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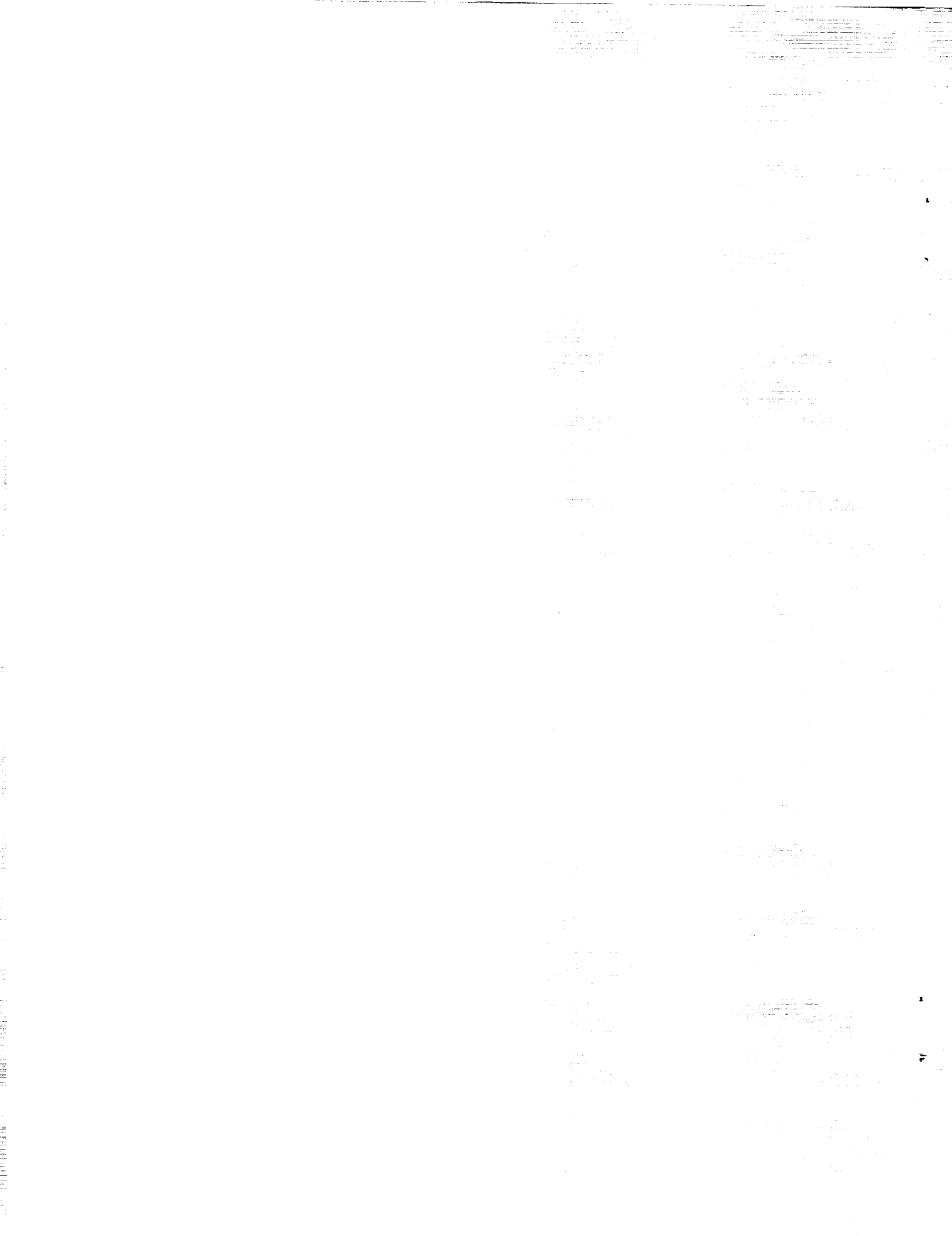
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Atomic and Molecular Data Needs for Astrophysics

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Atomic and Molecular Data Needs
for Astrophysics

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Abstract. We need a list of all the energy levels of all atoms and molecules that matter (qualifiers below). Except for the simplest species, it is impossible to generate accurate energy levels or wavelengths theoretically. They must be measured in the laboratory. From the list of energy levels can be generated all the lines. Given the low accuracy required, 1 - 10%, all the other data we need can eventually be computed or measured. With the energy levels and line positions known, one can measure gf values, lifetimes, damping, or one can determine a theoretical or semiempirical Hamiltonian whose eigenvalues and eigenvectors produce a good match to the observed data, and that can then be used to generate additional radiative and collisional data for atoms or molecules.

For atoms and ions, we need all levels, including hyperfine and isotopic splittings, for $n \leq 9$ below the lowest ionization limit and as much as practicable above. Lifetimes and damping constants depend on sums over the levels. Inside stars there are thermal and density cutoffs that limit the number of levels, but in circumstellar, interstellar, and intergalactic space, photoionization and recombination can populate high levels, even for high ions. We need all stages of ionization for elements at least up through Zn.

In the sun there are unidentified asymmetric triangular features that are unresolved multiplets of light elements with $n \leq 20$. Simple spectra should be analyzed up to $n = 20$. Levels that connect to the ground or to low levels should be measured to high n, say $n = 80$. The high levels are necessary to match line series merging into continua.

All the magnetic dipole, electric quadrupole, and maybe higher-pole, forbidden lines are required as well. Most of the universe is low density plasma or gas. If the Hamiltonian is well determined, forbidden lines should be reliably computable.

For molecules, we need all levels below the first dissociation limit and as much as is practicable above, especially levels of all states that connect to the ground state. Stars populate levels to high V and to high J. In the sun there are many broad bumpy features that are molecular bands that are not in the line lists. For the cooler stars we need all the diatomics among all the abundant elements, and, essentially, the hydrides and oxides for all elements (especially ScO, TiO, VO, YO, ZrO, LaO). For M stars triatomics also become important. Much more laboratory and computational work is needed for H_2O. In the brown dwarfs and "planets" methane is important and it needs more laboratory and computational work.

We can produce more science by investing in laboratory spectroscopy rather than by building giant telescopes that collect masses of data that cannot be correctly interpreted.

I am repeating the proposal abstract here to provide the context for the progress report:

I propose to continue providing observers with basic data for interpreting spectra from stars, novas, supernovas, clusters, and galaxies. These data will include allowed and forbidden line lists, both laboratory and computed, for the first five to ten ions of all atoms and for all relevant diatomic molecules. I will eventually expand to all ions of the first thirty elements to treat far UV and X-ray spectra, and for envelope opacities. I also include triatomic molecules provided by other researchers. I have made CDs with Partridge and Schwenke's water data for work on M stars. The line data also serve as input to my model atmosphere and synthesis programs that generate energy distributions, photometry, limb darkening, and spectra that can be used for planning observations and for fitting observed spectra. The spectrum synthesis programs produce detailed plots with the lines identified. Grids of stellar spectra can be used for radial velocity-, rotation-, or abundance templates and for population synthesis. I am fitting spectra of bright stars to test the data and to produce atlases to guide observers. For each star the whole spectrum is computed from the UV to the far IR. The line data, opacities, models, spectra, and programs are freely distributed on CDs and on my Web site and represent a unique resource for many NASA programs.

