## 1. Improvements to Continuum Lowering (CL) models at low temperatures

Prior to August 2023, Prism applications used the LTE population calculated with no CL to compute the electron density that determines the occupation probabilities and Ionization Potential Depression (IPD). However, at very low electron temperature $T_e$ and moderately high electron densities $n_e$, the LTE population without CL will produce near zero electron density $N_e$, resulting in little to no IPD at all. We implemented an improved model where the electron density and the amount of IPD are determined self consistently with a combination of iteration and bisection techniques to find the correct mean charge of the plasma. Figure 1.1 shows the mean charge of N plasma at temperatures of 0.1, 1, 10, and 100 eV in LTE conditions calculated with the self-consistent continuum lowering, and those calculated with the previous release of PrismSPECT, PrOpacEOS, SPECT3D, or HELIOS-CR. The results from an average atom model implemented in FAC are also shown. It demonstrates that the new results more closely resemble the average atom model, while the old version generally produces under ionized plasma.

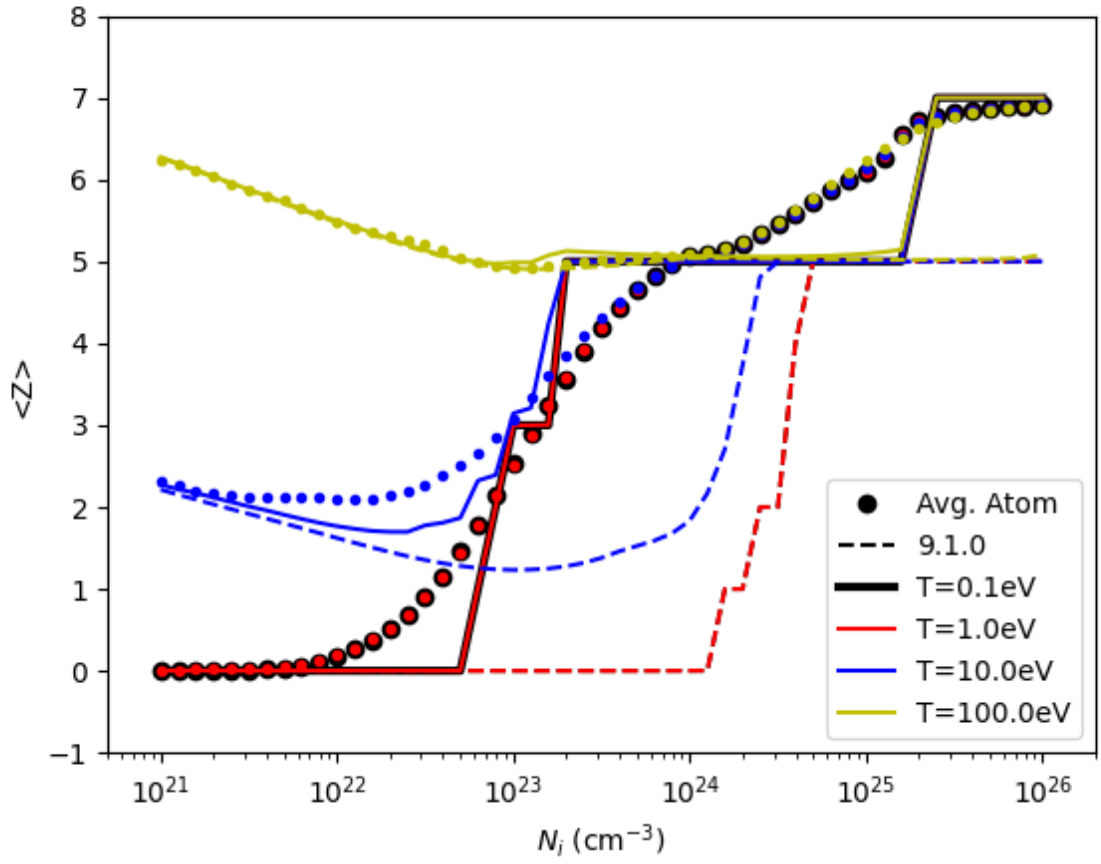


Figure 1.1. Mean charge of N plasma in LTE as functions of ion density $N_i$ from $10^{21}$ to $10^{26}$ cm$^{-3}$. The circle symbols are from the average atom model implemented in FAC. The solid lines are from the new self-consistent CL model at 4 different temperatures. The dashed lines are from PrismSPECT 9.1.0.

Figure 1.2 shows another example for Cu plasma in LTE. Note that even at room temperature, the mean charge is not necessarily zero near solid density, especially for metals like Cu. The level of ionization depends on the valence shell and the actual density. At high enough density, electrons eventually get ionized. It is difficult to model cold plasma near or above solid density. However, non-zero ionization in solid density metals at room temperature is plausible because the valence electrons are effectively free.

