

# IES

Integrated Energy Systems

## NEAMS Workbench and IES Holistic Energy Resource Optimization Network (HERON)

Hands on Working Lunch

5 April 2023

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# Purpose

- Context:
  - The NEAMS Workbench integration into FORCE is a new effort
  - Problem inputs and workflows are varied and can be complex
  - Workbench has features to help users
- Key goals:
  - Simplify problem input and workflow
  - Expose you to working examples of Workbench FORCE features as available in current releases
  - Open communication channels and obtain user feedback
  - Ultimately, improve problem input preparation, execution, and results visualization

# Outline

- Review Workbench + HERON requirements and setup
- Review the XML to EDDI input conversion step
  - Lightweight input format that preserves data without extra syntax
- Explore Workbench
- Conduct job launch
- Visualize results and explore visualization settings
- Discuss

# Requirements Review

- NEAMS Workbench 5.2
  - Available for download at <https://code.ornl.gov/neams-workbench/downloads/>
- Recent HERON release
  - Initial Workbench integration occurred March 10<sup>th</sup> 2023 via changeset [daca1335](#)
- Local installation or INL NCRC Access ([hpcondemand.inl.gov](http://hpcondemand.inl.gov))
- Conversion of HERON native XML input to EDDI-formatted input

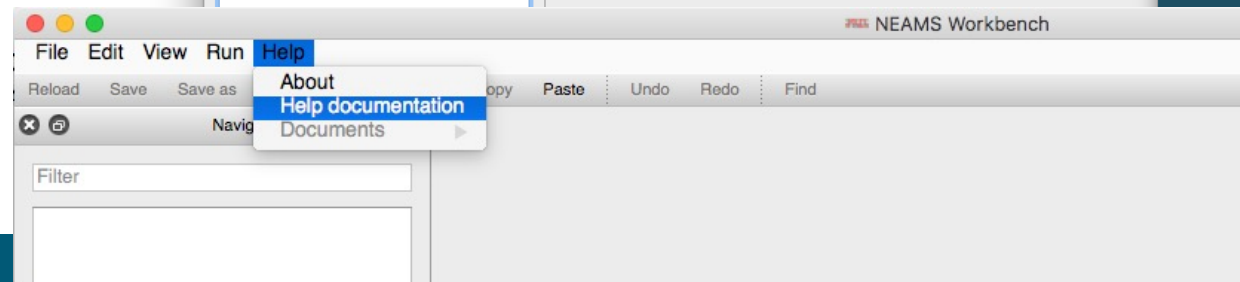
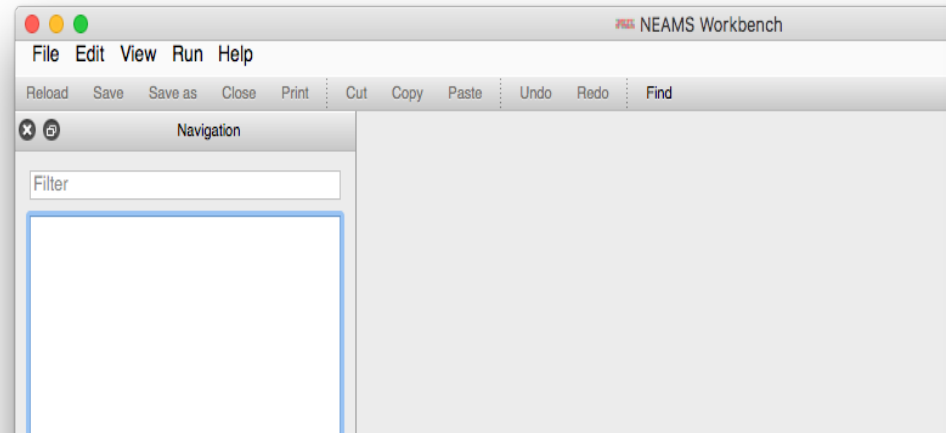
# Start Workbench

- NEAMS Workbench is available on INL's Nuclear Computation Resource Center (NCRC)
- Use default settings
- Ensure 5.2 is selected

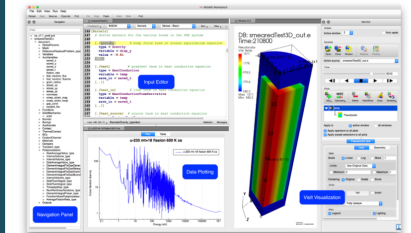
The screenshot displays the INL HPC OnDemand web interface. The top navigation bar includes links for 'INL HPC OnDemand', 'Files', 'Jobs', 'Clusters', 'Interactive Apps', 'Information', 'NCRC', 'Training', and 'My Interactive Sessions'. The 'NCRC' dropdown menu is open, showing a list of options: 'GUIs', 'NEAMS Workbench', 'Herd', 'Code Execution', 'Tests', 'Build Test Suite', 'Training Videos', and 'Bison Videos'. The 'NEAMS Workbench' option is highlighted with a red box. Below the navigation bar, the breadcrumb path is 'Home / My Interactive Sessions'. The main content area is divided into two columns. The left column, titled 'Interactive Apps', lists various desktop and IDE environments: 'Desktops', 'Linux Desktop', 'Linux Desktop with Visualization', 'IDE', 'Visual Studio Code Server', 'Jupyter', and 'Jupyter'. The right column, titled 'You have', lists available resources: 'NCRC', 'GUIs', 'NEAMS Workbench', 'Herd', and 'Code Execution'. The 'NEAMS Workbench' option in this column is also highlighted with a red box.

# Start the NEAMS Workbench

- Help documentation will display during the first startup
- Help documentation is accessible via **Help>Help Documentation**

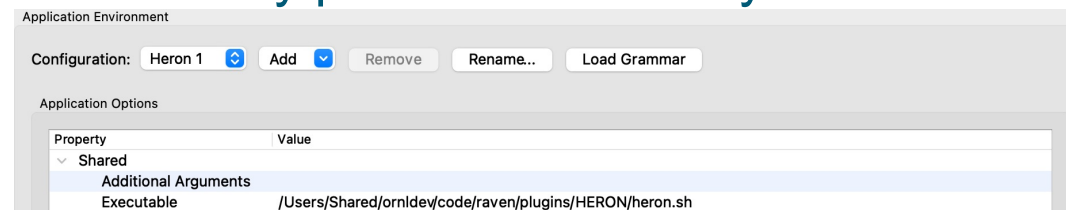


A screenshot of the "NEAMS Workbench User Documentation" web page. The page title is "NEAMS Workbench User Documentation". It includes a "Table of Contents" on the left, a "Next topic" section, and a "Quick search" field. The main content area contains a "Welcome to the NEAMS Workbench user documentation" message, followed by a list of supported applications and their descriptions. Below this is a "Getting Started with NEAMS Workbench and a supported Application" section, followed by "Requirements" and "Supported Operating Systems" sections. The "Supported Operating Systems" section lists Linux 64-bit (RHEL6), Mac OS X (Darwin) 10.9.5 or newer, and Windows 7, 10 64-bit. The "System Requirements" section lists minimum requirements (2 GB RAM, dual core processor), recommended requirements (4+ GB RAM, quad core processor), and recommended details models (16 GB RAM). The "Features" section lists the Document Navigator, Input Editor, Interactive Geometry Viewer, and Data Plots. At the bottom, there is a "Settings" section with options for Environment and Filter Set.