Kurucz and Fiorella Castelli in Trieste used Kurucz's new distribution function program to compute new opacity tables and then new grids of model atmospheres with improved convection. The grids of models, fluxes, and colors have been put on the Kurucz web site.

Kurucz has copied his extant test spectrum calculations to the web directory. The spectra were calculated either at resolving power of 500000 or 2000000 in Doppler space so that a shift in point number is a Doppler shift. Depending on effective temperature, the wavelengths range from 1 nm to 300μm. Some of the spectra have been broadened to lower resolution on the same point spacing. Eventually the resolutions will include 100000, 50000, 30000, 20000, 10000, 5000, 3000, 2000, 1000, 500, 300, 200, and 100. Oftentimes users can find what they need "off the shelf" on the web site. As Kurucz fills requests for new calculations the new spectra are added to the website. This is the current list: alphaCen, Arcturus, A spectral types, Betelgeuse, Procyon, Sirius, Vega, GL411.

Kurucz is now in full production of new line lists for atoms. He is computing all ions of all elements from H to Zn and the first 5 ions of all the heavier elements, about 800 ions. For each ion he does as many as 61 even and 61 odd configurations, computing all energy levels and eigenvectors. The Hamiltonian is determined from a scaled-Hartree-Fock starting guess by least squares fitting the observed energy levels. The average energy of each configuration is used in computing scaled-Thomas-Fermi-Dirac wavefunctions for each configuration which in turn are used to compute allowed and forbidden transition integrals. These are multiplied into the LS allowed and forbidden transition arrays. The transition arrays are transformed to the observed coupling to yield the allowed and forbidden line lists. Results are put on the web as they are finished. Kurucz expects to complete much of this work by August 2003. There will be more than 500 million lines. Kurucz will then

compare ion by ion, to all the laboratory and computed data in the literature
and make up a working line list for spectrum synthesis and opacity calcula-
tions with the best available data. As the laboratory spectrum analyses are
improved, the calculations will be redone with the new energy levels.

Bibliography for this performance period:

2002 A few things we do not know about the Sun and F stars and G stars.
      presented at the Workshop on Nearby Stars, NASA Ames Research Center,
      Moffett Field, California, June 24-26, 1999. Proceedings failed to
      be published. Published in Baltic Astronomy, 11, 101-111, 2002.

2002 Convective intensification of magnetic flux tubes in stellar
      photospheres. (S.P. Rajaguru, R.L. Kurucz, and S.S. Hasan)
      Astrophys. Journ., vol. 565, pp. L101-L104.

2002 A few things we do not know about stars and model atmospheres.
      Presented at the conference, New Quests in Stellar Astrophysics:
      The Link between Stars and Cosmology, 26-30 March, 2001, Puerto
      Vallarta, Mexico. in New Quests in Stellar Astrophysics:
      The Link between Stars and Cosmology, (eds. M. Chavez, A. Bressan,
      A. Buzzoni, and D. Mayya) Dordrecht: Kluwer, pp. 3-14, 2002. APPENDED

2002 The photospheric absorption lines in the UV spectrum of the multiple
      system HD 5980. (G. Koenigsberger, R.L. Kurucz, and L. Georgiev)
      Astrophys. Journ. vol. 581, pp. 598-609.

2002 Atomic and molecular data needs for astrophysics. Presented at
      The 3rd International Conference on Atomic and Molecular Data,
      Gatlinburg, Tennessee, April 24-27, 2002. in Atomic and Molecular
      Data and their Applications. (Ed. D.R. Schultz, P.S. Krstic, and
      F. Ownby) AIP Conf. Proc. 636, pp. 134-143. APPENDED

2002 A few things [we do not know about stars and model atmospheres].
      presented at IAU Symposium 210, Modelling of Stellar Atmospheres,
      17-23 June 2002, in Uppsala, Sweden. Abstract to be published in
      IAU Symposium 210, Modelling of Stellar Atmospheres, (eds. N.E. Piskunov,
      W.W. Weiss. and D.F. Gray) 2003.

2002 New grids of ATLAS9 model atmospheres. (F. Castelli and R.L. Kurucz)
      presented at IAU Symposium 210, Modelling of Stellar Atmospheres,
      17-23 June 2002, in Uppsala, Sweden. to be published in
      IAU Symposium 210, Modelling of Stellar Atmospheres, (eds. N.E. Piskunov,
      W.W. Weiss. and D.F. Gray) 2003.

2002 The progenitor of supernova 1993J revisited. (S.D. Van Dyk,
      P.M. Garnavich, A.V. Filippenko, P. Hoflich, R.P. Kirshner, R.L. Kurucz,
      P.M. Challis) Pub. Astron. Soc. of the Pacific, vol. 114, pp.1322-1332.

     Kurucz has avoided attending further meetings in order to finish the new
calculations on atoms and molecules as soon as possible. He attended
IAU Symposium 210, Modelling of Stellar Atmospheres, 17-23 June 2002,
in Uppsala, Sweden because much of the meeting dealt with his work.

INTRODUCTION

Astrophysicists work on "Important", "Big" problems and they think that the basic physics that they require to solve their problems has already been done, or, if it has not been done, it is easy and can be readily produced, as opposed to the hard problems they are working on. They have it backward. Getting the basic data is the hard part. When all the basic physics is known, pushing the "state-of-the-art" becomes straightforward.

Half the lines in the solar spectrum are not identified. All the features are blended. Most features have unidentified components that make it difficult to treat any of the identified components in the blend. And even the known lines have hyperfine and isotopic splittings that have not yet been measured. Is an asymmetry produced by a splitting. or by a velocity field, or both? It is very difficult to determine abundances, or any property, reliably when you do not know what you are working with.

For planetary and telluric atmosphere projects the solar irradiance spectrum is required as the input at the top of the atmosphere. It has never been observed. People ask me to compute it. I can compute it theoretically using both known and predicted lines and get agreement averaged over a nanometer but there is no way to predict the resolved spectrum when only half the lines are known. In other stars the situation is worse because the signal-to-noise and resolution of the observations are worse. Logically one has to know a priori what is in the spectrum in order to interpret it; there is not enough information in the observed spectrum itself.

