

Analysis of effects of interpolation on APEC models and fits

Adam Foster

November 22, 2019

1 Motivation

François Mernier sent a draft paper discussing fundamental issues with interpolation as a scheme for producing emissivities. The paper was quite detailed, but roughly speaking, he created a spectrum in SPEX and then fitted it with an `appec` model within SPEX at a range of temperatures and abundances. Significant differences appear on a 0.1dex grid temperature grid, maximizing at the midpoint of each of the APEC grid points. Essentially the abundances all agree quite well at the nodes on the APEC temperature grid, and the discrepancy becomes worse in between the nodes, up to 15%.

This analysis was repeated for a range of detectors, abundances, and temperatures. Depending on the instrument the effects were slightly different, but essentially things in the $E = 0.6 - 1.0\text{keV}$ range were most significantly affected.

2 Hypothesis

My initial assumption is that the main driver of this discrepancy is going to be the ionization balance. The APEC model is calculated on 51 temperatures from $10^4 < T < 10^9\text{K}$. The ionization balance and line emissivity are calculated at each temperature on this grid, and then multiplied together along with the elemental abundance and stored.

When calculating the spectrum for temperatures in between these 51 points, the adjacent temperature spectra are linearly interpolated. So for a temperature of 1keV, the spectrum is calculated as $0.38 * \text{Spectrum}(0.86\text{keV}) + 0.62 * \text{Spectrum}(1.08\text{keV})$. This calculation should occur in log-log space, as this is more relevant to the behaviour of the line emissivities as a function of kT , however this actually makes only a very minor difference.

My immediate suspicion is that the main issue we are facing is due to the ionization balance. Effectively, we are taking something which varies in a relatively smooth manner with temperature (the emissivity of the line) and multiplying it by the ion fraction, which is roughly an inverted parabola in log temperature space. Linear interpolation of this inverted parabola always results in values which are equal to, or lower than, the “real” value, resulting in effectively lowered emissivities, which is then compensated for by higher abundances.

A second question is whether the emissivities themselves can be usefully interpolated even if the ionization balance is sorted out.

Table 1: Plasma parameters for `tbabs * vrnei` model. Parameters marked with a † are free in the later fits

Parameter	Value	Units
nH	0.01	$\times 10^{22} \text{cm}^2$
kT†	varies	keV
kT_init	=kT	keV
H	1.0	
He	1.0	
C	=Fe	
N	=Fe	
O†	1.0	
Ne	=Fe	
Mg†	1.0	
Si†	1.0	
S†	1.0	
Ar	=Fe	
Ca	=Fe	
Fe†	1.0	
Ni	=Fe	
Tau	1e13	$\text{cm}^{-3} \text{s}$
Redshift	0.1	
norm†	1.0	$10^{14} \text{cm}^5 \text{s}^{-1}$

3 Ionization balance

I am starting with a simplified replication of the Mernier findings. I cannot easily incorporate SPEX into this analysis, so I'm working entirely with APEC/XSPEC. Under the assumption that calculations on the nodes are exact, and all other calculations are not (as they are interpolations), I am creating a fake spectrum using a `tbabs * vrnei`. This is a non-equilibrium plasma model, but by linking the initial and final temperatures, it is effectively turned into an equilibrium model.

The `rnei` model differs from the regular `apec` model significantly in the handling of the charge state distribution (CSD) of the ions. For the `apec` model, the ion fraction and emissivity are calculated at 51 temperatures, multiplied together, and then stored. Interpolation is therefore across both CSD*emissivity. For the `rnei` model, the line emissivities are calculated independent of the CSD, which is then calculated on the fly at each temperature and multiplied by the emissivity within XSPEC. Interpolation in this case is therefore only across the emissivity.

The model I have used is described in Table 1, and is an attempt to replicate the work in Section 3.1 of the Mernier proceedings. I have only used an abundance of 1 for all this work, and the canned MOS response file `m1_e14_im_p0_c.rmf` taken from the ESAS site.

Spectra were simulated with no counting statistics or background, for observation times of 100ks, and a norm of 1. This gives spectra with $> 100,000$ counts. This was done for 57 temperatures from $\log(T) = 6.8$ to $\log(T) = 8.1$ K (roughly $kT = 0.5$ to 10keV).