# Configure HERON in Workbench

- Configuring an application active in Workbench is only required once
- 2 primary routes for configuring HERON active in Workbench
  1. INL's NCRC preconfigured 'localhost' HERON activation
    1. Click **File > Localhosts...**
    2. Select the available application table **row** containing **NRCCHERON** and click **activate**
    3. Wait for activation to conclude as indicated by the message **Process finished with 0 return code**
    4. HERON is now activated
  2. Your own machine's installation
    1. Click **File > Configurations...**
    2. Click **Add...**
    3. Select **Heron** from the drop-down and click **OK**
    4. Update **Executable** property **Value** to be path to raven/plugins/HERON/heron and use enter key to capture the field – this may pause momentarily as the HERON grammar information is loaded
    5. HERON is now activated



# Review XML to EDDI

- What is EDDI and why?
  - Extra Definition Driven Input (EDDI) is a lightweight open-source input syntax that is supported in Workbench
  - It is used as an integration prototype to achieve the following:
    1. Enable Workbench integrators to programmatically survey existing HERON inputs
    2. Serve as a design iteration to the question *'is there a better user input format?'*
  - EDDI preserves all data structure but avoids the bothersome XML syntax
- Conversion script is available in Workbench
  - Takes XML file and emits EDDI-formatted equivalent



# XML to EDDI | Execution

## Example execution converting existing XML-formatted input to EDDI

### Linux and Mac OS invocation (terminal)

```
Workbench/rte/entry.sh Workbench/rte/util/xml2eddi.py path/to/heron_input.xml > path/to/heron_input.heron
```

### Windows invocation (CMD)

```
Workbench/rte/entry.bat Workbench/rte/util/xml2eddi.py path/to/heron_input.xml > path/to/heron_input.heron
```

- *Workbench*: Path to the Workbench installation
- *path/to/heron\_input.xml*: Path to favorite HERON input
- *> path/to/heron\_input.heron*: Output redirection to EDDI-formatted input (The file to be opened in Workbench)

**Note:** 'heron' extension is the default recognized HERON input in Workbench

**Note:** if performing the conversion on NCRC you will want to copy the HERON input *directory* to a location to which you can write

# XML2EDDI Conversion

- Go to Command line and convert XML to EDDI-formatted \*.heron file

- On INL HPC you will need to copy test files to a writable location
- Run the following commands in a HPC Terminal

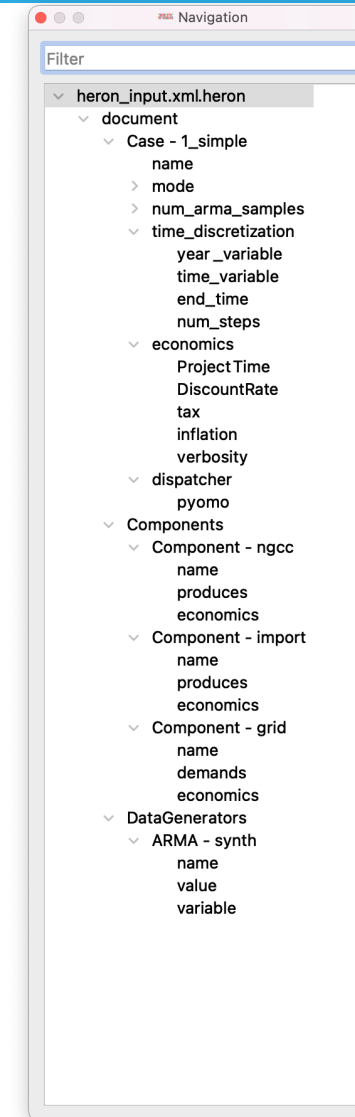
```
cp -r /apps/local/raven/raven_heron_20230327/plugins/HERON/tests/ ~/Downloads/heron_tests/
```

```
/apps/local/neams/Workbench-5.2.0/rte/entry.sh /apps/local/neams/Workbench-5.2.0/rte/util/xml2eddi.py  
~/Downloads/heron_tests/workshop/simple/heron_input.xml >  
~/Downloads/heron_tests/workshop/simple/heron_input.heron
```

- Open the \*.heron input file in Workbench

# NEAMS Workbench Document Navigation

- Hierarchical Listing of Document
  - Quick Navigation to input
  - Plot creation
- Filter
  - Regular expression-based item filtering
- Open Associated Files
  - Lists files with matching extension-less filename
  - Streamlines opening associated files
- Dockable
  - Dock to main NEAMS Workbench application
  - Float in separate window
  - Hide completely



