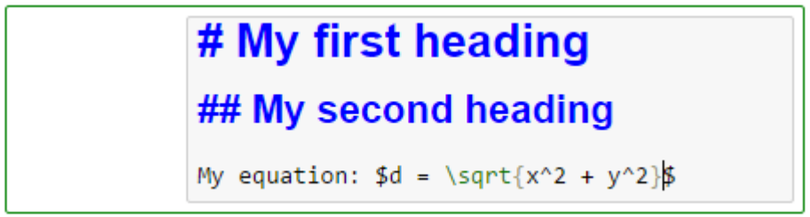
- The entire notebook can be run at once by using: Cell → Run All
- An individual cell can be run by using:
  - Cell → Run
  - Ctrl + Enter

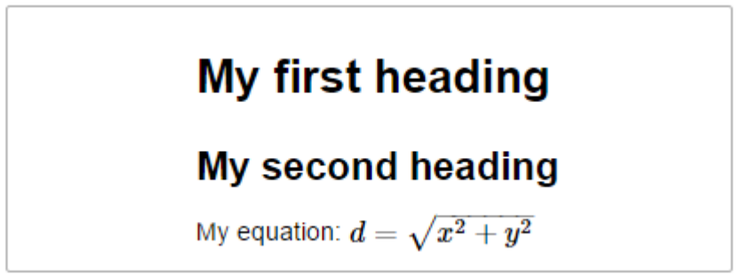


Other Notable Features of iPython Noteboook

- Tab-completion of commands and filenames
  - When typing, press Tab and a dropdown will appear with available options
- Markdown
  - Cell → Cell Type → Markdown
  - Allows you to document your work
  - Supports LaTeX equations
  - Supports headers and other formatting

