

Problems with Atomic and Molecular Data: Including All the Lines

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Abstract The line data available on my web site for computing opacities, model atmospheres, and spectra were computed or collected from the literature more than 25 years ago. I am recomputing the existing line lists including many more configurations and energy levels and producing many more lines. I am collecting more recent data from the literature, and I am extending the calculation to heavier elements and higher stages of ionization. I will produce more than 10 times as many lines which will significantly increase the opacity in the models and produce improved fits to observed spectra. All the new data are available on my website kurucz.harvard.edu.

1 Introduction

In 1965 I started collecting and computing atomic and molecular line data for computing opacities in model atmospheres and then for synthesizing spectra. I wanted to determine stellar effective temperatures, gravities, and abundances. I still want to.

I started using Cowan's (1968) atomic structure programs and managed to get them to work on a CDC 6400 computer instead of a supercomputer. I also computed linelists for diatomic molecules.

For 23 years I put in more and more lines but I could never get a solar model to look right, to reproduce the observed energy distribution.

In 1985 Sugar and Corliss at the National Bureau of Standards (NBS, now NIST) published a compilation of energy levels for the iron group elements. They gave me the tape that they used to typeset the book. I was able to decode it. I then applied for time at the San Diego Supercomputer Center.

By 1988 I finally produced enough lines, I thought. I completed a calculation of the first 9 ions of the iron group elements shown in Table 1 (Kurucz 1988). There

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were data for 42 million lines that I combined with data for 1 million lines from my earlier list for lighter and heavier elements including all the data from the literature. In addition I had computed linelists for diatomic molecules including 15 million lines of H₂, CH, NH, OH, MgH, SiH, C₂, CN, CO, SiO, and TiO for a total of 58 million lines.

Table 1 Iron group lines computed at San Diego Supercomputer Center 1988

	I	II	III	IV	V	VI	VII	VIII	IX
Ca	48573	4227	11740	113121	330004	217929	125560	30156	22803
Sc	191253	49811	1578	16985	130563	456400	227121	136916	30587
Ti	867399	264867	23742	5079	37610	155919	356808	230705	139356
V	1156790	925330	284003	61630	8427	39525	160652	443343	231753
Cr	434773	1304043	990951	366851	73222	10886	39668	164228	454312
Mn	327741	878996	1589314	1033926	450293	79068	14024	39770	147442
Fe	789176	1264969	1604934	1776984	1008385	475750	90250	14561	39346
Co	546130	1048188	2198940	1569347	2032402	1089039	562192	88976	15185
Ni	149926	404556	1309729	1918070	1971819	2211919	967466	602486	79627

I then tabulated 2 nm resolution opacity distribution functions (ODFs) from the line list for temperatures from 2000 to 200000K and for a range of pressure suitable for stellar atmospheres (Kurucz 1992a).

Using the ODFs I computed a theoretical solar model (Kurucz 1992b) with the solar effective temperature and gravity, the current solar abundances from Anders and Grevesse (1989), mixing-length-to-scale-height ratio $\ell/H = 1.25$, and constant microturbulent velocity 1.5 km s^{-1} . It generally matched the observed energy distribution from Neckel and Labs (1984).

I computed thousands of model atmospheres that I distributed on magnetic tapes, then on CDs, and now on my web site, kurucz.harvard.edu. They made observers happy and they made galaxy modellers happy and they made me happy. However, agreement with low resolution observations of integrated properties does not imply correctness.

2 Problems

In 1988 the abundances were wrong, the microturbulent velocity was wrong, the convection was wrong, and the opacities were wrong.

Since 1965 the Fe abundance has varied by over a factor of 10. In 1988 the Fe abundance was 1.66 times larger than today. There was mixing length convection with an exaggerated, constant microturbulent velocity. In the grids of models, the default microturbulent velocity was 2 km s^{-1} . My 1D models still have mixing-length convection, but now with a depth-dependent microturbulent velocity that scales with the convective velocity. 3D models with cellular convection do not have microturbulent velocity at all, but use the doppler shifts from the convective motions.

In 1988 the line opacity was underestimated because not enough lines were included in the linelists. Table 2 is an outline for the Fe II line calculation then. The higher energy levels that produce series of lines that merge into ultraviolet continua were not included. Those levels also produce huge numbers of weaker lines in the visible and infrared that blend and fill in the spaces between the stronger lines. Also lines of heavier elements were not systematically included. And then the additional broadening from hyperfine and isotopic splitting was not included. (In the following tables CI stands for configuration interaction and “good lines” are lines between measured levels.)

Table 2 Fe II in 1988. Based on Johansson (1978) and Sugar and Corliss (1985).

