

# Model Atmosphere Codes: ATLAS12 and ATLAS9

Robert L. Kurucz

**Abstract** I present three different treatments of opacity and the corresponding programs: Resolved spectra and SYNTHE; Sampled spectra and ATLAS12; Low resolution distribution functions and DFSYNTHE and ATLAS9. I also report on producing high-resolution, high signal-to-noise atlases for use in verifying the line data and spectrum calculations.

## 1 Introduction

I continue from my previous paper on "How to build a model of the atmosphere and spectrum". I gave a series of talks in Trieste in 2005 that can be found on my website [kurucz.harvard.edu/papers](http://kurucz.harvard.edu/papers).

/TRIESTEATLAS12 ATLAS12, SYNTHE, ATLAS9, WIDTH9, etc. (Kurucz 2005a)

/TRIESTELIMITS Physical, numerical, and computational limits for Kurucz codes. (Kurucz 2005b)

/TRIESTERAPID Rapid computation of line opacity in SYNTHE and DFSYNTHE. (Kurucz 2005c)

/TRIESTELINES Including all the lines. (Kurucz 2005d)

/TRIESTESOLAR New atlases for solar flux, irradiance, central intensity, and limb intensity. (Kurucz 2005e)

Here I present three different treatments of opacity and the corresponding programs: Resolved spectra and SYNTHE, and producing high-resolution, high signal-to-noise atlases for use in verifying the line data and spectrum calculations; Sampled spectra and ATLAS12; Low resolution distribution functions and DFSYNTHE and ATLAS9.

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## 2 SYNTHÉ

The original paper on SYNTHÉ was SAO Special Report No. 387 (Kurucz and Furenlid 1979) which is a sample atlas for Sirius showing both the observed and calculated spectrum with line identifications. It is on my website under **/papers/SAO387**. SAO Special Report No. 391 (Kurucz and Avrett 1981) added a few details about ultraviolet metal line series merging into continua and about including precomputed departure coefficients in the spectrum calculations. Gene Avrett would compute departure coefficients with his program PANDORA—and then I would compute spectra using those departure coefficients.

SYNTHÉ can compute only at high resolution because it sets up a grid of evenly spaced points in Doppler space and moves line centers to the nearest point on the grid. The Voigt profile is symmetric and only one wing need be computed, and I do that by table lookup. The grid can have more than a million points. I typically run at resolving power of 500 000 ( $0.6 \text{ km s}^{-1}$ ) if there are no telluric lines, as in satellite observations. If there are telluric lines I use 2 million ( $0.15 \text{ km s}^{-1}$ ) and I have gone up to as high as 10 million ( $0.03 \text{ km s}^{-1}$ ).

Some lines, such as autoionizing lines, can be specially treated with arbitrary profiles at their exact positions.

The Doppler point spacing allows Doppler shifts just by changing the point index. Radial velocity shifts between telluric and stellar spectra or between two components of a binary become simple. SYNTHÉ also allows depth-dependent Doppler shifts from convection or pulsation, but the shifts must be prespecified (a snapshot of pulsation.)

Another big timesaver is that SYNTHÉ begins each calculation by pretabulating the number densities of all atomic and molecular species and the continuum opacity at selected points (program XNFPELSYN). It then reads the line list and writes a new selected line list. For each line it reads it computes the line absorption coefficient and interpolates the approximate continuum opacity. If the line opacity is below a cutoff factor times the continuum opacity the line is rejected. The cutoff can be specified. I normally use 0.001 for stars and 0.0001 for the sun. You can try different numbers to find the value below which the spectrum does not change. This matters especially in molecular bands where there are sometimes 100 lines/Ångstrom.

The new selected line list is used for the detailed line profile calculations. Radiative, Stark, and van der Waals damping constants are included in the line list. The wings of each line are computed only out to the cutoff. That can be more than 100 nm for the strongest lines at high gravities.

All the lines that mattered in the spectrum calculation are saved in a file that can be read in as a new input line list. After comparison to observed spectra as described in Sec. 4, the wavelengths, gf values, and damping constants can be hand edited to improve the fits.