Basically we need a list of all the energy levels of all atoms and molecules that matter (qualifiers below). From that list can be generated all the lines. With the energy levels and line positions known, one can measure gf values, lifetimes, damping, or one can determine a theoretical or semiempirical Hamiltonian whose eigenvalues and eigenvectors produce a good match to the observed data, and that can then be used to generate additional radiative and collisional data for atoms or molecules.

For atoms and ions, we need all levels, including hyperfine and isotopic splittings, for $n \leq 9$ below the lowest ionization limit and as much as practicable above. Th is the only element that does not have splitting. Lifetimes and damping constants depend on sums over the levels. Inside stars there are thermal and density cutoffs that limit the number of levels, but in circumstellar, interstellar, and intergalactic space, photoionization and recombination can populate high levels, even for high ions.

One very important problem is diffusion of heavy elements inside stars because it changes the density and reaction rates. The radiative acceleration is computed by integrating over the line spectrum. At the surface some elements can be enhanced by a factor of 10^4. If the diffusion is deep inside the star, spectra for high stages of ionization are required.

In the sun I see unidentified asymmetric triangular features that are unresolved multiplets of light elements with $n \leq 20$. Simple spectra should be analyzed up to n = 20. Levels that connect to the ground or to low levels should be measured to high n, say n = 80. The high levels are necessary to match line series merging into continua.

All the magnetic dipole, electric quadrupole, and maybe higher-pole, forbidden

lines are required as well. Most of the universe is low density plasma or gas. If the Hamiltonian is well determined, forbidden lines should be reliably computable.

For molecules, we need all levels below the first dissociation limit and as much as is practicable above, especially levels of all states that connect to the ground state. Except for H_2(BX,CX), far ultraviolet bands have been ignored unless they appear as interstellar lines. We see H_2 lines in stars as hot as 8000K when the stars have low metal abundances so that the lines are not masked.

In the sun we see, and have linelists for, C_2(AX,ba,da,ea), CN(AX,BX), CO(AX,XX), H_2(BX,CX), CH(AX,BX,CX), NH(AX,ca), OH(AX,XX), MgH(AX,BX), SiH(AX), SIO(AX,EX,XX). The isotopomers are included. Some stellar spectroscopists have more recent linelists than I do. Mine are based on old laboratory data and were computed with rotationless RKR potentials. They all have to be brought up to date, or even further improved, and expanded to higher V and J levels. In many cases there are new analyses based on FTS spectra. Ions and a few minor molecules have to be added to the linelist as well. In the sun there are many broad bumpy unidentified features that are molecular bands that are not in the line lists. Most of them are probably just high-V transitions. It is important that the laboratory analyses include all the isotopomers. They are needed to interpret the stellar spectra. When they are not measured in the laboratory we have to make up our own predicted linelists for them.

For the cooler stars we need all the diatomics among all the abundant elements, and, essentially, the hydrides and oxides for all elements (such as ScO. TiO, VO, YO, ZrO, LaO, etc.). Ca appears as CaOH and CaH, not CaO. I use the TiO linelist from Schwenke (1998) [1] with 38 million lines.

Stars that are evolved and have high C abundances from nuclear burning can bind all the O into CO so that there are no other oxides, just C-bearing molecules. CN and C_2 bands are everywhere.

For M stars cooler than 3500K triatomics also become important. Much more laboratory and computational work is needed for H_2O. I currently use the linelist from Partridge and Schwenke (1997) [2] with 66 million lines.

In the brown dwarfs and "planets" methane is important and it needs more laboratory and computational work. This is too cool and too hard for me.

58, 154, 500 MILLION LINES

Here is the background starting with my calculations at the San Diego Supercomputer Center in the 1980s. I have computed line data for 42 million lines of the iron group elements [3] plus I have all the data from the literature for all elements. I have computed line data for 16 million diatomic molecular lines (Some as much as 20 years ago.) I have tabulated opacities for more than 30 abundances, for temperatures from 2000K to 200000K using all 58 million lines at 3.5 million wavelengths from 10 nm to 10000 nm. I have computed more than 9000 models for a wide range of abundances for 3500K to 50000K effective temperature. I have computed a solar model

that matches the observed energy distribution. I have computed fluxes and colors for the models. I have distributed all of this as it was produced, to supernova modelers, to galaxy modelers, to interior modelers, to stellar atmosphere modelers, to photometrists, etc. My line data are used as input to modelling codes for atmospheres, novas, and supernovas that are completely independent of my codes. They are basic data. Only 1 per cent (i.e., 600,000) of my computed lines have accurate wavelengths between known levels because the laboratory analyses have not yet found the levels and need improvement. When published theory or laboratory f values or broadening data seem better than mine, I use the better data. This "good" line list is the input for spectrum synthesis programs. I put the programs and data on CD-ROMs and I have distributed 26 titles so far. They are now on my web site.

I have added the TiO and H_2O line lists from Schwenke and I have thrown out my old TiO linelist. That leaves me with 154 million lines with which I can compute reasonable models for M stars down to 3500K.

To compute the iron group line lists I made Slater-expansion model Hamiltonians that included as many configurations as I could fit into the Cray. I used Hartree-Fock Slater integrals (scaled) for starting guesses and for higher configurations that had no laboratory energy levels. All configuration interactions were included. I then determined the Slater integrals for the observed configurations by least squares fitting the eigenvalues computed from the Hamiltonian matrix to the observed energies. The complication was that the eigenvalues and the observed energies had to be correlated by hand each iteration and more than a hundred interations were often required for convergence. My computer programs for these procedures have evolved from Cowan's (1968) programs [4]. Transition integrals were computed with scaled-Thomas-Fermi-Dirac wavefunctions and the whole transition array was produced for each ion. Radiative, Stark, and van der Waals damping constants and Landé g values were automatically produced for each line. The first nine ions of Ca through Ni produced 42 million lines. Eigenvalues were replaced by measured energies so that lines connecting measured levels have correct wavelengths. Most of the lines have uncertain wavelengths because they connect predicted rather than measured levels.

I am now computing or recomputing all the atoms and diatomic molecules. My old Cray programs from the 1980s were limited to 1100 x 1100 arrays in the Hamiltonian for each J. With my Alpha workstation I can easily run cases with 3000 x 3000 arrays so that I can include many more configurations and many more configuration interactions. The larger arrays produce about 3 times as many lines. At present I am limited to 61 even and 61 odd configurations and I try to include everything up through n = 9. I decided to test the new program on Fe I and Fe II to see whether there was any great difference in the low configurations compared to those from the Cray program. The major result was that the electric quadrupole transitions were 10 times stronger than before because the transition integrals are weighted by r^2 —they become very large for high n, and because there are numerous configuration interactions that mix the low and high configurations. As a check I was able to reproduce Garstang's (1962) lower results [5] by running his three configurations with my program. Since my model atom is still only a subset of a

real Fe II ion, the true quadrupole A values are probably larger than mine. The magnetic dipole lines are affected by the mixing but the overall scale does not change.

