

How does SCALE work?

SCALE 6.3

ORNL is managed by UT-Battelle, LLC for the US Department of Energy

Overview

- SCALE code system structure
- SCALE runtime environment and command line
- Graphical user interface (GUI)
- Manual is available online at scale-manual.ornl.gov

SCALE Structure

- SCALE has been built up from “**modules**”
 - Many originated in the 70s
 - KENO: criticality calculation module
 - ORIGIN: depletion/decay module
 - May have their own input, originating from their initial design
- SCALE has unified usage of modules into “**sequences**”
 - “Automatically” set up inputs for independent “modules” to run sequentially and to collect results and data to feed to the next module
 - “Sequences” are the top-level “applications” or “products” in modern terms
- Has **keyword-based input** with some position-dependent input needed to maintain backward compatibility

SCALE nomenclature

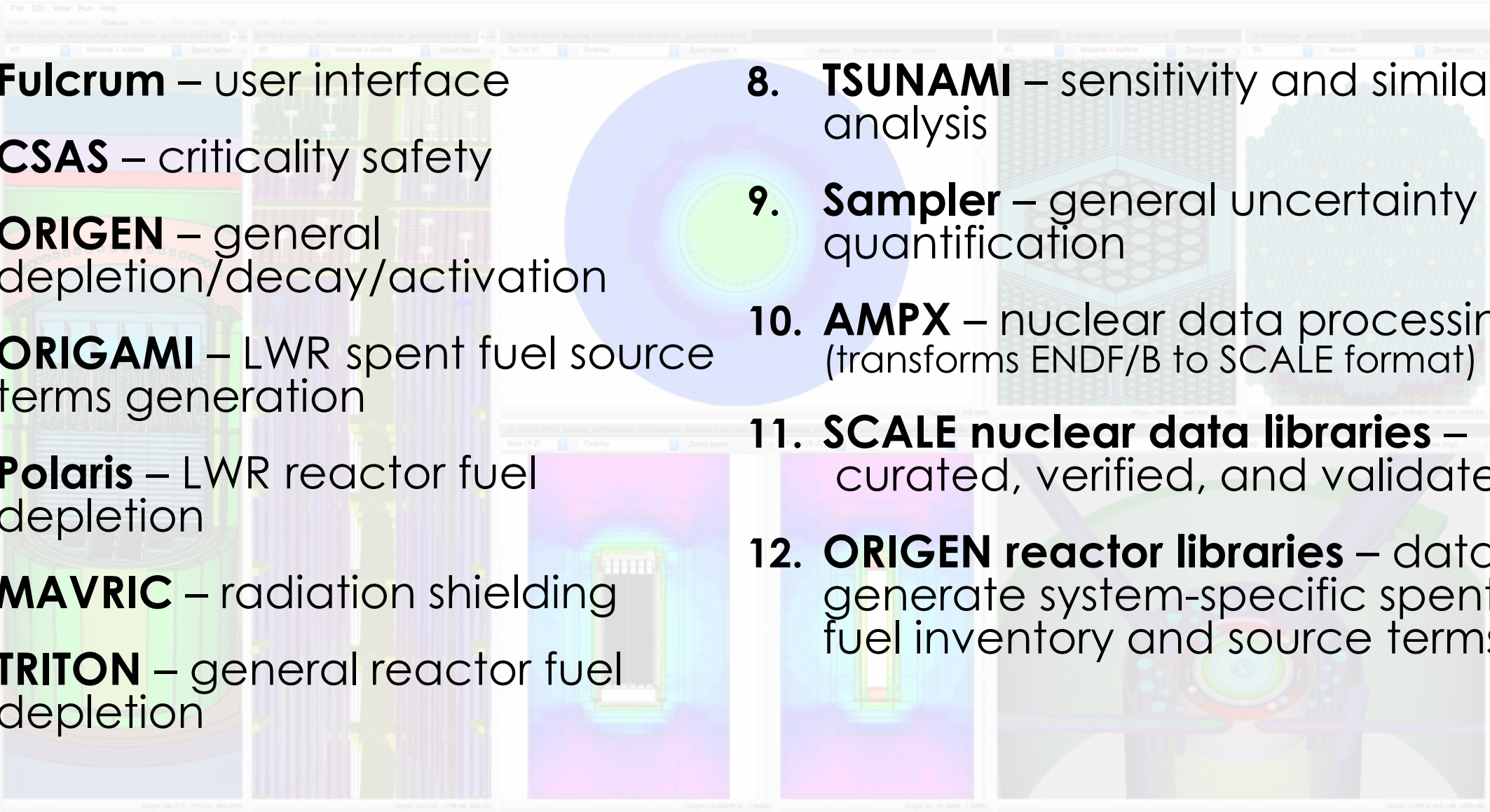
- **Library**
 - A collection of nuclear data (could be decay data or continuous-energy cross sections)
- **Module**
 - A fundamental code capability, which may or may not have a user input file
- **Sequence**
 - One or more modules running in “sequence,” each potentially reading user input files and data libraries
- **SCALE runtime environment (scalerte)**
 - The “**driver**” that sets up environment variables and calls each sequence in an input file

As SCALE moves to more flexible application programming interfaces (APIs) for modules, the idea of SCALE sequences is less useful because all the work happens in-memory.

Older sequences would write module inputs and read their outputs.

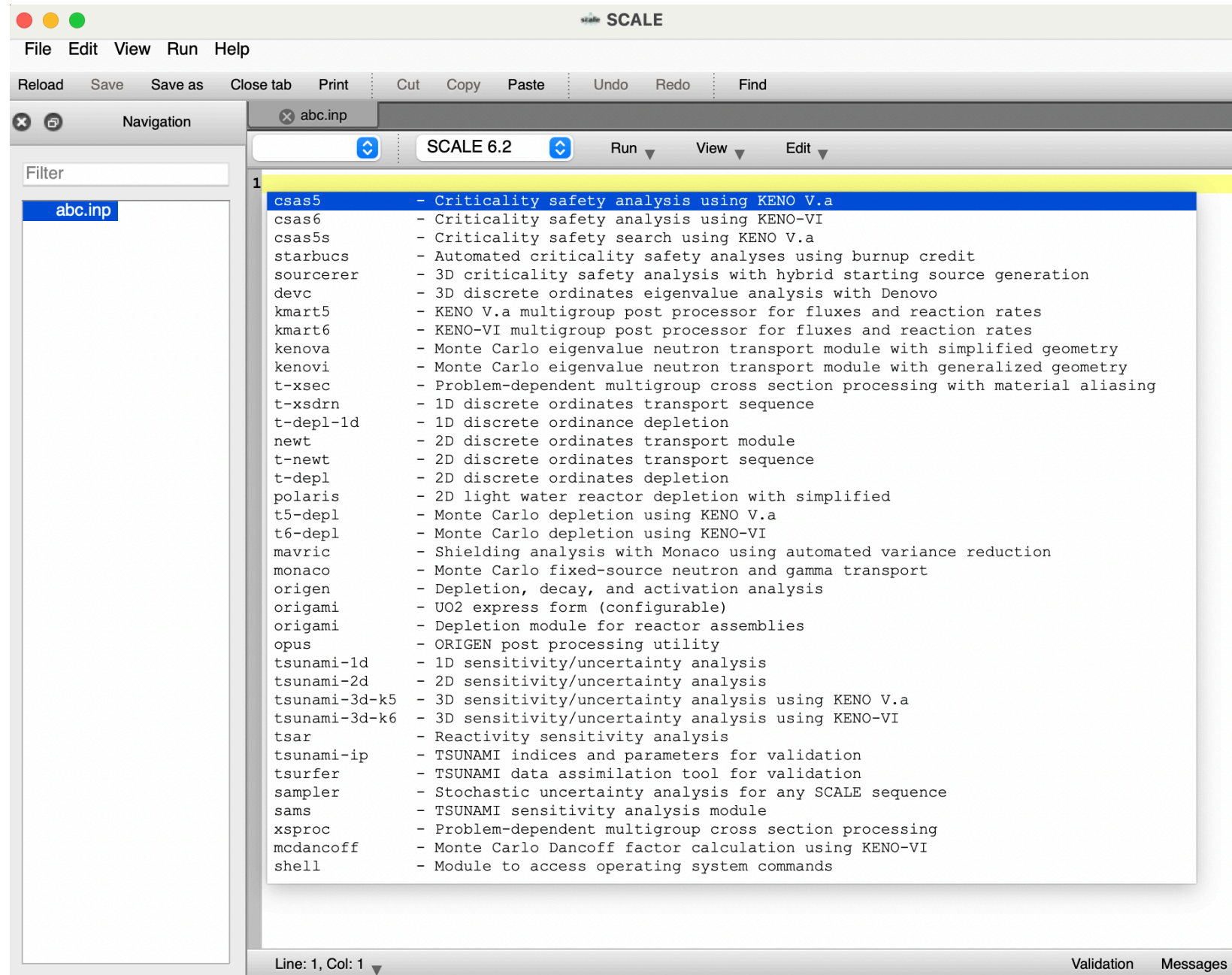
Moving forward, we prefer “**product**” or “**application**” for the end user “**sequences**” in SCALE.

SCALE contains 12 end user **products**

- 
1. **Fulcrum** – user interface
 2. **CSAS** – criticality safety
 3. **ORIGEN** – general depletion/decay/activation
 4. **ORIGAMI** – LWR spent fuel source terms generation
 5. **Polaris** – LWR reactor fuel depletion
 6. **MAVRIC** – radiation shielding
 7. **TRITON** – general reactor fuel depletion
 8. **TSUNAMI** – sensitivity and similarity analysis
 9. **Sampler** – general uncertainty quantification
 10. **AMPX** – nuclear data processing (transforms ENDF/B to SCALE format)
 11. **SCALE nuclear data libraries** – curated, verified, and validated
 12. **ORIGEN reactor libraries** – data to generate system-specific spent fuel inventory and source terms

SCALE sequences

- Within the Fulcrum GUI, **autocomplete** shows many “sequences”
- Sequences can be chained together in a single input file
- The “**shell**” sequence can be used to perform workflow steps, including copying files into and out of the working directory



Sequences usage example

- This input calls three SCALE sequences (called using **=**)
 - **origen** on line 1
 - **shell** on line 24
 - **opus** on line 29
- Each sequence calls one or more modules
- Every SCALE input is run with **scalerte** ...
 - E.g., **scalerte problem.inp**
- **scalerte** is the “glue” that
 - processes the input, finds each =ABC sequence, and calls the relevant code
 - sets up a temporary working directory for all files and performs numerous transfers between the working directory and other file locations
- Detailed output from the runtime environment can be enabled with **scalerte -v**

```
1 =origen
2 case{
3   lib{
4     file="end7dec"
5   }
6   mat{
7     iso[ pu238=1.0 ]
8     units=GRAMS
9   }
10  time{
11    t=[20L 1 1000]
12    units=YEARS
13  }
14  print{
15    nuc{ units=[WATTS GRAMS] }
16    ele{ units=[WATTS GRAMS] }
17  }
18  save=yes
19  % save=yes produces a file called ft71f001
20  % in the "working" directory.
21 }
22 end
23
24 =shell
25 ls ${TMPDIR}
26 end
27
28 'By default OPUS reads a file called ft71f001.
29 =opus
30 units=watt
31 end
32
33 'Here the SCALE driver, as it exits, performs
34 'various copies, moves, and renames of files
35 'like ft71f001 to pu238.f71.
36
```

SCALE execute options

scalerte [-options] inputfile(s)

where options include

- m Turn messages on
- T Specify the temporary directory. -T /dir/path/

Example: **scalerte inputfile.inp -m -T mytmp**

Many more runtime options are available. Simply type **scalerte** (no options or filenames) on the command line to see a list of the available options on your system.

