Mem. S.A.It. Suppl. Vol. 8, 14

Memorie della
Supplementi

ATLAS12, SYNTHE, ATLAS9, WIDTH9, et cetera

Robert L. Kurucz

Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA, USA
e-mail: `rkurucz@cfa.harvard.edu`

Abstract. The problem we address is including the opacity of millions or hundreds of millions of lines in model stellar atmosphere calculations, then generating detailed, realistic spectra from those model atmospheres, then modelling the observation process, and finally comparing the calculated spectra to observed spectra to determine the properties of stars so that we can understand their evolution and the evolution of galaxies. We describe the current status of Kurucz's programs and atomic and molecular line data.

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

1. Introduction

Once programs had been developed to compute a realistic opacity spectrum for large numbers of lines (SYNTHE, Kurucz and Avrett 1981) it became possible consider including all the lines in a model atmosphere calculation. I can do this directly but it would take about a month per model with the fastest Alpha workstation, and perhaps a day using the full power of a parallel supercomputer. More practical methods involve statistical treatments of the line opacity. I have programmed two different treatments. First, opacity distribution functions, ODFs, using DFSYNTHE to pretabulate the opacity, then ATLAS9 to compute the models and low resolution emergent flux, and finally SYNTHE and SPECTR to generate the high-resolution spectrum. Second, opacity sampling using ATLAS12 to compute both the opacity at a small number of points (30000) and a model that conserves energy but does not produce accurate fluxes. Then SYNTHE and SPECTR are used to generate the emergent high-resolution spectrum.

SYNTHE and SPECTR can also generate specific intensity spectra across the disk that ROTATE uses to produce rotationally broadened flux spectra. The intensity spectra themselves are the limb darkening. Spectra can be transmitted through the terrestrial atmosphere using the TRANSYNTHE suite of programs. The spectra can be convolved with filters to generate any color system using INTEGRATEFILTER. The spectra can be convolved with instrumental bandpasees to generate energy distributions, SEDs, or spectra at any resolution using BROADEN. The final computed spectra can be plotted together with the observed spectra with the lines labelled using PLOTSYN.

With a fast, large-memory workstation it is now possible to compute, for a fixed set of abundances, tables of ODF opacities in one day, and then to compute a whole grid of models in another day. A small section of spectrum, enough to calibrate a photometric system, or echelle orders, can be computed in another day for the whole grid of hundreds of models.

Alternatively, to work on individual stars with arbitrary abundances, including isotopic abundances, one can use ATLAS12 to generate in one day a small grid for one star that varies temperature, gravity, and abundances. In another day a small region of the spectrum can be computed for each model and compared to observation. The whole spectrum can be computed for the best fitting model.

2. ATLAS12 and SYNTHE

ATLAS12 still does not work as originally advertised (Kurucz 1995). It is supposed to be able to treat abitrary abundances, including depth-dependent isotopic abundances. At that time I had become interested in isotopes; I had isotopomeric molecular line lists that could show variation from dredge-ups, and also I was interested in isotopic splittings of atomic lines and diffusion. There were two problems, treating Rosseland opacities and treating the equation of state, that had to be solved to get ATLAS12 to work. All of my model atmosphere programs except the first few use a Rosseland opacity scale. This is the "natural" scale for coupling the structure of the atmosphere to the radiation field. Convective flux also depends on the Rosseland opacity. But for arbitrary, and espcially for depth-dependent abundances, the Rosseland opacity cannot be pretabulated. It has to be computed as the model is computed. It took me years to figure out how to generate a starting guess for the Rosseland opacity and to extrapolate from iteration to iteration as the temperature was changing. The guessing procedure worked and allowed ATLAS12 models to converge. At that point I started to let others use the program. Later it was pointed out to me by Tsymbal (Tsymbal & Shulyak 2003) that I could have chosen a continuum monochromatic optical depth scale that behaves similarly to the Rosseland depth scale, and that I could have computed the models on that depth scale. At each iteration I could compute the Rosseland opacity and use it to compute the convection. Once the model converged I could interpolate it to the Rosseland scale. This should work except in cases where there are big abundance changes that cause big opacity changes. Some users may wish to make a τ_{500nm} or τ_{1000nm} or $\tau_{whatever}$ version of ATLAS12.

Some of the equation of state routines date from the 1960s. If there were not good laboratory data for the energy levels, the partition functions generated then were wrong and the ionization potentials were uncertain, especially for the heavier elements, and they are still wrong. The molecules need a separate partition function for each isotopomer. I planned, and still plan, to write a new equation of state routine that uses partition function tables for each species including each isotopomer. Whenever I compute a new line list I automatically generate the energy levels and the partition function. When I computed an iron group line list (Kurucz 1988a), I generated a partition function table for each species. Those are stored in the file PFIRON. I am computing or recomputing all the atoms to fill out the line data so I will generate all the partition functions and the problem will be solved. However those calculations are going slowly, especially since I do not have funding. I have decided to try to do a quick Hartree-Fock calculation of the energy levels and the partition functions so that I can finish ATLAS12. Now that memory is not a problem, putting in the new partition functions and depth-dependent abundances should be simple.

