## 1. Photon energy grid refinement for both photo-absorption and spectral modeling

In previous versions of Spect3D, the photon energy grids used for integrating no-local radiative rates and for calculating spectral properties are based on the line width from the plasma grid cell with lowest electron density and temperature. For plasmas with non-uniform conditions, this can cause mismatch of line profiles and photon energy grid. In this release, we take into account the variation of line widths and photo-ionization edges across the plasma for determining the photon energy grid, resulting in better resolved bound-bound line profiles and bound-free edges, as shown in Figure 1.

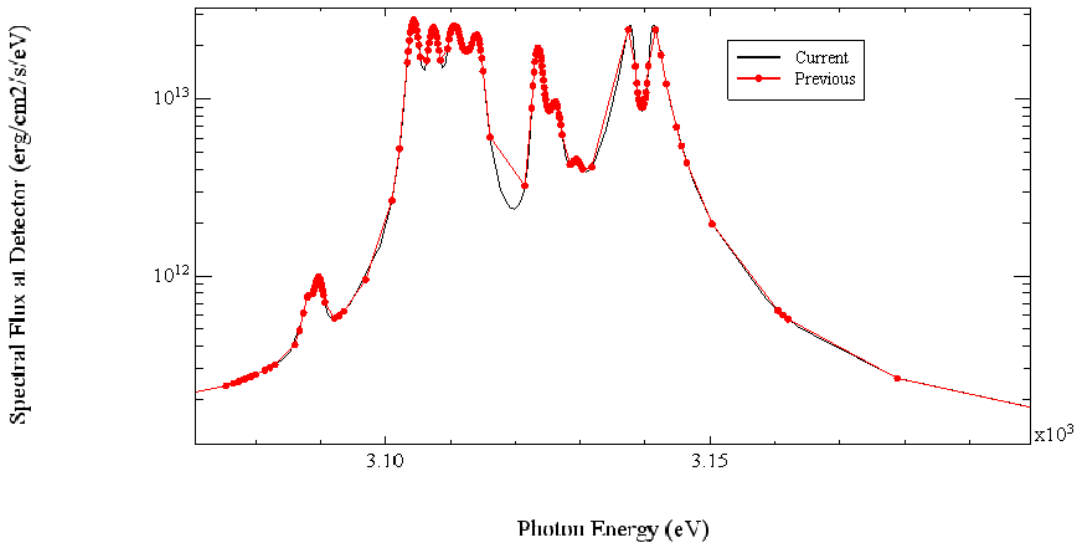


Figure 1. Spect3D example of Ar He-like alpha complex showing the inadequate photon energy resolution in some energy region as compared with the current release

## 2. Continuum lowering model avoids destroying transitions just below the ionization threshold

The updated continuum lowering model introduced in Spect3D 20.1.0 and PrismSPECT 9.5.0 tend to destroy the bound-bound transitions just below the depressed ionization edge. The is update avoids that behavior such that lines are not eliminated until they are above the ionization edge, which is how earlier versions of Spect3D and PrismSPECT behave. Figure 2 shows an example of this difference.