# NEAMS Workbench Input Editor Components

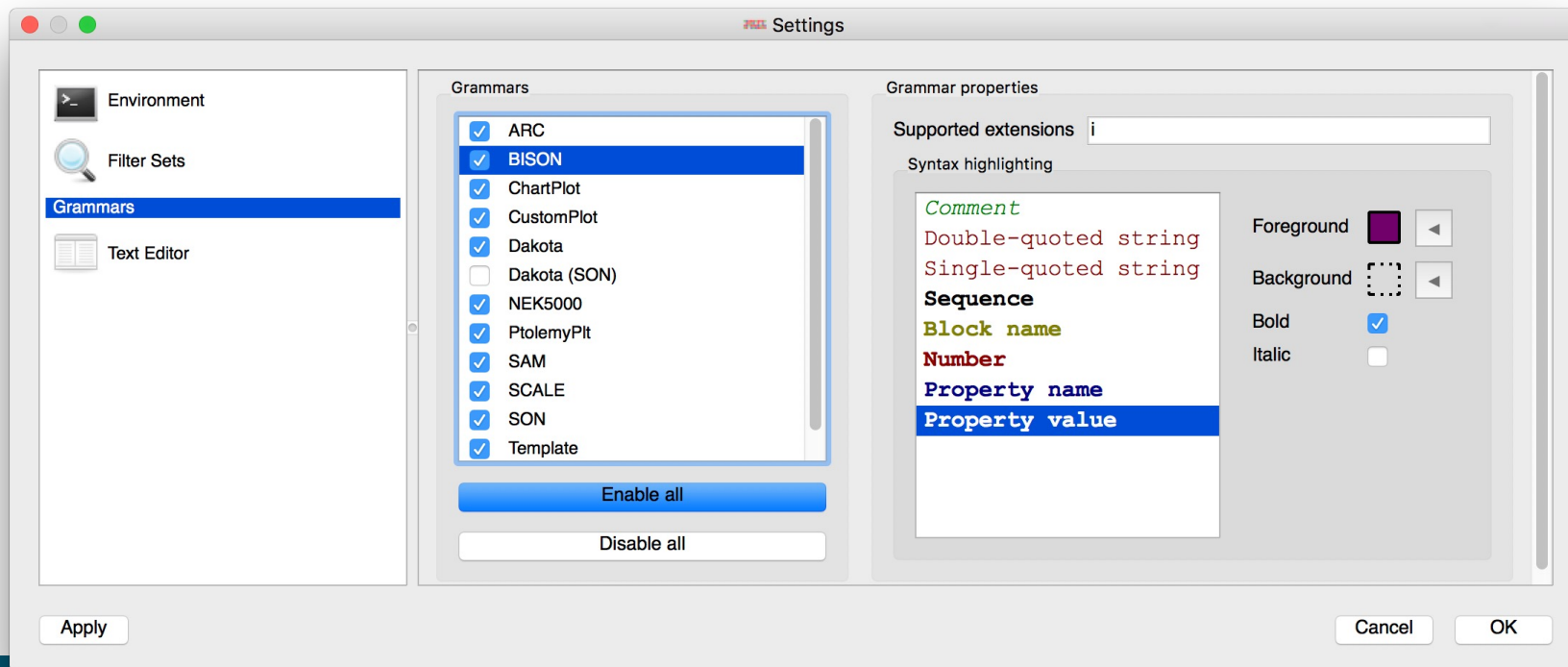
The image displays two side-by-side windows of the NEAMS Workbench Input Editor. The left window shows a code editor with a document titled 'document'. The right window shows a code editor with a document titled 'GlobalParams'. Both windows have a menu bar (File, Edit, View, Run, Help) and a toolbar (Reload, Save, Save as, Close tab, Print, Cut, Copy, Paste, Undo, Redo, Find). The code in both windows is color-coded and includes comments. Blue callout boxes with arrows point to various features: 'Syntax Highlights' points to color-coded code; 'Input Block Highlights' points to highlighted code blocks; 'Customizable Application Run Configuration' points to the 'Run' button in the toolbar; 'Synchronized Text Editors' points to the two editor windows; 'Execution Messages' points to a message box at the bottom; 'Context Aware Input Autocompletion' points to a dropdown menu; 'Document Type and Quick Navigation' points to the 'GlobalParams' document title; 'Cursor Context' points to the current cursor position; and 'Input Validation' points to error messages at the bottom of the editor.

```
199 # Define auxilliary kernels for each of the aux variables
200 [./fast_neutron_flux]
201   type = FastNeutronFluxAux
202   variable = fast_neutron_flux
203   block = clad
204   rod_ave_lin_pow = power_history
205   axial_power_profile = axial_peaking_factors
206   factor = 3e13
207   execute_on = timestep_begin
208 [../]
209
210 [./fast_neutron_fluence]
211   type = FastNeutronFluenceAux
212   variable = fast_neutron_fluence
213   block = clad
214   fast_neutron_flux = fast_neutron_flux
215   execute_on = timestep_begin
216 [../]
217
218 [./grain_radius]
219   type = GrainRadiusAux
220   block = pellet_type_1
221   variable = grain_radius
222   temp = temp
223   execute_on = linear
224
225 [./AuxKernels/GrainRadiusAux_type
226 active - If specified only the blocks named will be visited and made active
227 boundary - The list of boundary IDs from the mesh where this boundary conditio...
228 burnup - Burnup
229 control - Labels for accessing object parameters via contro...
230 error - Status of the MooseObject.
231 identifier - Identifiers matching these identifiers will be skipped.
232 instance - This is a MooseObjectAction.
233 seed - The seed for the master random number generator
234 use_displaced_mesh - Whether or not this object should use the displaced mesh for comput...
235 [./stress_yy]
236   type = MaterialTensorAux
237   tensor = stress
238   variable = stress_yy
239   index = 1
240   execute_on = timestep_end
241 [../]
242 [./stress_zz]
243   type = MaterialTensorAux
244   tensor = stress
245   variable = stress_zz
246   index = 2
247   execute_on = timestep_end
248 [../]
```

Validation Error: num\_radial value "-.80" is less than the allowed minimum inclusive value of 0.0001.
Validation Error: num\_axial value "-.11" is less than the allowed minimum inclusive value of 0.0001.
Validation Error: quantity value "wrong" is not one of the allowed values: [ ... "radial" "se

# Application Syntax Highlighting

- File extensions for which to automatically associate
  - Whitespace delimited list of file extensions for which to automatically associate the grammar rules.
- Syntax highlights for each grammar pattern
  - Edit Foreground and background color
  - Indicate bold and/or italic font face