The 30000 fluxes that ATLAS12 computes are accurate enough to compute the total flux but not good enough for intermediate band photometry such as uvby. It is necessary to make a separate flux calculation using SYNTHE after a model is converged. I use the following procedure:

I first run ATLAS12 only through the point where it selects the line data from the line list files. I write out and save the file. That file is in a packed format where all information not essential to the opacity calculation has been removed. The lines for any similar stars will be the same, so models for those stars can be computed from the same line list. Models with lower abundances will also work. Higher abundance models would need a new line selection.

To compute the spectrum for an ATLAS12 model with SYNTHE, use program RPACKEDLINE to read the line file. Since there are no identifications in the packed file, SYNTHE does not save any information about the lines. ATLAS9, or any other models, can be used with these line lists. A complete spectrum may have to be computed in pieces and patched together with MERGESYN. The packed line list can also be edited for computing shorter intervals for photomtery, etc.

These spectra do not reproduce real high resolution observed spectra. Stronger lines tend to have good data but the weaker lines are incomplete and they include the predicted lines with uncertain wavelengths that fill in the opacity between big lines. At lower resolution most of the wavelength errors should average out. Also models are generally computed with an overestimate of the Fe abundance and an overestimate of the microturbulent velocity to make up for some of the missing line opacity.

To make a detailed comparison to a high resolution spectrum, only the line lists with laboratory wavelengths should be used, and the gf values and damping constants need to be hand adjusted to match. The normal procedure is to work differentially by adjusting the line data to match a high resolution, high-signal-to-noise atlas for a star for which a good model atmosphere is available.

3. Depth-dependent microturbulent velocity

Microturbulent velocity is a parameter that is generally not considered physically except in the sun. Usually it is treated as the parameter that minimizes scatter among lines of the same ion in abundance analyses. Figure 1 shows the temperature versus optical depth for the empirical solar Model C of Fontenla, Avrett, and Loeser (1993). It also shows the empirical microturbulent velocity versus optical depth determined from (central intensity) line profiles. I have schematically divided it into microturbulent velocity that is produced by convective

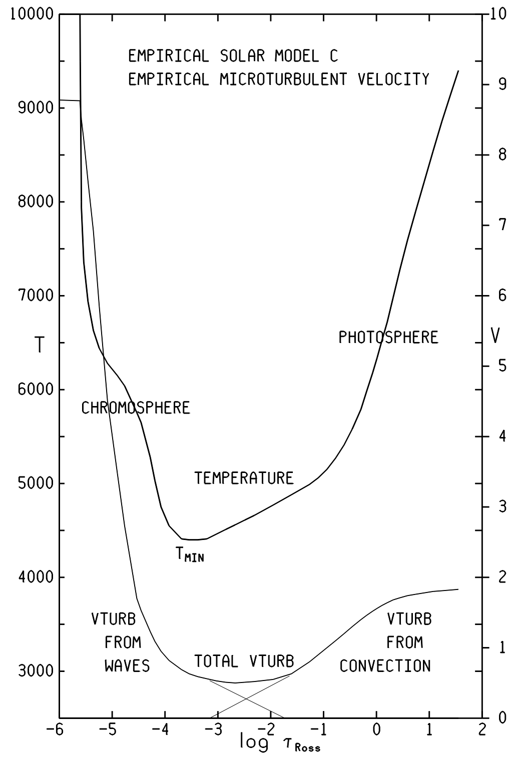

Fig. 1. The empirical solar model C by Fontenla, Avrett, and Loeser (1993) that has a chromosphere, a temperature minimum, and also an empirical microturbulent velocity distribution that I have divided into Vturb from convection and Vturb from waves.

motions that must go to zero at or below the temperature minimum, and into microturbulent velocity that is produced by the waves that heat the chromosphere. The minimum Vturb is about 0.28 of the maximum Vturb. The minimum temperature is about 0.76 Teff. I suggest that all "normally" convective cool stars have behavior like this.

This convective microturbulent velocity is not the microturbulent velocity found in equivalent width abundance analyses. In the sun an equivalent width determination of microturbulent velocity from the flux spectrum yields Vturb < 1 km s^{-1}. It is also not the Vturb of line opacity tables. My solar model, ASUN, (Kurucz 1992) has Vturb = 1.5 km s^{-1} in order to make up for missing lines that have not yet been included in the line list. We know for cer-

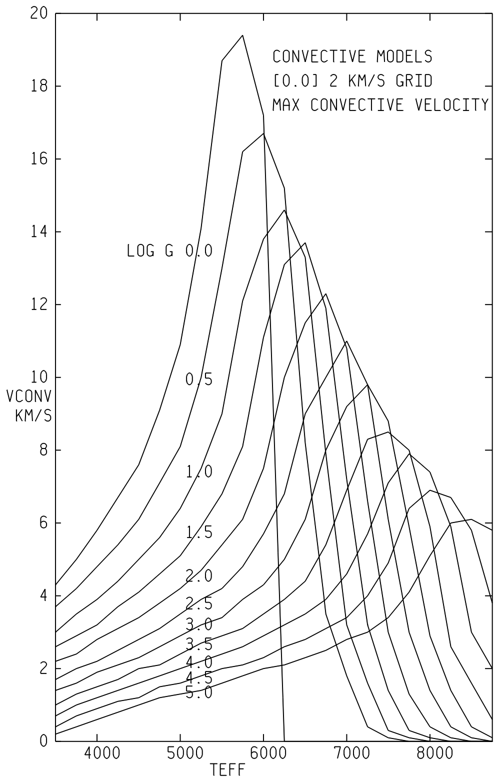

Fig. 2. Maximum convective velocity at any depth in each model for a solar abundance grid.