Once a spectrum has been computed it can be broadened with Gaussian or arbitrary profiles to any lower resolution. You can predict the appearance of the spectrum with various resolution spectrographs down to resolving power of 100.

I generally make a number of runs that cover the whole spectrum and merge them into one 4 million point spectrum for the whole SED (stellar energy distribution) from 1 nm to 300  $\mu\text{m}$ . For cool stars I start at 91 nm. You can find examples of various resolution spectra on my website at [/stars](#). Remember that these are computed photospheric spectra from models that do not include chromospheres. Real stars typically have chromospheric emission lines in the ultraviolet.

### 3 High Resolution Atlases

High-resolution, high-signal-to-noise spectra are needed to test the line data and the spectrum synthesis programs and to determine the stellar parameters.

There are no high quality solar spectra taken above the atmosphere in the ultraviolet, visible, or infrared out to 2.2  $\mu\text{m}$ . There is a recent central intensity atlas produced with an FTS on the ACE satellite (Hase et al. 2010) that covers from 2.2 to 14  $\mu\text{m}$ .

In the ultraviolet there are not even “good” quality solar spectra. There are various good quality solar spectra taken through the atmosphere in the visible and infrared. I have been trying to reduce the FTS spectra taken by Jim Brault from Kitt Peak to produce central intensity, limb intensity, flux, and irradiance atlases.

Fig. 1 shows the visible flux atlas from Kurucz (2005f). I have shown the telluric spectrum deduced from this atlas in my “How to” paper as part of the pipeline for atmospheric transmission.

Fig. 2 is the residual irradiance spectrum determined by removing the telluric lines from the flux spectrum (Kurucz 2005g). This is the spectrum at the top of the atmosphere.

Fig. 3 is the absolute irradiance spectrum determined by multiplying the residual irradiance times the continuum of my solar model ASUN seen from a distance of 1 AU (Kurucz 2005g). This is the spectrum of the sun as a star, the spectrum seen by all the bodies in the solar system. It is the spectrum studied by exoplanetary scientists on distant exoplanets searching unsuccessfully for habitable planets orbiting Sol.

Fig. 4 shows a sample residual irradiance spectrum for part of the H and K bands that I have worked on thus far (Kurucz 2008).

All of the above spectra can be found on my web site under [/sun](#).

And, of course, spectra of bright stars, Arcturus, Procyon, etc., are also needed for comparisons.

## 4 Validating Spectrum Calculations

Fig. 5 shows a detailed comparison of the solar calculations to 0.15 nm of the flux atlas shown in Fig. 1 at 599.1 nm. I have 10000 pages with comparisons like this. This is one of the least busy and and best fitting. Each spectrum is plotted twice: at normal scale, and at 10 times scale to emphasize discrepancies. The observed FTS spectrum is plotted in black. The computed telluric spectrum broadened to the FTS resolution is plotted in cyan. The computed solar spectrum broadened to the FTS resolution is plotted in red. The product of the solar and telluric spectra broadened to the FTS resolution is plotted in magenta. Comparing the magenta spectrum to the black spectrum tests the wavelengths, gf values, and damping constants. The left feature at 599.13 nm with depth 0.26 is mainly Fe II with some blending with CN, Fe I, Yb II, and telluric H<sub>2</sub>O. There are missing lines in both wings. The right feature at 599.185 nm with depth 0.05 is mostly 15 hyperfine components of a Co I line overlain by a telluric H<sub>2</sub>O line. There are also blends with CN, Cr I, and Ca I. There are missing lines in both wings; several beyond 599.21 nm. There are probably additional missing lines included in both features. Overall the comparison shows a tremendous improvement in the treatment of the Co I feature over my earlier solar calculations.

In these plots we compare only the 1% of my lines that have good wavelengths. Lines that are missing may be among the list of lines with predicted wavelengths. The predicted lines contribute statistically to the total opacity in model calculations.

Here are my conclusions from working with high quality spectra:

- Abundances are generally determined from blended features that must be interpreted by synthesizing the spectrum including every significant blending line.
- In general, one half the lines are missing from the list of lines with good wavelengths.
- Every line has to be adjusted in wavelength, damping constants, and gf value, and most are asymmetric from hyperfine and isotopic splitting. There are pressure shifts. There are depth-dependent Doppler shifts from motions.
- Most lines used in abundance analyses are not suitable.
- Including many lines reduces the accuracy.
- We do not know anything with certainty about the sun except its mass.

