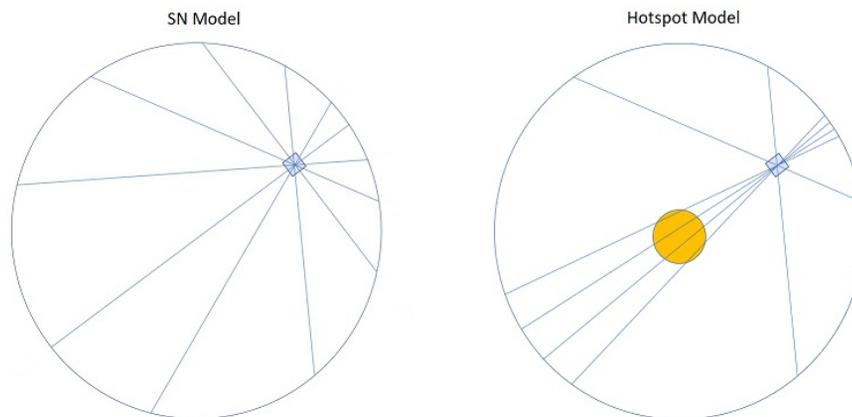


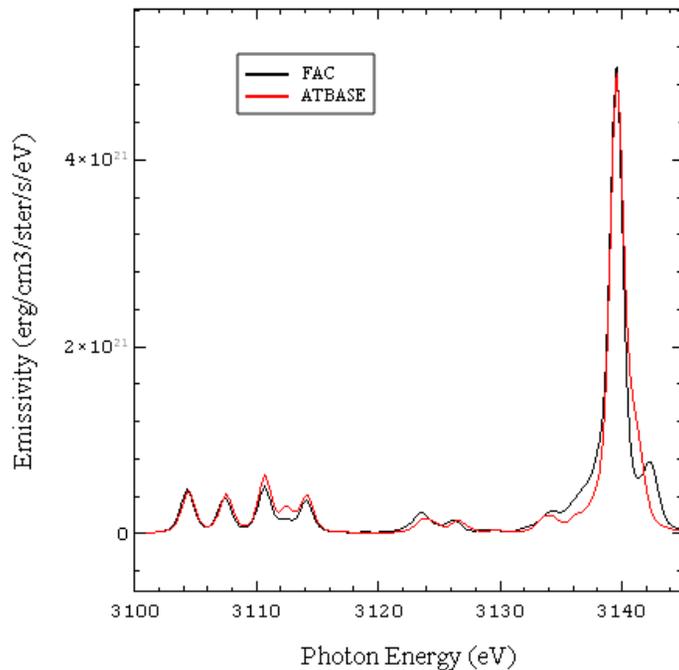
## SPECT3D version 19.0.0

### SPECT3D:

- Bound-bound and bound-free transitions now use separate photon energy grids, which saves a lot of computation time for some types of calculations. This new feature can be turned off by un-checking the box labeled "Separate photon energy grids for bound-bound and bound-free transitions" in the Simulations tab in Preferences (from the Edit menu).
- For 1D Geometries, image calculations now cache opacities and emissivities, resulting in faster calculations. This new feature can be turned off by un-checking the box labeled "Cache opacities and emissivities for image construction in 1D radiative transfer" in the Simulations tab in Preferences (from the Edit menu).
- Improvements have been made to the Short Characteristics radiation transport model, including:
  - A new correction to radiative transfer ray boundary conditions, based on effective path lengths of radiative transfer rays, along with weighted averaging over 3 angles, has been implemented. This results in much better agreement with analytical benchmarks in the optically thin regime. This new feature can be turned off by un-checking the box labeled "Use path length corrections for Short Characteristics ray boundary conditions" in the Simulations tab in Preferences (from the Edit menu).
  - Cartesian plane reflection symmetry (in the Geometry tab) are now supported. Previously, this was not allowed when using short characteristics.
  - Improved calculation speed, especially for K-alpha/beta calculations.
- A new Hotspot angle grid model is available for radiation transfer (both Short and Long Characteristics), for simulations where the standard method of discrete ordinates (SN angle grid model) is not sufficient for resolving a central radiation source.