EXAMPLES

Here I show sample statistics from my new semiempirical calculations for Fe II, Ni I, and Co I to illustrate how important it is to do the basic physics well and how much data there are to deal with. Ni, Co, and Fe are prominent in supernovas, including both radioactive and stable isotopes. There is not space here for the lifetime and gf comparisons. Generally, low configurations that have been well studied in the laboratory produce good lifetimes and gf values while higher configurations that are poorly observed and are strongly mixed are not well constrained in the least squares fit and necessarily produce poorer results and large scatter. My hope is that the predicted energy levels can help the laboratory spectroscopists to identify more levels and further constrain the least squares fits. From my side, I check the computed gf values in spectrum calculations by comparing to observed spectra. I adjust the gf values so that the spectra match. Then I search for patterns in the adjustments that suggest corrections in the least squares fits.

As the new calculations accumulate I will put on my web site the output files of the least-squares fits to the energy levels, energy level tables, with E, J, identification, strongest eigenvector components, lifetime, A sum, C_4, C_6, Landé g. The sums are complete up to the first (n = 10) energy level not included. There will be electric dipole, magnetic dipole, and electric quadrupole line lists. Radiative, Stark, and van der Waals damping constants and Landé g values are automatically produced for each line. Hyperfine and isotopic splitting are included when the data exist but not automatically. Eigenvalues are replaced by measured energies so that lines connecting measured levels have correct wavelengths. Most of the lines have uncertain wavelengths because they connect predicted rather than measured levels. Laboratory measurements of gf values and lifetimes will be included.

When computations with the necessary information are available from other workers, I am happy to use those data instead of repeating the work.

Fe II

Based on Johansson (1978) [6] and on more recent published and unpublished data. Johansson has data for more than 100 energy levels that I do not yet have.

d^7

$d^6 4s$	$d^5 4s^2$	$d^6 4d$	$d^5 4s4d$			$d^4 4s^2 4d$	$d^5 4p^2$	
$d^6 5s$	$d^5 4s5s$	$d^6 5d$	$d^5 4s5d$	$d^6 5g$	$d^5 4s5g$	$d^4 4s^2 5s$		
$d^6 6s$	$d^5 4s6s$	$d^6 6d$	$d^5 4s6d$	$d^6 6g$	$d^5 4s6g$			
$d^6 7s$	$d^5 4s7s$	$d^6 7d$	$d^5 4s7d$	$d^6 7g$	$d^5 4s7g$	$d^6 7i$	$d^5 4s7i$	
$d^6 8s$	$d^5 4s8s$	$d^6 8d$	$d^5 4s8d$	$d^6 8g$	$d^5 4s8g$	$d^6 8i$	$d^5 4s8i$	$d^5 4s9l$
$d^6 9s$	$d^5 4s9s$	$d^6 9d$	$d^5 4s9d$	$d^6 9g$	$d^5 4s9g$	$d^6 9i$	$d^5 4s9i$	$d^6 9l$

$$d^6 4p \quad d^5 4s4p \quad d^6 4f \quad d^5 4s4f \qquad\qquad\qquad\quad d^4 4s^2 4p \quad d^4 4s^2 4f$$
$$d^6 5p \quad d^5 4s5p \quad d^6 5f \quad d^5 4s5f \qquad\qquad\qquad\qquad\quad d^4 4s^2 5p$$
$$d^6 6p \quad d^5 4s6p \quad d^6 6f \quad d^5 4s6f \quad d^6 6h \quad d^5 4s6h$$
$$d^6 7p \quad d^5 4s7p \quad d^6 7f \quad d^5 4s7f \quad d^6 7h \quad d^5 4s7h$$
$$d^6 8p \quad d^5 4s8p \quad d^6 8f \quad d^5 4s8f \quad d^6 8h \quad d^5 4s8h \quad d^6 8k \qquad d^5 4s8k$$
$$d^6 9p \quad d^5 4s9p \quad d^6 9f \quad d^5 4s9f \quad d^6 9h \quad d^5 4s9h \quad d^6 9k \qquad d^5 4s9k$$

configurations	46 even	39 odd
levels	19771 even	19652 odd
largest J matrix	2965 even	3007 odd
known levels	403 even	492 odd
metastable levels	72 even	1 odd

[The odd metastable level $(^2I)4sp(^3P)\ ^4K_{8.5}$ is predicted at $103122 \pm 150\,\mathrm{cm}^{-1}$.]

Hamiltonian parameters	2645 even	2996 odd
free LS parameters	58 even	51 odd
standard deviation	$56\,\mathrm{cm}^{-1}$ even	$75\,\mathrm{cm}^{-1}$ odd

total E1 lines saved	7719063	old K88 [3] 1264969
between known levels	81225	old K88 45815

total M1 lines saved	1852641 even	2468074 odd
between known levels	28102 even	41374 odd
between metastable	1180 even	0 odd

total E2 lines saved	10347332 even	13179033 odd
between known levels	49019 even	71225 odd
between metastable	1704 even	0 odd

[My intuition tells me to keep all the forbidden lines, not just the ones connecting metastable levels. I do not have time to think about it now, but since the quadrupole A values get larger as n gets larger and since there are more than 10 million lines, they must somehow make our lives more complicated.]

isotopic components	^{54}Fe	^{55}Fe	^{56}Fe	^{57}Fe	^{58}Fe	^{59}Fe	^{60}Fe
fractional abundances	.059	.0	.9172	.021	.0028	.0	.0

There are 4 stable isotopes. ^{57}Fe has not yet been measured because it has hyperfine splitting. Rosberg, Litzén, and Johansson (1993) [7] have measured ^{56}Fe–^{54}Fe in 9 lines and ^{58}Fe–^{56}Fe in one line. I split the computed lines by hand.

Ni I

Ni I mostly based on Litzén, Brault, and Thorne (1993) [8] with **isotopic splitting**.

configurations	46 even	48 odd
levels	3203 even	4800 odd
largest J matrix	517 even	840 odd
known levels	130 even	153 odd
metastable levels	13 even	1 odd

[The odd metastable level is $(^3F)4sp(^3P)$ $^5G_6$ at 27260.894 cm^{-1}.]