Other SCALE execute options

- z Add the date to the output file name
 - t Use the last used temporary directory
 - o Override the default name *inputfile.out* for output file
- You can use wildcards to run multiple files or add multiple files to run to the command line

Examples:

```
scalerte mycase1.inp &
scalerte -m mycase1.inp mycase2.inp mycase3.inp
scalerte -m -T mycase*.inp
```

run in background

run multiple files

Other useful SCALERTE information

- Use the SCALE environment variables and the *shell* command to save files from the temporary directory
 - `OUTDIR`, `OUTBASE`, `TMPDIR`, and `BASENAME` are most common
 - Precede environment variable with “\$” and enclose the environment variable in curly braces: `${OUTDIR}`
 - Some Linux/UNIX shell commands are mapped to windows equivalents [cp, mv, rm, ln -s] allowing SCALE inputs to be semi-platform independent
- Example: use the *shell* command and the SCALE environment variables to save the ft71f001 file to the user directory. `OUTDIR/BASENAME` is equivalent to `OUTBASE`.

```
=shell
  cp "${TMPDIR}/ft71f001" "${OUTDIR}/${BASENAME}.f71"
  cp "${TMPDIR}/ft71f001" "${OUTBASE}.f71"
end
```

Key environment variables

1. **TMPDIR** – working directory used by SCALE for the calculations
2. **INPDIR** – input file directory (default is where input resides)
3. **OUTDIR** – output file directory (default is INPDIR)
4. **BASENAME** – the name of the input file minus the “.inp” extension
5. **OUTBASE** – the shorthand of OUTDIR/BASENAME
6. **DATA** – directory that contains the SCALE data files (e.g., libraries)

SCALE output files

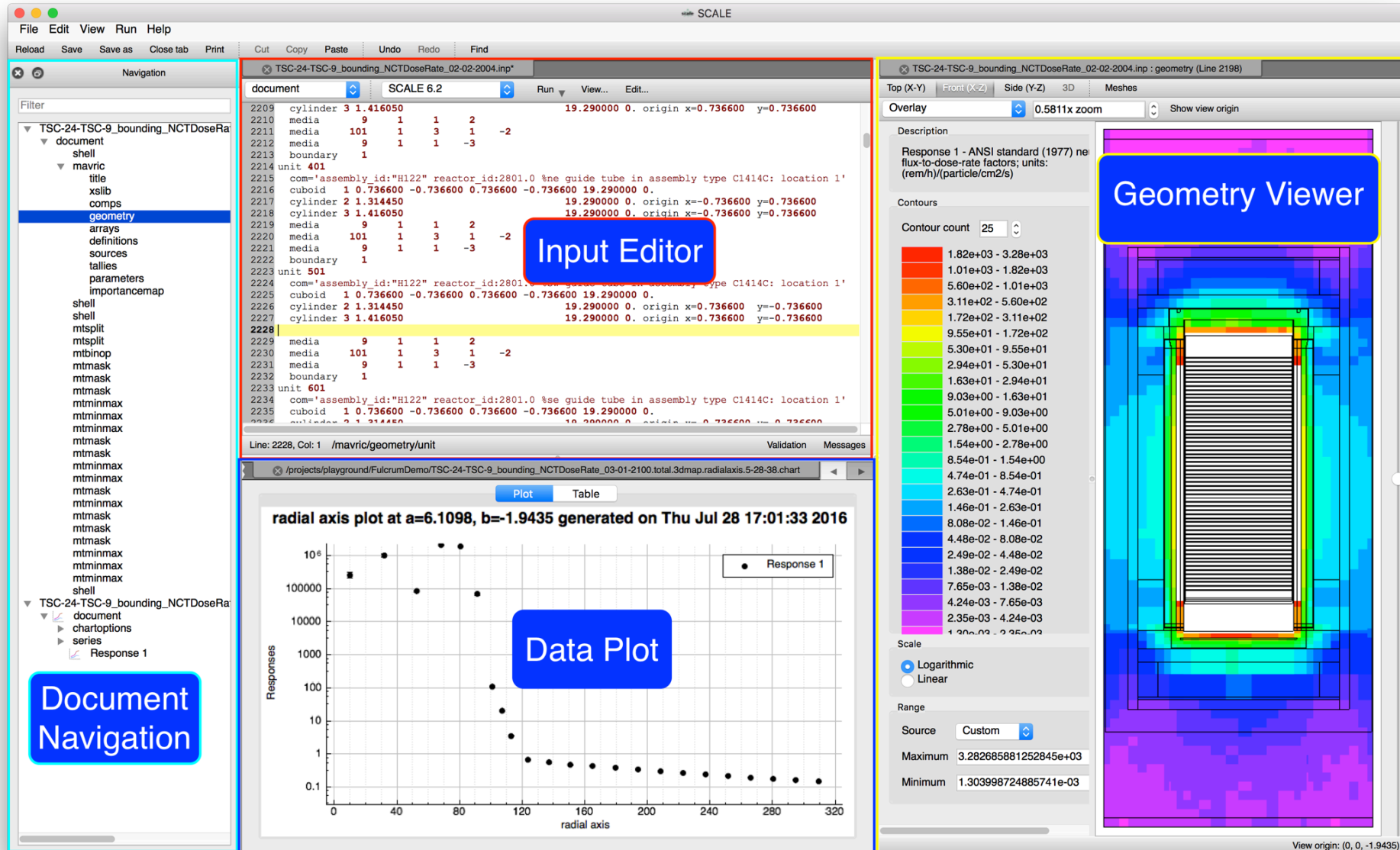
- Most of the important information can be found in the “.out” file
 - Every SCALE run creates a .out file, and most of the results are stored in this file, including most error messages
 - For KENO sequences, an HTML version of the output file can be opened in a browser
- The messages file “.msg” contains information printed to the screen
 - Can provide useful error messages that may not be contained in the “.out” file
- ORIGIN-specific files
 - “.plt” files contain selected isotopic information as a function of time
 - “.f71” files contains all isotopic information for the problem
 - “.f33” files contain ORIGIN 1-group cross sections
- Other output files – check Fulcrum’s open file for matching file extension

Fulcrum – SCALE's graphical user interface

- Platform-independent!
- GUI and integrated development environment for SCALE input files
- Looks like a text editor but is more powerful, with modular workspaces
- Syntax highlighting and input checking
- Integrated geometry visualization
- Run SCALE directly from Fulcrum
- View screen output in Fulcrum
- Integrated results visualization

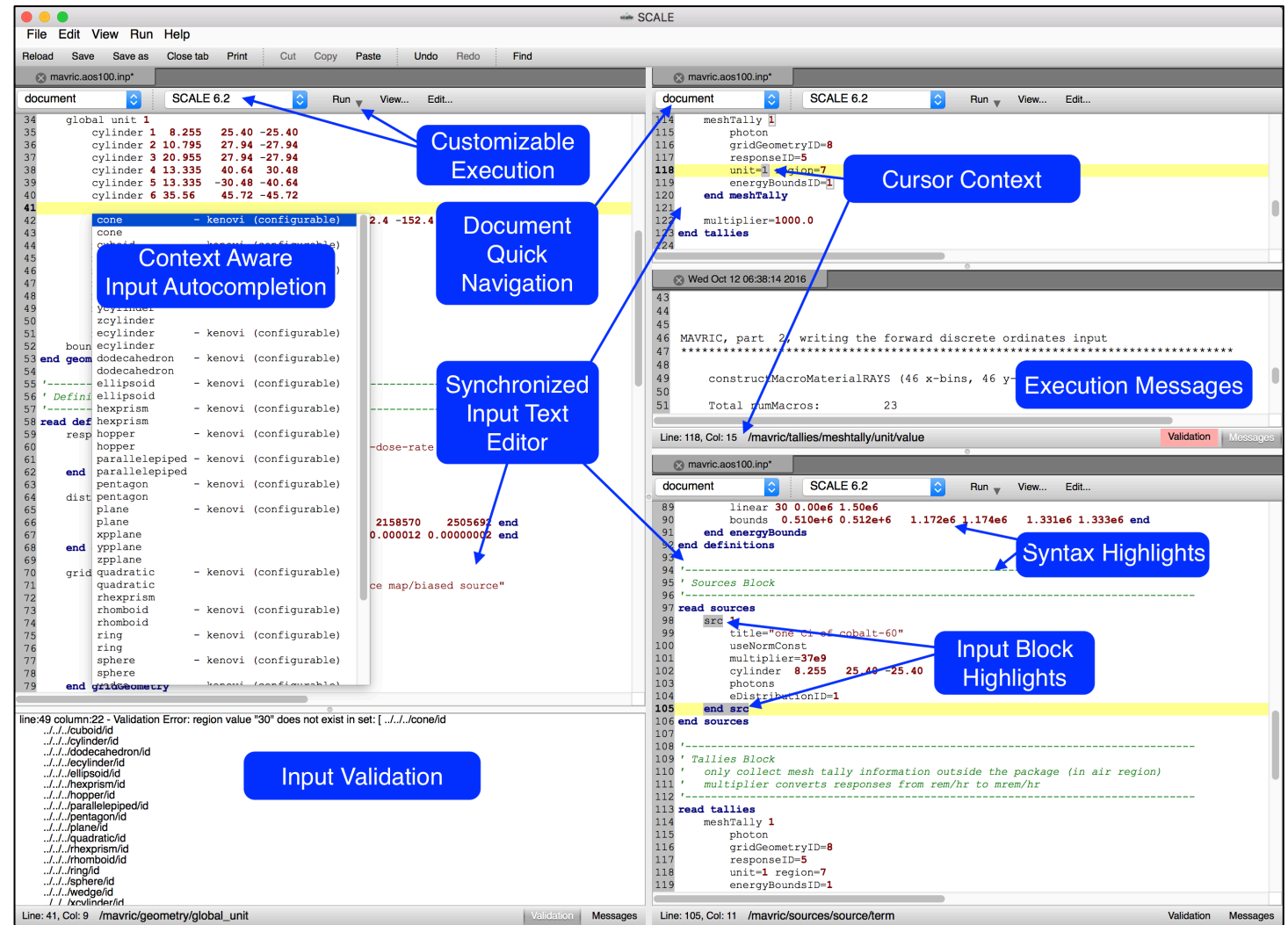


Fulcrum components overview



Fulcrum text editor features | Overview

- Customizable execution
- Quick navigation
- Cursor context
- Execution messages
- Input validity checks
- Syntax highlights
- Current block highlight
- Context-aware input auto completion
- Synchronized and split workspaces