- *Detector-Target Viewer*: The *Backlighter* (when present) is now shown in the *Detector Plot Objects List*. The *Backlighter* can be shown or hidden, and its radius in the graphics can be adjusted by right-clicking on it in the list.
- Implemented support for atomic data generated by FAC. For more details, see attachment titled "FAC Atomic Data in Prism Codes" in the main documentation.
- SPECT3D will be distributed with a standard set of FAC-generated data. Custom user-generated data are supported as well. The data need to be generated with the latest version of FAC available at GitHub.



Simulation results for Ar-doped DD plasma at 600 eV temperature and 1 g/cc density computed with FAC and ATBASE data. Ar He-alpha transition and associated Li-like satellites.

- Added support for Big Sur operating system on both Intel- and M1-based computers.
- When performing time-dependent collisional-radiative simulations, it is expected that the mass in each volume element (and therefore DCA atomic elements) does not change with time. If changes in the either number of volume elements in the grid, or in the mass of any of the volume elements is detected, a warning message is now displayed.
- For calculations using X-Ray Thomson scattering (XRTS), support has been implemented for hydro files containing a flag allowing individual cells to be omitted from the XRTS calculation. This flag must be an integer called "scatter\_flag", where a value of 0 will omit XRTS for a given cell, and 1 will allow it. If this variable exists in the hydro file, its usage is controlled by a checkbox labeled *Use XRTS flag from hydro file* in the *Plasma* tab of the XRTS setup interface. If this box is unchecked, the flag will not be used. The flag variable can also be plotted like other hydro variables.
- Linux users working in a KDE 5 desktop environment will likely experience very slow graphics performance. Use of KDE 5 is discouraged for the time being.
- Bug fixes:
  - When using X-Ray Thomson Scattering with table input for the source, in some previous versions, the table would not re-load when re-running a calculation in a single instance of Spect3D, even if the table was changed. This has been fixed, so the table will always be loaded when running a calculation.
  - *Detector-Target Viewer*:
    - Fixed bug that sometimes caused a crash when plotting isosurfaces after loading in a second *SPECT3D* workspace.
    - Fixed bug in *Hydro Data Plot Objects* list associated with mapping *Type* and *Definition* after a plot object was deleted.
  - Fixed crash that occurred when using radiation transport along with  $K\alpha/K\beta$  inner-shell transitions for grids with more than 1000 cells.
  - Previously, if a time-dependent simulation used the option to treat the grid as logically rectangular, time-dependent grid parameters could be overwritten by static parameters from the hydro file, which could give incorrect timing results if a coarse time grid is used. This has been fixed.
  - Previously, short characteristics could fail for certain grids, leading to error messages and stoppage of the calculation. Multiple issues have been fixed, resulting in smooth running for all cases tried.