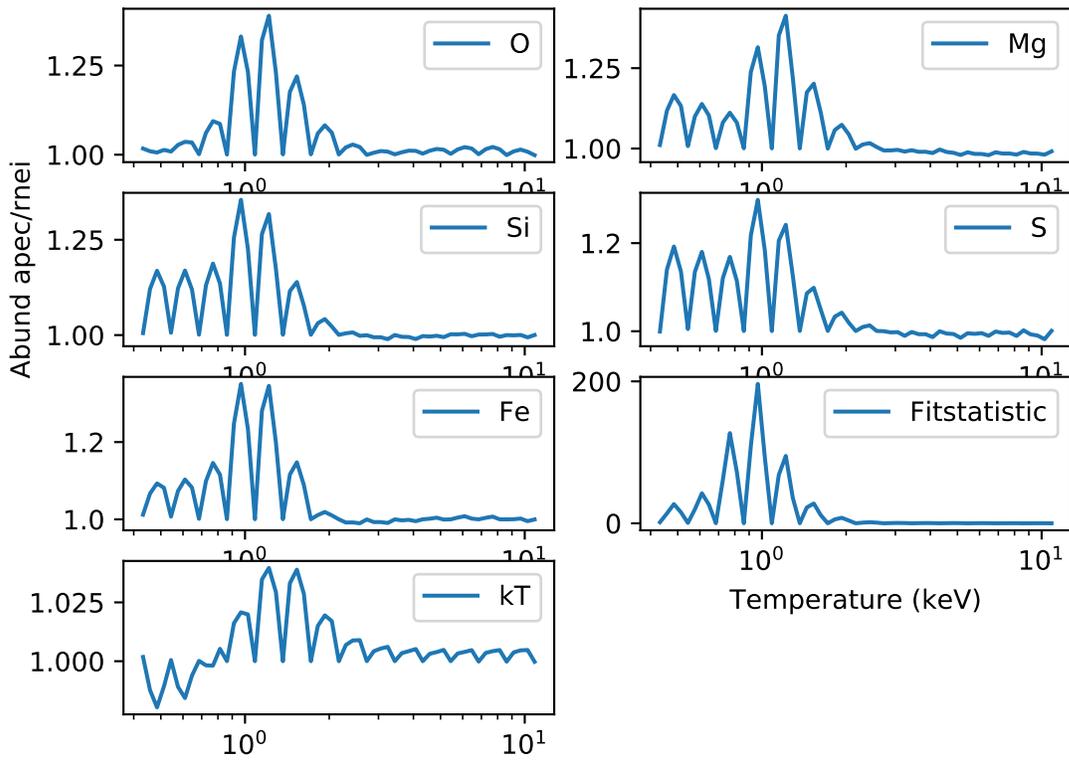


Figure 1: The abundances, temperatures and fit statistics from fitting the spectrum in Table 1 with a `tbabs * vapec` model.

