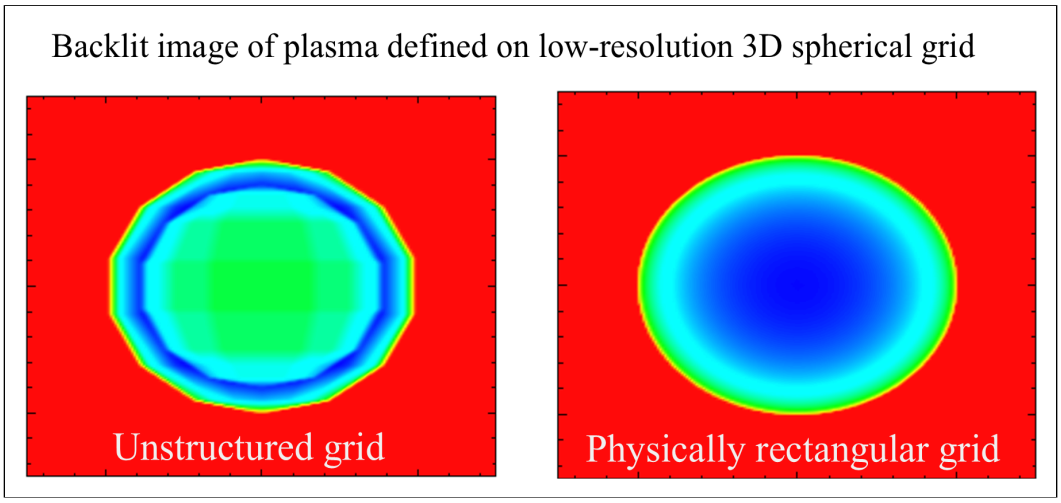
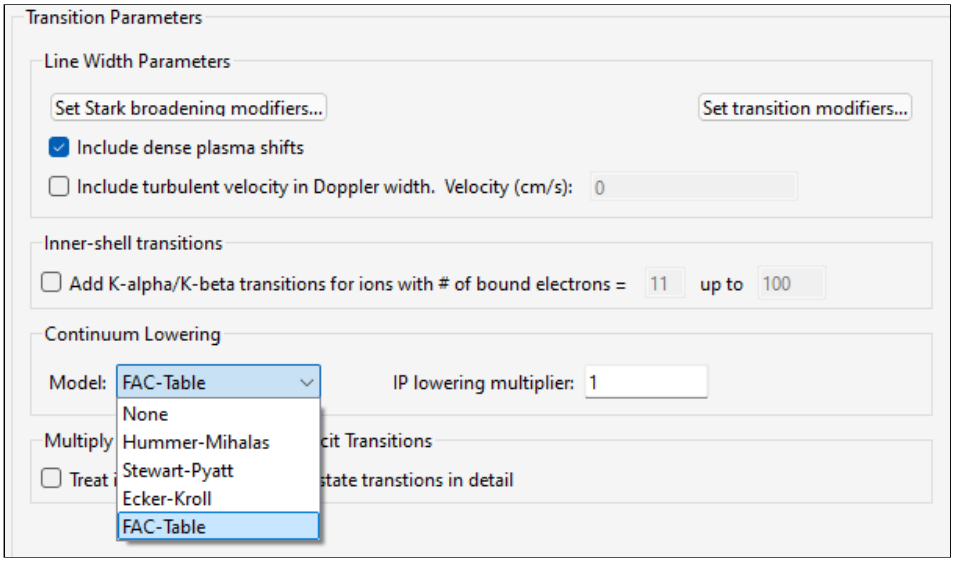
Revisions for SPECT3D 20.6.0

SPECT3D:

- Reading hydrocode data from *.exo files has been updated for Logically Rectangular and Physically Rectangular grids.
  - Connectivity array data in *.exo files are no longer utilized for both logically and physically rectangular grids.
  - For *physically rectangular* grids, the node arrays for written as 2 (if 2D) or 3 (if 3D) individual arrays (as opposed to using a 3D vector for each node). Physically rectangular model supports grid curvature.