## 5 ATLAS12

SYNTHE is the basis for ATLAS12. It provides the line and continuum opacity and the equation of state.

ATLAS12 can deal with more than 1 billion lines by sampling. It preselects into a smaller linelist the lines that are relevant for the model and also saves them in a file. That file can be used as the input line list for similar models. It can treat arbitrary depth-dependent abundances, isotopes, and velocities. It defaults to 30000 sampling

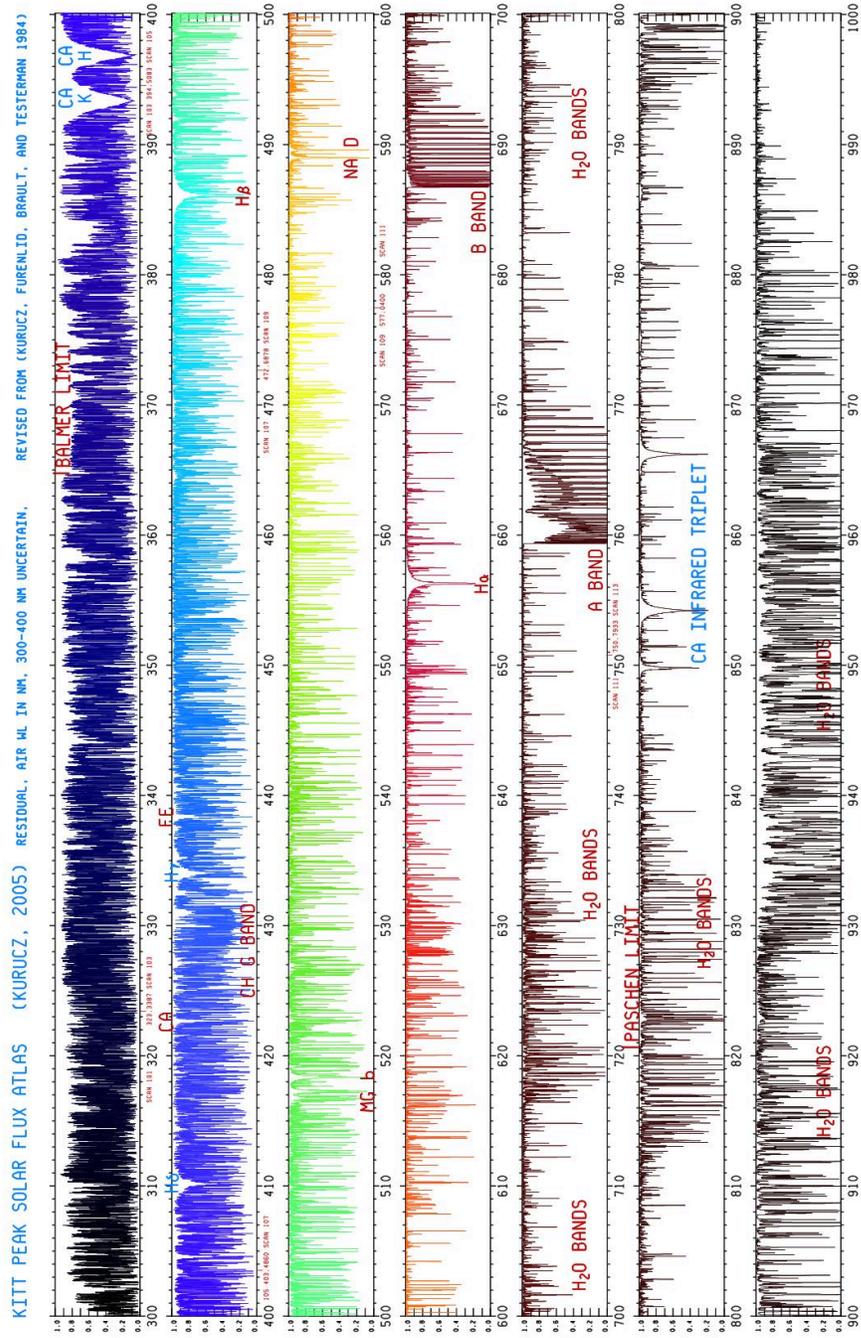


Fig. 1



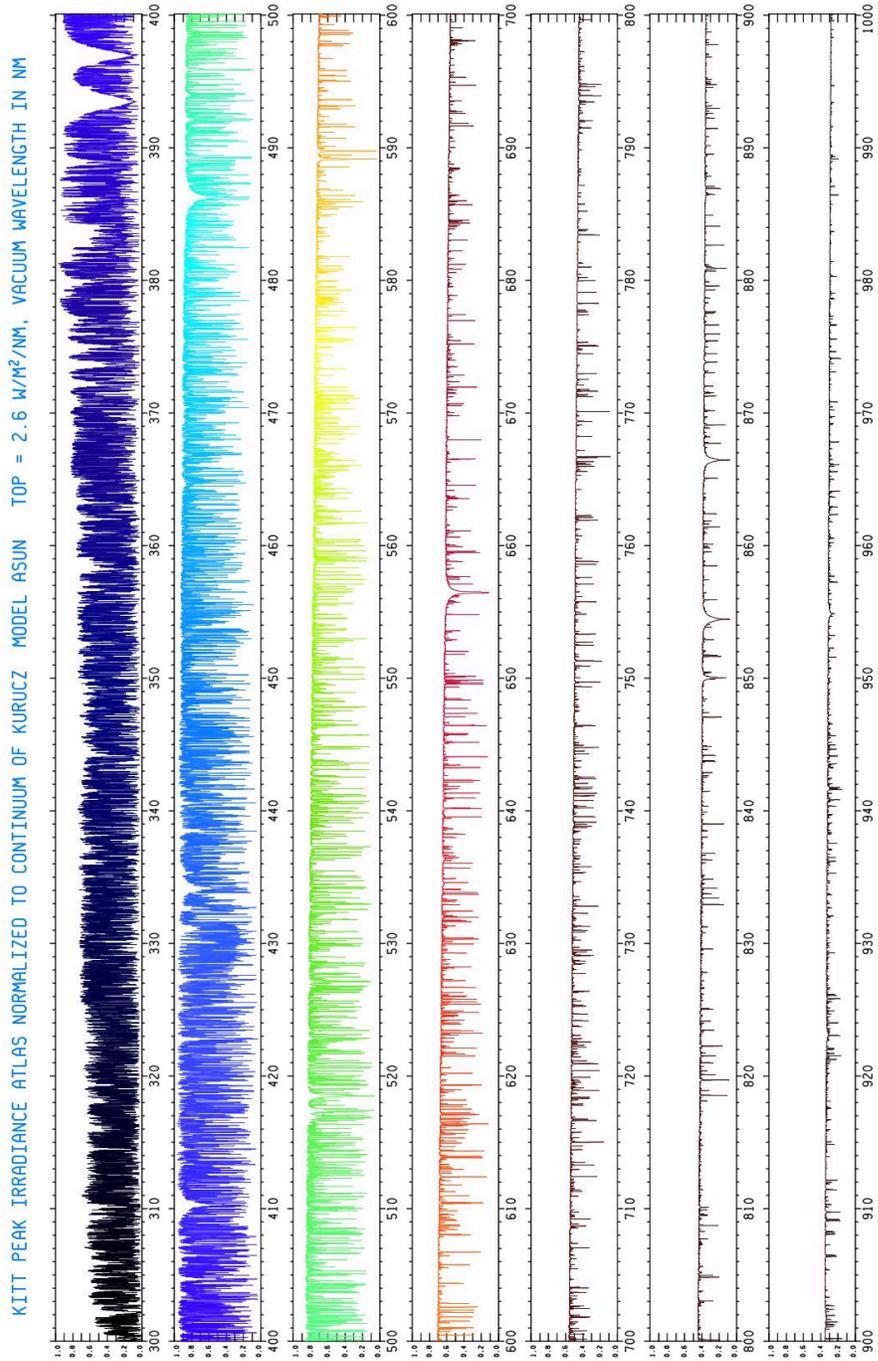


Fig. 3

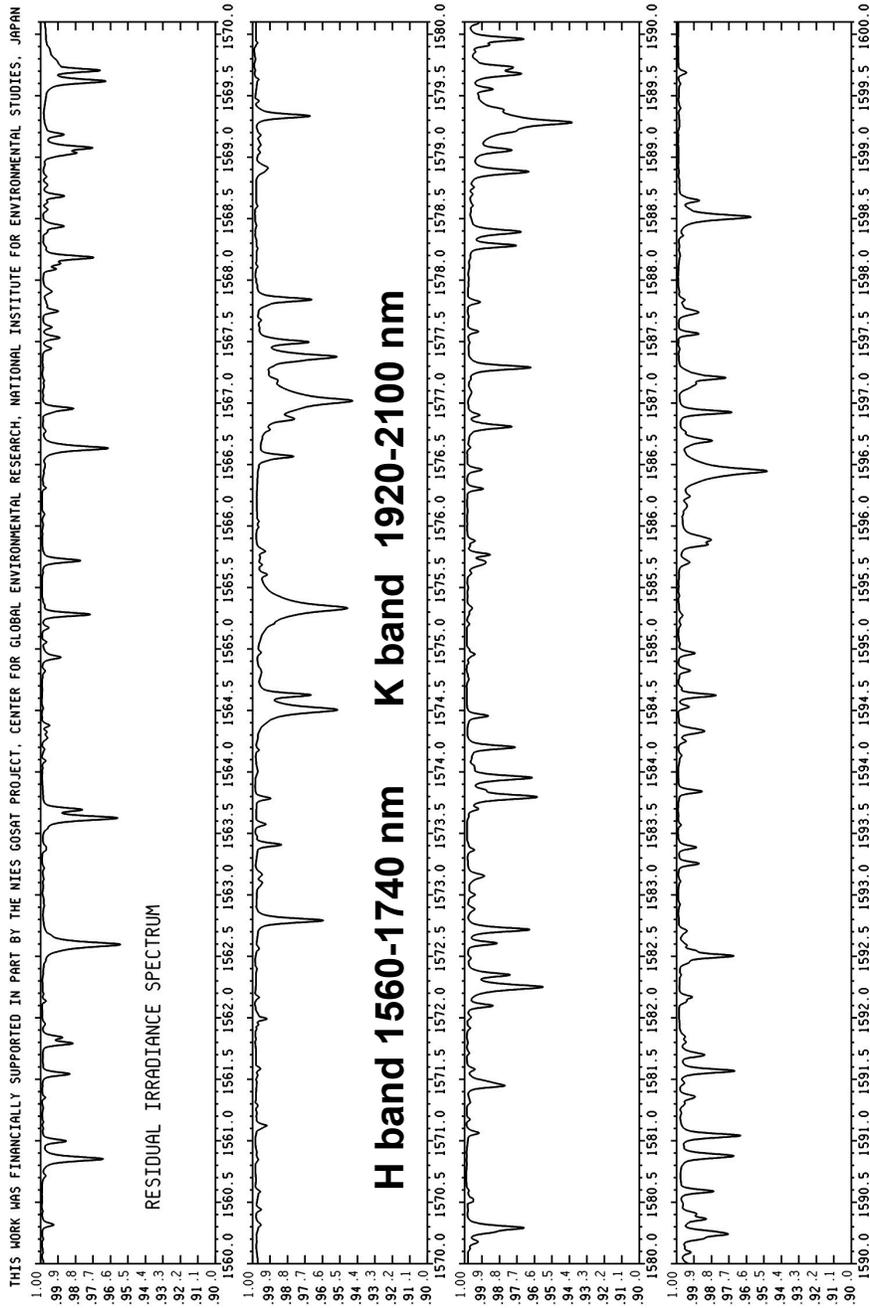


Fig. 4



points but it could sample more than a million. The points shift with effective temperature to give good coverage of the flux maximum. 30000 points are adequate for computing a flux-constant model but not for reliably predicting the SED over small intervals. For each model I make SYNTH runs at resolving power 500000 to compute the surface flux or intensities using the saved line file as input. I also compute spectra using only the lines with good wavelengths for comparison to observed spectra. Differences between the two computed spectra indicate how much more work needs to be done on the line list.