Hamiltonian parameters	2446 even	2996 odd
free LS parameters	33 even	33 odd
standard deviation	60 cm^{-1} even	88 cm^{-1} odd

total E1 lines saved	529632	old K88 149926
between known levels	9637	

total M1 lines saved	67880 even	159049 odd
between known levels	2227 even	5272 odd
betweem metastable	41 even	0 odd

total E2 lines saved	453222 even	929692 odd
between known levels	3776 even	7539 odd
between metastable	24 even	0 odd

isotope	^{56}Ni	^{57}Ni	^{58}Ni	^{59}Ni	^{60}Ni	^{61}Ni	^{62}Ni	^{63}Ni	^{64}Ni
fraction	.0	.0	.6827	.0	.2790	.0113	.0359	.0	.0091

There are 5 stable isotopes. There are measured splittings for 326 lines from which I determined 131 energy levels relative to the ground. These levels are connected by **11670 isotopic lines**. Hyperfine splitting was included for 61Ni but only 6 levels have been measured which produce 4 lines with 38 components. A pure isotope laboratory analysis is needed.

Ni I lines are asymmetric from the splitting. When the isotopic calculation was first checked against the solar spectrum it did not look right. Subsequently, I found a program error and recomputed the splittings. Now the profiles match the observed. Observed stellar spectra are generally not high enough quality to show that there are such errors.

Co I

Co I based on Pickering and Thorne (1996) [9] and on Pickering (1996) with **hyperfine splitting** [10]. This calculation was made before my programs were

expanded. I will rerun this with twice as many configurations.

configurations	32 even	32 odd
levels	3546 even	5870 odd
largest J matrix	748 even	1130 odd
known levels	139 even	223 odd
metastable levels	31 even	1 odd

[The odd metastable level is $(^4F)4sp(^3P)$ $z^6G_{6.5}$ at 25138.806 cm^{-1}.]

Hamiltonian parameters	1446 even	1762 odd
free LS parameters	27 even	26 odd
standard deviation	129 cm^{-1} even	126 cm^{-1} odd

total E1 lines saved	1729299	old K88 546130
between known levels	15481	

total M1 lines saved	396174 even	602458 odd
between known levels	3497 even	11993 odd
betweem metastable	286 even	0 odd

total E2 lines saved	1218019 even	2468646 odd
between known levels	5094 even	15943 odd
between metastable	410 even	0 odd

isotopic components	^{56}Co	^{57}Co	^{58}Co	^{59}Co
fractional abundances	.0	.0	.0	1.00

^{59}Co is the only stable isotope. Hyperfine constants have been measured in 297 levels which produce **244264 component E1 lines**. I have not yet computed the M1 or E2 components. The new calculation greatly improves the appearance of the Co I lines in the solar spectrum.

U I

In this volume, Wyart and Hubbard describe their web site for actinides. The U I directory is a good example of what can be accomplished with hard work. There are 1426 even levels and 536 odd levels, many with Landé g and isotopic splitting U^{238}-U^{235}.

Cr IV, Mn IV-V, Fe IV-VI, Co IV-VII, Ni IV-VIII

Sugar and Corliss (1985) [11] found no laboratory energy levels for n = 5, 6, 7, 8, 9 for these ions. The laboratory sources used were not able to populate the high upper

levels to produce emission lines. However in hot stars lines to the excited levels appear in absorption shortward of Lyman α and through the Lyman continuum. For absorption it is necessary to populate only the lower level of a transition. The observed lines cannot be identified or analyzed. When I compute all these excited levels the uncertainty in the energies is too great. This is a problem that has to be solved by building new laboratory sources and by measuring the spectrum from the infrared to the extreme ultraviolet.

TiO

Schwenke calculated energy levels for TiO including in the Hamiltonian the 20 lowest vibration states of the 13 lowest electronic states of TiO (singlets a, b, c, d, f, g, h and triplets X, A, B, C, D, E) and their interactions. He determined parameters by fitting the observed energies or by computing theoretical values. Using Langhoff's transition moments [12] Schwenke generated a linelist for J = 0 to 300 for the

isotopomers	$^{46}Ti^{16}O$	$^{47}Ti^{16}O$	$^{48}Ti^{16}O$	$^{49}Ti^{16}O$	$^{50}Ti^{16}$
fractional abundances	.080	.073	.738	.055	.054 .

My version has 37744499 lines.

Good laboratory analyses and a similar semiempirical treatment are needed for CaOH, ScO, VO, YO, ZrO, LaO, etc. Better laboratory data could be used to further improve TiO.

I_2

I_2 is not an astronomical molecule but it is dear to the hearts of people who search for planets [13]. I_2 absorption cells are the standard against which radial velocities are measured. The I_2 transmission spectrum [14] is imposed on the stellar spectrum by passing the light from the star through an absorption cell maintained at a constant temperatue above 300K. By various reduction techniques the motion of the stellar spectrum relative to the I_2 spectrum is determined as a function of time. Since thousands of lines are compared, weak signals can be found. However a problem that people ignore is that the resolved spectrum of I_2 has never been observed. $^{127}I_2$ has 1/3 the doppler width of $^{16}O_2$. The resolving power required is in the millions but FTS spectra are in the range 300000 to 500000. Observers have been using FTS I_2 templates to reduce their data but the templates are so underresolved that an FTS line that has a depth of 1/3 is black in reality. A number of techniques have produced high resolution spectra of I_2 [15] that show the hyperfine structure in small wavelength intervals. We need a list of all the hyperfine energy levels. It would be absolutely fabulous if someone then would write a computer program that can generate the resolved transmission spectrum of an I_2 absorption cell for any temperature.

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A Few Things We Do Not Know About Stars and Model Atmospheres

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Abstract. We list a few things that we do not understand about stars and that most people ignore. These are all hard problems. We can learn more cosmology by working on them to reduce the systematic errors they introduce than by trying to derive cosmological results that are highly uncertain.

1. Optimism and Pessimism

People sometimes complain that I am too pessimistic and that I criticize too much. In fact I am the most optimistic person. I believe that the human race is tremendously improvable and that humans can solve any problem. But the most important step in solving a problem is to realize that the problem exists. When I identify a problem I tell, or try to tell, the people who are capable of doing something about it. I also work on correcting the problem myself, if I am capable.

A pessimist does not believe that problems can be solved so does not question the present and does not search for errors. A pessimist acts so "optimistically" about the present that a pessimist prevents progress. Why worry about basic physics when everything is fine as it is?

The papers below are on my web site kurucz.harvard.edu. Some of them are also on the ASTRO-PH preprint server at Los Alamos.

A Few Things We Do Not Know About the Sun and F Stars and G Stars. I gave part of this talk at The Workshop on Nearby Stars at Ames two years ago. They wanted to know the state of the art in computing model atmospheres and spectra to determine whether they could see small abundance effects in the nearby stars or any spectral signature of planets. (I doubt it.)

Radiatively-Driven Cosmology. Most cosmologists never took a stellar atmospheres course and do not have experience with radiation. They do not realise the power of radiative acceleration compared to gravity.

A Correction to the pp Reaction. What if the pp reaction is a three-body reaction, two protons and an electron?