Input autocompletion : Static text

- Static text autocompletion facilitates abbreviated input to include the component's description, allowing users to discover and/or more quickly recall the necessary input components for their analysis
- Cursor context allows the autocompletion popup to show what is legal and has not already been specified

Access Autocomplete via
* CTRL+SPACE Keys, or,
* Edit...>Autocomplete

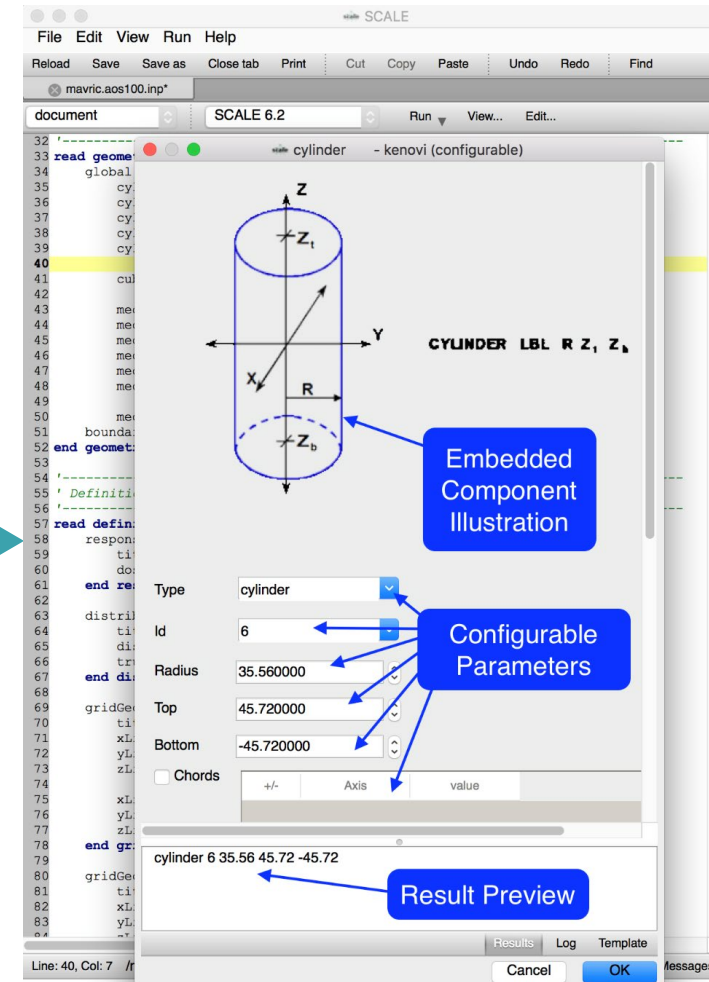
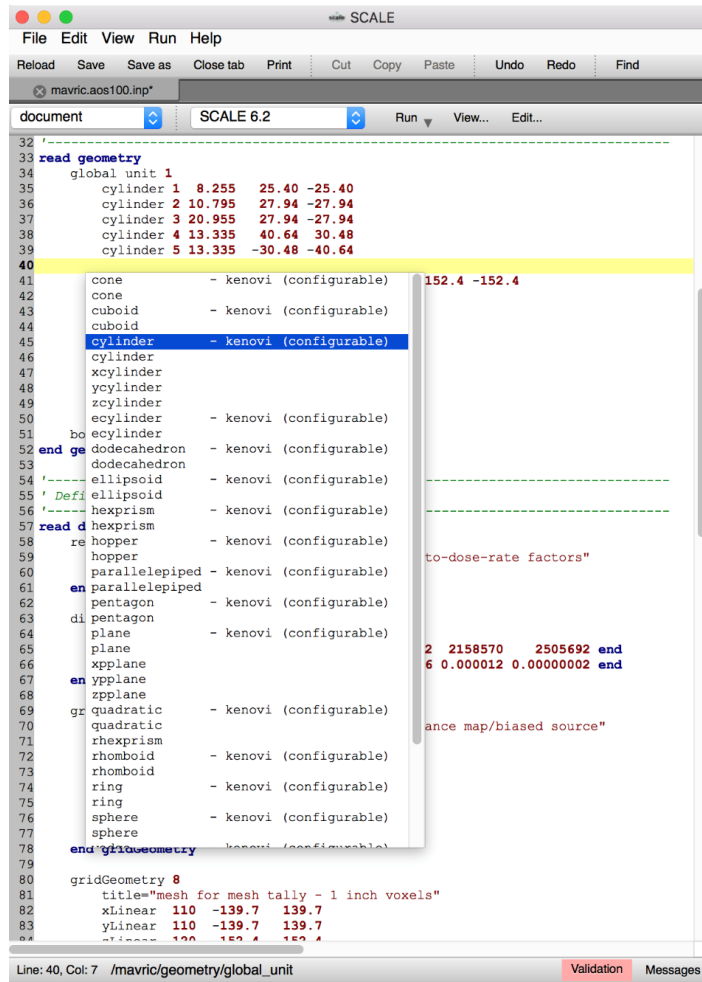
The screenshot shows the SCALE 6.2 application window. The menu bar includes File, Edit, View, Run, and Help. Below the menu bar is a toolbar with buttons for Reload, Save, Save as, Close tab, Print, Cut, Copy, Paste, Undo, Redo, and Find. The main window displays a code editor with a file named 'csas6_7.inp'. The code is written in a syntax-highlighted format, with parameters and their descriptions listed. A blue box highlights the text 'Parameters with descriptions'.

Parameter	Description
rnd	- random number
tme	- execution time (min)
tba	- batch time (min)
wt	- average weight
wt	- wt. for splitting
wtl	- russian roulette wt.
sig	- deviation limit
msh	- size of flux mesh
ttl	- ce temperature tol.
dbh	- upper dbrc energy cutoff
dbl	- lower dbrc energy cutoff
gen	- no. of generations
npg	- no. per generation
nsk	- generations skipped
res	- gens. between restart
nbk	- neutron bank positions
xnb	- extra bank entries
nfb	- fission bank positions
xfb	- extra bank entries
xld	- no. of extra l-das
beg	- restart at this gen.
nb8	- blocks for d.a. unit
nl8	- length of d.a. block
nqd	- quadrature order for angular fluxes moments
ngp	- number of energy groups for tallying
pnm	- order of flux moments
cxm	- reaction rate tallying mode
cep	- continuous energy directory file
fno	- output restart file identifier
fni	- input restart file identifier
dbx	- use dbrc for scattering
app	- doppler broadening method
flx	- collect and print
fdn	- fission densities
adj	- adjoint calculation
ptb	- use probability tables

Input autocomplete : Configurable text

- Allows user to configure values prior to inserting into input

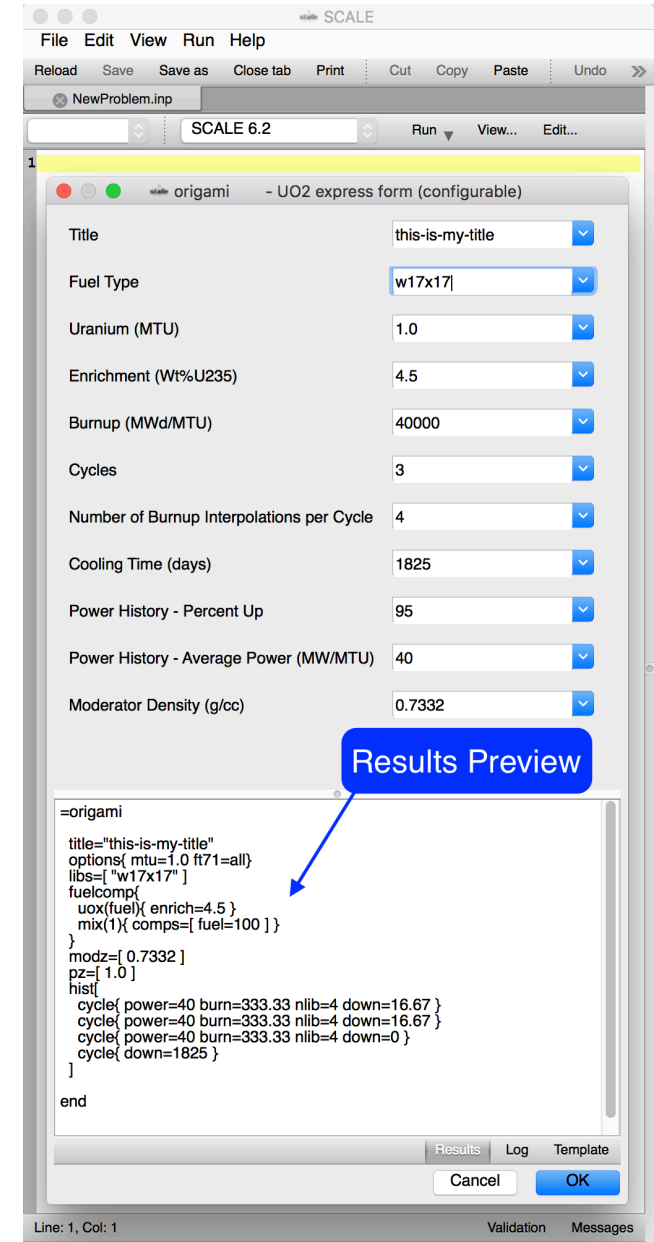
Access Autocomplete via
* CTRL+SPACE Keys, or,
* Edit...>Autocomplete