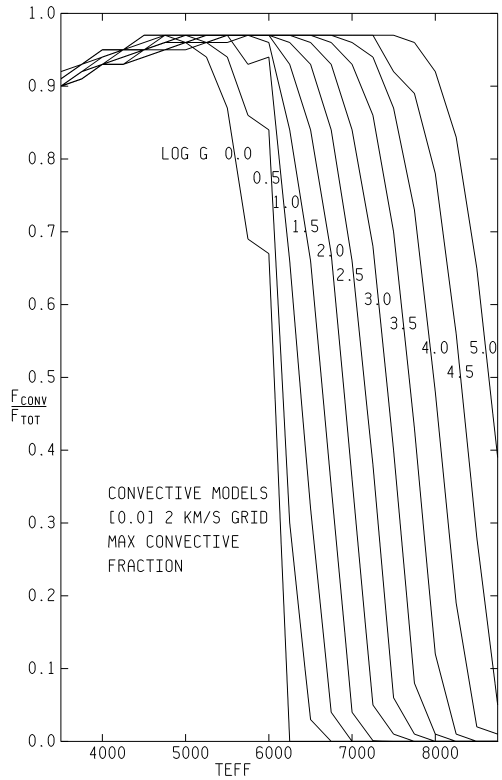

Fig. 3. Maximum fraction of convective flux at any depth in each model for a solar abundance grid.

tain that the microturbulent velocity varies with depth, that the opacity is strongly dependent on microturbulent velocity, and that the model atmospheres do not include depth-dependent microturbulent velocity.

In Figure 2 I show the maximum convective velocity for a grid of solar abundance convective models. In Figure 3 I show the maximum fraction of convective flux at any depth for each model in Figure 2. In Figure 4 I have weighted the maximum convective velocity by the maximum convective fraction. I treat this weighted velocity V_W as the microturbulent velocity at the bottom of the atmosphere. It agrees with the empirical value in the sun. Then I take the depth dependence of the microturbulent velocity produced by convection in the sun and I scale to V_W. I ignore outwardly increasing Vturb from waves and set the minimum Vturb to max(Vturb, 0.28 V_W) as in the sun. Figure 4 then gives the variation of microturbulent velocity with temperature and gravity as long as we stay on the cool side of the maximum. And, since we do not understand what is happening on the hot side, let us blindly do the same there. One thing we know for certain is that there can be no microturbulent velocity produced by convective motions if there is no convection. Convection deeper in the star can generate waves that propagate through the atmosphere and produce a "wave" Vturb. One can also guess that the "mean" microturbulent velocity must be on the order of $V_W/2$ which should roughly correspond to the number found from curves of growth.

Microturbulent velocity varies with effective temperature and gravity and abundance because convection varies with effective temper-

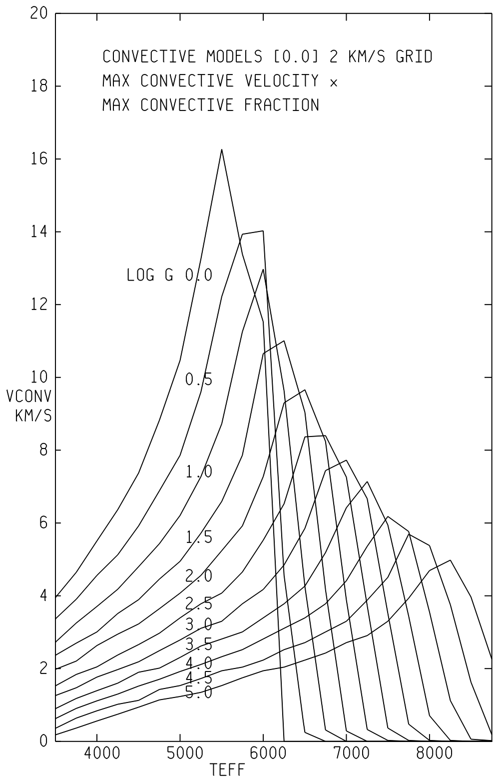

Fig. 4. The product of Fig. 2 times Fig. 3, the flux-weighted convective velocity, which I use as the estimator of Vturb at the bottom of a model.

ature, gravity, and abundance. When comparing the properties of two stars, the difference in microturbulent velocity must be accounted for. When comparing two stages along an evolutionary track, the change in microturbulent velocity must be accounted for. By using grids with depth-dependent microturbulent velocity as described here, this effect is automatically included. Vturb is no longer a free parameter. This may not be true for low-gravity stars hotter than the sun that have only weak convection.