Vegan Astrophysics. This is a gedanken experiment to show the importance of basic physics.

2. We do not know how to make realistic model atmospheres; we do not understand convection

Recently I have been preoccupied with convection because the model atmospheres are now good enough to show shortcomings in the convective treatment. Here I will outline what I have learned. I will mainly list the conclusions I have come to from examining individual convective models and from examining grids of convective models as a whole. Eighteen figures illustrating the points made here can be found in Kurucz (1996).

Every observation, measurement, model, and theory has seven characteristic numbers: resolution in space, in time, and in energy, and minimum and maximum energy. Many people never think about these resolutions. A low resolution physics cannot be used to study something in which the physical process of interest occurs at high resolution unless the high resolution effects average out when integrated over the resolution bandpasses.

What does the sun, or any convective atmosphere, actually look like? We do not really know yet. There is a very simplified three-dimensional radiation-hydrodynamics calculation discussed in the review by Chan, Nordlund, Steffen, and Stein (1991). It is consistent with the high spatial and temporal resolution observations shown in the review by Topka and Title (1991). Qualitatively, there is cellular convection with relatively slowly ascending, hot, broad, diverging flows that turn over and merge with their neighbors to form cold, rapidly descending, filamentary flows that diffuse at the bottom. The filling factor for the cold downward flowing elements is small. The structure changes with time. Nordlund and Dravins (1990) discuss four similar stellar models with many figures. Every one-dimensional mixing-length convective model is based on the assumption that the convective structure averages away so that the emergent radiation depends only a one-dimensional temperature distribution.

There is a solar flux atlas (Kurucz, Furenlid, Brault, and Testerman 1984) that Ingemar Furenlid caused to be produced because he wanted to work with the sun as a star for comparison to other stars. The atlas is pieced together from eight Fourier transform spectrograph scans, each of which was integrated for two hours, so the time resolution is two hours for a given scan. The x and y resolutions are the diameter of the sun. The z resolution (from the formation depths of features in the spectrum) is difficult to estimate. It depends on the signal-to-noise and the number of resolution elements. The first is greater than 3000 and the second is more than one million. It may be possible to find enough weak lines in the wings and shoulders of strong lines to

map out relative positions to a few kilometers. Today I think it is to a few tens of kilometers. The resolving power is on the order of 522,000. This is not really good enough for observations made through the atmosphere because it does not resolve the terrestrial lines that must be removed from the spectrum. (In the infrared there are many wavelength regions where the terrestrial absorption is too strong to remove.) The sun itself degrades its own flux spectrum by differential rotation and macroturbulent motions. The energy range of the atlas is from 300 to 1300 nm, essentially the range where the sun radiates most of its energy.

This solar atlas is of higher quality than any stellar spectrum taken thus far but still needs considerable improvement. If we have difficulty interpreting these data, it can only be worse for other stars where the spectra are of lower quality by orders of magnitude.

To analyze this spectrum, or any other spectrum, we need a theory that works at a similar resolution or better. We use a plane parallel, one-dimensional theoretical or empirical model atmosphere that extends in z through the region where the lines and continuum are formed. The one-dimensional model atmosphere represents the space average of the convective structure over the whole stellar disk (taking account of the center-to-limb variation) and the time average over hours. It is usually possible to compute a model that matches the observed energy distribution around the flux maximum. However, to obtain the match it is necessary to adjust a number of free parameters: effective temperature, surface gravity, microturbulent velocity, and the mixing-length-to-scale-height-ratio in the one-dimensional convective treatment. The microturbulent velocity parameter also produces an adjustment to the line opacity to make up for missing lines. Since much of the spectrum is produced near the flux maximum, at depths in the atmosphere where the overall flux is produced, averaging should give good results. The parameters of the fitted model may not be those of the star, but the radiation field should be like that of the star. The sun is the only star where the effective temperature and gravity are accurately known. In computing the detailed spectrum, it is possible to adjust the line parameters to match many features, although not the centers of the strongest lines. These are affected by the chromosphere and by NLTE. Since very few lines have atomic data known accurately enough to constrain the model, a match does not necessarily mean that the model is correct.

From plots of the convective flux and velocity for grids of models I have identified three types of convection in stellar atmospheres:

• normal strong convection where the convection is continuous from the atmosphere down into the underlying envelope. Convection carries

more than 90% of the flux. Stars with effective temperatures 6000K and cooler are convective in this way as are stars on the main sequence up to 8000K. At higher temperature the convection carries less of the total flux and eventually disappears starting with the lowest gravity models. Intermediate gravities have intermediate behavior. Abundances have to be uniform through the atmosphere into the envelope. The highly convective models seem to be reasonable representations of real stars, except for the shortcomings cited below.

• atmospheric layer convection where, as convection weakens, the convection zone withdraws completely up from the envelope into the atmosphere. There is zero convection at the bottom of the atmosphere. Abundances in the atmosphere are decoupled from abundances in the envelope. For mixing-length models the convection zone is limited at the top by the Schwarzschild criterion to the vicinity of optical depth 1 or 2. The convection zone is squashed into a thin layer. In a grid, this layer continues to carry significant convective flux for about 500K in effective temperature beyond the strongly convective models. There is no common-sense way in which to have convective motions in a thin layer in an atmosphere. The solution is that the Schwarzschild criterion does not apply to convective atmospheres. The derivatives are defined only in one dimensional models. A real convective element has to decide what to do on the basis of local three-dimensional derivatives, not on means. These thin-layer-convective model atmospheres may not be very realistic.

• plume convection. Once the convective flux drops to the percent range, cellular convection is no longer viable. Either the star becomes completely radiative, or it becomes radiative with convective plumes that cover only a small fraction of the surface in space and time. Warm convective material rises and radiates. The star has rubeola. The plumes dissipate and the whole atmosphere relaxes downward. There are no downward flows. The convective model atmospheres are not very realistic except when the convection is so small as to have negligible effect, i.e. the model is radiative. The best approach may be simply to define a star with less than, say, 1% convection as radiative. The error will probably be less than using mixing-length model atmospheres.

Using a one-dimensional model atmosphere to represent a real convective atmosphere for any property that does not average in space and time to the one-dimensional model predictions produces systematic errors. The Planck function, the Boltzmann factor, and the Saha equation are functions that do not average between hot and cold convective elements. We can automatically conclude that one-dimensional convective models must predict the wrong value for any parameter that has strong exponential temperature dependence from these functions.