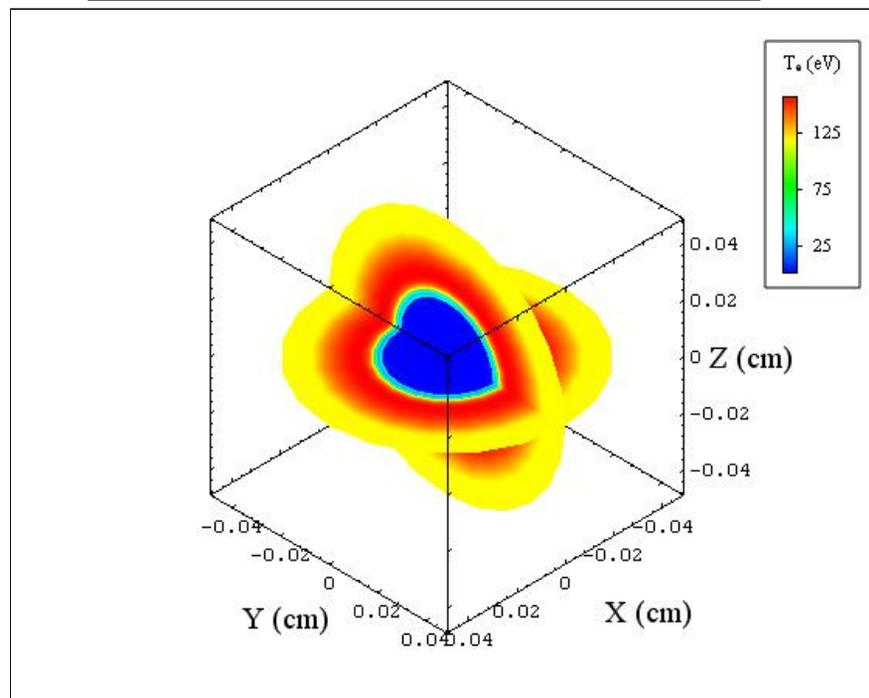
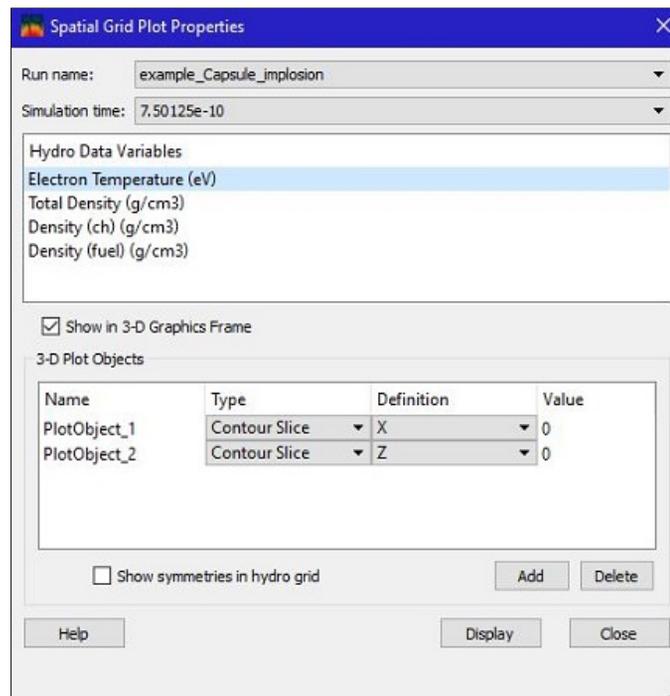
- Fixed bug which occurred when writing binned spectral data for each LOS to its output file. The bug occurred in cases where the photon energy range for the bins exceeded the range for the spectral calculation.
- Fixed error that occurred when using inner-shell transitions ( $K\alpha/K\beta$ ) along with combining DCA and non-DCA materials.
- Fixed possible crashes when running time-dependent calculations with more than one detector.
- Fixed inconsistent information in the populations files for non-primary detectors.
- Fixed a problem with loading the "Use AMR gridding data in Hydrocode file if available" checkbox in Preferences. Previously, if this was checked (or un-checked) *after* loading a workspace, it was not recognized when running.

## VISUALIZER:

- Bug fixes:
  - *Drilldown* plots: fixed problem that occurred when computing *Ionization Fractions* for atomic elements residing in volume elements that contained both DCA and non-DCA materials.
  - *Time-Integrated Spectra* plots: the units for the y-axis has been fixed ("/s" removed).