If two stars have the same effective temperature and gravity, the one with the higher abundances will have higher microturbulent velocity because it is more convective. I have not yet computed the grids to work out the numbers. I expect that in ATLAS12 the Vturb varies with the convection, the convection varies with the Rosseland opacity at τ=1, and the Rosseland opacity at τ=1 varies with the abundances.

4. Rotation and differential rotation

Rotational broadening is computed in program ROTATE by generating intensity spectra for a range of angles (currently 17, μ = 1.0, .9, .8, .7, .6, .5, .4, .3, .25, .2, .15, .125, .1, .075, .05, .025, .01), then defining a rectilinear grid over the disk of the star (currently 200x200, or 100x100 quadrant), then interpolating the spectrum for the angle and projected velocity at each point, and finally summing all the points. There are two more approximations. First the spectra are interpolated to 100 angles (μ = 0.005 to 0.995 by .010) and pretabulated. The spectrum at each point on the disk is found by choosing the nearest angle in the pretabulation. Second, the spectrum is Doppler shifted by the nearest integral number of points. If the resolving power is 500000 the shift can have an error of one part in one million. Most of the errors are random and cancel but they should be checked for critical work. Increase the resolving power or the grid size or the number of angles and see if the output spectrum is affected.

More physics can be put in. I have added differential rotation using the empirical fit for the sun from Libbrecht and Morrow 1991 for latitude ϕ and $R_\odot$ in km,

$V_{rot}(\phi)=$

$$(462 - 75\sin^2\phi - 50\sin^4\phi)10^{-9}\ 2\pi R_\odot,$$

$V_{rot}(0)$ = 2.020 km/s at the equator,

$V_{rot}(1)$ = 1.474 km/s at the pole,

$V_{rot}(\phi)/V_{rot}(0)$ =

$$(1 - 75/462\ \sin^2\phi - 50/462\ \sin^4\phi).$$

The parameter read by ROTATE is the stellar equitorial velocity. Differential rotation is assumed to have the same behavior for all stars. It is computed only if it is explicitly turned on.

As long as physical variables can be defined on an array of points and there is a procedure for interpolating in a grid of spectra that vary in those physical variables, one can treat any shape star, or binaries, spots, rapid rotators, etc. using similar methods.

5. Interstellar transmission

In order to compare to observation we convolve the spectra computed with the SYNTHE suite of programs with a theoretical model of the observation. One can model the transmission of any material between the star and the observer.

I have not yet written the programs to model the reddening, the diffuse interstellar bands, and the interstellar lines, but it would be easy for the user to do it. In the meantime, I check for such absorption before comparing to observed spectra. There are diffuse interstellar band catalogues, for example, Herbig (1995). Since the interstellar lines are also stellar lines, they would be on my website in the line list if the line list were complete. Just search for lines with lower energy level < 1000 cm^{-1}. An interstellar package will eventually be included with SYNTHE.

6. Telluric emission

I have also not yet written the programs to model airglow and anthropogenic pollution emission lines, but those would also be easy for the user to do. For now, I check for such emission in observed spectra. There are catalogues by Osterbrock et al. (2000) for airglow lines and by Slanger et al. (2003) for pollution lines that will eventually be included in SYNTHE.

7. Atmospheric transmission

In 1988 (Kurucz 1988b) I discovered that there were broad features in Kitt Peak FTS solar spectra (taken by James Brault) that were produced by ozone and by $[O_2]_2$ (O_2 dimer) that I had not known about and had not considered in the reduction of the Solar Flux Atlas (Kurucz, Furenlid, Brault, and Testerman 1984). The $[O_2]_2$ number density is quadratic in O_2 so is concentrated near the ground. It produces strong features at sunset and sunrise. Figure 5, 6, and 7 show the features produced by O_3, $[O_2]_2$, and their product in the visible. There are also many lines of O_2 and H_2O that blend with, or that mask, solar lines in the FTS spectra shown in Figure 8.

This figure is available in electronic form only. Also available from the site of R.L. Kurucz It will be mailed by post on request, by R.L. Kurucz.

Fig. 8. Telluric lines of O_2 and H_2O that were computed for the flux scans in the Kitt Peak Solar Flux Atlas (Kurucz 2005) and pieced together in the solar laboratory frame with gravitational red shift removed.

Much of the research on atmospheric transmission has been done by the United States Air Force (Air Force Research Laboratory, formerly Air Force Geophysics Laboratory, formerly Air Force Cambridge Research Laboratory). They have produced empirical model atmospheres, line data (HITRAN), and computer programs for calculating transfer through the atmosphere (LOWTRAN, MODTRAN). These programs are not designed for doing the whole spectrum at once in high resolution.

Astronomers should measure the atmosphere over their heads and determine the run of temperature, pressure, O_3, and H_2O with altitude because it affects their observations, but they do not care. The Air Force had a program of measuring these quantities and has produced averaged models for the whole year, or quarterly, or monthly, for temperate latitudes, tropical latitudes, etc. (Anderson et al. 1986). From those models I have made up four models MODMIDWIN, MODSPRING, MODMIDSUM, and MODAUTUMN that I use to represent the atmosphere above Kitt Peak. They can be used as starting guesses at any observatory except in Antarctica. The temperatures, pressures, O_3, and H_2O, must be adjusted to get a good fit for any observed spectrum. MODMIDSUM is listed in Table 1.

