Revisions for SPECT3D 21.0.0

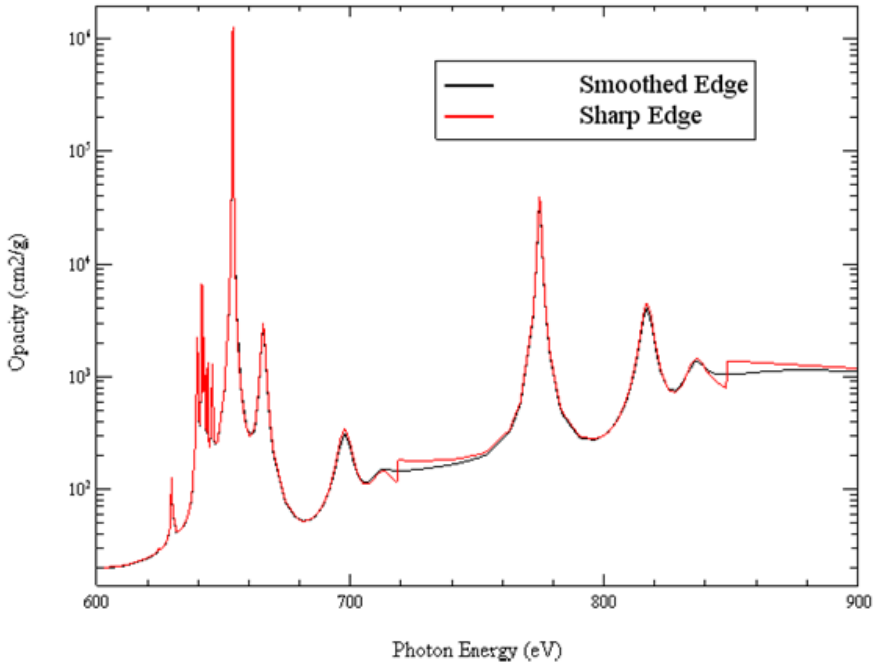
SPECT3D:

- Support for utilizing JSON-formatted workspaces has been added.
  - This option provides better support for reading/writing workspaces that use different versions of *SPECT3D*.
  - JSON-formatted files can be readily modified using scripting tools such as Python.
  - To turn this option off, check the "Use non-JSON format" button on the *Directories/Files* tab of *Preferences*. By default, this option is now turned on.
  - When saving a workspace that was originally read in using the old (non-JSON) format, a warning is presented notifying the user that it is now being saved to a JSON-formatted file. (This warning can be turned on/off in the *Warnings* tab of *Preferences*.)

- The OpenGL graphics in each of *SPECT3D* graphics widgets has been updated to utilize virtual buffer objects. This was done in order for *SPECT3D* to work effectively on more modern computer monitors and graphics acceleration hardware.
- When using native *FLASH* hydro files in Spect3D via the *FLASH* log file, if no FLASH checkpoint (chk) files are found, it will instead try using *FLASH* plot (plt) files.
- Photoionization edge smoothing. With continuum lowering, the photoionization edge is shifted lower relative to the isolated atom values. This shift is sometimes called ionization potential depression, or IPD. However, experimental results have shown the edges are also likely to have a smooth and round edge, rather than a sharp step used in previous versions of the code. In this release, we have implemented a smoothing procedure for photoionization cross sections. The procedure involves two steps. First the photoionization cross sections of an isolated atom is extrapolated toward the depressed ionization threshold in the log-log scale, and extended further below the threshold at a constant value. We then determine the multiplicative smoothing factor

$$S(E, E_{th}) = \int_{-\infty}^{E} \phi(E', E_{th}, w) dE'$$

where $\phi(E,E_{th},w)$ is the Stark line profile for a bound-bound transition close in energy to the depressed ionization threshold E_{th} with corresponding broadening FWHM w. The product of this factor and the extrapolated photoionization cross section provide the smoothed absorption edges. An example of the smoothing is shown below for the opacities of He-like and H-like Oxygen ions.