Even: 22 configurations; 5723 levels; 354 known levels; 729 Hamiltonian parameters, all CI; 46 free LS parameters; standard deviation 142 cm^{-1}

d^7

$d^6 4s \ d^5 4s^2 \ d^6 4d \ d^5 4s 4d \ d^4 4s^2 4d \ d^5 4p^2$
 $d^6 5s \ d^5 4s 5s \ d^6 5d \ d^5 4s 5d \ d^6 5g$
 $d^6 6s \ d^5 4s 6s \ d^6 6d \ d^5 4s 6d \ d^6 6g$
 $d^6 7s \ d^6 7d \ d^6 7g$
 $d^6 8s \ d^6 8d$
 $d^6 9s$

Odd: 16 configurations; 5198 levels; 435 known levels; 541 Hamiltonian parameters, all CI; 43 free LS parameters; standard deviation 135 cm^{-1}

$d^6 4p \ d^5 4s 4p \ d^6 4f \ d^5 4s 4f \ d^4 4s^2 4p$
 $d^6 5p \ d^5 4s 5p \ d^6 5f$
 $d^6 6p \ d^5 4s 6p \ d^6 6f$
 $d^6 7p \ d^5 4s 7p$
 $d^6 8p \ d^5 4s 8p$
 $d^6 9p$

Total E1 lines saved 1254969
 E1 lines with good wavelengths 45815

In 1988 the opacities were low but were balanced by high abundances that made the lines stronger and high microturbulent velocity that made the lines broader. Now the abundances, the convection, and the opacities are still wrong, but they have improved. I am concentrating on filling out the line lists.

3 Examples of new calculations

Here I show sample statistics from my new semiempirical calculations for Fe II, Ni I, and Co I in Tables 3 to 5 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 supernovae, 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 (E1), magnetic dipole (M1), and electric quadrupole (E2) line lists. Radiative, Stark, and van der Waals damping constants and Landé g values are automatically produced for each line. Branching fractions are also computed. Hyperfine and isotopic splitting will be 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. Measured or estimated widths of autoionizing levels will be included when available. The partition function will be tabulated for a range of densities.

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

Once the linelist for an ion or molecule is validated it will be incorporated into the wavelength sorted linelists on my website for computing opacities or detailed spectra. The web directories are kurucz.harvard.edu/atoms and [/molecules](http://kurucz.harvard.edu/molecules) for the details, and [/linelists](http://kurucz.harvard.edu/linelists) for the completed linelists.

Table 6 presents line statistics from some of my recent calculations that show an order of magnitude increase over my earlier work because I am treating about 3 times as many levels. Considering only the ions in the table, there are about 257 million lines compared to 26 million in the 1988 calculation. Table 7 shows my estimate (individual ions only to astronomical accuracy) that my linelists will have several billion atomic and molecular lines if I can continue my work. I expect to update and replace all my previous calculations for lighter elements and for the iron group in the near future. Then I will concentrate on extending the work to heavier elements and higher ions.

Table 3 Fe II based on Nave and Johansson (2013) and on Castelli and Kurucz (2010). ^{57}Fe has not yet been measured because it has hyperfine splitting. Rosberg, Litzén, and Johansson (1993) have measured ^{56}Fe – ^{54}Fe in 9 lines and ^{58}Fe – ^{56}Fe in one line. I split the computed lines by hand.

Even: 46 configurations; 19771 levels; 466 known levels; 2645 Hamiltonian parameters, all CI; 57 free LS parameters; standard deviation 48 cm^{-1}

d^7

$d^6 4s \ d^5 4s^2 \ d^6 4d \ d^5 4s 4d \ d^4 4s^2 4d \ d^5 4p^2$
 $d^6 5s \ d^5 4s 5s \ d^6 5d \ d^5 4s 5d \ d^6 5g \ d^5 4s 5g \ d^4 4s^2 5s$
 $d^6 6s \ d^5 4s 6s \ d^6 6d \ d^5 4s 6d \ d^6 6g \ d^5 4s 6g$
 $d^6 7s \ d^5 4s 7s \ d^6 7d \ d^5 4s 7d \ d^6 7g \ d^5 4s 7g \ d^6 7i \ d^5 4s 7i$
 $d^6 8s \ d^5 4s 8s \ d^6 8d \ d^5 4s 8d \ d^6 8g \ d^5 4s 8g \ d^6 8i \ d^5 4s 8i \ d^5 4s 9i$
 $d^6 9s \ d^5 4s 9s \ d^6 9d \ d^5 4s 9d \ d^6 9g \ d^5 4s 9g \ d^6 9i \ d^5 4s 9i \ d^6 9i$