Laboratory ozone cross-sections for the ultraviolet Hartley and Huggins (Bass & Paur 1981, Griggs 1968, Freeman et al. 1983) and the visible Chappuis & Wulf (tabulated by Shettle & Anderson 1995) bands are tabulated for several temperatures and interpolated. Widths and strengths of individual O_2 dimer features have been measured in the laboratory (Greenblatt et al. 1990; Dianov-Klokov 1959) and computed from those parameters.

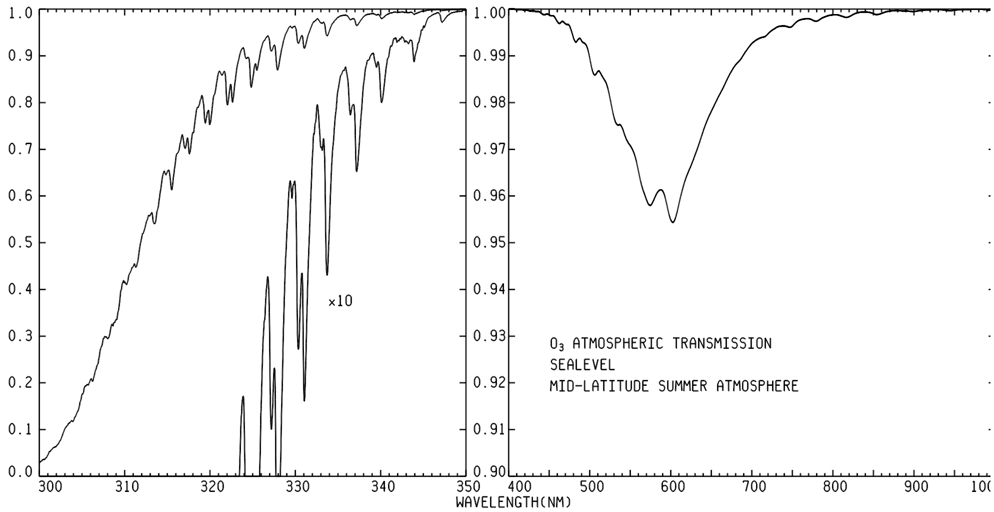

Fig. 5. Telluric O_3 transmission from 300 to 1000 nm.

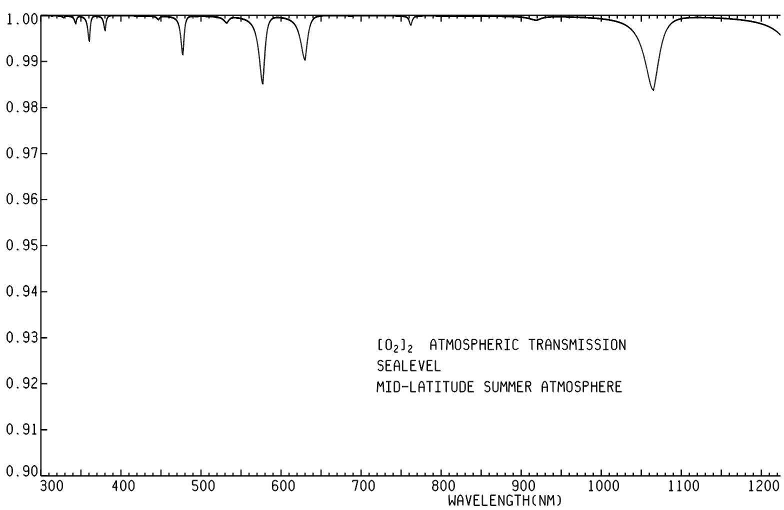

Fig. 6. Telluric $[O_2]_2$ transmission from 300 to 1500 nm.

The main source of line data is the HITRAN (HIgh-resolution TRANsmission) database (Rothman et al. 2005). Smithsonian Astrophysical Observatory has taken over management of the database from the Air Force. Historically the Air Force concentrated on infrared data beyond 1μm aiming for very accurate line positions, strengths, pressure-shifts, and damping constants. Researchers all over the world work on and with HITRAN, not just the Air Force. The visible data were poor quality. Much of it was missing or wrong. Now about half of the O_2 and H_2O are good. I have tried to fill in missing lines for O_2 by calculating them and by fitting them in solar spectra. There are calculations available for H_2O but they do not work very well. I have tried to adjust many of the lines by hand. One of the main problems with these lines, one that astronomers have not yet had to face, except in Stark broadening, is pressure shifts. The measured positions of telluric lines in the solar spectra are not the real line positions. If they are used to generate molecular constants, they