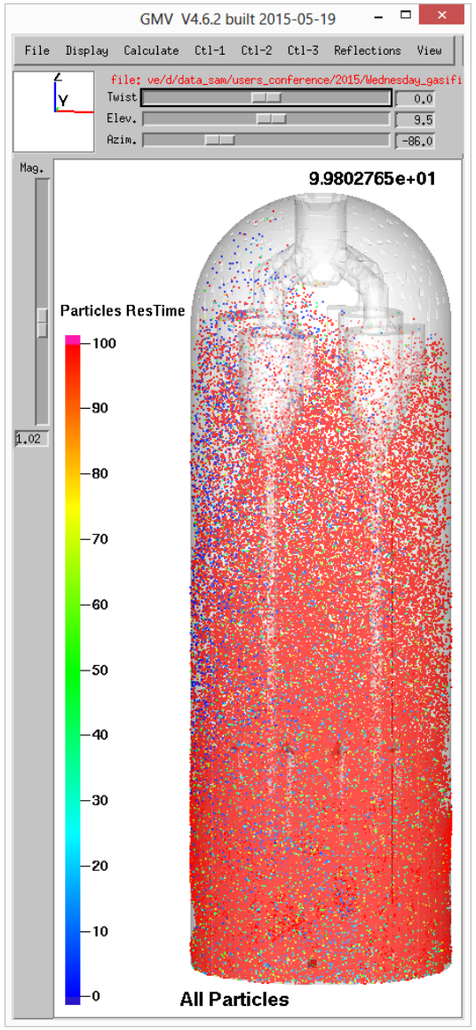


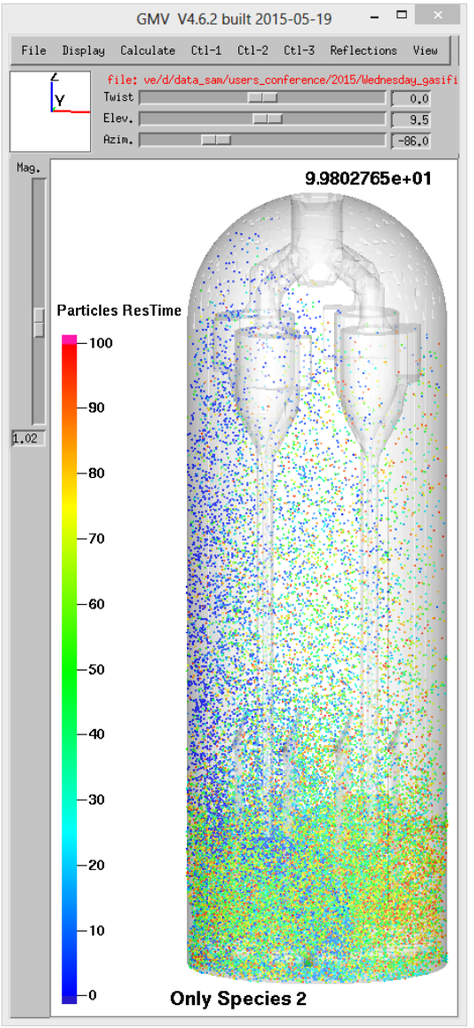


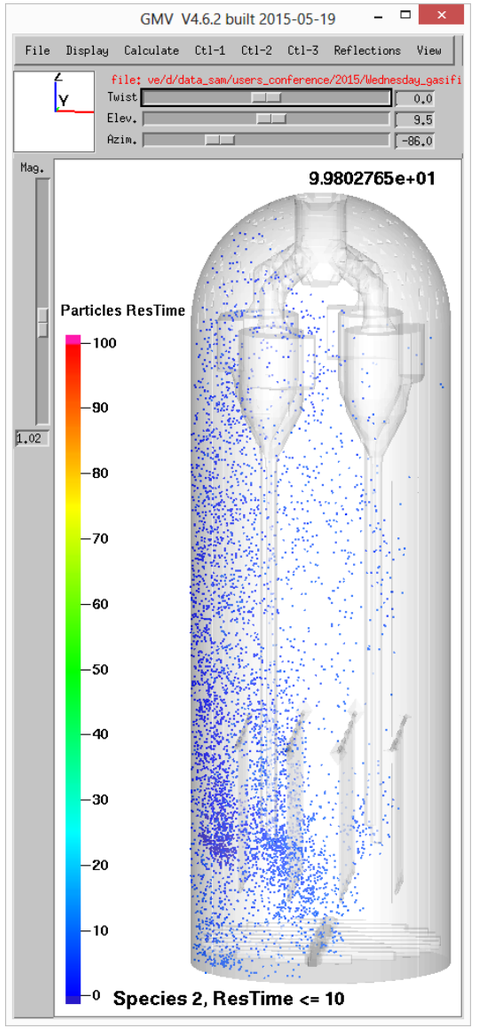


Goal 3: Viewing a Single Particle Species in GMV

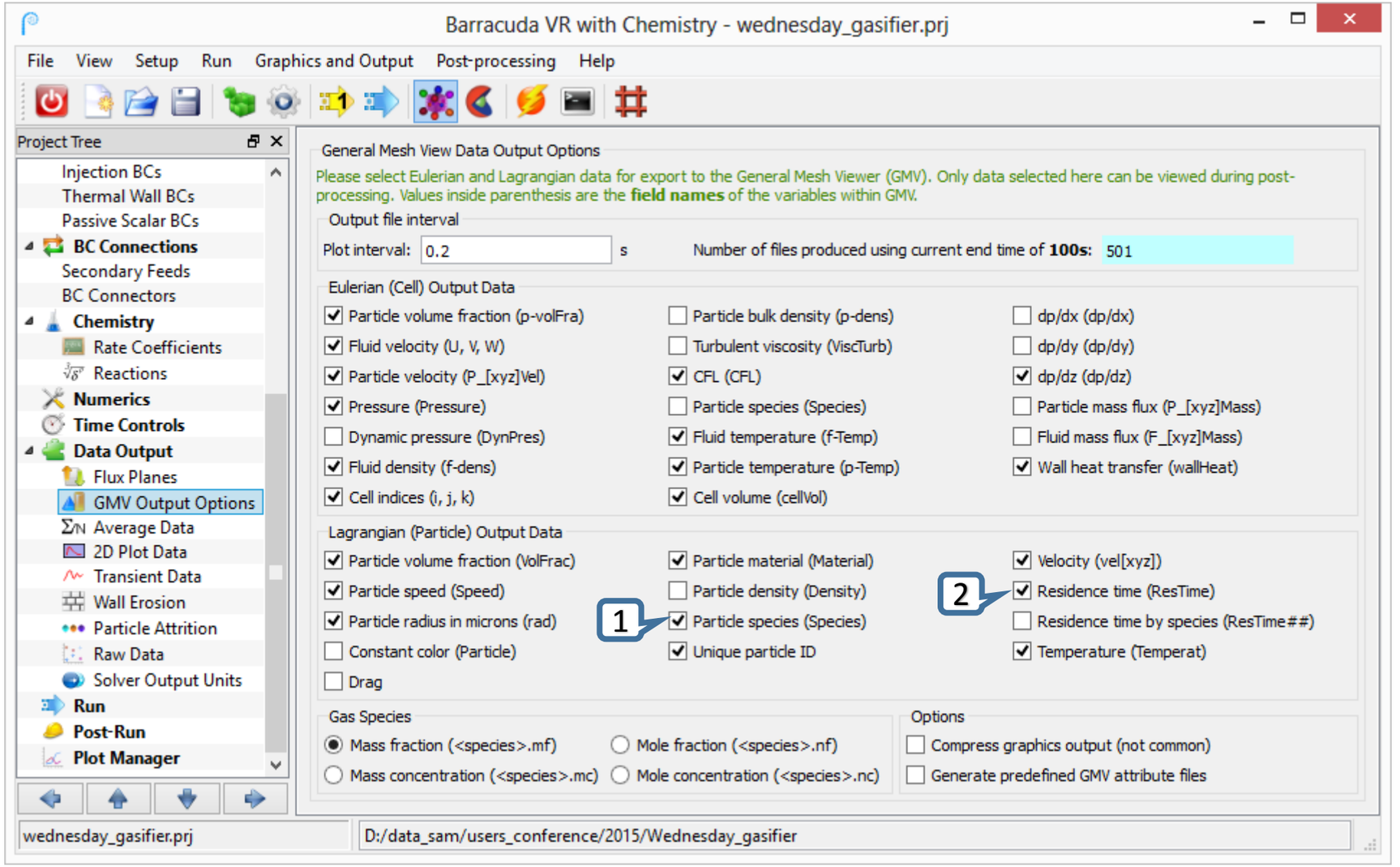
- Achieving Goal 3: Using **Particle Select** in GMV
  - Introduction to Particle Select
  - Selecting based on multiple criteria