Odd: 39 configurations; 19652 levels; 643 known levels; 2996 Hamiltonian parameters, all CI; 47 free LS parameters; standard deviation 63 cm^{-1}

$d^6 4p \ d^5 4s 4p \ d^6 4f \ d^5 4s 4f \ d^4 4s^2 4p \ d^4 4s^2 4f$
 $d^6 5p \ d^5 4s 5p \ d^6 5f \ d^5 4s 5f \ d^4 4s^2 5p$
 $d^6 6p \ d^5 4s 6p \ d^6 6f \ d^5 4s 6f \ d^6 6h \ d^5 4s 6h$
 $d^6 7p \ d^5 4s 7p \ d^6 7f \ d^5 4s 7f \ d^6 7h \ d^5 4s 7h$
 $d^6 8p \ d^5 4s 8p \ d^6 8f \ d^5 4s 8f \ d^6 8h \ d^5 4s 8h \ d^6 8k \ d^5 4s 8k$
 $d^6 9p \ d^5 4s 9p \ d^6 9f \ d^5 4s 9f \ d^6 9h \ d^5 4s 9h \ d^6 9k \ d^5 4s 9k$

Total E1 lines saved 7834681 new 1254969 old ratio = 6.1
 E1 lines with good wavelengths 124920 new 45815 old ratio = 2.3

Forbidden lines	M1 even	M1 odd	E2 even	E2 odd
Total lines saved	2702418	3651124	10856977	13551054
with good wavelengths	46846	80161	72075	131362
between metastable	1250	0	1853	0

Isotope	^{54}Fe	^{55}Fe	^{56}Fe	^{57}Fe	^{58}Fe	^{59}Fe	^{60}Fe
Fraction	.059	.0	.9172	.021	.0028	.0	.0

Table 4 Ni I based on Litzén, Brault, and Thorne (1993) with **isotopic splitting**. There are measured isotopic 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 ^{61}Ni 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 and they now agree in shape with lines in the solar spectrum.

Total E1 lines saved 732160 new 149926 old ratio = 4.9
 E1 lines with good wavelengths 9663 new 3949 old ratio = 2.4

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

Table 5 Co I based on Pickering and Thorne (1996) and on Pickering (1996) with **hyperfine splitting**. Hyperfine constants have been measured in 297 levels which produce **244264 component E1 lines**. The new calculation greatly improves the appearance of the Co I lines in the solar spectrum.

Total E1 lines saved 3771908 new 546130 old ratio = 6.9
 E1 lines with good wavelengths 15441 new 9879 old ratio = 2.4

Isotope ^{56}Co ^{57}Co ^{58}Co ^{59}Co ^{60}Co
 Fraction .0 1. .0 .0 .0

Table 6 Sample recent atomic calculations. This is one page worth. The current list including lighter and heavier elements is in kurucz.harvard.edu/atoms/completed.

	config.		levels		----- E1 lines -----		
	even	odd	even	odd	good	wl	total
Sc I	61	61	2014	2318	15546	737992	191253
Sc II	61	61	509	644	3436	116491	49811
Sc III	39	38	134	147	1313	5271	1578
Ti I	61	61	6628	7350	33815	4758992	867399
Ti II	61	61	2096	2318	8188	835027	264867
Ti III	73	68	3636	3845	4090	499739	23742
V I	61	61	13767	15952	23342	7043556	1156790
V II	61	61	6740	7422	18389	3932853	925330
V III	61	61	2094	2318	9892	966528	284003
Cr I	47	40	18842	18660	35315	2582957	434773
Cr II	61	61	13767	15890	58996	6970052	1304043
Cr III	61	61	6580	7526	23150	5535931	990951
Mn I	44	39	18343	19652	16798	1481464	327741
Mn II	50	41	19686	19870	31437	4523390	878996
Mn III	61	61	13706	15890	17294	10525088	1589314
Fe I	61	50	18655	18850	93508	6029023	789176
Fe II	46	39	19771	19652	124654	7834553	1264969
Fe III	49	41	19720	19820	37199	9548787	1604934
Fe IV	61	54	13767	14211	8408	14617228	1776984
Fe V	61	61	6560	7526	11417	7785320	1008385
Fe VI	73	73	2094	2496	3534	9072714	475750
Fe VII	85	86	7132	7032	2326	2816992	90250
Fe VIII	52	52	1365	1244	233	220166	14561
Co I	61	61	10920	13085	15441	3771900	546130
Co II	61	50	18655	19364	23355	10050728	1361114
Co III	44	39	18343	19652	9356	11515139	2198940
Ni I	61	61	4303	5758	9663	732160	149925
Ni II	61	61	10270	11429	55590	3645991	404556
Ni III	61	50	18655	19364	21251	11120833	1309729
Ni IV	44	39	18343	19517	5659	15152636	1918070
Ni V	46	41	10637	19238	10637	15622452	1971819
Ni VI	61	61	13706	15792	12219	17971672	2211919
Ni VII	73	73	24756	19567	3502	28328012	967466
Ni VIII	73	73	12714	8903	758	12308126	602486
Ni IX	85	86	7132	7032	253	2671345	79627
Ni X	52	52	1365	1208	235	285029	
Cu I	61	61	920	1260	5720	28112	
Cu II	61	61	4303	5758	14959	622985	
Cu III	61	61	10270	11429	17539	5258607	