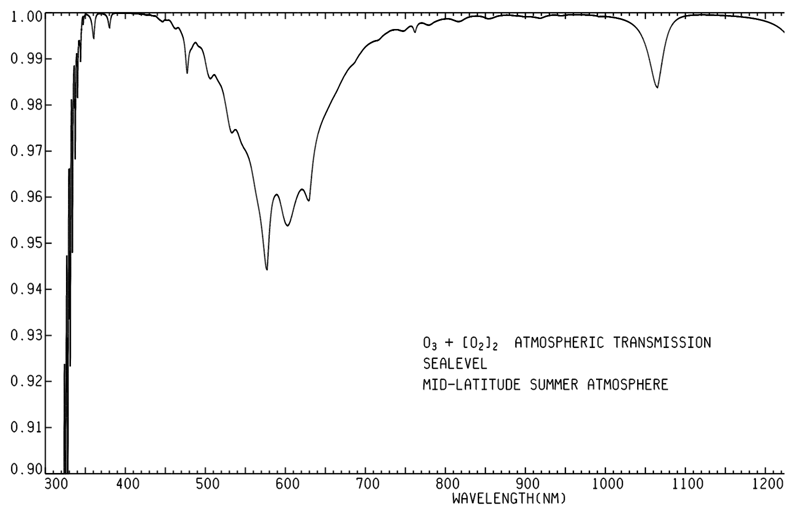

Fig. 7. Telluric O_3 and $[O_2]_2$ transmission from 300 to 1500 nm.

introduce systematic errors. Laboratory work is required to measure the line positions as a function of pressure and to extrapolate to zero pressure. Only the strongest bands of O_2 have been well measured.

I have written subroutines OZONE and O2DIMER for computing the transmission spectra of the broad features and the TRANSYNTHE suite of programs for treating telluric lines. The cause of the delay, as for solar lines, is that the telluric data are still not good enough to treat the problem without hand adjustment, even for O_2, and there are many missing lines.

Files AIR1, AIR2, AIR3, ..., AIR10, AIR20, AIR100, AIREND have telluric line data for 0 to 1 μm, 1 to 2 μm, etc. Most of the data except in AIR1 are from HITRAN reformatted like other data in the Kurucz linelists. Some of the data have hand corrections. The overall quality at short wavelengths is not good. Every line should be checked for critical work.

TRANSYNBEG reads the input parameters. The wavelength range and resolution must be the same as in any subsequent stellar spectrum calculation. The lines are shifted by the radial velocity of the star which must be specified. In wavelength regions where sharp telluric lines are present, the resolving power of the calculation must be at least 2 million to treat the sub-300K doppler width. Any computed stellar spectra must have the same resolution.

RMOLAIR reads the line data from the AIR* files.

TRANSYNTHE computes the opacity spectrum.

TRANSPECTR computes the mean transmission spectrum from the given starting and stopping airmass, starting and stopping hour angle, mean declination, latitude, and altitude. It also computes the residual depth of each line. The line data and depth are passed along with the spectrum for labelling plots.

TRANSMIT multiplies a stellar spectrum by the transmission spectrum.

8. Spectrophotometry

Once the computed spectrum has been computationally transmitted from the star to the instrument it is instrumentally broadened for comparison to observation. Program BROADEN convolves a Gaussian, sin(x)/x, or rectangular profile specified by FWHM in velocity, wavelength, wavenumber, or resolving power. It also can use instrumental pro-

Table 1. Mid-Latitude summer (July) atmosphere. after Anderson et al. (1985)

H(km)	P(Mb)	T(K)	Ntot(/cm3)	H2O(ppmv)	O3(ppmv)
0.	1013.	294.2	2.496E+19	1.88E+04	3.02E-02
1.	902.	289.7	2.257E+19	1.38E+04	3.34E-02
2.	802.	285.2	2.038E+19	9.68E+03	3.69E-02
3.	710.	279.2	1.843E+19	5.98E+03	4.22E-02
4.	628.	273.2	1.666E+19	3.81E+03	4.82E-02
5.	554.	267.2	1.503E+19	2.23E+03	5.51E-02
6.	487.	261.2	1.351E+19	1.51E+03	6.41E-02
7.	426.	254.7	1.212E+19	1.02E+03	7.76E-02
8.	372.	248.2	1.086E+19	6.46E+02	9.13E-02
9.	324.	241.7	9.716E+18	4.13E+02	1.11E-01
10.	281.	235.3	8.656E+18	2.47E+02	1.30E-01
11.	243.	228.8	7.698E+18	9.56E+01	1.79E-01
12.	209.	222.3	6.814E+18	2.94E+01	2.23E-01
13.	179.	215.8	6.012E+18	8.00E+00	3.00E-01
14.	153.	215.7	5.141E+18	5.00E+00	4.40E-01
15.	130.	215.7	4.368E+18	3.40E+00	5.00E-01
16.	111.	215.7	3.730E+18	3.30E+00	6.00E-01
17.	95.0	215.7	3.192E+18	3.20E+00	7.00E-01
18.	81.2	216.8	2.715E+18	3.15E+00	1.00E+00
19.	69.5	217.9	2.312E+18	3.20E+00	1.50E+00
20.	59.5	219.2	1.967E+18	3.30E+00	2.00E+00
21.	51.0	220.4	1.677E+18	3.45E+00	2.40E+00
22.	43.7	221.6	1.429E+18	3.60E+00	2.90E+00
23.	37.6	222.8	1.223E+18	3.85E+00	3.40E+00
24.	32.2	223.9	1.042E+18	4.00E+00	4.00E+00
25.	27.7	225.1	8.919E+17	4.20E+00	4.80E+00
27.5	19.07	228.5	6.050E+17	4.45E+00	6.00E+00
30.	13.2	233.7	4.094E+17	4.70E+00	7.00E+00
32.5	9.30	239.0	2.820E+17	4.85E+00	8.10E+00
35.	6.52	245.2	1.927E+17	4.95E+00	8.90E+00
37.5	4.64	251.3	1.338E+17	5.00E+00	8.70E+00
40.	3.33	257.5	9.373E+16	5.10E+00	7.55E+00
42.5	2.41	263.7	6.624E+16	5.30E+00	5.90E+00
45.	1.76	269.9	4.726E+16	5.45E+00	4.50E+00
47.5	1.29	275.2	3.390E+16	5.50E+00	3.50E+00
50.	.951	275.7	2.500E+16	5.50E+00	2.80E+00
55.	.515	269.3	1.386E+16	5.35E+00	1.80E+00
60.	.272	257.1	7.668E+15	5.00E+00	1.30E+00
65.	.139	240.1	4.196E+15	4.40E+00	8.00E-01
70.	.0671	218.1	2.227E+15	3.70E+00	4.00E-01
75.	.0300	196.1	1.109E+15	2.95E+00	1.90E-01
80.	.0120	174.1	4.996E+14	2.10E+00	2.00E-01
85.	.00448	165.1	1.967E+14	1.33E+00	5.70E-01
90.	.00164	165.0	7.204E+13	8.50E-01	7.50E-01
95.	.000625	178.3	2.541E+13	5.40E-01	7.00E-01
100.	.000258	190.5	9.816E+12	4.00E-01	4.00E-01