## SpectraPLOT:

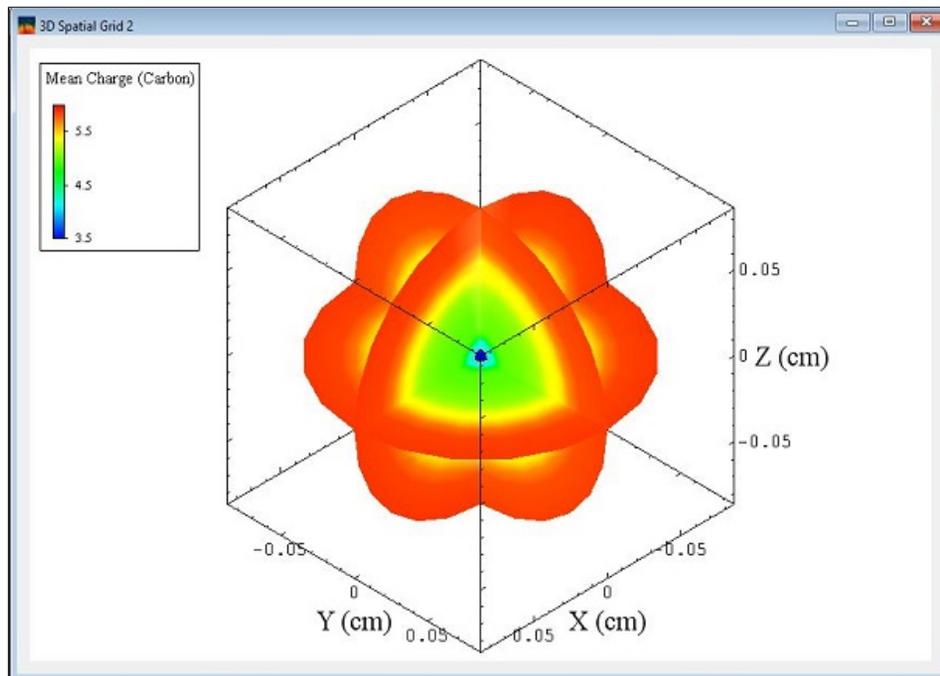
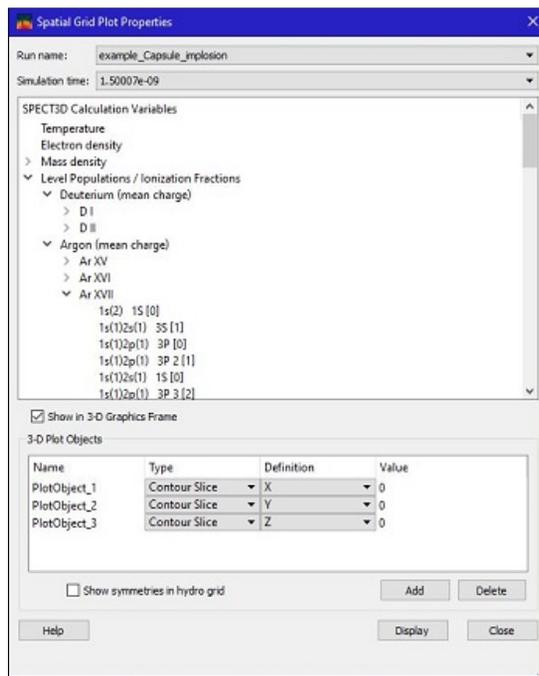
- The capability to show two new types of data on the *SPECT3D* spatial grid is now supported:
  - Hydrodynamics data (*i.e.*, data that is *input* into a *SPECT3D* calculation) can be displayed using either the geometry of the original hydro grid (*e.g.*, 1-D spherical, 2-D cylindrical R-Z, ...), or using a 3-D spatial grid. The simulation times available are those contained in the hydro data file. To plot in 3-D, check the *Show in 3-D Graphics Frame* check box (see below)..



When displaying in 3-D, one or more contour slices and/or isosurfaces can be added to the plot window. The above example shows contour slices of the electron temperature in the  $x = 0$  and  $z = 0$  planes.

- Ionization plot windows are used to show various quantities associated with ionization results from a *SPECT3D* calculation, including mean charge, ionization fractions, and atomic level populations. The temperature, electron density and material mass densities can also be displayed. The simulation times available are those used in the *SPECT3D* calculation (in *SPECT3D* calculations with time-dependent kinetics, the simulation time grid is generally different than the time grid of the hydro data file).

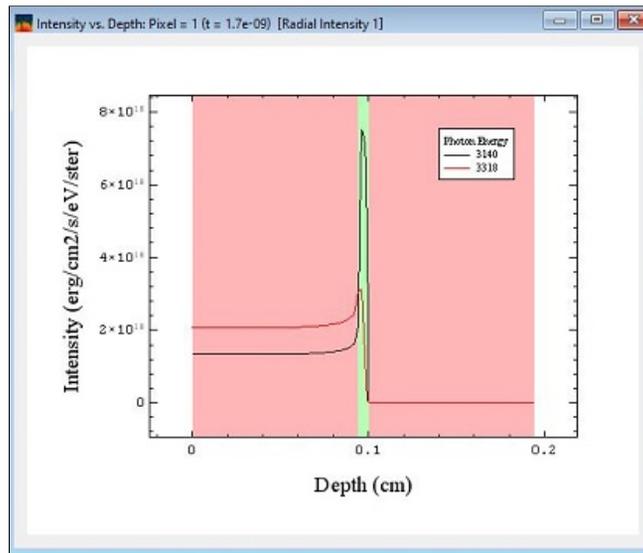
Like the displays of hydro data (above), results can be displayed using either the geometry of the original hydro grid, or using a 3-D spatial grid.