Input autocomplete : Configurable text

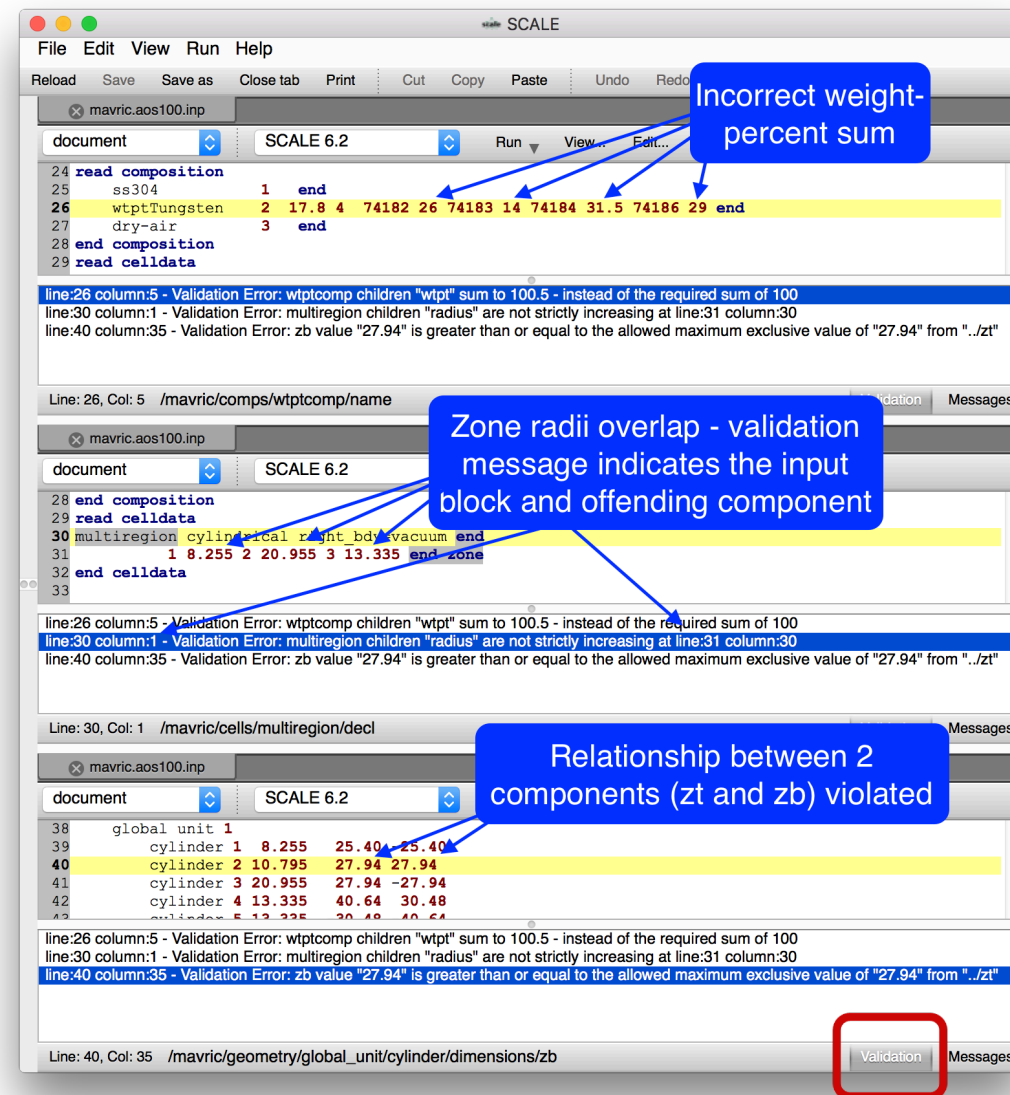
- Configurable autocomplete allows creation of entire input
- Results preview facilitates learning input syntax
- Attributes can be labeled even when the actual input attribute may not have a label
- Attributes can have a drop-down listing the available or common values to specify

Access Autocomplete via
* CTRL+SPACE Keys, or,
* Edit...>Autocomplete



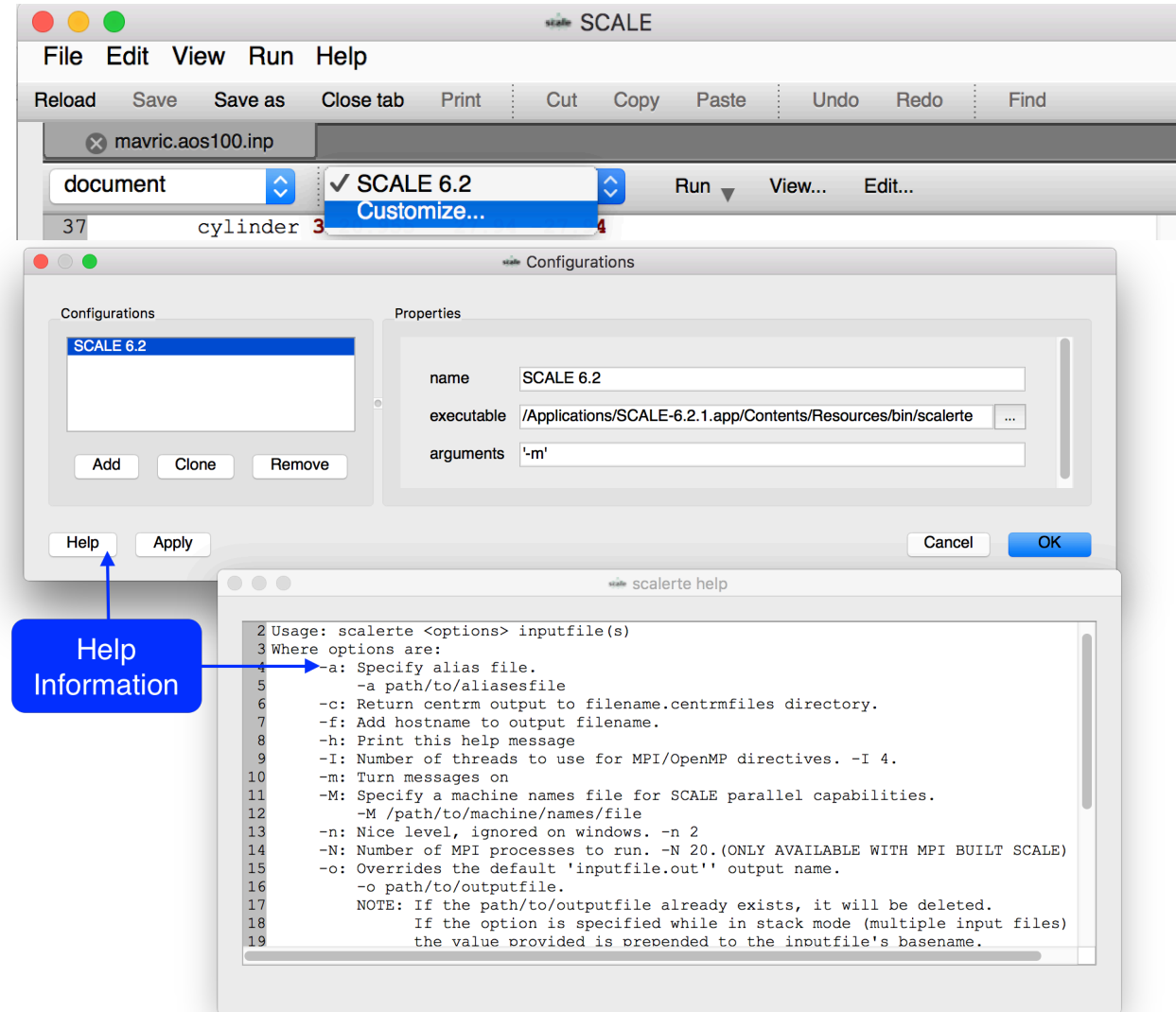
Input validation | Automatic input checking

- Fulcrum applies numerous input checks to your input while you are editing
 - Results of input checks are listed in the text editor's **Validation** panel located in the lower right corner, adjacent to the **Messages** panel
 - Left-clicking the message quick-navigates to the error location



Input Execution: Customized run configurations

- Add new
- Clone existing
- Remove existing
- Modify existing
- Show executable help
- Provide additional arguments



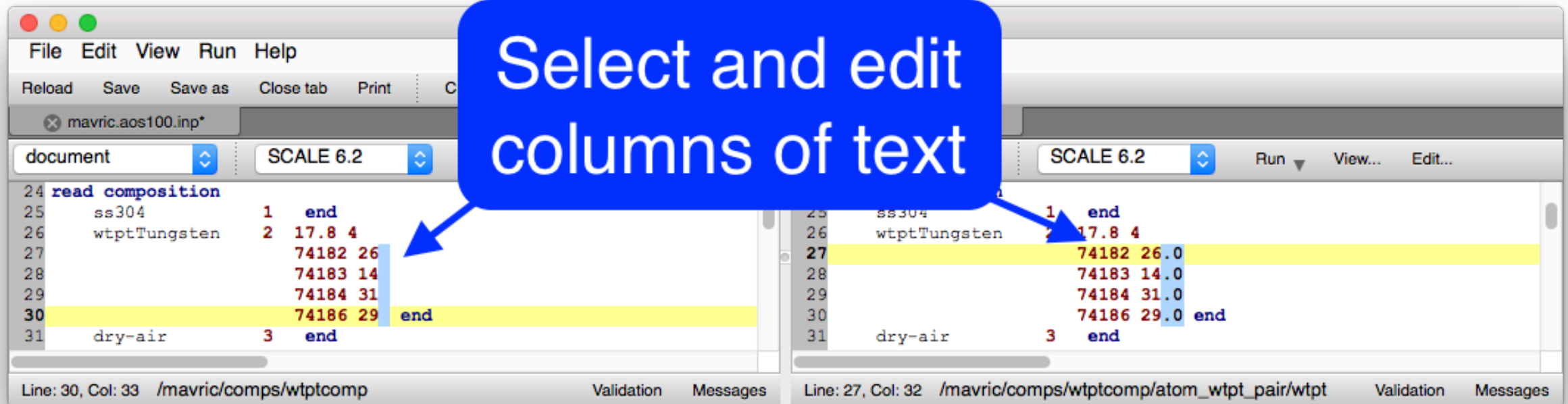
Miscellaneous features

- 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
 - Evaluate selected text as a math expression – replaces selection with expression's result
- Comment toggle
 - Comment/uncomment selected lines
- Indent/unindent
 - Indent/unindent selected lines
- Auto-saves – automatic backup to *inputname.fulcrum.autosave*

Column text selection and editing

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

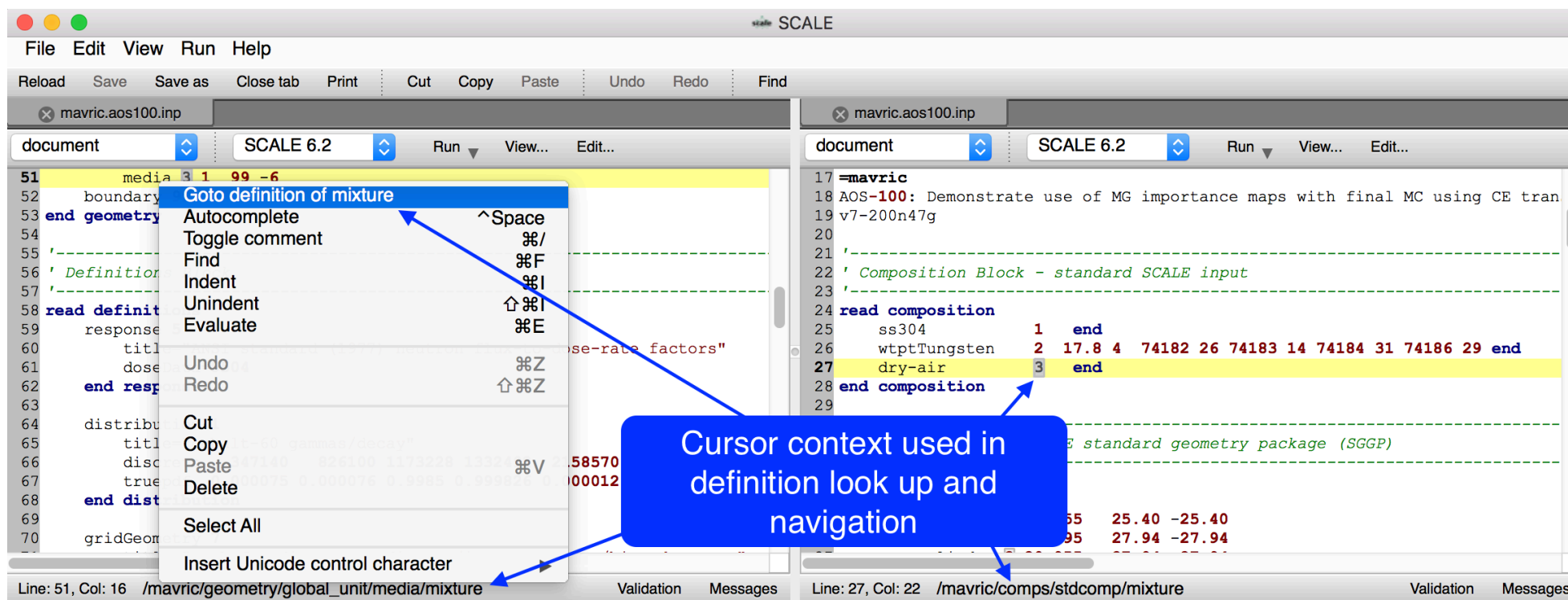
- Column selection via **ALT+MOUSE SELECTION**
- With column selection made, any edits are made to all columns for each row
- E.g., update all isotope weight percent values to have a decimal digit