files specified at the computed point spacing. When the profile is rapidly changing, program BROADENX linearly interpolates between profiles specified at the ends of a wavelength interval.

Now, when I compute a model that I think might be of general interest, I compute the spectrum as far to the ultraviolet and infrared as I can. Then I broaden it to resolving powers of 500000, 100000, 50000, 30000, 20000, 10000, 5000, 3000, 2000, 1000, 500, 300, 200, and 100 and put those spectra on my website in the STARS directory so people can find predictions"off the shelf" to compare to their observations. It takes about one day per model.

9. Photometry

Photometry is computed by convolving the spectra output from the SYNTHE suite of programs with a theoretical model of the observation. That model would include detector response, filter transmission, transmission of the obtical system, and, for an observation from the ground, transmission of the atmosphere. I have written a simple program INTEGRATEFILTER that convolves SYNTHE output spectrum with a response function in this way. INTEGRATEFILTER will read any number of response functions. The Asiago Database (Moro & Munari 2000) has the most photometric systems so I suggest that some user make up a general input file from it and a program to generate all the colors.

The atmospheric transmission is computed with the TRANSYNTHE suite of programs and is applied to the spectra before INTEGRATEFILTER is used. Most filter systems in the visible and near infrared are insensitive to the atmospheric transmission, while ultraviolet and infrared systems are sensitive.

10. Limb darkening

Limb darkening is automatically produced when I generate a spectrum for a rotating star but the files are so big that I have been throwing them away. The rotation program computes the intensity spectrum at a number of angles across the disk (currently 17 angles) and interpolates the spectrum at each point on a rectangular mesh overlaid on the disk. Those spectra are tabulated at all the angles for each wavelength. If the file is transposed to all the wavelengths at each angle, limb darkening is computed by convolving those spectra with a theoretical model of the observation. That model would include detector response, filter transmission, transmission of the obtical system, and, for an observation from the ground, transmission of the atmosphere. I have written simple programs SPLIT17SYN and

INTEGRATEFILTER that convolve a SYNTHE output spectrum with a response function in this way. INTEGRATEFILTER will read any number of reponse functions. The atmospheric transmission is computed with the TRANSYNTHE suite of programs and is applied to the intensity spectra before INTEGRATEFILTER is used. Most filter systems in the visible and near infrared are insensitive to the atmospheric transmission.

11. PLOTSYN

I make large plots that compare computed and observed spectra and that actually show errors and provide information to the reader. The features are labelled and the wavelengths and energy levels can actually be read off the plots, and there is a file giving complete information for each labelled line. In addition there is a hand-editable file that gives the input data for evey line that contributed to the spectrum. That file can be read back in to iterate on the fit.

My plotting software was written before Postscript was invented. At present PLOTSYN writes a binary vector file that must be translated to Postscript. I am going to rewrite the plotting utilities, PLOTPACK, to write Postscript directly. (It is simple.) This will make the files smaller, scalable, and editable. I am considering ways to put plots on CDs or DVDs. Perhaps solar spectra at 1 Å per page with line identifications to be used as a reference, or big continuous plots that can be windowed.

12. WIDTH9

At solar abundances there are very few isolated single lines. Most lines are blended with other species, or with telluric lines in spectra taken from the ground, and almost all lines have isotopic or hyperfine splitting. At infinite signal-to-noise the equivalent width of a weak line on the linear part of the curve of growth is independent of the resolution of the observation. But that is not true for noisy observations where the continuum level is uncertain. Also in the presence of noise, blends that are not understood do not have a well defined equivalent width. Lines that are not on the linear part of the curve of growth are subject to large systematic uncertainties from errors in the physics in the model atmospheres, in the microturbulent velocity, and in the treatment of damping. In stars with low abundances the uncertainties from blending are reduced but even though a blend is buried in the noise it still offsets the continuum level.