ATLAS12 is slow by design for treating individual stars with individually determined abundances and parameters. I compute a grid of models for each star I work on varying all the parameters. There is a big investment in quality.

## 6 DFSYNTH and ODFs

If you are working on huge numbers of stars and want to interpolate in large grids of models to determine parameters, it is more efficient to pre-tabulate the opacities for a fixed set of abundances and then to compute the grid, or as many models as you need, using ATLAS9 because it is fast.

DFSYNTH is the program you use to compute the line opacity spectra and from them to tabulate opacity distribution functions, ODFs.

First let me describe ODFs. Fig. 6 shows a schematic line opacity profile and a schematic spectrum extending over an interval  $\Delta\lambda$ . An integral of some property of the radiation over that interval is independent of the wavelength order of the points in the spectrum as long as the source function, which is the Planck function  $B_\nu$ , does not vary significantly over the interval. You can rearrange the line profile or spectrum in order of increasing opacity. If you then normalize by the width of the interval, you have a distribution function that tells you the fraction of the interval that has opacity less than a given value of the line opacity,  $\ell_\nu$ .

Fig. 7 shows a set of distribution functions computed for the region on the blue side of the Balmer discontinuity for a range of electron number densities. The interval included about 10000 wavelength points. In this case I approximated the distribution function with a 10 point step function. The average radiation field over this interval is then calculated at 10 distribution function points instead of 10000 wavelength points, a saving of a factor of 1000. Using a step function introduces some numerical error and some physical error. The smallest step represents the width of the line cores so if the real line cores are narrower it smooths them and reduces the maximum optical depth. Fiorella Castelli (Castelli and Kurucz 2004) uses 12 steps to better represent the cores.

Another physical error is shown in Fig. 8. Using ODFs assumes that the opacity spectrum has similar appearance at every depth in the atmosphere as in the left panel. Then the optical depth is computed correctly even when the spectrum is rearranged in an ODF. But if the opacity spectrum significantly changes shape because of ionization or molecular bands that introduce strong temperature dependence, the

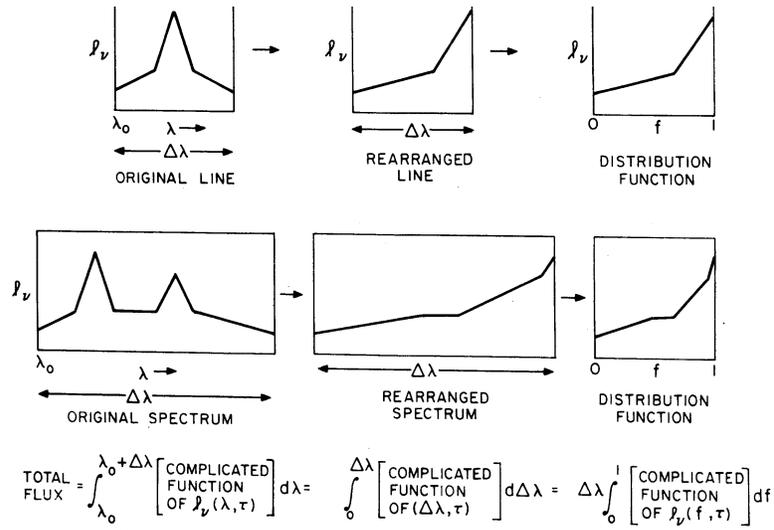


Fig. 6 Schematic opacity distribution functions, ODFs.

