

Revisions for SPECT3D v. 20.1.0

SPECT3D:

• In the previous versions of SPECT3D, for NLTE calculations with radiation-dependent rates included, the steady state solution of statistical equilibrium are obtained by a time-dependent solver to let the system of ordinary differential equations evolve until equilibrium is reached. In the current release, we implemented a new solver where a true steady state solution is obtained in each iteration for a given set of collisional and radiative rates. This new solver is more efficient for a broad range of problems because it often requires fewer iterations to converge, and needs less time per iteration. The choice of solver method for the populations can be specified in the preferences. The default is the new steady-state iterative solver.

comic Data	User Directories	Default Directories	Simulations	
-Multi-threa	ding			
Perform	multi-threaded sim	ulations		
	mit max number of t	nread to: 1		
Grid model				
🔽 LIce AM	Paridding data in h	hydrocode file if availab	le l	
Cost All	it ground data in t	lydrocode me n dvanab		
Advanced R	adiation Physics Par	ameters		
🔽 Use pat	h length correction	s for Short Characteristi	cs ray boundary conditions	
Cache o	pacities and emissiv	vities for image constru	tion in 1D radiative transfer	
Senarat	e photon energy ar	ids for bound-bound a	nd hound-free transitions	
	e prioton energy gr	han as madel		
Se qua	asi-contiguous imes	napes model		
Solver Meth	nod for Steady-State	Populations		
O Pseudo	-time-dependent	Max. num. iterations	: 150	
-	stata itarativa	May num iteration	. 500	
Chan des	state iterative	Max. num. iterations	: 500	

- For NLTE calculations, consistency checks were added for extrapolating atomic cross-sections to high energies.
- Consistency checks were added to occupation probability model to prevent possible scenarios where the occupation probability of an excited state is greater than that of the ground state within the same ionization.
- Improved computational efficiency for pressure broadening algorithms of transitions in neutral atoms.
- Improved computational efficiency for 1D NLTE simulations with high-resolution detectors by chaching emissivities and opacities for each zone.
- Improved computational efficiency for image calculations when all materials are non-DCA.
 - Reduced memory consumption for simulations where the "Logically rectangular grid model" is specified.
- Bug fixes:
 - On some Windows computers that use scaled desktop resolution, corruption of graphics could occur. This behavior has been fixed.
 - Fixed graphics distortion issues on Windows computes with high-resolution (4K) monitors.
 - Problem occurring when displaying the data of picked volume elements when displaying hydro data from 3D hydro grids on a 2D contour plot has been fixed.
 - Fixed potential crashes when using "Treat implicit multiply exited transitions in details" option for the elements with a large number of implicit transitions.
 - Fixed potential crash when using all non-DCA elements with Doppler shifts.
 - Fixed potential problems with extrapolating photoionization cross-sections. This may affect opacities at very high photon energies.
 - Fixed erroneous "invalid collapse mode" warning for time-dependent calculations with more than one detector.

VISUALIZER:

• Visualizer is no longer distributed with SPECT3D.

SpectraPLOT:

- Updates were made to better support viewing the results from different *SPECT3D* runs within the same *SpectraPLOT* workspace. This primarily affects accessing the data for drilldown plots, ionization/populations plots, and viewing rate coefficient data.
- Improved efficiency of getting non-DCA ionization fractions from tables. This can significantly affect cases with a very large number of volume elements.
- The list of windows on the left side of the SpectraPLOT Main Window is now static. It is no longer reordered based on their stacking order.
- The names of plot windows can be edited. To do this, right-click on the plot widget in the Window List, and select the Rename menu item.
- Viewing and exporting data from Space-Resolved Spectra plots is now supported.
- Support saving shaded material region plot parameters in Drilldown plots to workspace file.
- Plot widgets that contain no plot items are now deleted when saving SpectraPLOT workspace files.
- Batch mode has several improvements, including new options for auto-scaling plots, and better file naming.
- Bug fixes:
 - Fixed crash that occurs when the DCA population file is inconsistent with the atomic model file. A warning message is now provided when this occurs.
 - Fixed graphics distortion issues on Windows computes with high-resolution (4K) monitors.