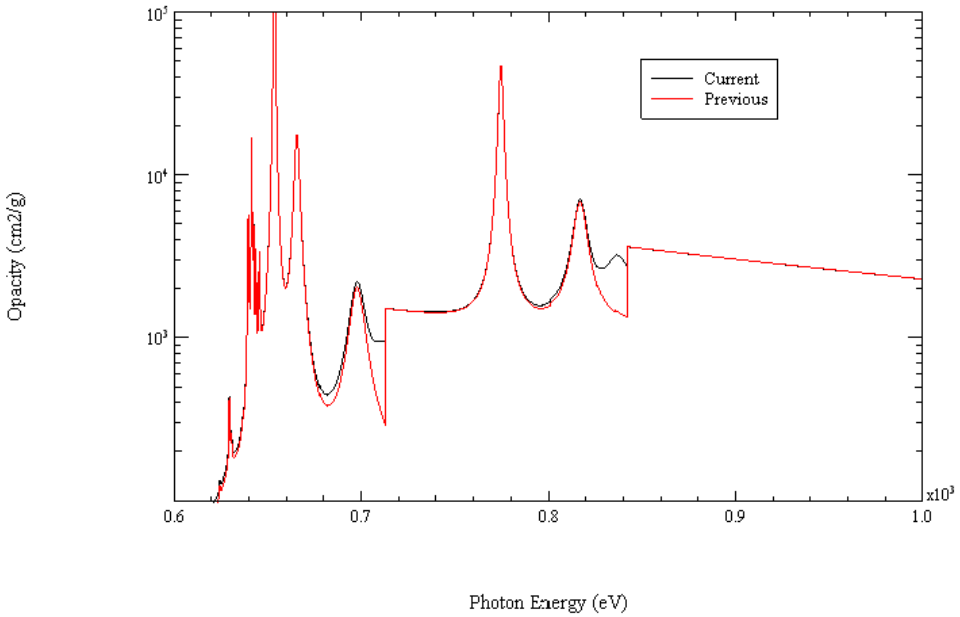


Figure 2. Opacity of Oxygen near He-like and H-like edge showing differences in the lines just below the ionization potential at same plasma conditions

## 3. Including more line wings in bound-bound emissivities

Previous versions of Spect3D and PrismSPECT have a temperature dependent cutoff of the Lorentzian wings of bound-bound transitions. This can cause incorrect line profiles at low temperatures. This update corrects this behavior by ensuring the cutoffs are at least several Stark widths away from the line center. Figure 3 shows an example of this difference.

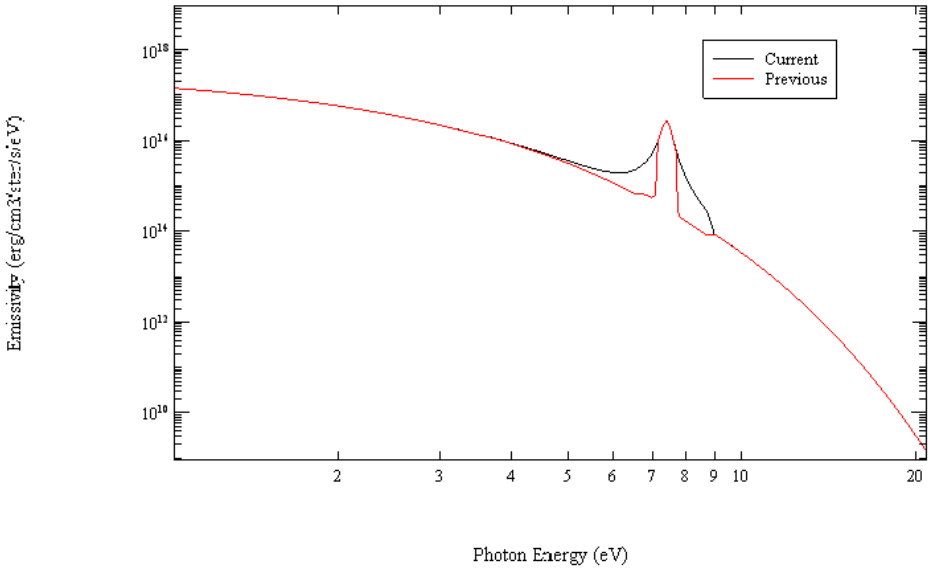


Figure 3. Al plasma at T=1 eV and mass density of 0.27 g/cc, showing the line profile differences in the current release

## 4. Extrapolation of photo-ionization cross sections below depressed ionization potential

The behavior of photo-ionization cross sections at energies between the depressed and original ionization potential is updated. In Spect3D versions prior to 20.1.0 and PrismSPECT versions prior to 9.5.0 takes the constant value of the original threshold cross section, while Spect3D 20.1.0 and PrismSPECT 9.5.0 introduced a shift of the cross sections that also affected the values above the original ionization threshold. The new release introduces a new method where the cross sections below the original ionization edge are obtained by extrapolating the cross sections above the edge. This results in more smooth behavior of bound-free opacities and emissivities.