# Input Autocompletion Overview

- **What is it?**

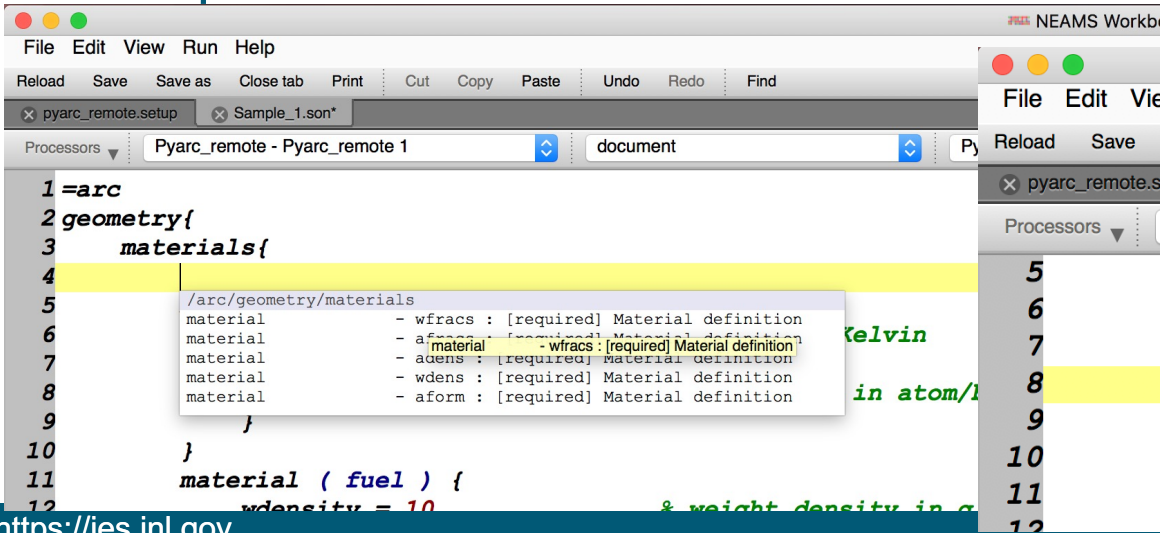
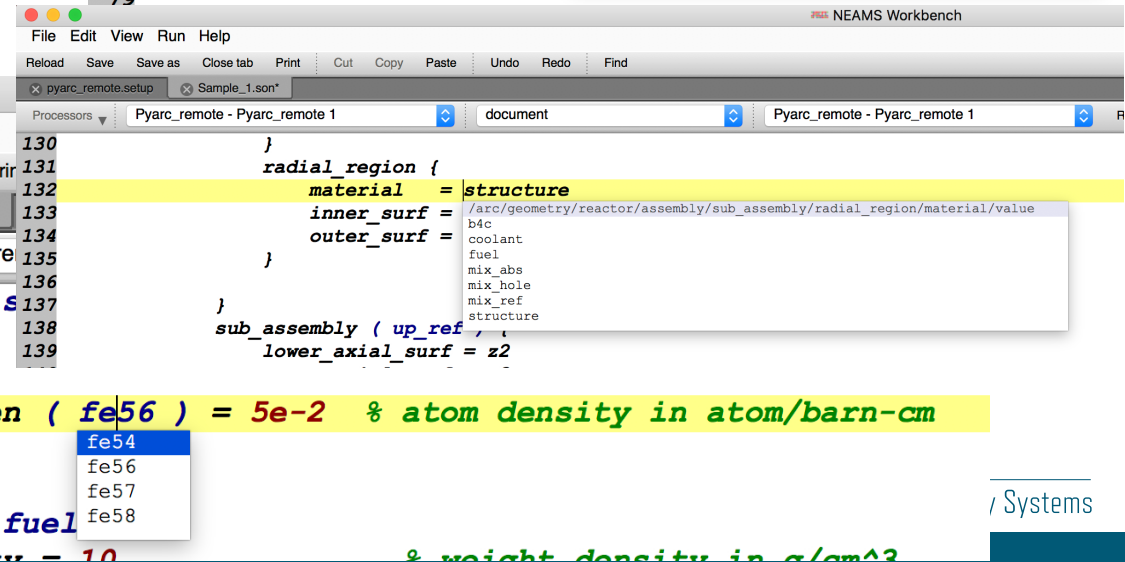
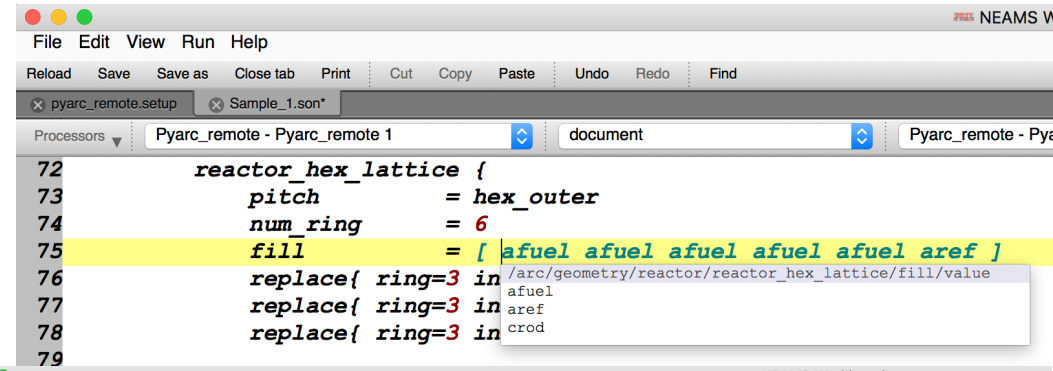
- Autocompletion is the ability for Workbench to generate parts of the input on demand

- **Why is it needed?**

- Autocompletion listings communicate to the user what input parts are available for insertion which accelerates input creation

- **Where is it available?**

- Everywhere, unless all valid input has been specified



# Output Text File Viewing

- Easy to access from the Input file's list of associated files popup context menu.
- Output file Can be drag-n-dropped onto NEAMS Workbench from a file browser
  - Any application file with an extension, (\*.inp, \*.out, etc.) can be dropped onto NEAMS Workbench
  - Open directory assists in identifying files for drag-n-drop

The screenshot displays the NEAMS Workbench interface. The top menu bar includes File, Edit, View, Run, and Help. Below it are sub-menus for Reload, Save, Save as, Close, Print, Cut, Copy, Paste, Undo, Redo, and Find. The main window shows a file browser on the left with a tree view containing 'textbook\_uq\_sampling.in'. A context menu is open over this file, listing options: Reload, Close, Open directory, Open associated files (highlighted), Copy directory path to clipboard, and Copy file path to clipboard. A blue callout box points to the 'Open associated files' option with the text: 'Associated files available via right click on document'. The main editor area shows the content of 'textbook\_uq\_sampling.in', which includes a header line '# Dakota Input File: textbook\_uq\_sampling.in', followed by 'environment' and 'tabular\_data' sections. The 'tabular\_data' section contains a table of response levels: 

response_levels =	0.1	0.2	0.6
	0.1	0.2	0.6
	0.1	0.2	0.6

. Below this is a list of associated files, with 'textbook\_uq\_sampling.out' highlighted. A second blue callout box points to this list with the text: 'Plain text output with supported text Processors'. The bottom pane shows the content of 'textbook\_uq\_sampling.out', which is a plain text file containing a partial correlation matrix and other output details, including a date '1-08) built Nov 9 2017' and a start time 'Start time: Mon Feb 19 11:24:42 2018'. The status bar at the bottom indicates 'Line: 2, Col: 27'.