My recommendation for making or checking an abundance analysis are the following: Using stronger lines that are not on the linear part of the curve of growth just increases the real error because the errors are not random. There is no improvement from using many lines. Throw out all lines that are not on the linear part of the curve of growth. Get a high-signal-to-noise high-resolution atlas of a slowly rotating star that has the lines that are in your star. (Fast rotators have similar equivalent widths although the lines may not be discernable.) Look up every line left in your line list and throw out any that are significantly blended. Synthesize the spectrum for the atlas and for your star. Try to understand the blending and the continuum level for each of the lines that remain. Throw out any lines that you do not understand to the 95 percent level.

When I did this for the Fe I lines that were used to determine the solar Fe abundance by Grevesse & Sauval (1999) only three lines remained. The three lines produced the same Fe abundance which was 10 percent less than the abundance found by Grevesse & Sauval from all the lines. You have to measure only those three Fe I lines to determine the Fe abundance relative to the sun for any star like the sun. There is a complication, of course. Fe I is not the principal ionization stage for Fe. Most of the Fe is Fe II. A dominant ion is much less sensitive to errors in the model than a minor ion so dominant ions should always be used in an abundance analysis if there is a choice. Going through the same elimination procedure for Grevesse & Sauval's Fe II lines leaves only one "reliable" line. It gives the same abundance as the three Fe I lines.

WIDTH9 computes line profiles and curves of growth for individual lines and it can derive an abundance from an observed equivalent width. It can be used to determine the sensitivity of lines to the model, to a chromosphere, to the microturbulent velocity, and to the damping. (Weak lines can have strong damping.) WIDTH9 can be used to determine the equivalent width at which a line is no longer on the linear part of the curve of growth which varies throughout the spectrum. It can be used to investigate the choice of continuum level on apparent equivalent width. I have an advantage because I have the atlases, and the computed spectra with the line identifications, and the line data, and the computer programs so it is easy for me to make these tests. I am giving you the solar atlases. I am giving you the line data. I will eventually give you the atlases with the line identifications. I am giving you the programs. Use them.

References

Anderson, G. P., et al. 1986 AFGL-TR-86-0110.

Bass, A.M. & Paur, R.J. 1981. J. Photochem. 17, 141

ianov-Klokov, V.I. 1959 Optics and Spectroscopy, 6, 290

Fontenla, J. M., Avrett, E. H., & Loeser, R. 1993, ApJ, 406, 319

Freeman, D. E., Yoshino, K., Esmond, J. R., & Parkinson, W. H. 1984, Planet. Space Sci., 32, 239

Greenblatt, G. D., Orlando, J. J., Burkholder, J. B., & Ravishankara, A. R. 1990, J. Geophys. Res., 95, 18577

Grevesse, N., & Sauval, A. J. 1999, A&A, 347, 348

Griggs, M. 1968, JCP 49, 857

Herbig, G. H. 1995, ARA&A, 33, 19

Kurucz, R.L. 1988a. in *Trans. IAU XXB*. M.McNally, ed., Dordrecht: Kluwer, p. 168

Kurucz, R.L. 1988b. in *Infrared Extinction and Standardization*, E.Milone, ed., Berlin: Springer-Verlag, p. 55

Kurucz, R.L. 1992. in *Stellar Population of Galaxies*, (eds. B. Barbuy and A. Renzini) Dordrecht: Kluwer, p. 225

Kurucz, R.L. 1995. in *Stellar Surface Structure*, (ed. K.G. Strassmeier & J.L.Linsky) Dordrecht:Kluwer, p. 523

Kurucz. R.L. 2005. *Kitt Peak Solar Flux Atlas 300 to 1000 nm*, in preparation

Kurucz, R.L. & Avrett, E.H. 1981. Solar spectrum synthesis. I. A sample atlas from 224 to 300 nm. SAO Spec. Rep. 391

Kurucz, R.L., Furenlid, I., Brault, J., & Testerman. L. 1984. *Solar Flux Atlas from 296 to 1300nm*. National Solar Observatory, Sunspot, NM

Libbrecht, K.G. and Morrow, C.A. 1991. in *The Solar Interior and Atmosphere*, eds. A.N. Cox, W.C. Livingston, and M. Matthews, Tucson: University of Arizona Press, p. 479

Moro, D., & Munari, U. 2000, A&AS, 147, 361

Osterbrock, D. E., Waters, R. T., Barlow, T. A., Slanger, T. G., & Cosby, P. C. 2000, PASP, 112, 733

Rothman, L.S. et al. 2005 JQSRT 96, 13

Shettle, E.P. & Anderson, S.M. 1995 PL-TR-95-2060.

Slanger, T. G., Cosby, P. C., Osterbrock, D. E., Stone, R. P. S., & Misch, A. A. 2003, PASP, 115, 869

Tsymbal, V., & Shulyak, D. 2003, IAU Symposium, 210, 15P