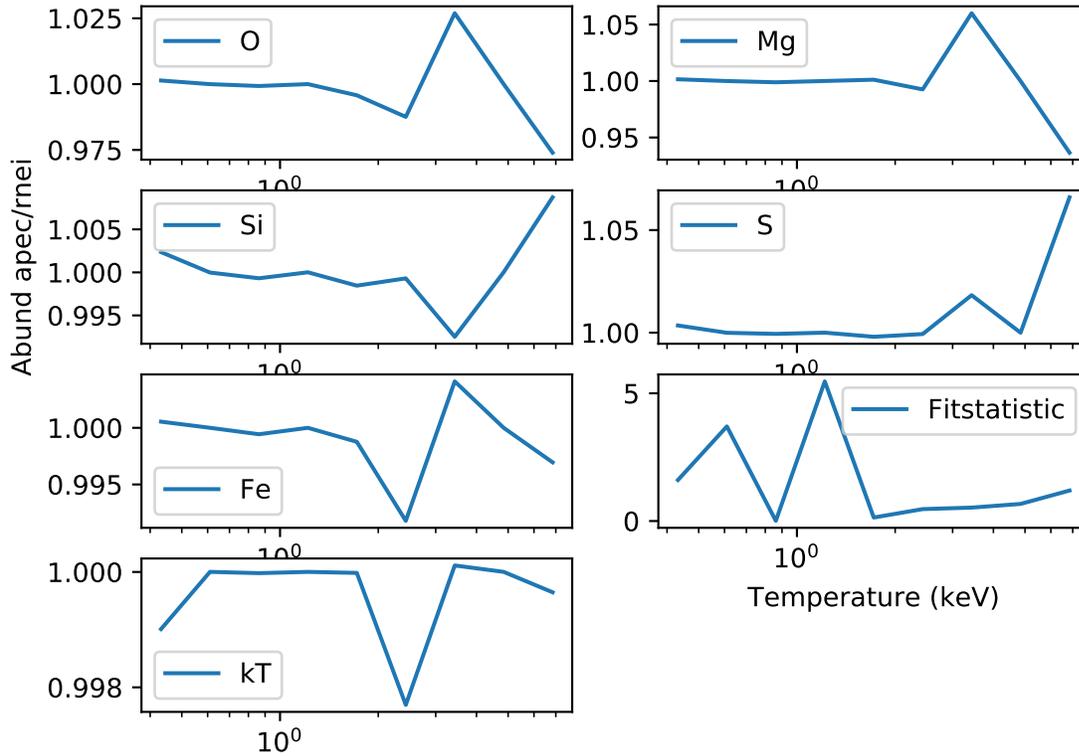


Figure 2: The abundances, temperatures and fit statistics from fitting the spectrum in Table 1, created on an offset temperature grid, with a `tbabs * vrnei` model.

The same model was then loaded up, except as a `tbabs * vapec` model, the initial parameters were set to the correct answer, and the spectrum was fit using Cash statistics. In theory, everything should return 1. The results are shown in Figure 1. The “ringing” can be seen, in which the data matches the exact calculations well but gets worse at the midpoint between the two. Abundance differences can be up to 30%, and the fit statistic gets substantially worse. Also, all the abundances change in the expected positive direction in an attempt to fill in the missing flux due to the reduced ionization balance.

4 Emissivity vs Ionization Balance

The next question is whether this is due solely to the ionization balance. I have approached this by trying to remove the ionization balance as a factor and studying the effect of interpolating the emissivities.

I re-ran the APEC code to calculate exact emissivities at temperatures between the existing APEC grid. So instead of $10^4 < T < 10^9\text{K}$ in 0.1 dex steps, it was instead done from $10^4.05 < T < 10^8.95\text{K}$ in 0.1 dex steps. This provides the exact emissivity, based on accurately querying

the atomic database and the correct ionization balance on this offset temperature grid.¹

I've taken these data, and simulated the spectrum as above, using a `tbabs*vapec` model, abundances fixed to 1, and the temperatures from the offset grid between 0.5 and 8 keV.

I have then loaded up a `tbabs*vrnei` model, which is still on the original temperature grid, and fitted it to these spectra with, again, the O, Mg, Si, S, Fe, norm and temperature free (kT_{init} and kT were linked as before to give effectively an equilibrium spectrum), and the faked spectrum were fit.

The results are shown in Figure 2. As can be seen, the variation is now much much smaller - less than 1%, excluding the $kT > 3\text{keV}$ range for O, Mg and S when there is no significant emission from these elements to constrain the fit.

5 Conclusions

Based on this work, and the paper from François Mernier, it is clear that the `apec` model in XSPEC should be retired, or at least replaced with a link to the `rnei` model to remove the effects of the ionization balance.

However, it seems that the general scheme of interpolating emissivities is, while not perfect (you may always land on an inflection point, and you will always be interpolating under the curve, effectively), a very minor contributor to emissivity and abundance issues given the scale of uncertainties in atomic data, and the sparseness of the temperature grid on which the fundamental atomic data is typically calculated.

We should keep an eye on this, and welcome further test suggestions.

¹Note that due to a typo, I actually ran it on 0.15 dex grid, which means only every other point is actually on the offset grid. I can re-run this, but I think there is plenty of data here to show the point I am making