- Extending maximum number of levels in atomic models. Previous versions of atomic model file (atm) file format had a hard limit on the maximum number of levels. This new release removes this limitation. The formats of several input (atm file) and output (population) files have been extended such that data columns involving level and transition indices now have a larger width to avoid overflow. As a result, the new atm files cannot be read by older versions of *AtomicModelBuilder*, *PrismSPECT*, *PROPACEOS*, and *Spect3D*.
- Bug fixes:
  - When using *OPLIB* opacity files:
    - No longer receive improper error message about wrong *PROPACEOS* format.
    - Previously, a bug could occur when outputting space-resolved spectra, causing *SpectraPLOT* to crash when attempting to plot the result. This has been fixed.
  - When using SDF hydro input, if density units were kg/m3, *and* volume fractions were used for the material(s), material densities were incorrect in the simulation. This has been fixed.
  - Previously, using VisRad-formatted flux files for a backlighter was causing a crash. This has been fixed. Now, either a VisRad-formatted flux file or a simple 2-column file can be used.
  - Fixed incorrect termination of the simulations with time-dependent kinetics and more than one detector.
  - Convergence improvement of steady state block matrix solver. Previous version of *SPECT3D* introduced a block matrix solver for steady state solution to handle larger atomic systems more efficiently. The solver was found to occasionally fail for complex atomic systems. *SPECT3D* 21.0.0 includes improvements to the stability of the solver.
  - Improvement to photon energy grid construction method. Previous versions may fail for large atomic models when number of transitions are very large, such that resolving bound-bound transitions with sufficient accuracy requires number of photon energy points to exceed the preset limit. *SPECT3D* 21.0.0 implements an iterative procedure to relax the resolution requirement such that the total number of photon energy points always stay close to the preset limit.

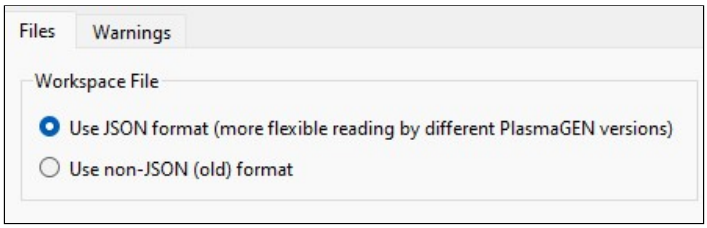
SpectraPLOT:

- Support for utilizing JSON-formatted workspaces has been added.
  - This option provides better support for reading/writing workspaces that use different versions of *SpectraPLOT*.
  - JSON-formatted files can be readily modified using scripting tools such as Python.
  - To turn this option off, check the "Use non-JSON format" button on the *Files* tab of *Preferences*. By default, this option is now turned on.
  - When saving a workspace that was originally read in using the old (non-JSON) format, a warning is presented notifying the user that it is now being saved to a JSON-formatted file. (This warning can be turned on/off in the *Warnings* tab of *Preferences*.)

- The OpenGL graphics in each of *SpectraPLOT* graphics widgets has been updated to utilize virtual buffer objects. This was done in order for *SpectraPLOT* to work effectively on more modern computer monitors and graphics acceleration hardware.

Plasma Grid Generator:

- Support for utilizing JSON-formatted workspaces has been added.
  - This option provides better support for reading/writing workspaces that use different versions of *PlasmaGEN*.
  - JSON-formatted files can be readily modified using scripting tools such as Python.
  - To turn this option off, check the "Use non-JSON format" button on the *Directories/Files* tab of *Preferences*. By default, this option is now turned on.
  - When saving a workspace that was originally read in using the old (non-JSON) format, a warning is presented notifying the user that it is now being saved to a JSON-formatted file. (This warning can be turned on/off in the *Warnings* tab of *Preferences*.)



- When writing to JSON-formatted workspace files, color bar and text box properties are now saved.
- The OpenGL graphics in each of *SPECT3D* graphics widgets has been updated to utilize virtual buffer objects. This was done in order for *SPECT3D* to work effectively on more modern computer monitors and graphics acceleration hardware.
- Support for *Preferences* have been added. To edit *Preferences*, select the *Edit* | *Preferences* menu item. This initial setup has been added to support options for JSON-formatted workspaces described above.
- The ability to duplicate *Spatial Regions* has been added. To do this, right-click on an item in the *Regions List* and select *Duplicate*.
- A new tool button has been added to reset the viewing area (). The check box to "Automatically adjust viewing area to fit regions to window" has been removed.
- Support for reading in recent workspaces has been added to the *File* menu.