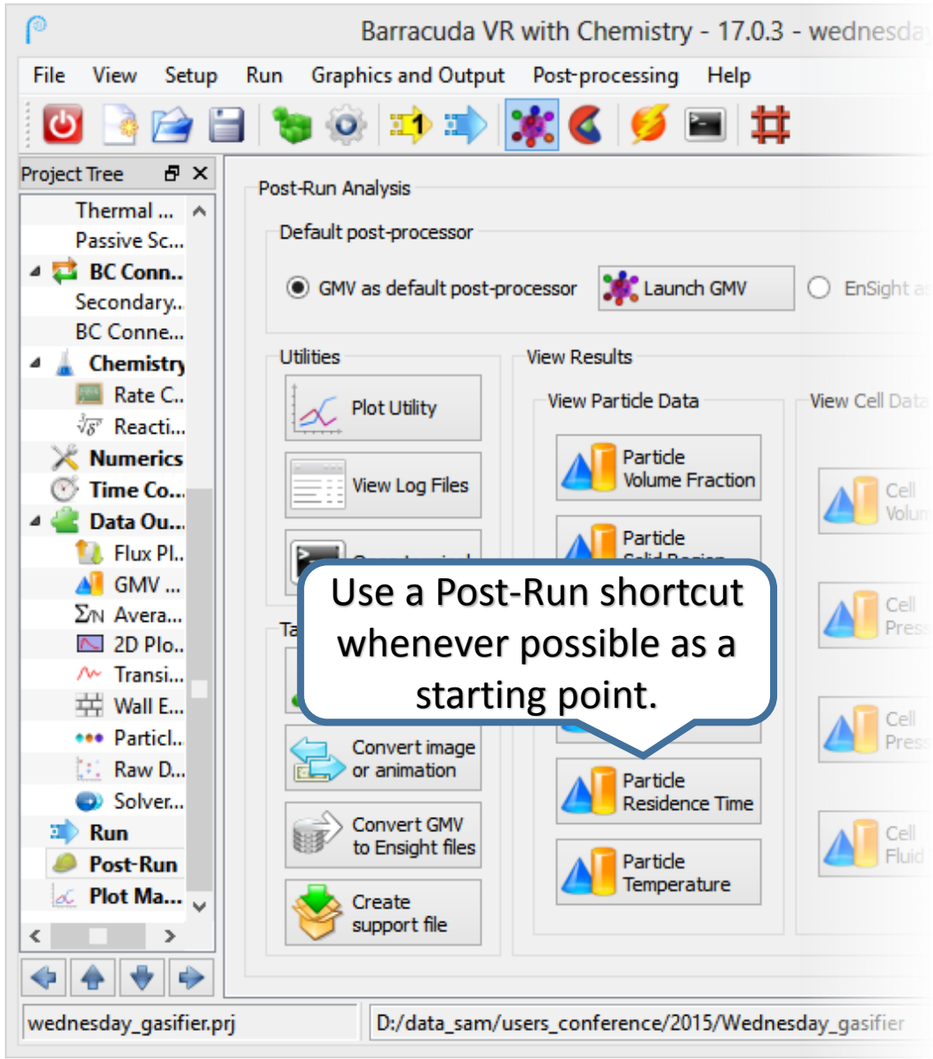


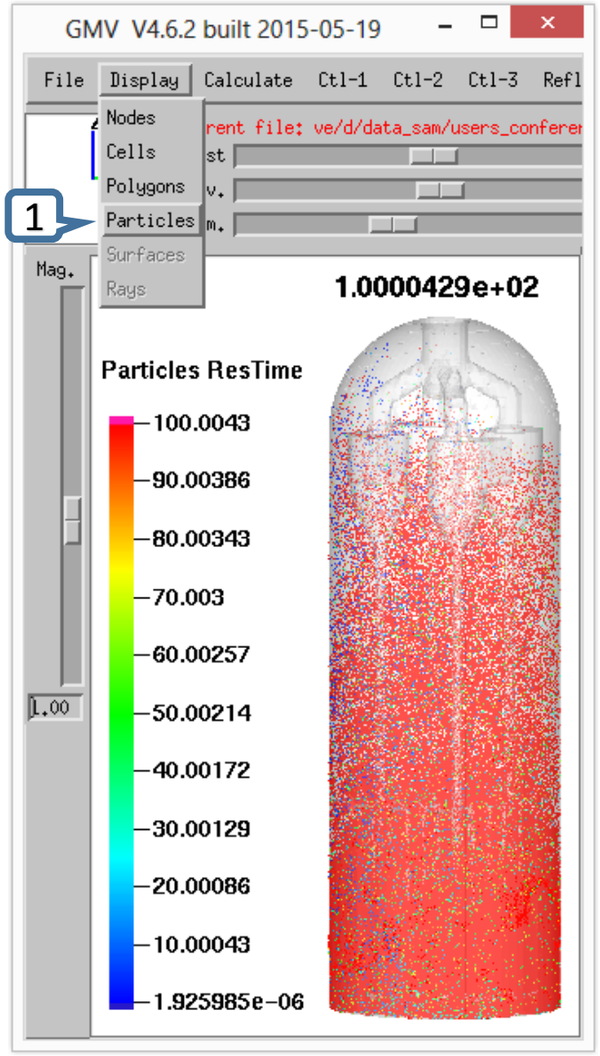


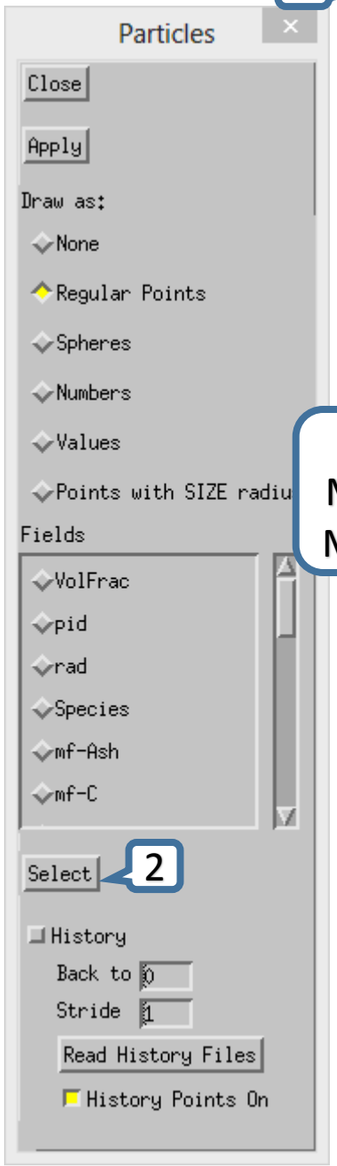
Variables Used in GMV Must Be Selected in GMV Output Options

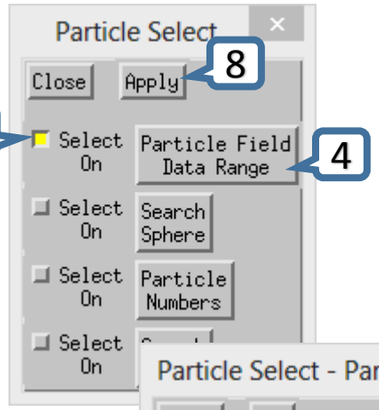


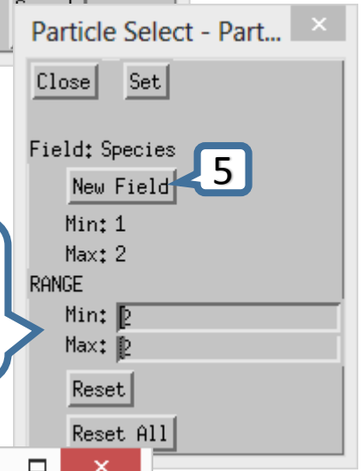