Starting with the Planck function, ultraviolet photospheric flux in any convective star must be higher than predicted by a one-dimensional model (Bikmaev 1994). Then, by flux conservation, the flux redward of the flux maximum must be lower. It is fit by a model with lower effective temperature than that of the star. The following qualitative predictions result from the exponential falloff of the flux blueward of the flux maximum:

- the Balmer continuum in all convective stars is higher than predicted by a one-dimensional model;
- in G stars, including the sun, the discrepancy reaches up to about 400nm;
- all ultraviolet photoionization rates at photospheric depths are higher in real stars than computed from one-dimensional models;
- flux from a temperature minimum and a chromospheric temperature rise masks the increased photospheric flux in the ultraviolet;
- the spectrum predicted from a one-dimensional model for the exponential falloff region, and abundances derived therefrom, are systematically in error;
- limb-darkening predicted from a one-dimensional model for the exponential falloff region is systematically in error;
- convective stars produce slightly less infrared flux than do one-dimensional models.

The Boltzmann factor is extremely temperature sensitive for highly excited levels:

- the strong Boltzmann temperature dependence of the second level of hydrogen implies that the Balmer line wings are preferentially formed in the hotter convective elements. A one-dimensional model that matches Balmer line wings has a higher effective temperature than the real star;
- the same is true for all infrared hydrogen lines.

The Saha equation is safe only for the dominant species:

- neutral atoms for an element that is mostly ionized are the most dangerous because (in LTE) they are much more abundant in the cool convective elements. When Fe is mostly ionized the metallicity determination from Fe I can be systematically offset and can result in a systematic error in the assumed evolutionary track and age.
- in the sun convection may account for the remaining uncertainties with Fe I found by Blackwell, Lynas-Gray, and Smith (1995);
- the most striking case is the large systematic error in Li abundance determination in extreme Population II G subdwarfs. The abundance is determined from the Li I D lines which are formed at depths in the highly convective atmosphere where Li is 99.94% ionized (Kurucz 1995b);

• molecules with high dissociation energies such as CO are also much
more abundant in the cool convective elements. The CO fundamental
line cores in the solar infrared are deeper than any one-dimensional
model predicts (Ayres and Testerman 1981) because the cooler convec-
tive elements that exist only a short time have more CO than the mean
model.

Given all these difficulties, how should we proceed? One-dimensional
model atmospheres can never reproduce real convective atmospheres.
The only practical procedure is to compute grids of model atmospheres,
then to compute diagnostics for temperature, gravity, abundances, etc.,
and then to make tables of corrections. Say, for example, in using the
Hα wings as a diagnostic of effective temperature in G stars, the models
may predict effective temperatures that are 100K too high. So if one
uses an Hα temperature scale it has to be corrected by 100K to give
the true answer. Every temperature scale by any method has to be
corrected in some way. Unfortunately, not only is this tedious, but it is
very difficult or impossible because no standards exist. We do not know
the energy distribution or the photospheric spectrum of a single star,
even the sun. We do not know what spectrum corresponds to a given
effective temperature, gravity, or abundances. The uncertainties in so-
lar abundances are greater than 10%, except for hydrogen, and solar
abundances are the best known. It is crucial to obtain high resolution,
high signal-to-noise observations of the bright stars.

3. We do not consider the variation in microturbulent velocity

Microturbulent velocity in the photosphere is just the convective mo-
tions. At the bottom of the atmosphere it is approximately the maxi-
mum convective velocity. At the temperature minimum it is zero or
near zero because the convecting material does not rise that high.
There is also microturbulent velocity in the chromosphere increasing
outward from the temperature minimum that is produced by waves
or other heating mechanisms. In the sun the empirically determined
microturbulent velocity is about 0.5 km/s at the temperature mini-
mum and about 1.8 km/s in the deepest layers we can see. In a solar
model the maximum convective velocity is 2.3 km/s. The maximum
convective velocity is about 0.25 km/s in an M dwarf and increases
up the main sequence. The convective velocity increases greatly as the
gravity decreases. I suggest that a good way to treat the behavior of
microturbulent velocity in the models is to scale the solar empirical

distribution as a function of Rosseland optical depth to the maximum convective velocity for each effective temperature and gravity.

Why does this matter? Microturbulent velocity increases line width and opacity and produces effects on an atmosphere like those from changing abundances. At present, models, fluxes, colors, spectra, etc are computed with constant microturbulent velocity within a model and from model to model. This introduces systematic errors within a model between high and low depths of formation, and between models with different effective temperatures, and between models with different gravity. Microturbulent velocity varies along an evolutionary track. If microturbulent velocity is produced by convection, microturbulent velocity is zero when there is no convection, and diffusion is possible.

By now I should have computed a model grid with varying microturbulent velocity but I am behind as usual.

4. We do not understand spectroscopy; we do not have good spectra of the sun or any star

Very few of the features called "lines" in a spectrum are single lines. Most features consist of blends of many lines from different atoms and molecules. All atomic lines except those of thorium have hyperfine or isotopic components, or both, and are asymmetric (Kurucz 1993). Low resolution, low-signal-to-noise spectra do not contain enough information in themselves to allow interpretation. Spectra cannot be properly interpreted without signal-to-noise and resolution high enough to give us all the information the star is broadcasting about itself. And then we need laboratory data and theoretical calculations as complete as possible. Once we understand high quality spectra we can look at other stars with lower resolution and signal-to-noise and have a chance to make sense of them.

5. We do not have energy distributions for the sun or any star

I get requests from people who want to know the solar irradiance spectrum, the spectrum above the atmosphere, that illuminates all solar system bodies. They want to interpret their space telescope observations or work on atmospheric chemistry, or whatever. I say, "Sorry, it has never been observed. NASA and ESA are not interested. I can give you my model predictions but you cannot trust them in detail, only in, say, one wavenumber bins." The situation is pathetic.

I am reducing Brault's FTS solar flux and intensity spectra taken at Kitt Peak for .3 to 5 μm. I am trying to compute the telluric spectrum and ratio it out to determine the flux above the atmosphere but that will not work for regions of very strong absorption. Once that is done the residual flux spectra can be normalized to low resolution calibrations to determine the irradiance spectrum. The missing pieces will have to be filled in by computation. Spectra available in the ultraviolet are much lower resolution, much lower signal-to-noise, and are central intensity or limb intensity, not flux. The details of the available solar atlases can be found in two review papers, Kurucz (1991; 1995a).

6. We do not know how to determine abundances; we do not know the abundances of the sun or any star

One of the curiosities of astronomy is the quantity [Fe]. It is the logarithmic abundance of Fe in a galaxy, cluster, star, whatever, relative to the solar abundance of Fe. What makes it peculiar is that we do not yet know the solar abundance of Fe and our guesses change every year. The abundance has varied by a factor of ten since I was a student. Therefore [Fe] is meaningless unless the solar Fe abundance is also given so that [Fe] can be corrected to the current value of Fe.

For an example I use Grevesse and Sauval's (1999) solar Fe abundance determination. I am critical, but, regardless of my criticism, I still use their abundances. There are scores of other abundance analysis papers, including some bearing my name, that I could criticize the same way.

