Hi Joe:

As a result of the conversation we had several weeks ago in Madison concerning the Liedahl et al. 1990 paper on X-ray spectral signatures of photoionized plasmas, I have begun work on trying to replicate the two main figures in that paper using PrismSPECT 2.2.0. I started by using Atomic Model Builder 2.5.0 to construct atomic models for Iron in the coronal and XPN cases. For both cases, I attempted to use all of the configurations used in the paper, as listed in the tables (`coronal_table.gif` and `xpn_table.gif`). The first problem I encountered was the inability to select all configurations (and consequently the levels) that Liedahl et al. selected for their models. I have provided for you the `*.atm` files I constructed (`iron_coronal_1.atm` and `iron_xpn_1.atm`), but for quick reference, I'll give you a quick summary of what I was able and unable to do.

Since Liedahl et al. do not list the 1s shell in any of their configurations, we assumed that for each configuration the inclusion of 1s(2) was implicit.

`iron_coronal_1.atm`

For all ionization stages I selected the ground state **only**, except for the following stages:

Species	Levels	Configurations
Fe XVI	48	2s(2)2p(6)3l, 2s(2)2p(5)3l3l'
Fe XVII	42	2s(2)2p(6), 2s(2)2p(5)3l, 2s(2)2p(5)4l
		Not available: 2s(1)2p(6)3l, 2s(1)2p(6)4l
Fe XVIII	60	2s(2)2p(5), 2s(1)2p(6), 2s(2)2p(4)3l
		Not available: 2s(1)2p(5)3l, 2p(6)3l
Fe XIX	86	2s(2)2p(4), 2s(1)2p(5), 2p(6), 2s(2)2p(3)3l
		Not available: 2s(1)2p(4)3l, 2p(5)3l

`iron_xpn_1.atm`

For all ionization stages I selected the ground state **only**, except for the following stages:

Species	Levels	Configurations
Fe XVII	57	2s(2)2p(6), 2s(2)2p(5)3l, 2s(2)2p(5)4l, 2s(2)2p(5)5l

		Not available: 2s(1)2p(6)3l, 2s(1)2p(6)4l
Fe XVIII	90	2s(2)2p(5), 2s(1)2p(6), 2s(2)2p(4)3l, 2s(2)2p(4)4l
		Not available: 2s(1)2p(5)3l, 2p(6)3l
Fe XIX	127	2s(2)2p(4), 2s(1)2p(5), 2p(6), 2s(2)2p(3)3l, 2s(2)2p(3)4l
		Not available: 2s(1)2p(4)3l, 2p(5)3l
Fe XX	15	2s(2)2p(3), 2s(1)2p(4), 2p(5)

Is my assumption of 1s(2) for all configurations a wrong one, or did I simply miss these configurations when I made my selections in the model? Is PrismSPECT 2.2.0 missing these configurations?

Though these models do not conform to the models established by Liedahl et al., I went ahead anyway and used them to set up PrismSPECT workspaces for the coronal case, `iron_coronal.psi`, and the XPN case, `iron_xpn.psi`. At first for both `*.atm` files I used the most detailed structure collapse model for both the populations and spectra in an effort to produce the most detailed and accurate spectra possible. For the coronal workspace, I used the Liedahl et al. electron temperature of $T_e = 500$ eV and for the XPN workspace I used $T_e = 10$ eV. In both workspaces, I set the density to 10^{11} cm^{-3}.

At first, I used LTE for both simulations, but the spectrum for each was a straight line, since all of the iron was mostly ionized (in both cases). I then tried using NLTE, since the plasma should not be so ionized for the NLTE atomic level population model given the same temperature and density, but each time I tried to run the simulation with this change it crashed. See the image `prismspect_error_message.gif` for the error message. I did several things to try to avoid this error, including:

(1)   Created a `*.atm` file with only ground states selected for **all** ionization stages;

(2)   Changed collapse model of populations and spectra to Configuration Averaged, and then later to Least Detailed Structure;

(3)   Modified the Advanced parameters of NLTE so that only the relevant rate processes were selected.

Unfortunately, each one of the efforts resulted in the same error in the simulation. I wondered if the same error would occur for an NLTE PrismSPECT simulation of a different element, so I set up a workspace for neon using `neon_1_small.atm` (which was used for all of the Helios and Spect3D simulations) and the parameters $T_e = 35$ eV

and $n_{ion} = 10^{18}$ cm^{-3}. Surprisingly, this simulation ran without error, and produced a believable emission rate spectrum.

Is the problem with my Iron `*.atm` files, or is PrismSPECT having trouble with the low ion densities?

Obviously, I am in no rush to hear back from you, but if you have some time to look at this in the near future, I would appreciate any comments and suggestions you could provide me.

Thanks.

--Nate