# Miscellaneous Features

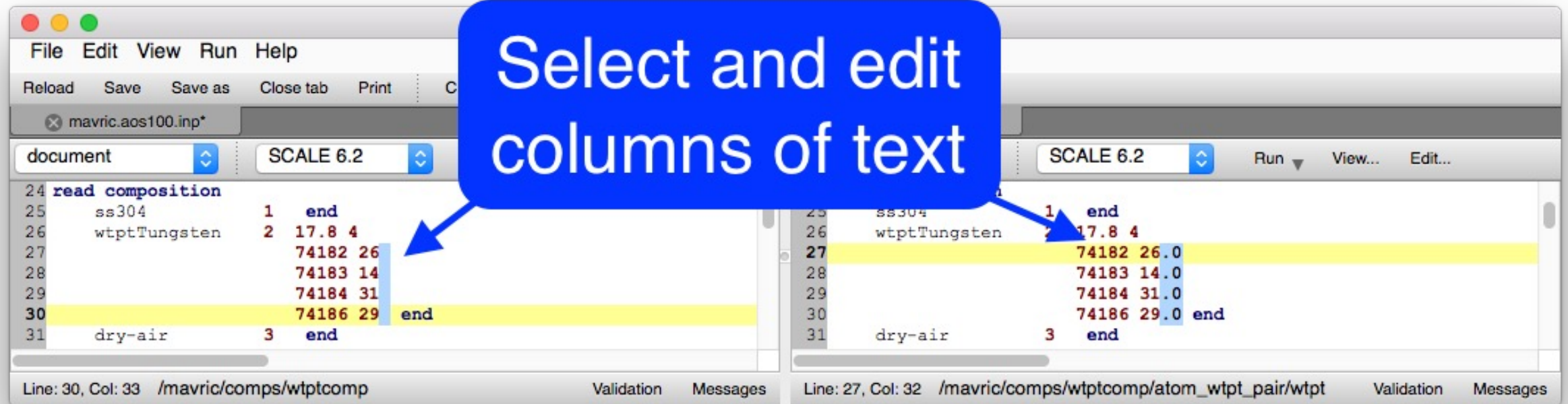
- Column select/edit
  - via ALT+left click+mouse drag key and mouse combo
- Go to definition – allows quick navigation to input components definition via a right click popup context menu.
  - E.g., anywhere an identifier is used to reference another input component.
- Math evaluator
  - Ability to evaluate selected text as a math expression – replaces selection with expression's result.
- Comment toggle
  - Ability to comment/uncomment selected lines
- Indent/unindent
  - Ability to indent/unindent selected lines
- Auto saves – automatic back up to *inputname.wb.autosave*.
  - File exists only while there are unsaved document changes
- Features illustrated on following slides



# Miscellaneous : Column Selection/Edit

Formatting related text into aligned columns allows for faster recognition and column-wise text operations.

- NEAMS Workbench provides column selection via ALT+MOUSE SELECTION.
- With column selection made, any edits are made to all columns for each row.
  - E.g., Update all isotope weight percent values to have a decimal digit.



# Miscellaneous : Go To Definition

The 'Go To Definition' feature is intended to facilitate the user in quickly navigating to the component being referencing.

- New users can discover input component relationships.
- Experienced users can have their navigation accelerated, especially in larger inputs.
- Referenced Geometry Surface identifiers goes to the surface definition.
- Accessible via right clicking an input component

The screenshot shows the NEAMS Workbench interface with two panes. The left pane displays a code snippet with line 82 highlighted: `lower_axial_surf=z0`. A context menu is open over this line, with the 'Goto definition of value' option selected. A blue callout box with the text 'Goto definition of component' has an arrow pointing from the menu option to the right pane. The right pane shows the definition of the surface `plane ( z0 ) { z = 0.0e-2` on line 55, which is also highlighted. The status bar at the bottom indicates the current location: 'Line: 45, Col: 19 /arc/geometry/surfaces/plane/id'.

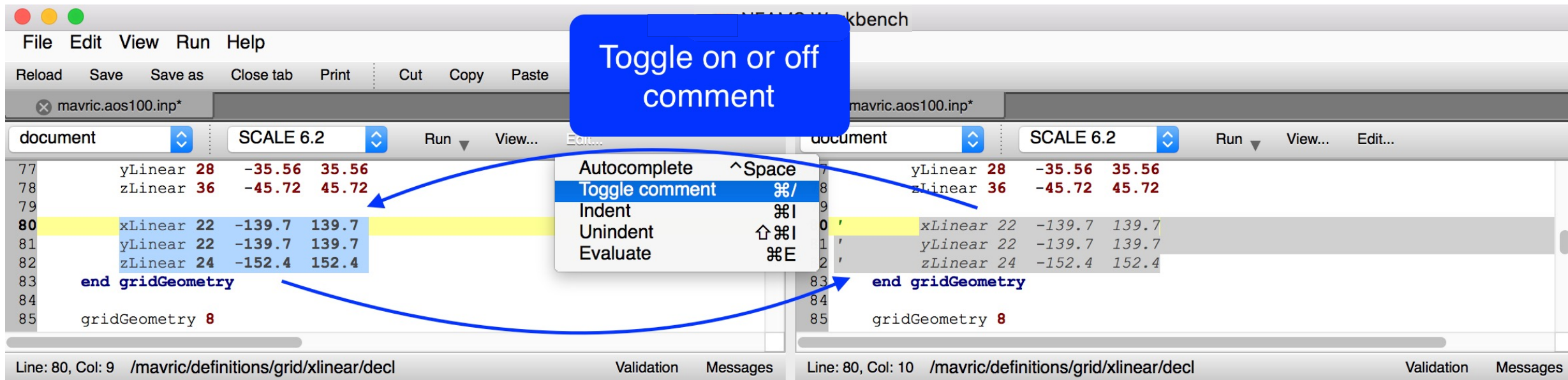
# Miscellaneous : Math Evaluations

- Mitigates typographical errors
- Encourages documentation of engineering specifications that require conversion
- Full complement of math functions available :
  - +, -, \*, /, ^, sqrt, cos, sin, root, abs, min, max, avg, sum, mul, floor, ceil, exp, log, logn, log10, hyp, if, clamp, inrange, sign, deg2rad, tan, equal, acos, asin, atan, cosh, tanh, sec, csc, cot, sinh, round, roundn, d2g, g2d, r2d
- Evaluation occurs on selected text

# Miscellaneous : Comment Toggle

Comment toggling allows users to quickly comment or uncomment pieces of input.