Grevesse and Sauval included 65 Fe I "lines" ranging in strength from 1.4 to 91.0 mÅ and 13 Fe II "lines" ranging from 15.0 to 87.0 mÅ. They found an abundance log Fe/H + 12 = 7.50 ± 0.05.

Another curiosity of astronomy is that Grevesse and Sauval have decided a priori that the solar Fe abundance must equal the meteoritic abundance of 7.50 and that a determination is good if it produces that answer. If the solar abundance is not meteoritic, how could they ever determine it?

There are many "problems" in the analysis. First, almost all the errors are systematic, not statistical. Having many lines in no way decreases the error. In fact, the use of a wide range of lines of varying strengths increases the systematic errors. Ideally a single weak line is all that is required to get an accurate abundance. Weak lines are relatively insensitive to the damping treatment, to microturbulent velocity, and to the model structure. The error is reduced simply by throwing out all lines greater than 30 mÅ. That reduces the number of Fe I lines

from 65 to 25 and of Fe II lines from 13 to 5. As we discussed above, the microturbulent velocity varies with depth but Grevesse and Sauval assume that it is constant. This problem is minimized if all the lines are weak.

As we discussed above "lines" do not exist. The lines for which equivalent widths are given are all parts of blended features. As a minimum we have to look at the spectrum of each feature and determine how much of the feature in the "line" under investigation and how much is blending. Rigorously one should do spectrum synthesis of the whole feature. We have solar central intensity spectra and spectrum synthesis programs. For the sun we have the advantage of intensity spectra without rotational broadening. In the flux spectrum of the sun and of other stars there is more blending. The signal-to-noise of the spectra is several thousand and the continuum level can be determined to on the order of 0.1 per cent so the errors from the spectrum are small. With higher signal-to-noise more detail would be visible and the blending would be better understood. Most of the features cannot be computed well with the current line data. None of the features can be computed well without adjusting the line data. Even if the line data were perfect, the wavelengths would still have to be adjusted because of wavelength shifts from convective motions.

Fe has 4 isotopes. The isotopic splitting has not been determined for the lines in the abundance analysis. For weak lines it does not affect the total equivalent width but it does affect the perception of blends.

It is possible to have undetectable blends. There are many Fe I lines with the same wavelengths, including some in this analysis, and many lines of other elements. We hope that these blends are very weak. The systematic error always makes the observed line stronger than it is in reality so they produce an abundance overestimate.

There are systematic errors and random errors in the gf values. With a small number of weak lines on the linear part of the curve of growth it is easy to correct the abundances when the gf values are improved in the future.

We are left with 3 relatively safe lines of Fe I and 1 relatively safe line of Fe II. These have the least uncertainty in determining the blending by my estimation. Grevesse and Sauval found abundances of 7.455, 7.453, and 7.470 for the Fe I lines and 7.457 for the Fe II line. Thus from the same data the Fe abundances is 7.46 instead of 7.50.

7. We do not have good atomic and molecular data; one half the lines in the solar spectrum are not identified

It is imperative that laboratory spectrum analyses be improved and extended, and that NASA and ESA pay for it. Some of the analyses currently in use date from the 1930s and produce line positions uncertain by 0.01 or 0.02 Å. New analyses with FTS spectra produce many more energy levels and one or two orders of magnitude better wavelengths. One analysis can affect thousands of features in a stellar spectrum. Also the new data are of such high quality that for some lines the hyperfine or isotopic splitting can be directly measured. Using Pickering (1996) and Pickering and Thorne (1996) I am now able to compute Co I hyperfine transitions and to reproduce the flag patterns and peculiar shapes of Co features in the solar spectrum. Using Litzen, Brault, and Thorne (1993) I am now able to compute the five isotopic transitions for Ni I and to reproduce the Ni features in the solar spectrum. These new analyses also serve as the basis for new semiempirical calculations than can predict the gf values and the lines that have not yet been observed in the lab but that matter in stars. I have begun to compute new line lists for all the elements and I will make them available on my web site, kurucz.harvard.edu.

8. Cepheids have convective pulsation but the models do not; we do not have high quality spectra over phase for any Cepheid

Cepheids are convective with velocities the same order of magnitude as the pulsation velocities. The sum of the velocities is supersonic and the difference is order zero. It is completely unphysical to try to compute the convection and the pulsation independently. Convective pulsation is a 3-dimensional radiation-hydrodynamics problem that must be solved as a whole.

If a hot Cepheid has a radiative phase, it becomes convective as it cools. The transition phase has space-time-random outward plumes that become supersonic. The surface is covered with spikes or bumps that cool by radiating toward the side.

All of this physics is displayed in the spectra of nearby Cepheids that are bright enough to be observed at 1 km/s resolution and S/N 3000. It would be perfectly feasible to make an atlas of such high resolution spectra every hour through the phases and then to read out the story, and also to use it to estimate boundary conditions for convective pulsation calculations.

9. We do not understand abundance evolution in early type stars

This is a simplified, qualitative outline. Since there is no convection the atmosphere and upper layers mix very slowly. The bulk of the material of the star has approximately scaled solar abundances, [Fe] $\geq$ 0. When the star is formed the material in the atmosphere is the last to be accreted. It consists of dregs of the infall material that has been depleted of elements that are able to condense into grains. A young star has low metal abundances in the atmosphere and so appears to have [Fe] $<<$ 0. As the star ages heavy elements with many lines are levitated into the atmosphere by radiative acceleration. Some elements, such as He, settle inward from gravity. The abundances become closer to solar, [Fe] $\leq$ 0. The star grows older and the abundances continue to increase in the atmosphere so that the star becomes a metallic line star with [Fe] $>$ 0. If the star has strong magnetic spots, the abundances can be selectively enhanced by many orders of magnitude in the spots. The star is called "peculiar". A radiative wind selectively reduces abundances in the atmosphere because radiative acceleration affects some elements more than others. The only safe way to investigate early type stars is to obtain high quality spectra and spectrophotometry and to compute models and spectra for each star individually. Colors integrate away too many details. Astroseismology may be able to show abundance variation with depth.

From an evolutionary point of view, all main sequence early-type stars in our galaxy have slightly over solar abundances.

10. Many early type stars are oblate fast rotators

Early-type stars that are not in binaries are generally fast rotators. They are oblate because of the reduced gravity at the equator. The temperature can be several thousand degrees hotter at the poles than at the equator. Plane-parallel models like mine can be found that represent some average behavior but rigorously one must compute three dimensional rotating models. The real star has more ultraviolet flux from the poles and more infrared flux from the equator than the plane-parallel models so the ionizing radiation field around an early-type star is prolate. It is probably not safe to use any unary early-type star as a photometric standard for calibrating theoretical photometry.

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