Miscellaneous: Go to definition

Feature is available via right-clicking an input component and facilitates quick navigation to the component being referenced. New users can discover input component relationships. Experienced users can accelerate their navigation, especially in larger inputs.

- Referenced mixture identifier – goes to the mixture's definition
- Referenced Geometry unit identifiers (holes) – goes to the unit definition



Expression evaluation | Embedded calculator

- An integrated expression evaluation engine is available in Fulcrum
- Accessible via **Edit > Evaluate** or **CTRL+E** (Windows/Linux) **CMD+E** (Mac)
- Arithmetic operators: +, -, *, /, ^ and supports typical functions
- Example:

Calculate the fuel area given the fuel diameter of 0.8357

Enter a comment with **pi*(fueld=0.8357/2.0)^2**

```
20 end composition
21 ' The cell processing
22 ' pi*(fueld=0.8357/2.0)^2
23 read celldata
24 latticecell
25 squarepitch pitch 1.2598 8
26 fueld 0.8357 1
27 cladd 0.94996 2 end
```

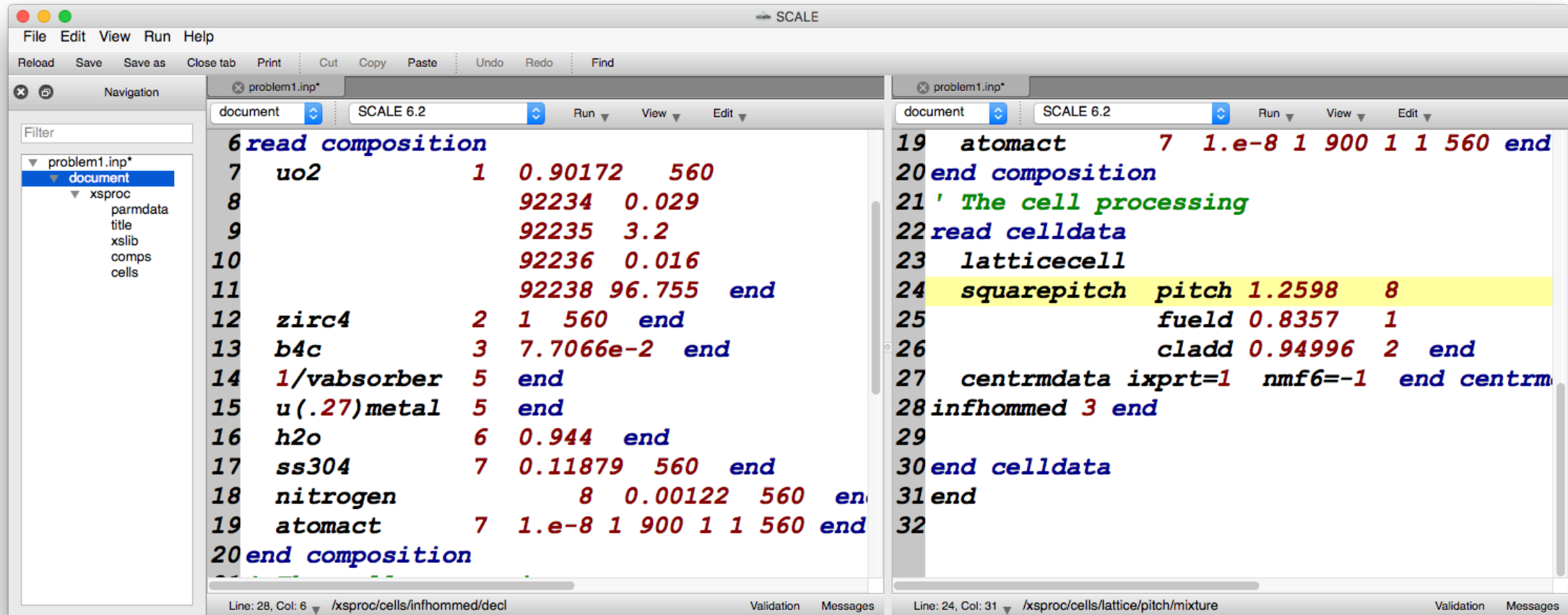
Select the text and evaluate it

I.e., **Edit > Evaluate** or
CMD+E (Mac) or
CTRL+E (Windows/Linux)

```
20 end composition
21 ' The cell processing
22 ' 0.548518
23 read celldata
24 latticecell
25 squarepitch pitch 1.2598 8
26 fueld 0.8357 1
27 cladd 0.94996 2 end
```

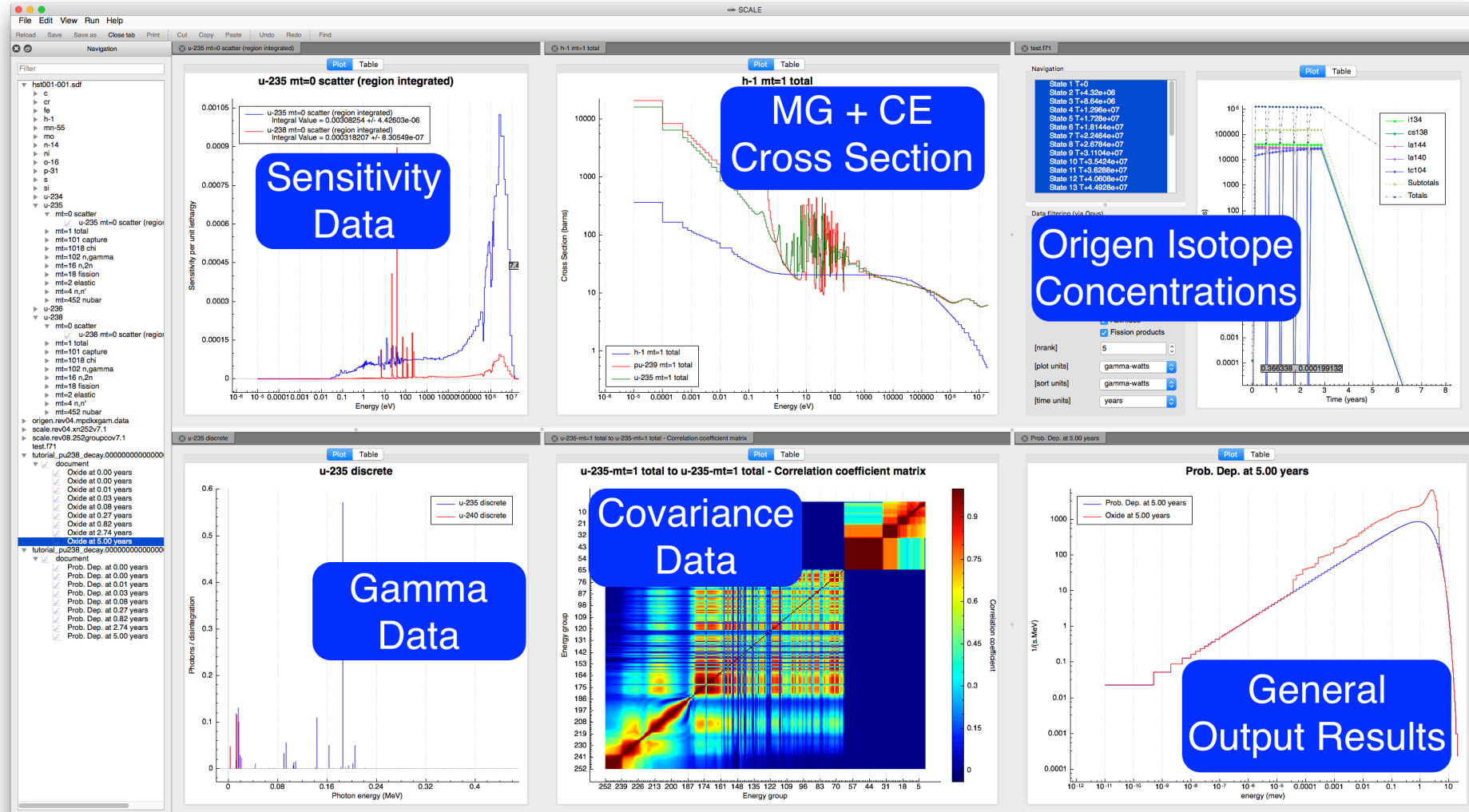
Workspaces | Split editor

- Split editor allows for viewing and editing associated input sections
- Rearranging workspaces is facilitated by **click-and-drag** of the desired tab to the new location