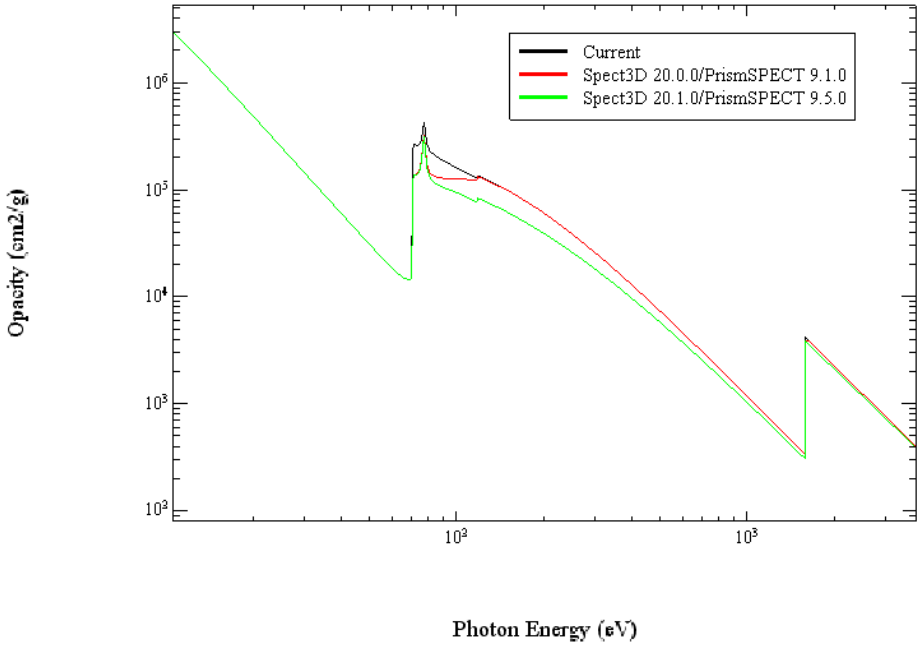


Figure 4. Photoionization cross sections below depressed ionization potential have different behaviors between different Spect3D and PrismSPECT versions, illustrated by Al LTE opacity at T=1eV and solid density

## 5. Automatic adjustment of time steps for non-local time dependent population solver

For time dependent calculations with non-local radiative transfer, the time grid specified in the Spect3D and PrismSPECT input are the points where radiative rates are calculated. Although the population solver can reduce the time step used in the integration routine, the radiative rates are not recalculated between the input time grid points. For cases where radiative rates change rapidly, this causes incorrect population solutions. This release introduces a new option to automatically adjust the time steps where non-local radiative rates recomputed. Figure 5 shows an example where this option makes a significant difference.

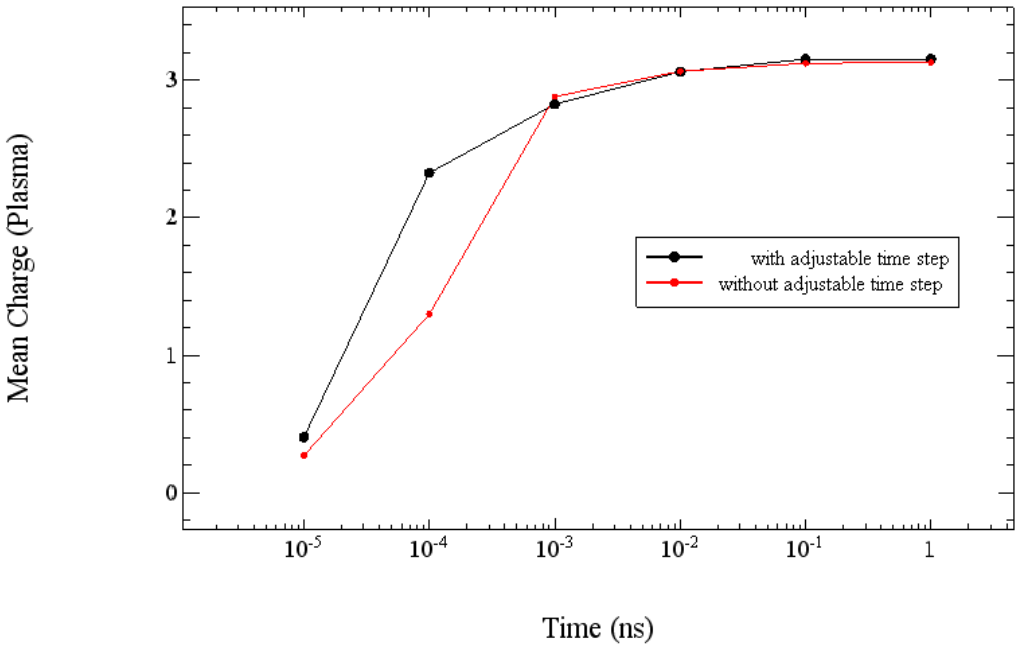


Figure 5. Time evolution of Al mean charge in a time dependent run, with and without adjustable time step

## 6. A new output file for line profile data

For PrismSPECT runs, a new output file is introduced to tabulate line profile parameters with individual broadening components, including Stark, Doppler, natural, and UTA width, and if enabled, Stark and UTA shifts. This file has the same number of rows as the existing *transpwr* file, where each row corresponds to one bound-bound transition.