PROGRESS ON MODEL ATMOSPHERES AND LINE DATA
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ABSTRACT
I can compute arbitrary-abundance models and spectra at high resolution using millions of atomic and diatomic molecular lines. I am improving the input line data.

ATLAS12 is an opacity sampling program that I originally wrote in 1992 to allow computation of models with individual abundances. The program reads data for 58 million atomic and diatomic molecular lines from my CD-ROMs 1 and 15. I have computed sample models for Sirius (Kurucz 1993) (Figure 1), Vega (Castelli and Kurucz 1993), Sakurai’s object, and various B stars. ATLAS12 can be used to model exciting stars for H II regions with abundances consistent with those of the H II region. I have recently fixed problems with convection and have computed models for the Sun, Arcturus (Figure 2), and Betelgeuse (Figures 3-5). As I do not yet have line data for tritomic molecules, I cannot yet compute cooler models.

The fluxes predicted by ATLAS12 are not accurate in intermediate or narrow bandpass intervals because the sample size is too small. A stripped version of the spectrum synthesis program SYNTHETE (Kurucz and Avrett 1980) is used to generate resolution 500000 flux for the converged model using the same line data that were used in the model calculation. The interval can be as large as 10 nm to 300 μm or just a small region of interest. As most of the line positions are predicted, the computed flux spectrum is not realistic when compared to a high resolution observed spectrum. For that case the spectrum can be computed using the full SYNTHETE program with only the subset of lines with accurate wavelengths (Figure 5). The spectrum calculations are not coupled to ATLAS12; any model can be used.

The high resolution spectrum can be used directly or can be instrumentally broadened to compare to low resolution observations. It is now feasible to compute grids of “observables” by computing sections of spectra for every model in a grid. A version of SYNTHETE is being developed for pretabulating distribution function opacity so that grids of models can be produced quickly with ATLAS9 (CD-ROM 13). In 1995 I published CD-ROM 23, Atomic Line Data (Kurucz and Bell) with all the laboratory and computed line data with good wavelengths sorted into one file, and then also divided into 10 nm or 100 nm blocks for convenience. I have made no significant progress on the line data in the last two years because of problems with office space and computers. I now have an Alpha and several Vaxes with 60 GB of disk, a CD writer, and a web server. There are directories for every atom and diatomic molecule. I will soon begin large scale production of atomic and molecular line data. I will continue to distribute the results on CD-ROMs, and I will make them available on the World Wide Web.

Figure 1 shows the spectrum of Sirius out to 13 μm computed with SYNTHETE using all the atomic line data for a model computed with ATLAS12 using all the line data. The calculation extends to 300 μm. (Flux units are arbitrary in all figures.)

Figure 2 shows a similar calculation for Arcturus using all the atomic and molecular line data. The molecular bands are labelled in the region from 2.2 to 12.5 μm. This is not a final model for Arcturus but one of a grid of models that are being tested.

Figure 3 shows a similar calculation for Betelgeuse using all the atomic and molecular line data. The molecular bands are labelled in the region from 1.05 to 1.9 μm. This is not a final model for Betelgeuse but one of a grid of models that are being tested. This figure illustrates the effect of decreasing resolution on the appearance of the spectrum. The stellar physics and the radiation transfer take place at high resolution. Low resolution observations are of limited value for understanding the star.

Figure 4 is the same spectrum as in Figure 3 but with the scale approximately doubled 9 times to give an impression of the complexity and information content that is lost at low resolution.

Figure 5 repeats the largest scale panel from Figure 4. Most of the lines in the line list connect predicted energy levels that are uncertain. Here the spectrum of Betelgeuse is computed with the same model but with only lines with reliable wavelengths from the line list. All the significant lines are labelled. The features are actually blends of lines, usually of different species. The spectrum can be interpreted only by detailed spectrum synthesis.

Castelli, F. and Kurucz, R.L. 1993. pp. 496-501 in
Kurucz, R.L. 1993. pp. 87-97 in
Peculiar versus Normal Phenomena in A-type and Related stars (eds. M.M. Dworetsky, F. Castelli, and R. Faraggiana), A.S.P. Conference Series 44.
Question from Giovanni Strazzulla

Question: One of the most interesting puzzles in the physics of the ISM is the (non)-identification of species responsible for the so called diffuse interstellar bands. Have you ever attempted to use the enormous number of atomic and molecular data you have to identify some of those species?

Answer: No. I have seen bumps in the spectra that have always turned out to be stellar autoionizing lines or bandheads of molecules. I do not think the diffuse bands are so simple.

Question from Christian Muller

Question: How could the ATMOS spectrum shown be improved?

Answer: The observations are only a few minutes in duration. They should be hours or days. The wavelength range should be extended. The spectra are not actually central intensity but integrations over a large circular diaphragm. There is significant rotational broadening. With a smaller diaphragm the lines would be narrower and better resolved.