Using Particle Select to Show Only Species 2



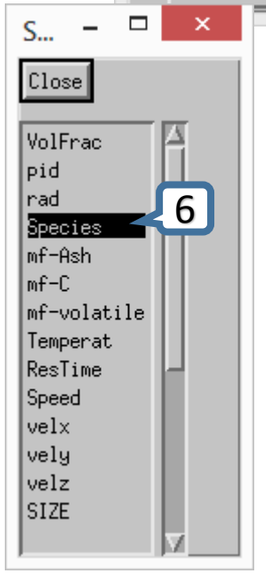




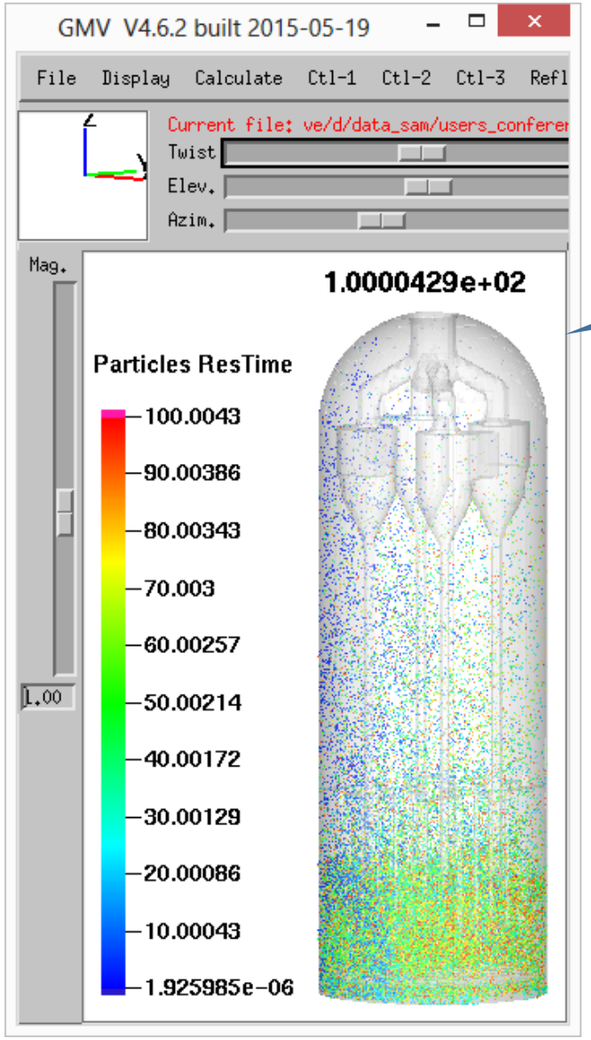




7
Min=2
Max=2

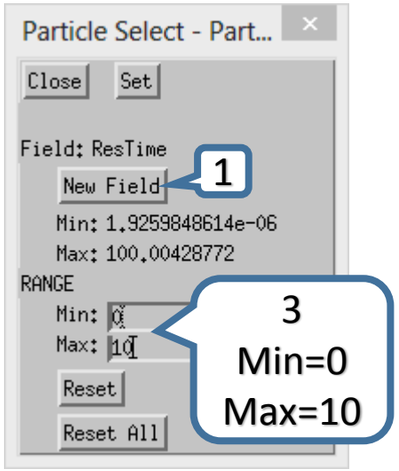


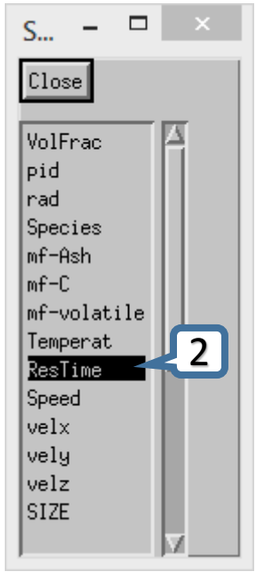
Selecting Particles Based on Multiple Criteria