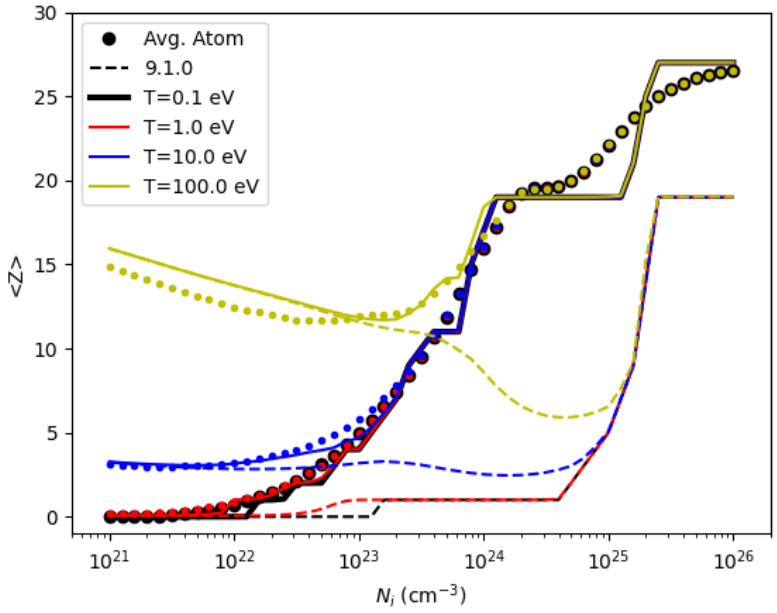


Figure 1.2. Same as Figure 1.1, but for Cu plasma in LTE.

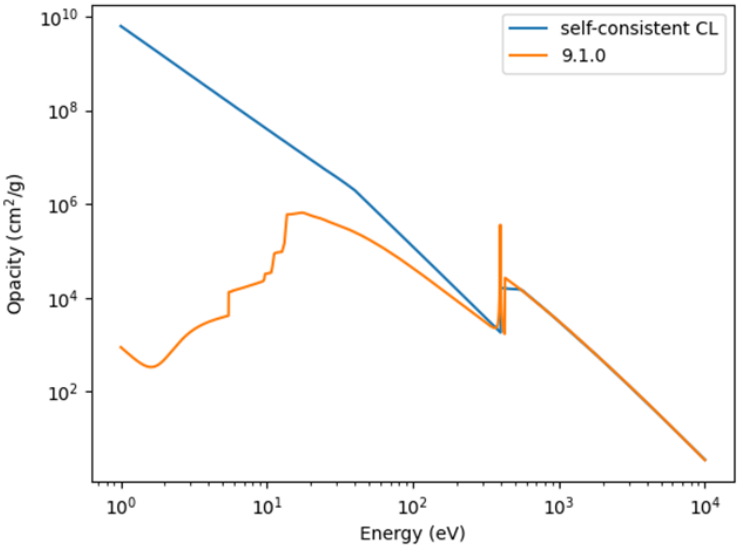


Figure 1.3. Opacities of N plasma at temperature of 1eV and ion density of $4 \times 10^{23}$ cm$^{-3}$ in LTE.

In Figure 1.3, we show the frequency dependent absorption opacity of N in LTE conditions at temperature of 1 eV and density of $4x10^{23}$ $cm^{-3}$. Differences in the spectral features are due to the differences in the charge state distributions. In the old model, the near zero mean charge results in little free-free opacity.

The new release of Prism codes also handles the ionization mixture plasma better, such as a minor dopant embedded in a dense H plasma. The previous release does not take into account the effect of H atoms on the occupation probability of the dopant energy levels fully. Figure 1.4 shows the mean charge of 0.1% Ar embedded in H. The old release produces low Ar ionization at very high H densities, while the new release shows the effects of pressure ionization, and agrees better with the results of average atom model.