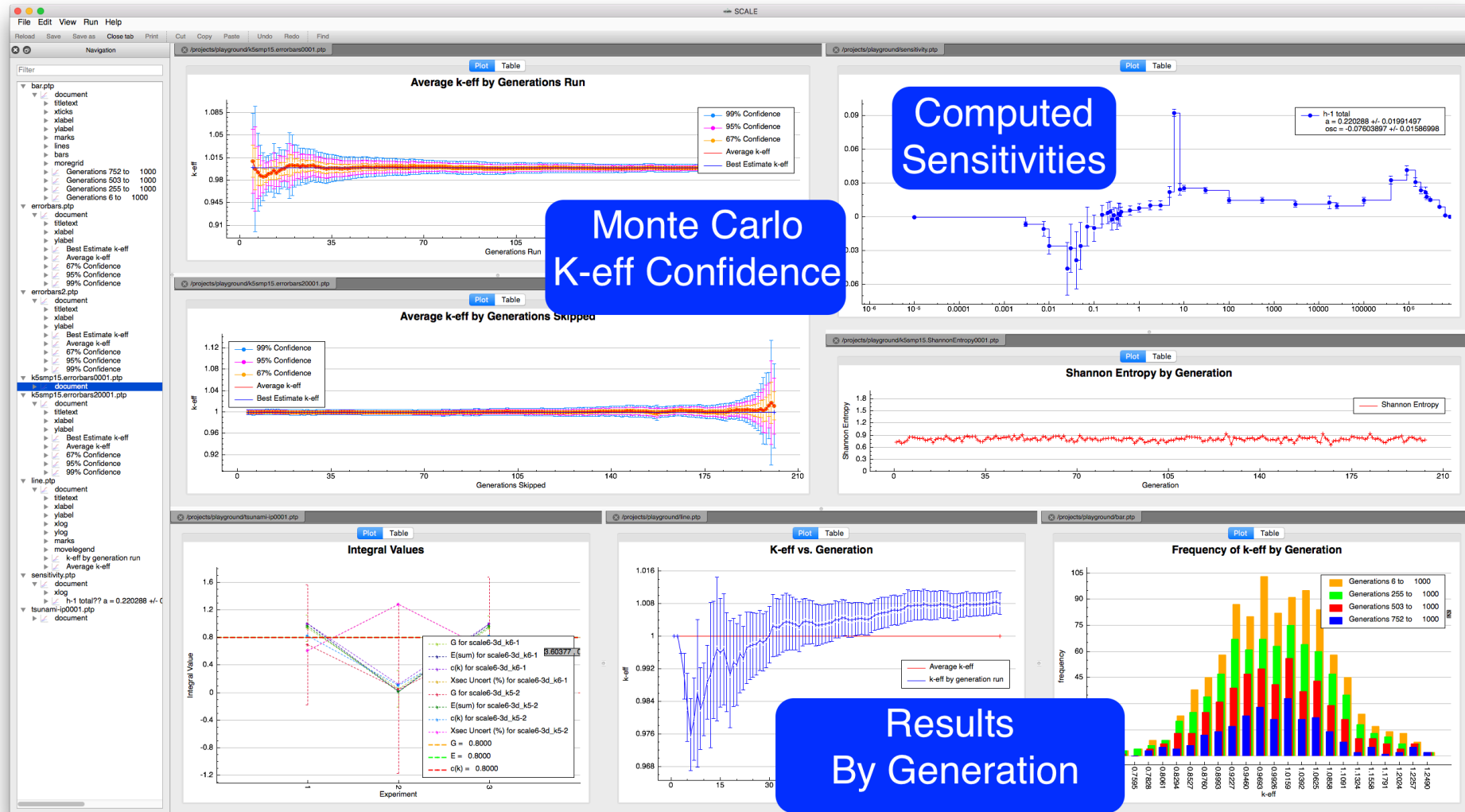


Fulcrum plot data

- Supports most major SCALE data formats
- Export to image (supports scalar vector graphics)

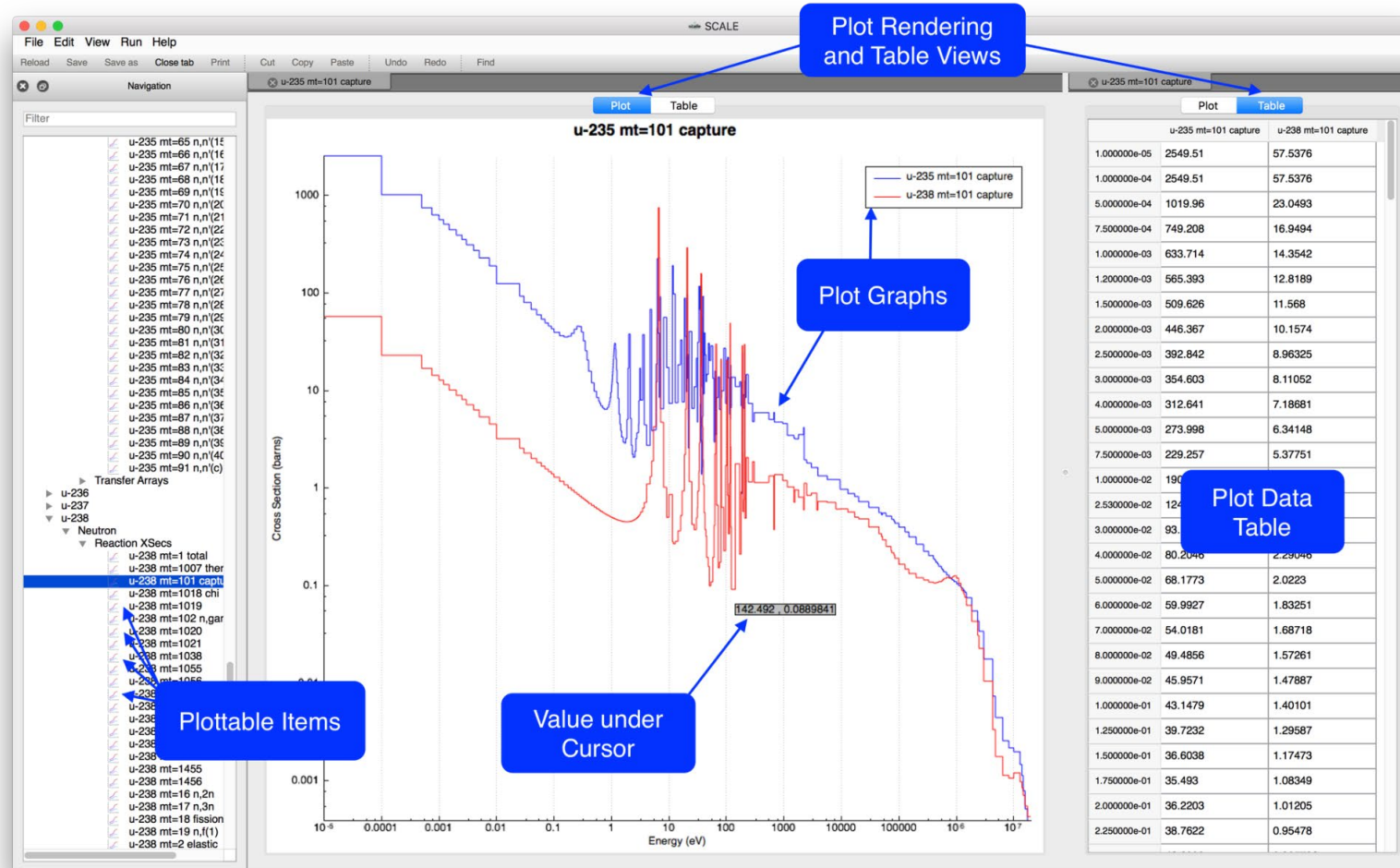


Fulcrum general output result plots



General plot overview

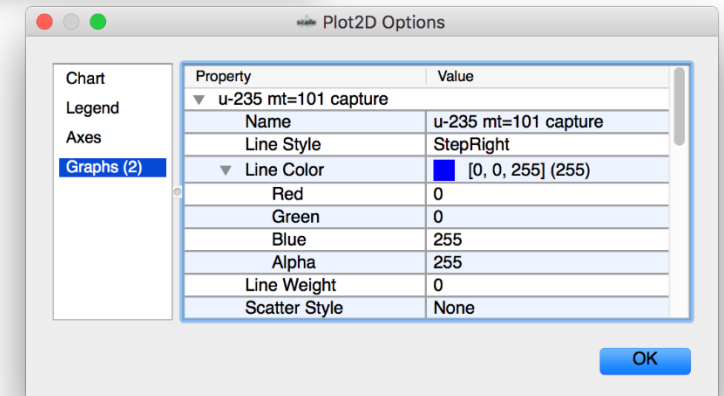
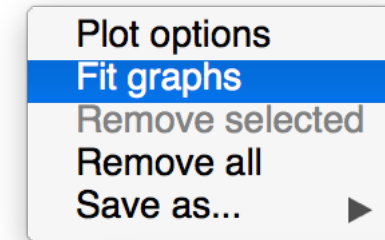
- Interactive and configurable plot rendering
- Plot data table displays graph data (allows row and table copy to clipboard)