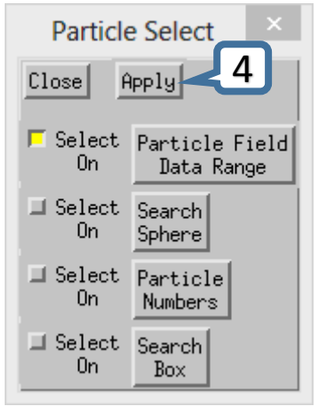


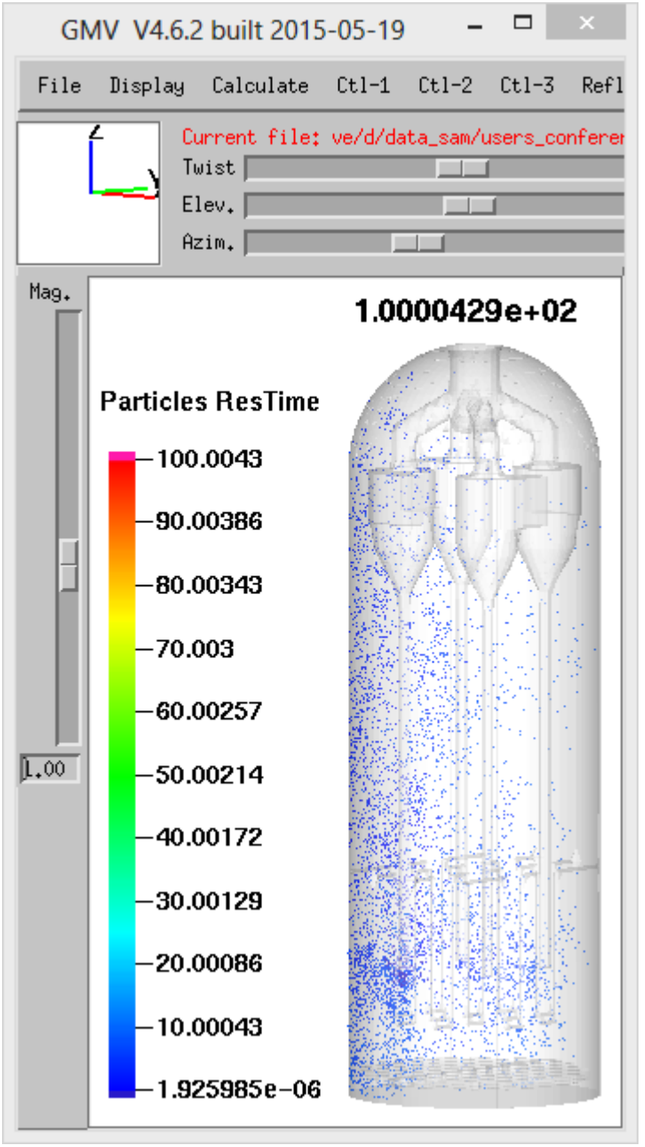
View resulting from steps shown on previous slide. Only particles with Species = 2 are shown.

View resulting from steps shown on this slide. Only particles with Species = 2 **and** ResTime ≤ 10 are shown.