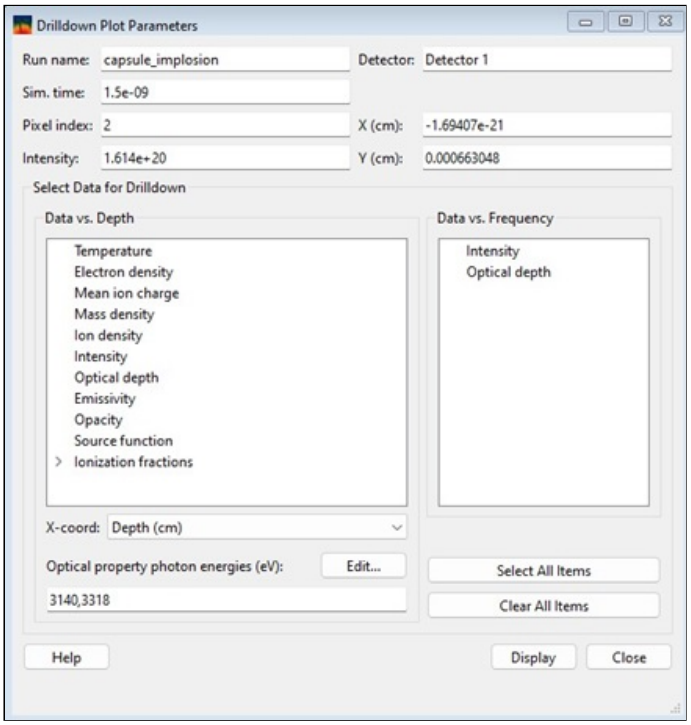
- The name used to identify the *LOS-Grid Intersection Model* for unstructured grids has be changed from "Evaluate for individual elements" to "Unstructured grid (Individual volume elements)".
- Prism developed a set of Python scripts that converts arbitrary hydro data into NetCDF format suitable for SPECT3D. The scripts will be distributed to all SPECT3D users.
- Additional option for continuum lowering models (*Atomic Processes -> Advanced -> Transitions*) and for dense plasma shifts. FAC Table option and dense plasma shifts require *.es atomic data files. The data will be distributed to all SPECT3D users. A systematic calculation of plasma screening effects on atomic structure for all ions of Z=1 to 36 has been carried out using the Flexible Atomic Code. The screening potential is obtained within the framework of Stewart-Pyatt model. The shifts in ionization potentials of bound electron radial orbitals up to principal quantum number 10 and all orbital angular momenta are tabulated on a grid of electron densities and temperatures. Due to the slight differences in the screening effects on different radial orbitals, this tabulated database enables to not only determine the continuum lowering of the ground states, but also transition energy shifts within the same ionization stages. The database of ionization potential shifts is a significant improvement over analytical formulas often employed for ionization potential depression.



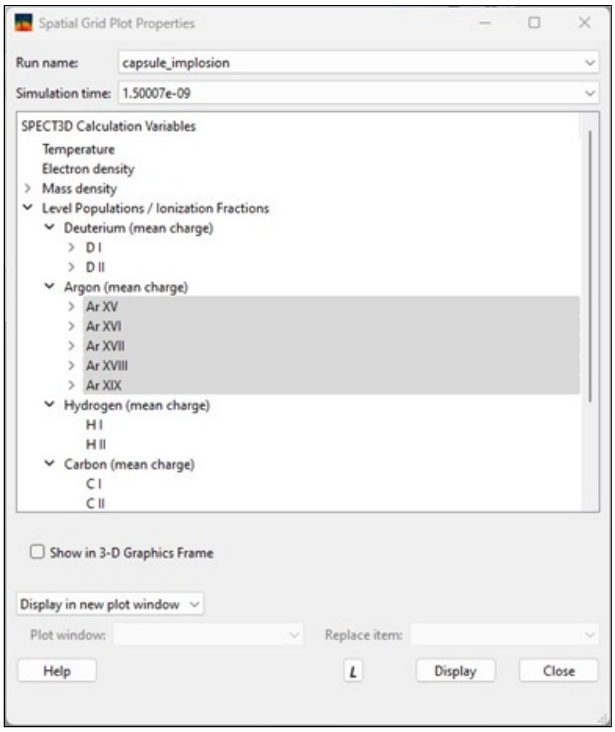
- Improved convergence stability for NLTE simulations with large optical depths. Note that this may increase the simulation time for some calculations.
- Bug fixes:
  - When displaying energetic electron data from hydro data files (*Display* | *Hydro Data* menu item), plotting data shown in the *Hot Electron Energy Bins* box has been fixed.
  - The *Detector-Target Viewer* is now updated properly when a detector name is changed in the *Detector Setup* widget.
  - Displaying hydro data for binned hot electron distributions: fixed bug displaying too many windows when multiple bins are selected.
  - Displaying hydro data: fixed color bar tick labels when units changed on *Plasma Properties Setup* widget after plot was originally shown.