- Allows comment creation
- Mitigates user needing to recall what a comment looks like
- Assists in input development iterations
- CMD+/ on OS X and CTRL+/ on Windows and Linux



# Miscellaneous : Input Indent/Unindent

- Hierarchical input (Application > Block > Record) can be depicted using levels of indentation
- Input indent and unindent facilitates quick formatting to visually depict hierarchy
- Indentation operates on selected text, 4 spaces per indent/unindent
- In inputs without terminators, indentation is used to prioritize autocompletion suggestions

The image displays three side-by-side screenshots of the NEAMS Workbench interface, illustrating the use of indentation in code. The code is organized into hierarchical blocks, with each block's content indented relative to its parent block. A context menu is open over the code in the first screenshot, showing options like 'Indent', 'Unindent', 'Copy', and 'Paste'. The second and third screenshots show the code after indentation adjustments, with blue and yellow highlights indicating the changes.

```
106 [Functions]
107
108 [./power_history]
109 type = PiecewiseLinear
110 data_file = powerhistory.csv
111 scale_factor = 1
112 [../]
113
114 [./axial_peaking_factors]
115 type = ParsedFunction
116 value = '1'
117 [../]
118
119 [./pressure_ramp]
120 type = PiecewiseLinear
121 x = '-200 0'
122 y = '0 1'
123 [../]
124
125 [./q]
126 type = CompositeFunction
127 functions = 'power_histo
128 [../]
129 []
130
```

# Miscellaneous : File Autosaves

Any file NEAMS Workbench edits - currently only text files - are immediately backed up to a *filename.wb.autosave*. In the scenario that the NEAMS Workbench or computer crashes the autosave file will persist.

- Upon NEAMS Workbench restart, reloading the original file will check for *filename.wb.autosave* and load this instead, mitigating any lost progress
- A save of the file will remove the autosave

# Workbench HERON Input

- Demonstrate HERON input features in Workbench
- Launch HERON input
  - Workbench's HERON runtime converts \*.heron to native HERON XML and executes HERON and RAVEN as needed
  - \*.heron becomes \*.heron.xml and can be reviewed for completeness
- Open opt\_soln\_0.csv and plot results

# General Plot Overview

- Interactive and configurable plot rendering
- Plot data table displays graph data.
  - Allows row, column, and table copy to clipboard

The screenshot displays the NEAMS Workbench interface. On the left is a 'Navigation' pane with a list of 'Plottable Items' including various isotopes and capture reactions for u-235. The central plot, titled 'u mt=101 capture', shows the cross-section in barns on a logarithmic y-axis (0.001 to 1000) versus energy in eV on a logarithmic x-axis (10<sup>-5</sup> to 10<sup>7</sup>). Two data series are plotted: 'u-235 mt=101 capture' (blue line) and 'u-238 mt=101 capture' (red line). On the right, a 'Table' view shows the data points for these two series. A menu at the top of the plot area allows switching between 'Plot' and 'Table' views. Blue callout boxes highlight the 'Plottable Items' list, the 'Plot Render and Table Views' menu, the 'Plot Graphs' legend, and the 'Plot Data Table'.

	u-235 mt=101 capture	u-238 mt=101 capture
1.000000e-05	2549.51	57.5376
1.000000e-04	2549.51	57.5376
5.000000e-04	1019.96	23.0493
7.500000e-04	749.208	16.9494
1.000000e-03	633.714	14.3542
1.200000e-03	565.393	12.8189
1.500000e-03	509.626	11.568
2.000000e-03	446.367	10.1574
2.500000e-03	392.842	8.96325
3.000000e-03	354.603	8.11052
4.000000e-03	316.367	7.3681
5.000000e-03	280.139	6.7148
7.500000e-03	224.842	5.37751
1.000000e-02	190.139	4.55082
2.530000e-02	124.928	3.21795
3.000000e-02	93.2524	2.57105
4.000000e-02	80.2046	2.29046

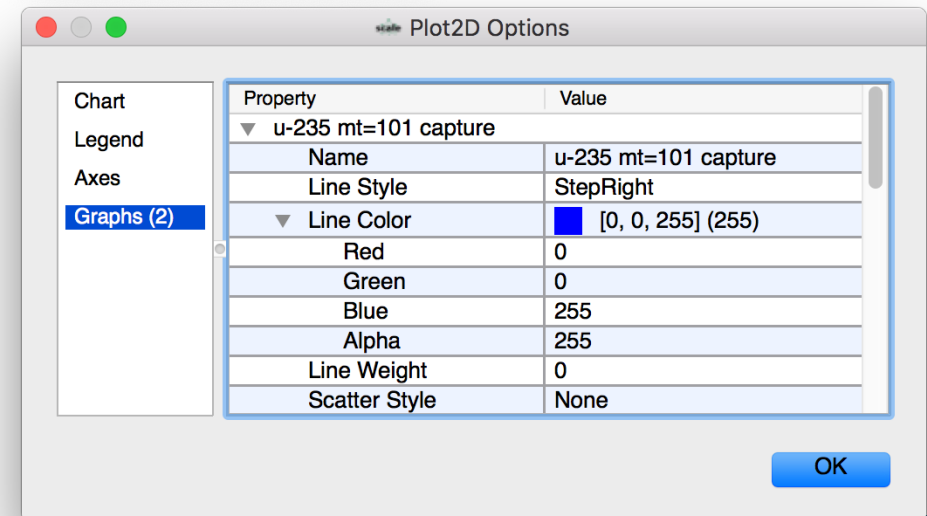
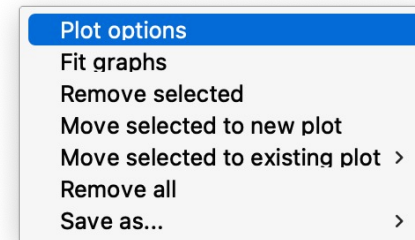


# Plot Controls

NEAMS Workbench plots consist of graph, bars, or color maps, which can be manipulated as follows.

- Select graph via left click in plot or legend.
  - Remove or move selection via context menu
- Zooming is performed via the mouse scroll action.
  - Zoom in by scrolling up.
  - Zoom out by scrolling down.
- Reset to original via context menu Fit graphs.
- Panning is performed via a click and drag.
  - Pan right by left clicking and dragging left.
  - Pan up by left clicking and dragging down.
- Save Plot as
  - PDF (includes scalable vector graphics SVG),
  - PNG and JPG image format
  - Interactive Scale Plot Format (SPF)

- Plot attributes (color, style, etc.) can be changed via context menu Plot options.
- Plot Legend can be drug to 9 positions via left-click and drag.



# Plot Controls : Plot Options

- Chart – Allows changing the plot title and title visibility.
- Legend – Allows changing the legend's font and visibility.
- Axis – Allows changing axis visibility, label text, label text font, axis scale, axis range, axis grid, tick label font and tick text attributes (rotation, precision, etc.).
- Graphs – Allows changing graph name, line style, line color, line weight, scatter style, scatter size, pen style, adaptive sampling\*, errors bars.
- Bars – Allows changing bar graph name.
- Color Map – Allows changing color map graph name and color gradient.

\* adaptive sampling – conducts intelligent sampling of the data points providing significant speed up when many data points are involved. Default is on.