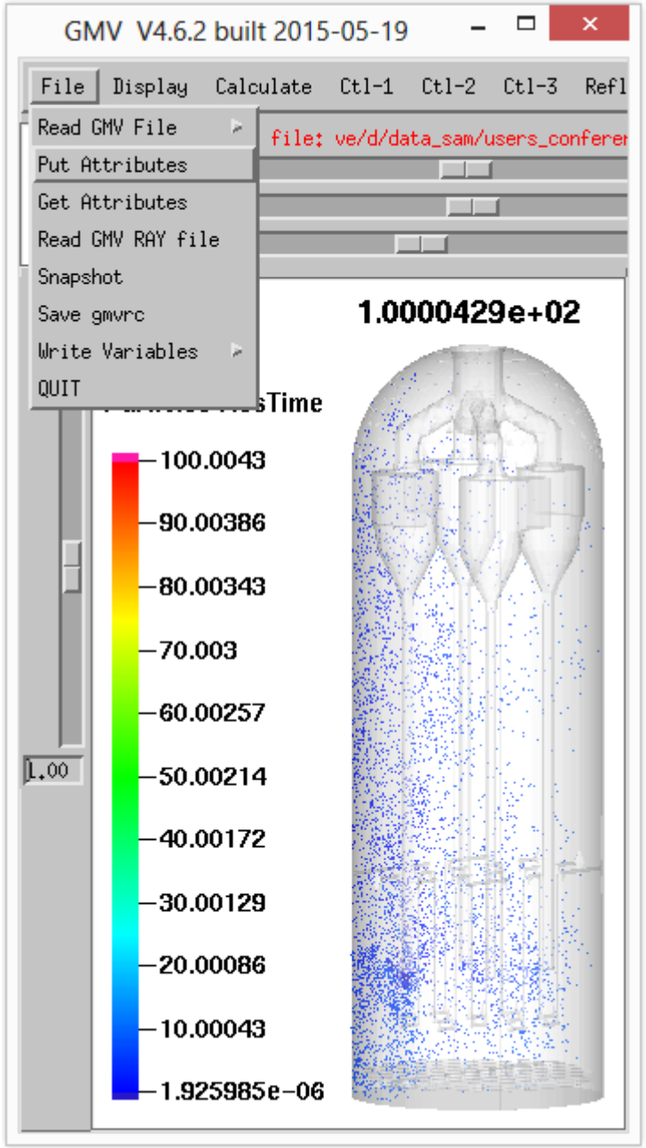


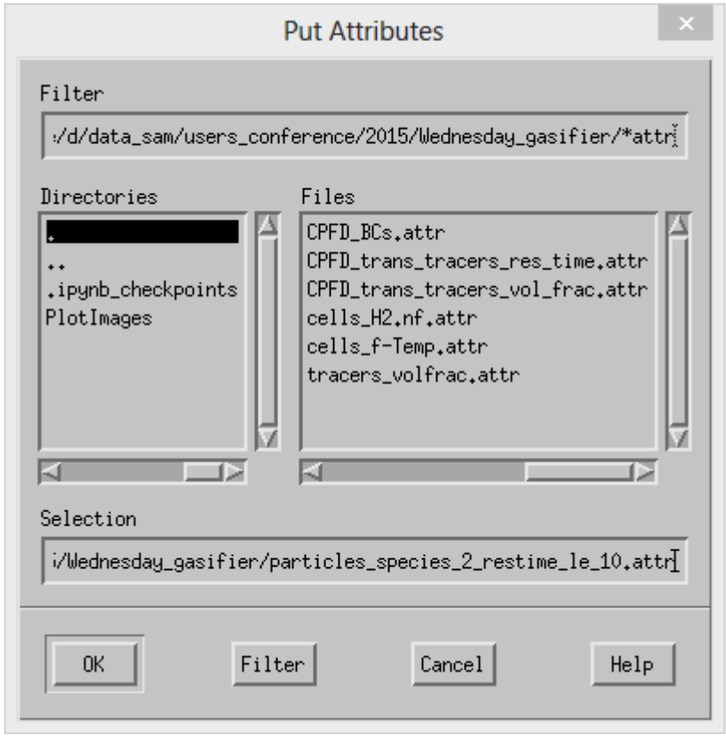
Goal 4: Creating a Spinning Movie

- Achieving Goal 4: Using BATCHMOVIE.sh
  - Introduction to BATCHMOVIE.sh
  - Creating a spinning movie using the `-azim` flag in BATCHMOVIE.sh

Save an Attribute File

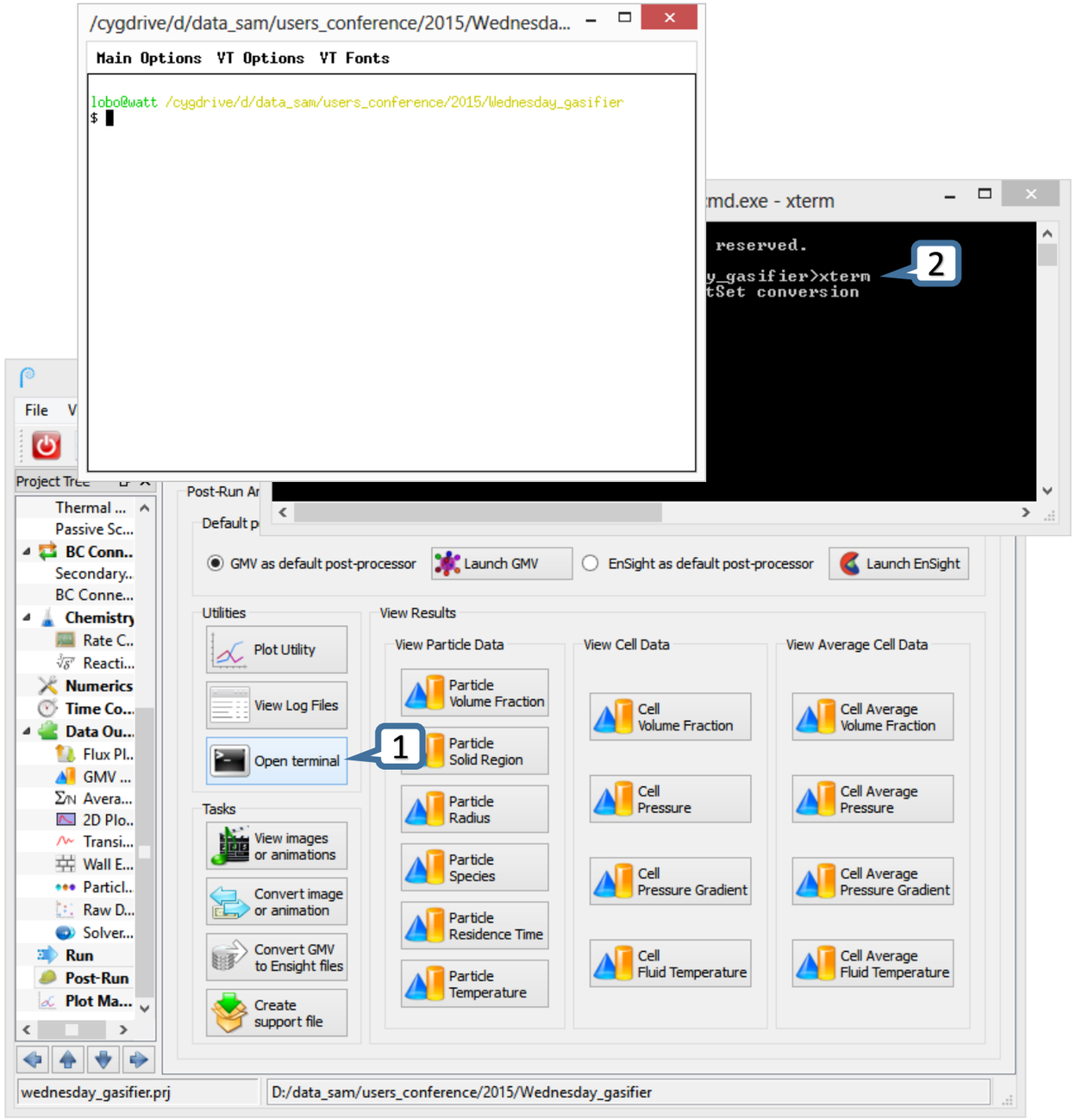
- BATCHMOVIE.sh creates images for each Gmv* file by using an **attribute file** describing the view.
- Create the view you want in GMV, then use the menu: File → Put Attributes
- Use a good, descriptive name (with no spaces) for the attribute file.