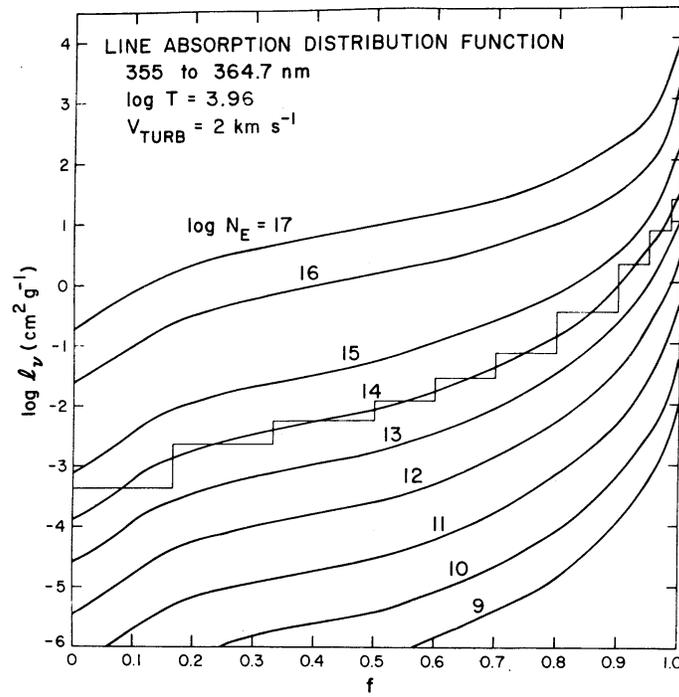
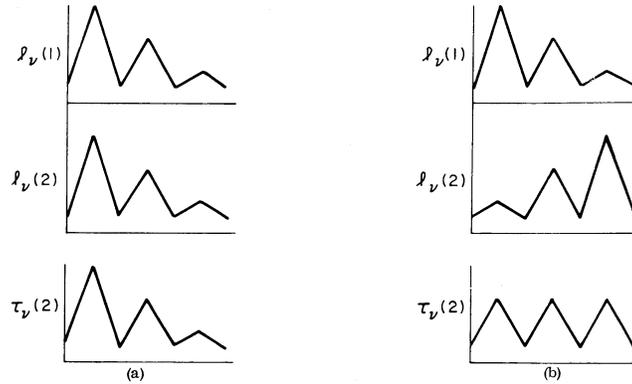


Fig. 7 Computed opacity distribution functions.

optical depth will be underestimated and overestimated by the ODF. The spectra in the right panel have the same ODFs as those in the left but different optical depths. In practice, in general, ATLAS9 models with ODFs look the same as ATLAS12 models with sampling which do not have any rearrangement. It must be that the errors average out. However, no one has yet computed a complete ATLAS12 grid to compare to a complete ATLAS9 grid to look for peculiar cases.



**Fig. 8** ODFs can produce errors in optical depth; see text.

DFSYNTH is a version of SYNTH that can compute the LTE opacity spectrum of more than 1 billion lines, at more than 4 million frequencies, for more than 1200 temperature-pressure pairs, for a range of  $V_{\text{turb}}$ , on a workstation (or a super-computer). These spectra can be statistically processed into ODF tables as they are computed. Or the spectra can be saved directly if you have enough disk space. Then you can work out any kind of opacity representation you want with them.

## 7 ODFs and ATLAS9

ATLAS9 works with two different sets of ODFs. One with 337 “big” wavelength intervals covering the whole spectrum and one with 1221 “little” wavelength intervals covering the whole spectrum. The ODFs use a 12-step representation. There is one time-saving modification. The radiation field is computed starting with the highest step and working down. If a lower step does not matter because the line opacity is small relative to the continuum at all depths, all the lower steps are lumped together and not computed.

The big ODFs run faster while the little ODFs show more detail. I usually compute models with the big and then compute final fluxes with the little.

The original writeup for ATLAS, which describes ATLAS5, SAO Special Report 309 (Kurucz 1970), gives a general overview of other details of the program and how to compute models as of 40 years ago. It is on my website [/papers/SAO309](#).

You can get the Castelli ODFs and grids of models computed with those ODFs from Fiorella Castelli's web site [www.user.oat.ts.astro.it/castelli](http://www.user.oat.ts.astro.it/castelli). She has the Linux versions of ATLAS9, ATLAS12, SYNTHÉ, and DFSYNTHÉ, and manuals. You may never have to compute the ODFs yourself unless you want your own personal set of abundances. Start with hers and then learn how to compute your own models. Szabolcs Mészáros has followed that path and computed ODFs and massive grids of models using the Linux versions (Mészáros et al. 2012) and put them on his website [www.iac.es/proyecto/ATLAS-APOGEE](http://www.iac.es/proyecto/ATLAS-APOGEE).

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