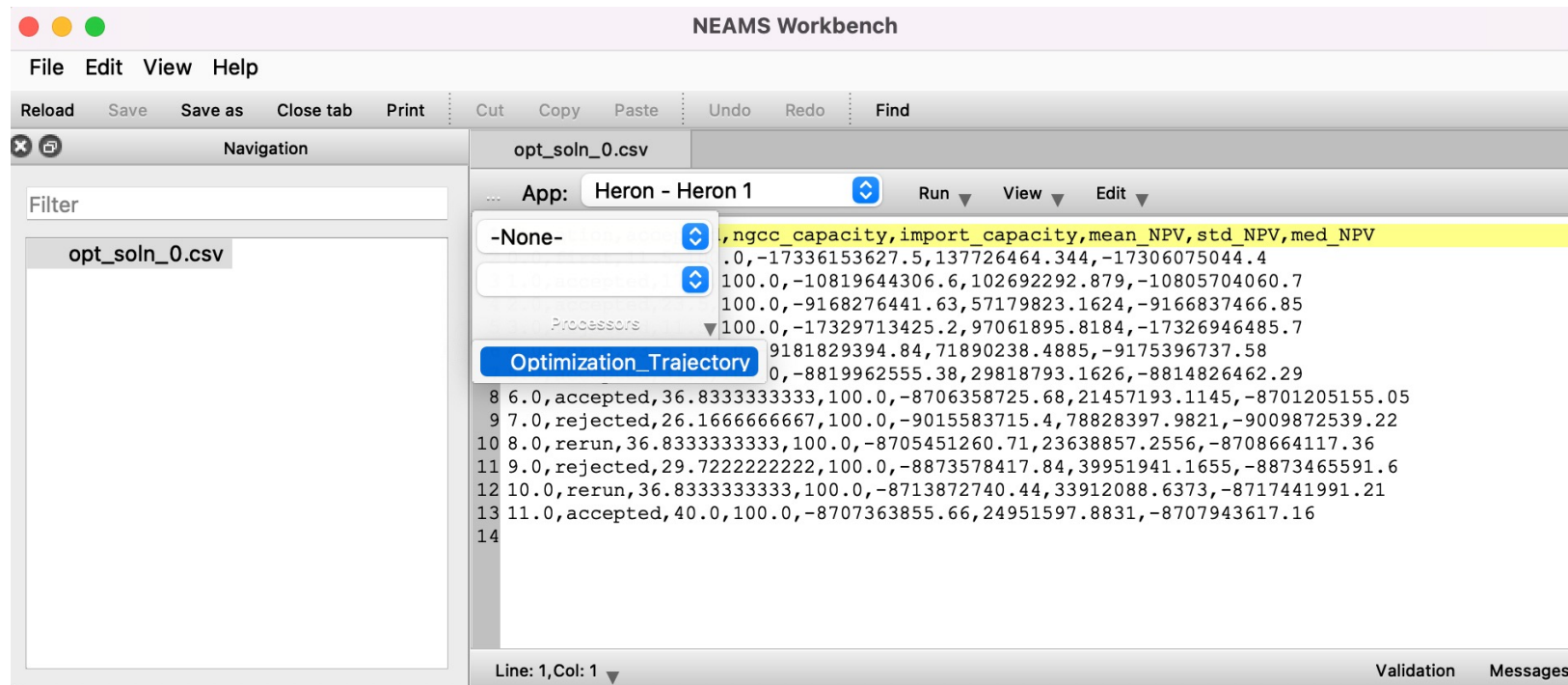


**IES**

Integrated Energy Systems

# Processor Generated Result Plots

- Automates data plot generation
  - Streamlines typical excel spreadsheet workflow of extracting data to charts.
- User-extensible
  - Can execute user specified logic