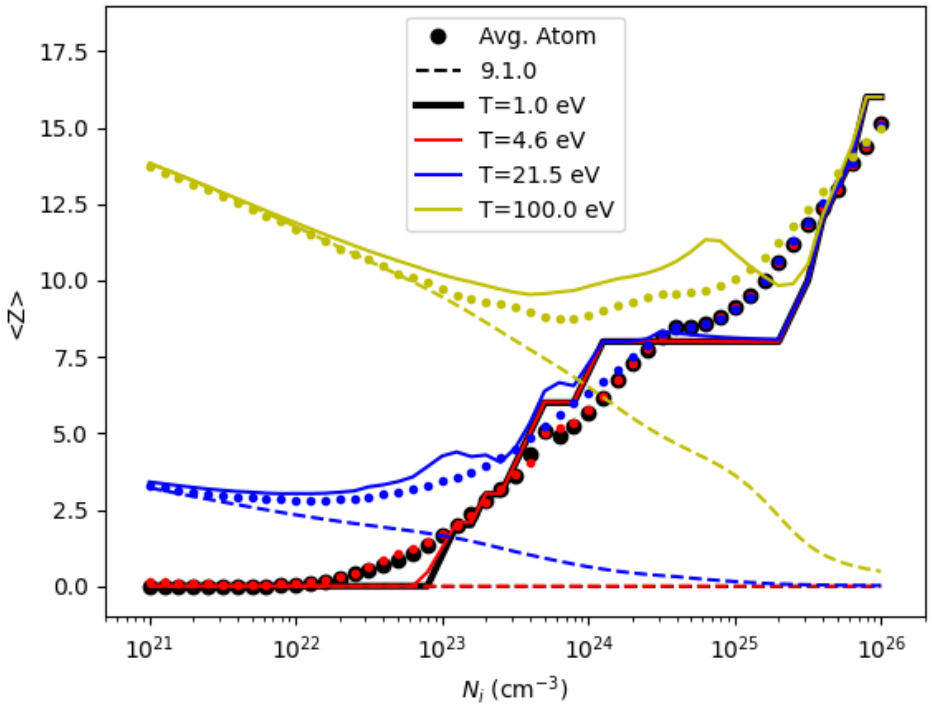


Figure 1.4. Same as Figure 1.1, but for a mixture plasma with 0.1% Ar embedded in H in LTE conditions

## 2. New block matrix population solver for large atomic systems

The solution to the collisional radiative equilibrium model is obtained by solving a system of linear equations. For small to moderately large systems with up to a few thousand levels, the standard method provided by LAPACK is generally adequate. However, with the number of levels $n > 10000$, both memory and CPU consumption pose significant challenges. A new custom

designed linear equations solver was developed recently to handle such large systems. First the rate coefficients are stored in a sparse matrix to reduce the memory foot-print. Since the coupling between levels are mostly restricted within neighboring ionization stages, the new matrix storage scheme can reduce memory usage by more than an order of magnitude. The atomic levels are then grouped into blocks to form a block matrix with much smaller dimension. Each block typically consists of one ionization stage, but levels from a single ion can be further split into multiple blocks if it contains a large number of levels. The solution to the original system of linear equations is obtained iteratively by solving the populations of blocks starting with an initial estimate of the individual level populations within each block. Once the block populations are known, the smaller system of equations for individual levels in each block are solved one block at a time. The iteration continues until the solution to all level populations is converged. To further improve the efficiency, we examine the ionization balance after each iteration, and drop the ions with abundances smaller than a set threshold from the system of equations.

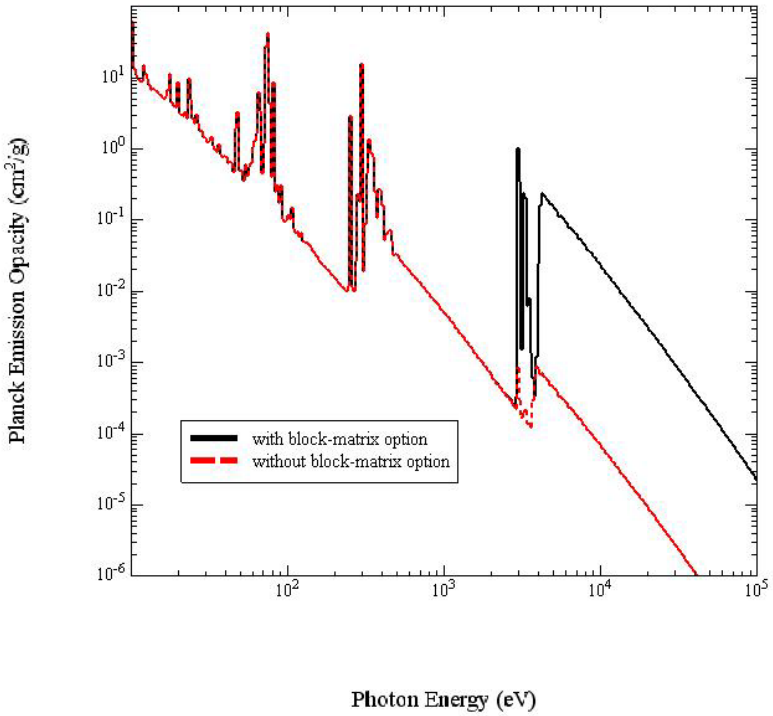


Figure 2.1 Planck emission opacity of an Ar dopped Deuterium plasma at T=63 eV and $N_i$=4.6x$10^{18}$cm$^{-3}$ computed with and without the block-matrix option.

For atomic models containing over 20000 levels, the new solver is expected to use significantly less memory, and faster by at least a factor of few. However, the solution to the populations of ions with very small abundances may differ in the two methods. This would affect weak emissivity features from these minor ions. In NLTE PrOpacEOS calculations of plank emission opacities, the emissivities are converted into opacities by Planckian weighting functions,

which amplifies the weak emission at photon energies where $hv/kT >> 1$. These differences in weak emission therefore look more pronounced in the emission opacity plots. Figure 2.1 shows such an example, where the Planck emission opacities of an Ar dopped Deuterium plasma at $T$ = 63 eV and $N_i = 4.6\text{x}10^{18}\text{cm}^{-3}$ computed with two different matrix solvers are compared. The large difference at $hv >$ 2keV are due to the population differences in the ions with small abundances. However, at these energies, the Planckian weighting factor is nearly zero, the actual emissivities are very small. Such differences are therefore of little practical concern.