Start a Terminal

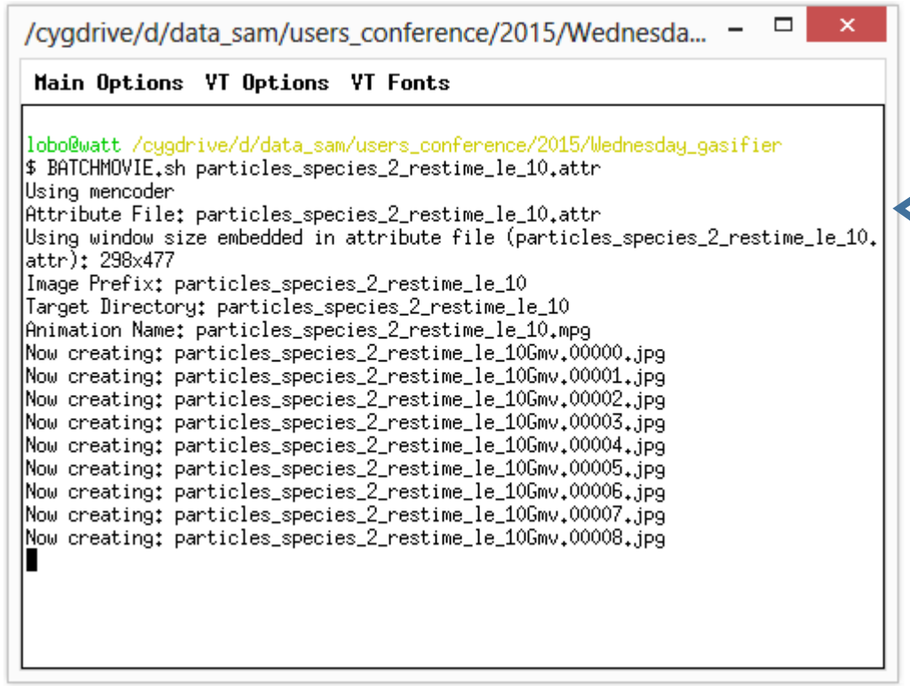
- BATCHMOVIE.sh is a command-line utility, so we need to open a terminal in the current project's directory to use it.
- In Windows:
  - Post-Run → Open Terminal
  - In cmd.exe enter: xterm
- In Linux:
  - Post-Run → Open Terminal



Basic BATCHMOVIE.sh Command

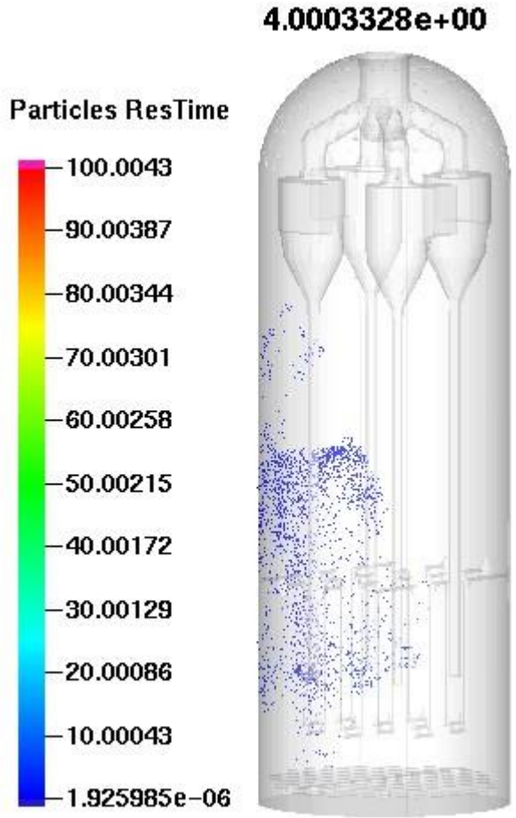
- Create a “regular” movie:

`BATCHMOVIE.sh particles_species_2_restime_le_10.attr`



BATCHMOVIE.sh will process all Gmv* files in the current directory, creating images and a final animation based on the specified attribute file.