Plot controls

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

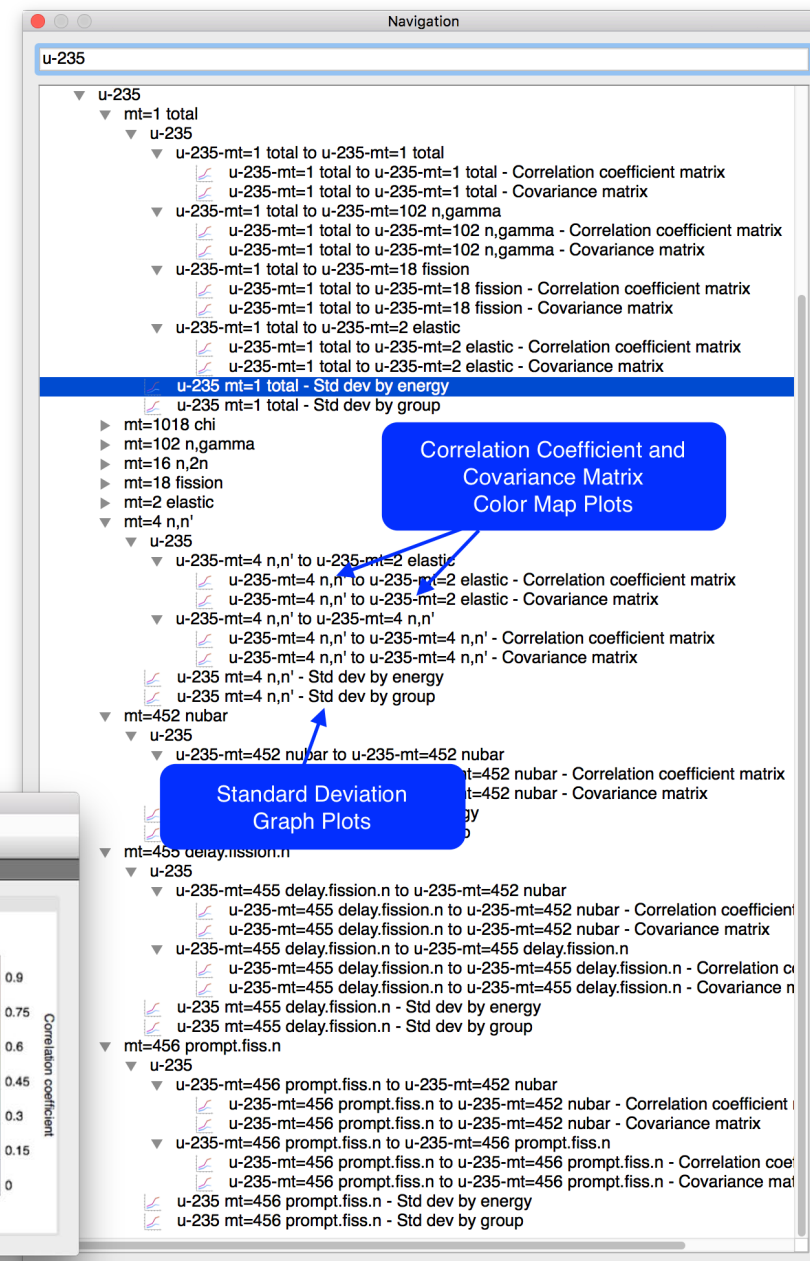
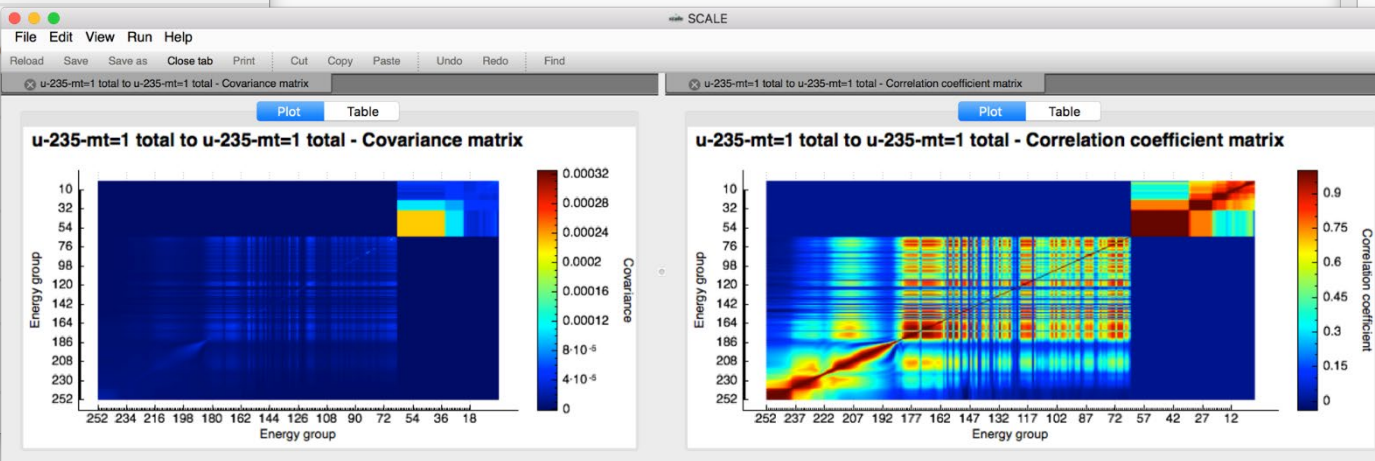
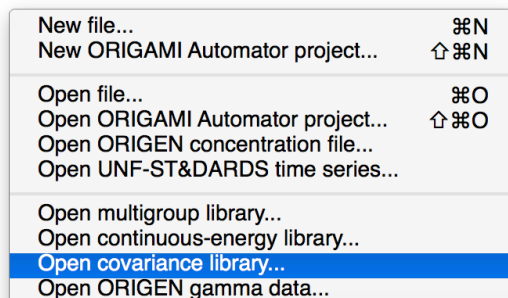
- Select graph via left-click in plot or legend
 - Remove selection via context menu 'Remove selected'
- Zooming is performed via the mouse scroll action
 - Zoom in by scrolling up; zoom out by scrolling down
- Reset to original via context menu Fit graphs
- Panning is performed via a click and drag.
 - 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 formats
 - **Interactive Scale Plot Format (SPF)**
- Plot attributes (color, style, etc.) can be changed via context menu Plot options
- Plot Legend can be dragged to 9 cardinal positions via left-click and drag



Covariance data

Covariance data are available in SCALE/data. Because the files do not have a unique extension, the user must load them specifically by type.

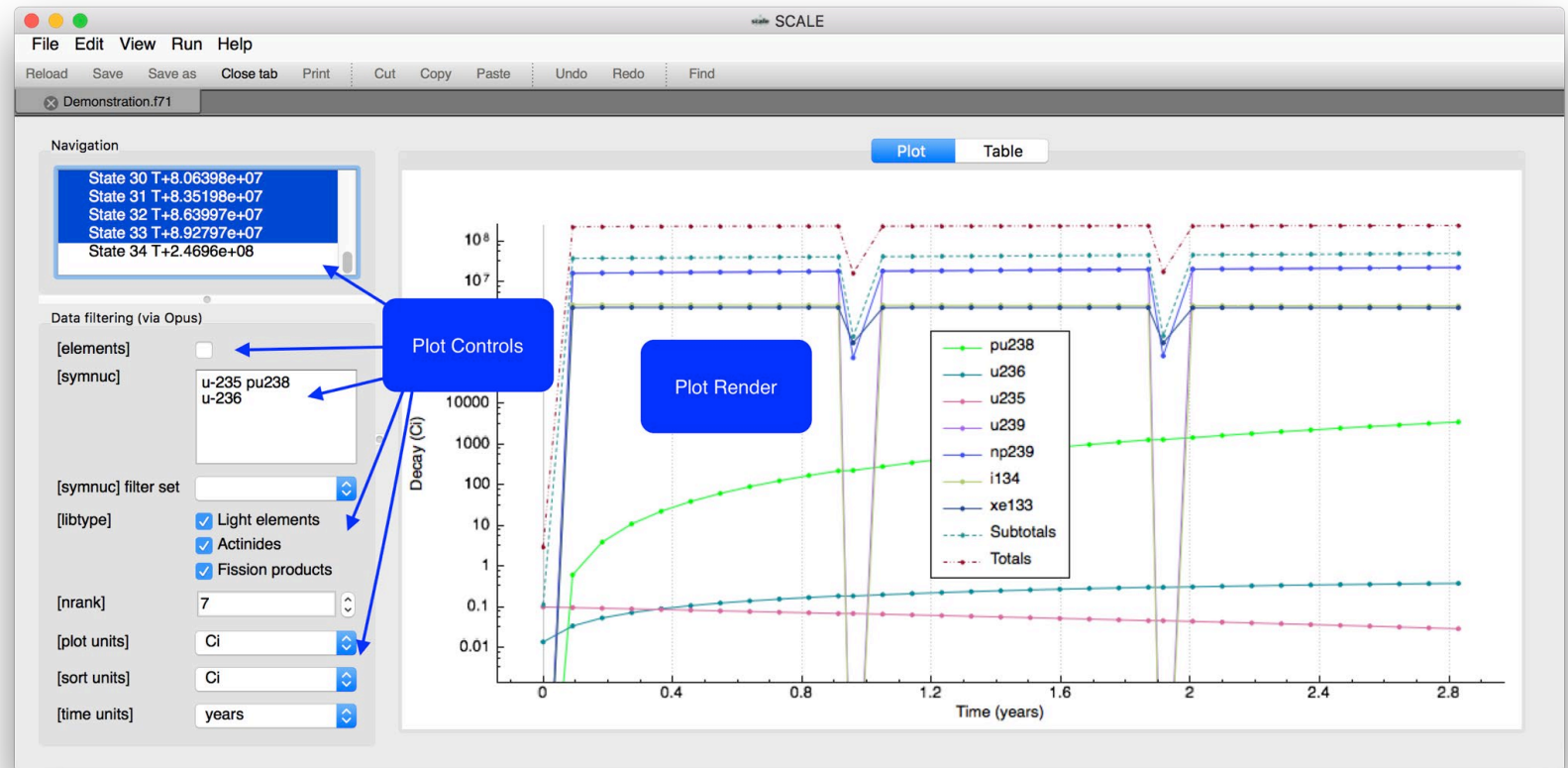
- Correlation coefficient matrix color map plots
- Covariance matrix color map plots
- Isotope Reaction Standard Deviation by energy or group graph plots



ORIGEN nuclide concentration data (F71)

ORIGEN concentration data contain results from depletion, decay, and activation calculations.

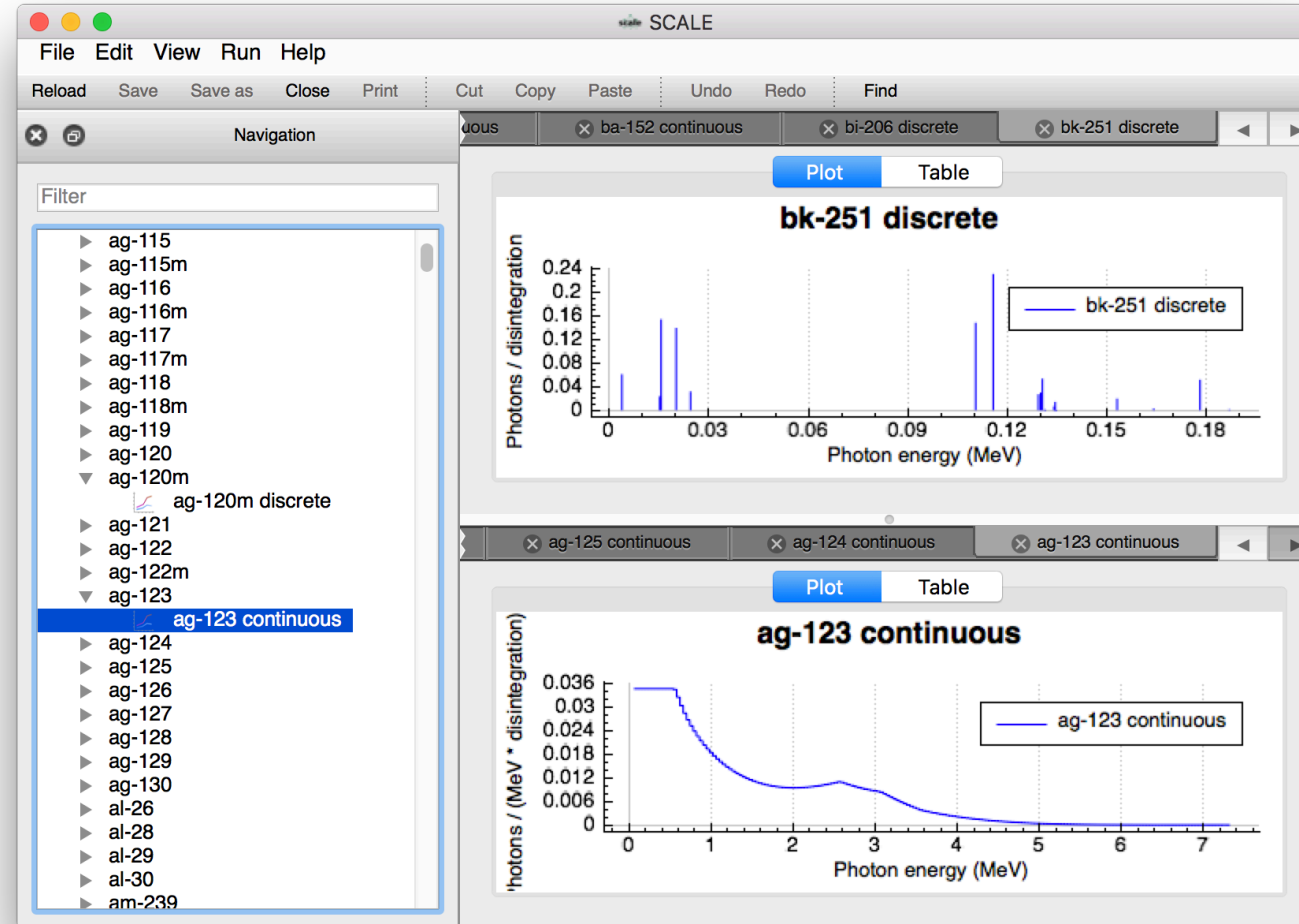
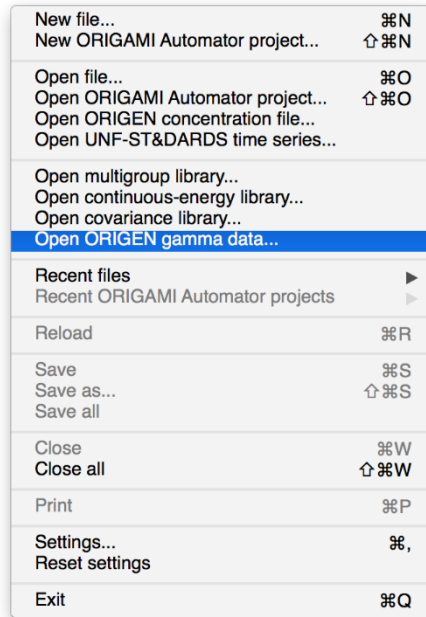
- Easy selection of state information to display
- Easy display of nuclides or elements by identifier or category
- Easily display using different units
- **NOTE:** if Plot rendering is empty, then the decay data are missing and must be configured in the **File > Settings > Environment > DecayData** field