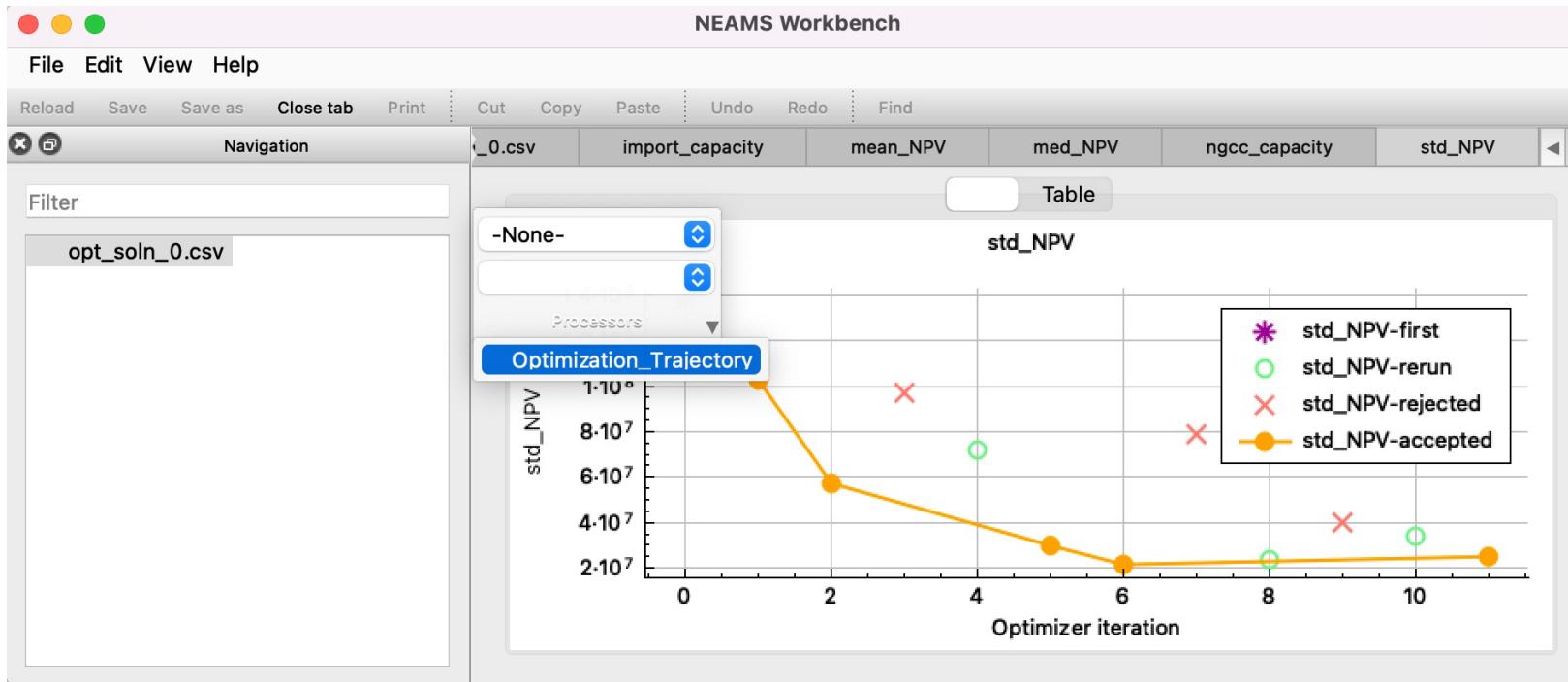


The screenshot displays the NEAMS Workbench interface. The main window shows a data table for 'Heron - Heron 1' with columns for 'ngcc\_capacity', 'import\_capacity', 'mean\_NPV', 'std\_NPV', and 'med\_NPV'. The table contains 14 rows of data, with the first row highlighted in yellow. The interface includes a menu bar (File, Edit, View, Help), a toolbar (Reload, Save, Save as, Close tab, Print, Cut, Copy, Paste, Undo, Redo, Find), and a navigation pane on the left with a filter and a list of files (opt\_soln\_0.csv). The status bar at the bottom indicates 'Line: 1, Col: 1' and 'Validation Messages'.

	ngcc_capacity	import_capacity	mean_NPV	std_NPV	med_NPV		
1	.0	-17336153627.5	137726464.344	-17306075044.4			
2	100.0	-10819644306.6	102692292.879	-10805704060.7			
3	100.0	-9168276441.63	57179823.1624	-9166837466.85			
4	100.0	-17329713425.2	97061895.8184	-17326946485.7			
5	9181829394.84	71890238.4885	-9175396737.58				
6	0	-8819962555.38	29818793.1626	-8814826462.29			
8	6.0	accepted	36.8333333333	100.0	-8706358725.68	21457193.1145	-8701205155.05
9	7.0	rejected	26.1666666667	100.0	-9015583715.4	78828397.9821	-9009872539.22
10	8.0	rerun	36.8333333333	100.0	-8705451260.71	23638857.2556	-8708664117.36
11	9.0	rejected	29.7222222222	100.0	-8873578417.84	39951941.1655	-8873465591.6
12	10.0	rerun	36.8333333333	100.0	-8713872740.44	33912088.6373	-8717441991.21
13	11.0	accepted	40.0	100.0	-8707363855.66	24951597.8831	-8707943617.16
14							

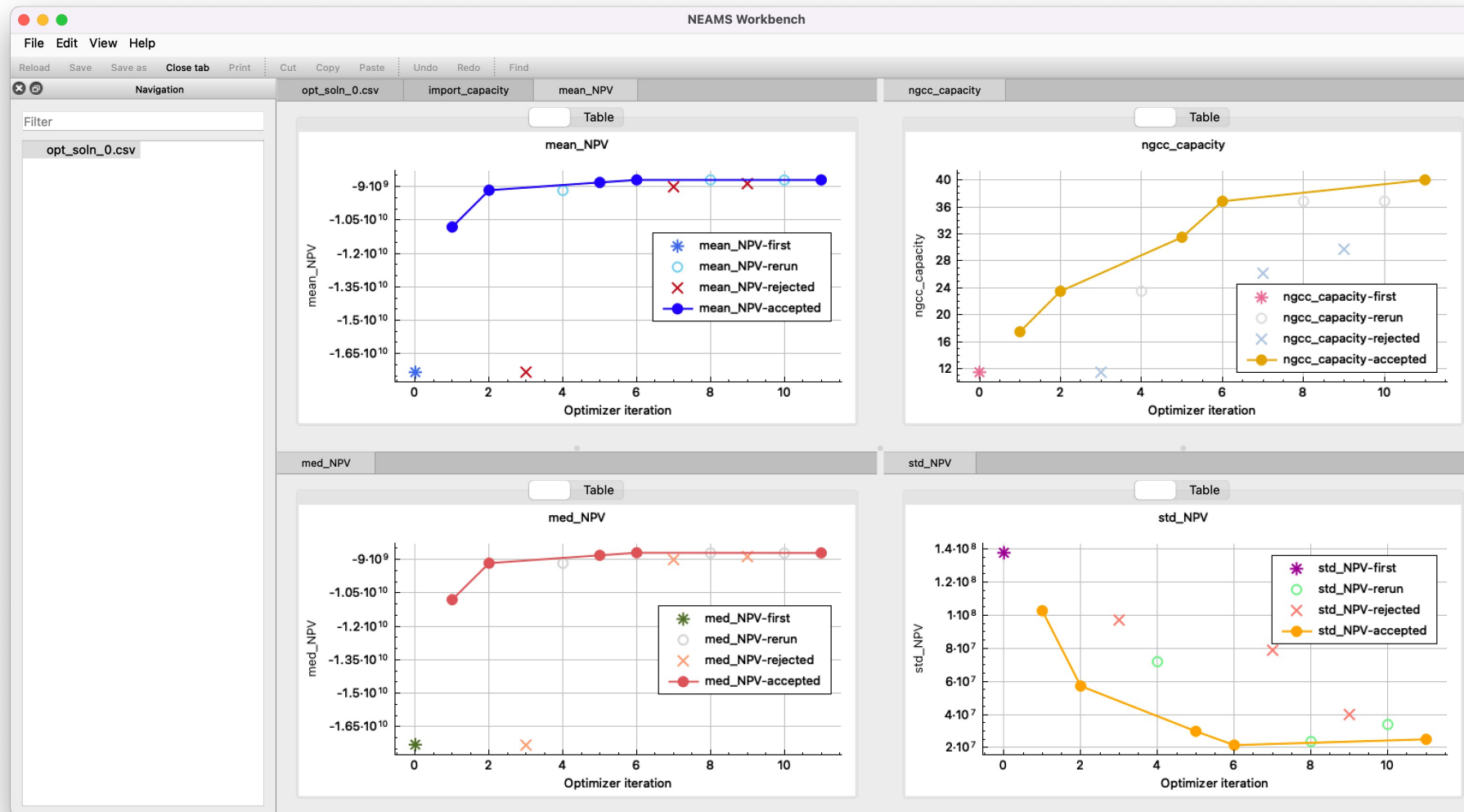
# Processor Generated Results Plots

Clicking the Optimization\_Trajectory will generate plot tabs



# Processor Generated Results Plots

Tabs can be rearranged for broader viewing experience of results



# Questions & Discussion

Special thanks to Mark Baird (ORNL) and Brandon Biggs (INL) for facilitating the use and demonstration of the NEAMS Workbench and HERON on INL's NCRC

Reminder: integration effort is new. User input and feedback is valuable.