The resulting movie will match the view defined in the attribute file, including particle selection. Only particles with Species = 2 and ResTime ≤ 10 will be shown.



Using the `-azim` Option to Create a Spinning Movie

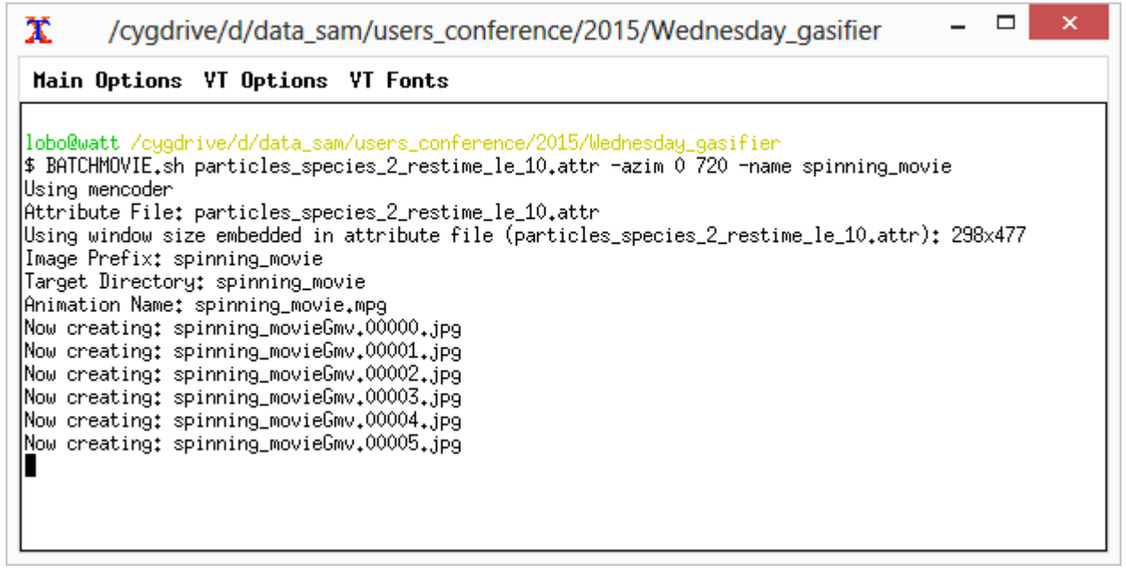
- BATCHMOVIE.sh has a `-azim` option to rotate the movie as time progresses. In this example, let's spin the geometry two full turns over the course of the 100 s of simulation time.
  - In order to use the `-azim` option in Windows, the `tclsh` package must be installed in Cygwin. If this package is not already on your system, see this knowledge base post for details about how to install it.
- Let's also use the `-name` option, to give the resulting images and movie a different prefix than they would have by default.

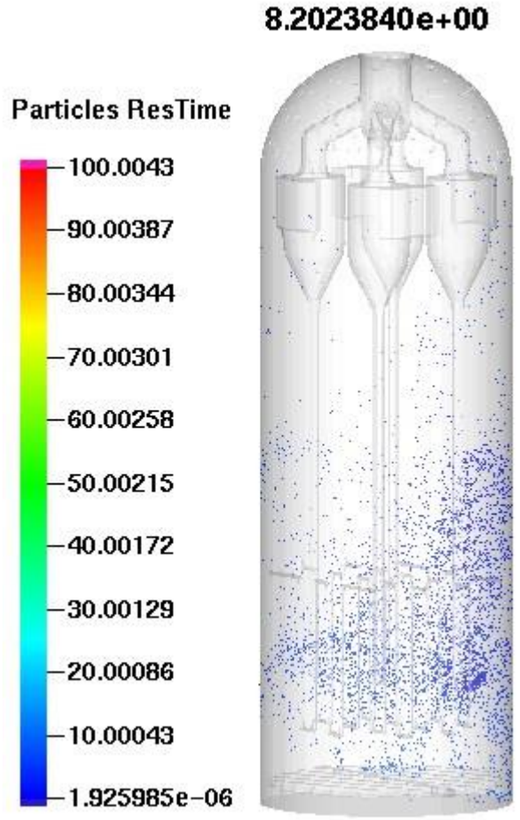
```
BATCHMOVIE.sh particles_species_2_restime_le_10.attr -azim 0 720
-name spinning_movie
```

Put this BATCHMOVIE.sh command on a single line in the terminal.

Final Spinning Movie

- BATCHMOVIE.sh will run, creating the images and final movie with spinning geometry.





Further Tools for Creating Fancy Movies

- `-mp4` flag for BATCHMOVIE.sh, and standalone script `jpg2mp4`
  - The .mpg files generated by BATCHMOVIE.sh sometimes cannot be played by Windows Media Player or Microsoft PowerPoint
  - You can create a .mp4 file instead, which will usually be able to play successfully on Windows
- MULTIFRAME.tcl
  - Script distributed with Barracuda VR
  - Can combine frames from multiple animations into a single final animation
  - See Barracuda VR Training Materials for details, or this support site post.
- CEI EnSight
  - Alternative post-processor that supports GMV files
  - Modern GUI design with many features
  - Also scriptable through a built-in Python interface
  - Sold and distributed by CEI