SpectraPLOT:

- Several upgrades were made to support *Drilldown*:
  - The pixel index can now be entered by the user (previously, this set only by picking a pixel in an *Image* plot window.)
  - The efficiency of retrieving data from calculations involving non-local radiation fields has been improved.
  - Three new optical quantities that can be displayed vs. depth:
    - Emissivity
    - Opacity
    - Source function
  - The photon energies at which optical properties vs. depth can be displayed can be edited by the user. Previously, these were constrained to the values specified when setting up a *SPECT3D* simulation (in the *Photon Energies* tab of the *Output* parameters widget). These photon energies are now shown near the bottom left of the *Drilldown Plot Parameters* window (see below).



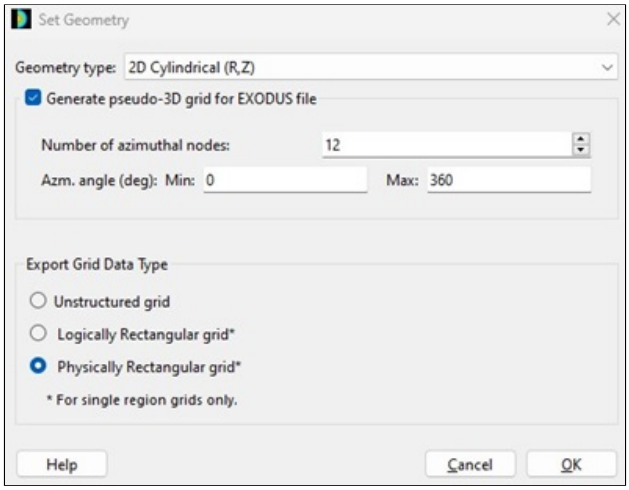
- The default *SPECT3D* run name is now specified when setting up a new plot window by clicking on the *New Plot Window* button. Previously, the default run name was based on the run that was selected in the *SPECT3D Run Results List*. The default run name has implications for what types of plots are available (*e.g.*, when using a *Disk* detector in a *SPECT3D* run, it is possible to view the *Image* intensity either in a contour plot or a radial line plot).
- *Ionization Plots*: For 1-D spatial grids:
  - Selecting multiple items of the same type (*e.g.*, element, ion, atomic level) is now supported.
  - The option to replace individual plot items has been removed. Instead, users can add and delete plot items as needed.
  - To utilize the name of the element, ion, or energy level in the legend name, check the appropriate box in *Preferences*.



- Bug fixes:
  - The units for the *y*-axis are now updated when the *x*-quantity is changed between wavelength and photon energy in the *Window Quantities / Units* box.
  - The line integration tool has been fixed for cases when the x-axis quantity is in units of wavelength (as opposed to photon energy).
  - Fix for crashes when plotting ionization for runs where local populations are not written for all hydro zones.
  - Fixed bug for legend strings when reading in a *SpectraPLOT* workspace.

Plasma Grid Generator:

- Upgrades have been made to generate *.exo files that better support logically and physically rectangular grids.
  - Connectivity array data are no longer written to *.exo files for both logically and physically rectangular grids.
  - For 3D physically rectangular grids, the node position are written as:
    - Cartesian: *x(i), y(j) ,z(k)*
    - Cylindrical: *r(i), z(j), φ(k)*
    - Spherical: *r(i), θ(j), φ(k)*
  - For 2D physically rectangular grids, the node position are written as:
    - Cartesian: *x(i), y(j)* for *Rectangle* objects when using 2D Cartesian XY geometry
    - Cylindrical: *r(i), θ(j)* for *Disk* objects when using 2D Cartesian XY geometry
    - Cylindrical: *r(i), z(j)* for *Rectangle* objects when using 2D Cylindrical RZ geometry
    - Spherical: *r(i), θ(j)* for *Disk* objects when using 2D Cylindrical RZ geometry
  - The parameter indicating that the grid is continuous in the *k*-dimension (*i.e.*, the azimuthal angle wraps around full 360 degrees) has been removed.
- When exporting grid data to *.exo files, an option is now available to export the data as either *Logically Rectangular*, *Physically Rectangular*, or *Unstructured*.



- Bug fixes:
  - Fixed crash associated with running in batch mode.

GridConvert:

- Grid Convert has been updated to generate multi-timestep NetCDF files based on PlasmaGEN files with logically and physically rectangular grids.