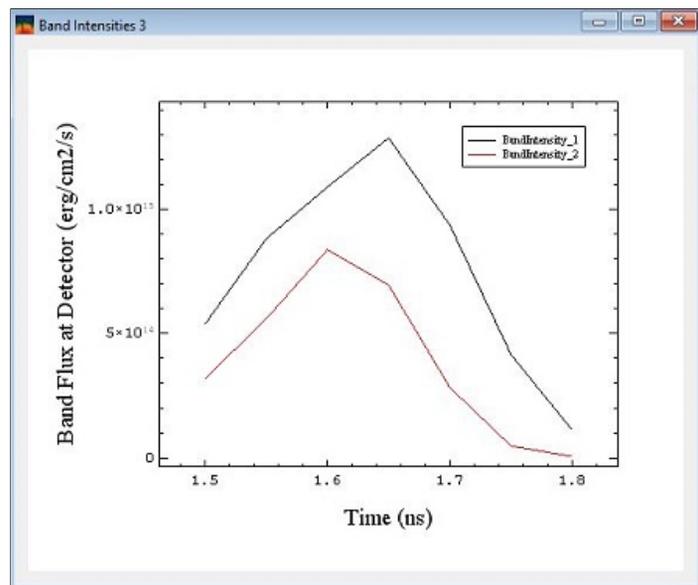
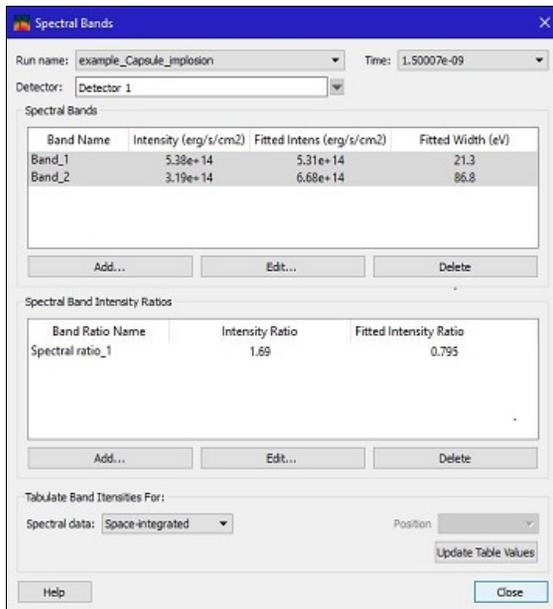
The example above shows the spatial distribution of the carbon mean charge state in the  $x = 0$ ,  $y = 0$ , and  $z = 0$  planes.

When viewing atomic level population results, the Atomic Rate Coefficient data for a particular volume element can be displayed by picking the element after clicking on the  button in the toolbar.

- The appearance of the drilldown toolbutton has been changed to .
- *Drilldown* is now supported when viewing *Radial Image* plots. When clicking on the drilldown toolbutton when a *Radial Image* plot is shown, the symbols are shown for each point along the line plot. Select one of the points to get the drilldown plots associated with the line-of-sight at that radius.
- Materials region locations can now be shown on *Drilldown* plots use the *Show Material Locations* toolbutton . For any *Drilldown* plot where a quantity is plotted vs. depth, clicking on the toolbutton will toggle the visibility of shaded regions for each material.



- Displaying *Spectral Band Intensities* and *Band Intensity Ratios* is now supported in *SpectraPLOT*. To do this, select *Band Intensities* when setting up a new plot window. Then in the *Plot Settings* widget, select the *View Bands* button to set up spectral bands to analyzed. Spectral intensities integrated over a frequency band can then be displayed.



- Multi-threading is now supported for some calculations performed in *SpectraPLOT* (e.g., generating *Contour Slice* and *Isosurface* data). To set the parameters for multi-threading, select the *Edit | Preferences* menu item, and set the parameters in the *Simulations* tab.
- When specifying a non-zero time resolution for streaked spectra, the time grid for the plot is adjusted to show more detail.
- Bug fixes:
  - Fixed bug for *Optical Depth Isosurface* plots where z-axis title was not being saved correctly.
  - If a new *Optical Depth Isosurface* plot, is requested, but the *Plot Item Properties* widget is closed without saving the item, the item no longer appears in the legend.
  - *Drilldown Plot Parameters* dialog: the *Intensity* of the picked pixel is now shown correctly.
  - *Drilldown* plots: fixed problem that occurred when computing *Ionization Fractions* for atomic elements residing in volume elements that contained both DCA and non-DCA materials.
  - Fixed problem that occurred when reading in *Spaced-Resolved Spectra* data when having only one pixel in a spatial dimension.

- Fixed crash that occurred when attempting to read in *Detector Image* data from a *SPECT3D* run that did not successfully complete
- Fixed "file not found" bug that occurred when attempting to display spatially-resolved spectra when only vertically-resolved spectra were computed.