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Physical, Numerical, and Computational Limits for Kurucz Codes

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Abstract. We outline physical, numerical, and computational limits on Kurucz's codes, for model atmospheres, ATLAS12 and ATLAS9, spectrum synthesis, SYNTHE, and abundance analysis, WIDTH9.

Key words. Stars: atmospheres – Stars: abundances – Atomic data – Molecular data – Techniques: spectroscopic

In astronomy observations are often made that are too noisy and with resolution too low to show the real physics, and then these observations are interpreted using approximate physics that gives unreliable answers. Sometimes there is no choice, but we have seen in this meeting that it is possible to take high quality spectra of bright stars that can actually show us some of the real physics. My programs are designed to do approximate physics for approximate observations. But they can also be used to eke out some real physics from high quality observations, physics that can be used in more realistic programs in the future.

ATLAS12 and ATLAS9 are one-dimensional, plane-parallel model atmosphere programs that assume LTE and hydrostatic equilibrium, have only radiative-convective energy transport, no waves, no magnetic energy or pressure, and assume time and horizontal-space averaging. Real stars do not look like that.

In real stars convection produces waves that heat the temperature minimum and the chromopshere. There the waves produce Doppler shifts that are treated as microturbulent velocity increasing upward. The minimum temperature occurs at about T=0.76*Teff. If you compute the blue and ultraviolet spectrum of a model and then make the temperature constant above .76*Teff to the surface and then recompute the spectrum, the spectra will show differences where a real star would have chromospheric and non-LTE effects. Redward of these differences the spectrum is not systematically wrong for these reasons except in the cores of strong lines.

You should never trust the computed depths and cores of strong lines unless you make a non-LTE calculation and unless you include a chromosphere if the star is convective. For the sun you can use an empirical model such as model C by Fontenla, Avrett, and Loeser (1993) in LTE, or in non-LTE with their departure coefficients for the low energy levels of abundant elements. I have non-LTE versions of SYNTHE and SPECTR that can use pre-existing departure coefficients but they do not work very well. Lines without departure coefficients must be treated with scattering source functions in the chromosphere to keep them from going into emission. Historically, as more and more lines have been included in the calculations, non-LTE effects have become weaker. At depths below the temperature minimum in the sun, LTE is generally a good approximation.

Someone should generate ad hoc chromospheres for convective models.

Even in supergiants the difference between plane-parallel and spherical models is not that great where most of the flux is produced. It becomes very important for intensity or limbdarkening calculations near the limb.

For pulsation one can assume some sort of quasi-equilibrium pulsation where each phase is represented by an equilibrium ATLAS9 or ATLAS12 model. SYNTHE allows a depth-dependant velocity shift. Or snapshot models can be taken from a pulsation calculation where the models are not in hydrostatic equilbrium and run through SYNTHE.

The distribution function opacities are tabulated from 2000 to 200000K. The equation of state is not valid for Population I abundances at low temperatures. Also the line list is missing low temperature molecules. Below 3500K Population I stars have VO bands but VO is not in the line list, nor are other molecules that matter at lower temperatures. I will add more molecules. The opacities probably work for extreme Population II abundances at lower temperatures. But, there are physical/numerical/programming problems with H_2 convection in M stars. It is especially bad for Population II M dwarfs. You may have to solve these problems yourself if you need the models.

Some of the partition functions for the lanthanides and other heavy elements date from the 1960's when the laboratory analyses were very poor. There can be huge errors in the ionization equilibirum. They essentially all need to be replaced. When I compute the energy levels for an atom, I automatically compute the partition function, but that has been going slowly. I am considering computing Hartree-Fock energy levels for all elements and generating the partition functions so I can update the equation of state in all my programs. Cowley and Barisciano (1994) have already done this for the third spectra of the lanthanides. Also ionization potentials and dissociation energies keep changing with time as calculations and measurements improve. The only number that is fixed is the speed of light, by definition. Energies, wavelengths, and other numbers we deal with change over time. Since some of my data are even from the pre-computer age, you should check that they are still current.

The equation of state does not include high enough ionization stages for the iron group so the ion populations are wrong at high temperatures ($\sim$ 200000K). In an early type star the temperature at the bottom of a model is several times the effective temperature; there might be a problem above Teff $\sim$ 60000K. I will fix the equation of state when I compute the line lists and partition functions for higher ions.

In real stars convection is three-dimensional, and there are hot and cold regions that contribute to the radiation field. In the ultraviolet the radiation field does not average out to the mean of the temperatures but is weighted toward the hotter elements. Therefore a real star radiates more than a one dimensional model in the ultraviolet. The wavelength where this starts to matter varies with effective temperature and the peak of the Planck function. In an M star, it matters in the visisble.

If you determine abundances from equivalent widths, use only weak lines on the linear part of the curve of growth to averages out as much of the bad physics in the model as possible. There are problems if the ion or molecule occurs only in a thin layer so that there is no averaging over depth. If the species occurs mainly in cool convective elements or mainly in hot convective elements, the species effectively occupies only a fraction of the area of the star so there has to be a large systematic error.

Abundances can be very uncertain unless the ion is the dominant stage of ionization or the molecule is not overly sensitive to temperature and pressure changes.

Computing a model atmosphere is a physical experiment. If you ask the programs to work outside their normal range, they do not have to converge, but may. If you ask the programs to compute models for stars that have never existed in nature, they do not have to converge. If you ask for models of stars that exist, or have existed, or will exist, the programs are supposed to work. If they do not, fix them.

1. References

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