ORIGEN gamma data

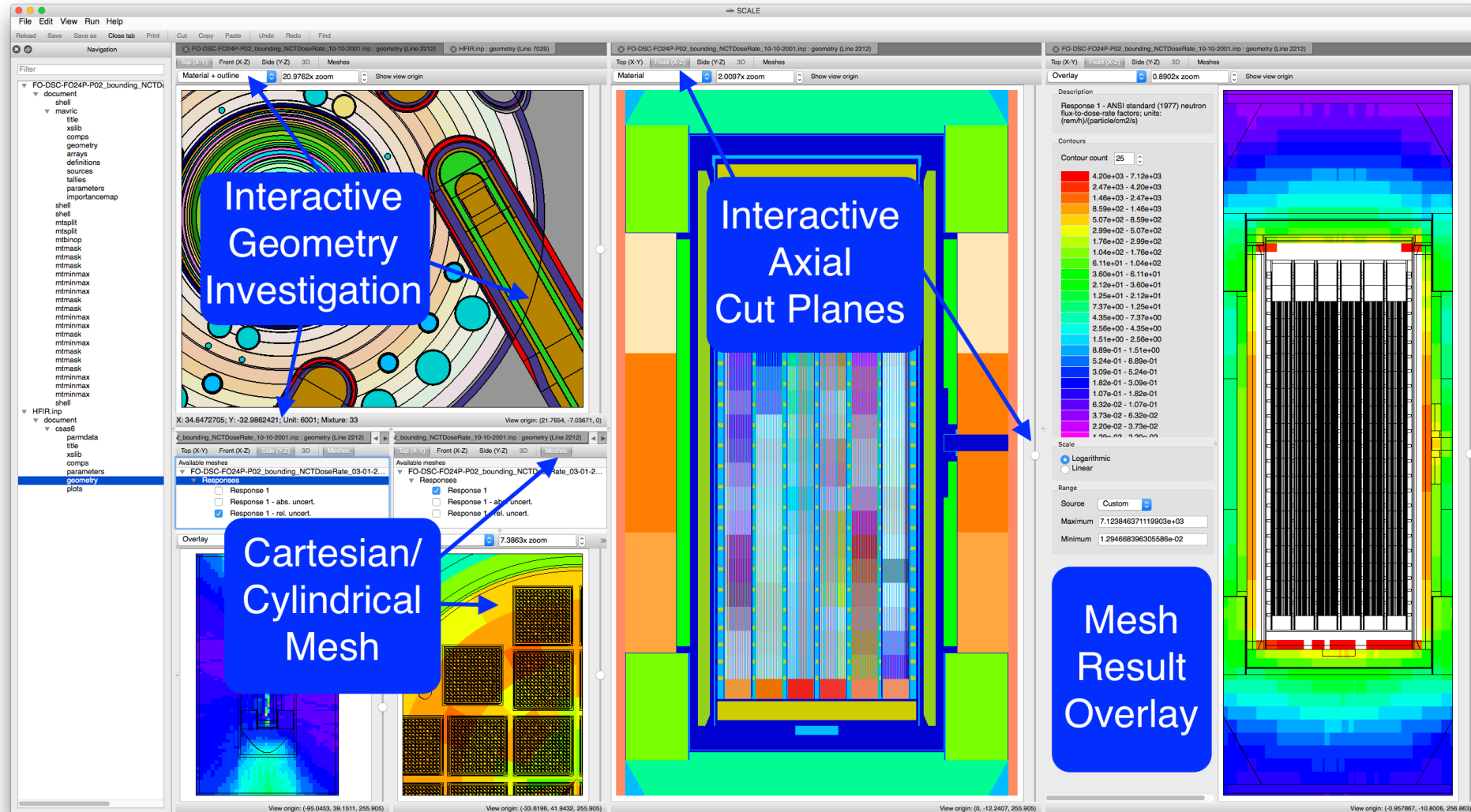
Master photon data library provides both discrete and continuous-energy gamma lines. Located at SCALE/data/origen_data/origen.rev##.mpdkxgam.data.

- Open via **File > Open ORIGEN gamma data...**



Fulcrum geometry visualization

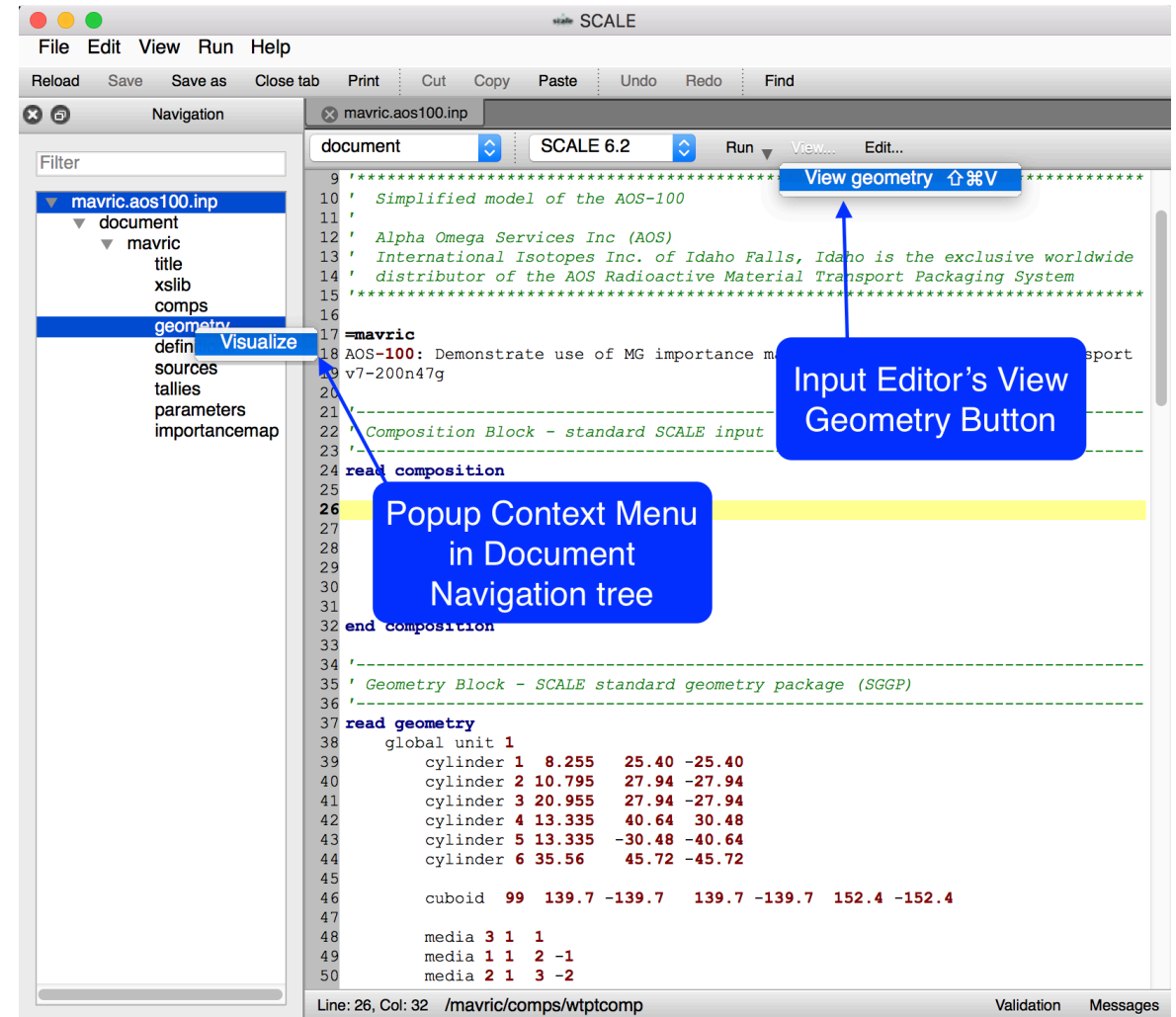
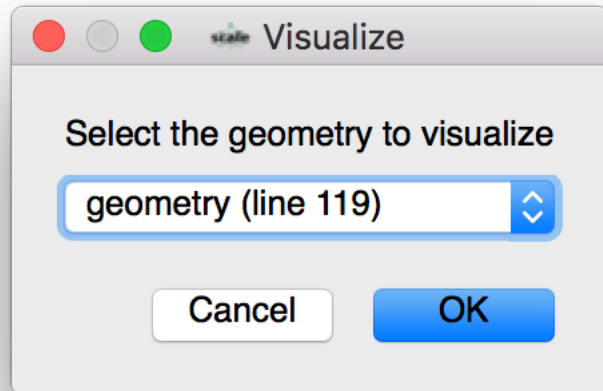
- Interactive geometry visualization
- Support for most mesh data*



*Currently supports: 3dmap, Mesh Importance Map, Mesh Source Map, and Denovo Flux File

Activating the geometry viewer

- Via the Input Editor's **View...>View geometry** button or the Document Navigation geometry item's popup context menu
- If multiple geometry input blocks exist in the document, a selection will be provided



Questions and discussion

- Future questions or issues can be sent to scalehelp@ornl.gov