Table 7 Estimated lines in 3d and 4d group sequences (in millions)

	I	II	III	IV	V	VI	VII	VIII	IX	X	...
Ca	.05										
Sc	.7	.05									
Ti	5	.7	.05								
V	14	5	.7	.05							
Cr	10	14	5	.7	.05						
Mn	1.5	10	14	5	.7	.05					
Fe	6	7	10	14	5	.7	.05				
Co	4	10	7	10	14	5	.7	.05			
Ni	.7	4	10	7	10	14	5	.7	.05		
Cu	.03	.6	4	10	7	10	14	5	.7	.05	
Zn	.1	.03	.6	4	10	7	10	14	5	.7	...
Ga		.1	.03	.6	4	10	7	10	14	5	...
Ge			.1	.03	.6	4	10	7	10	14	...
As				.1	.03	.6	4	10	7	10	...
Se					.1	.03	.6	4	10	7	...
Br						.1	.03	.6	4	10	...
Kr							.1	.03	.6	4	...
Rb								.1	.03	.6	...
Sr	.05								.1	.03	...
Y	.7	.05								.1	...
Zr	5	.7	.05								...
Nb	14	5	.7	.05							...
Mo	10	14	5	.7	.05						...
[Tc]	1.5	10	14	5	.7	.05					...
Ru	6	7	10	14	5	.7	.05				...
Rh	4	10	7	10	14	5	.7	.05			...
Pd	.7	4	10	7	10	14	5	.7	.05		...
Ag	.03	.6	4	10	7	10	14	5	.7	.05	...
Cd	.1	.03	.6	4	10	7	10	14	5	.7	...
In		.1	.03	.6	4	10	7	10	14	5	...
Sn			.1	.03	.6	4	10	7	10	14	...
Sb				.1	.03	.6	4	10	7	10	...
Te					.1	.03	.6	4	10	7	...
I						.1	.03	.6	4	10	...
Xe							.1	.03	.6	4	...
Cs								.1	.03	.6	...
Ba									.1	.03	...

Total 3d > 500 million

Total 4d > 500 million

+ lanthanide sequences > 1000 million

+ all the other element sequences

4 Molecules, TiO and H₂O

These are examples of incorporating data from other researchers.

Schwenke (1998) 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 (1997) transition moments he generated a linelist for $J = 0$ to 300 for the isotopologues $^{46}\text{Ti}^{16}\text{O}$, $^{47}\text{Ti}^{16}\text{O}$, $^{48}\text{Ti}^{16}\text{O}$, $^{49}\text{Ti}^{16}\text{O}$, and $^{50}\text{Ti}^{16}\text{O}$ with fractional abundances .080, .073, .738, .055, and .054. My version has 37,744,499 lines.

Good analyses and a similar semiempirical treatment are needed for CaOH, ScO, VO, YO, ZrO, LaO, etc. I am adding linelists for VO, CaH, CrH, and FeH to extend my opacities through the M stars.

Partridge and Schwenke (1997) treated H₂O semiempirically. They included isotopologues H₂¹⁶O, H₂¹⁷O, H₂¹⁸O, and HD¹⁶O. My version has 65,912,356 lines.

Barber, Tennyson, Harris, and Tolchenov (2006) have massively treated H₂¹⁶O. My version of their linelist has 335,767,086 lines. I left out the very weak lines and added in the Partridge and Schwenke isotopologues. Linelists for many molecules are available or referenced on their website www.exomol.com that I do not hesitate to appropriate.

5 Spectrum Analysis Using Stellar Atlases as the Laboratory Source

Chemically peculiar or CP stars are early type stars with large over- and underabundances. They can have very small projected rotation velocities, hence narrow lines. HR6000 has $T_{\text{eff}} = 13450\text{K}$, $\log g = 4.3$, and projected rotation velocity about 1.5 km s^{-1} from Castelli and Hubrig (2007). The abundances (log relative to solar) are Fe [+0.9], Xe [+4.6], P [$>+1.5$], Ti [+0.55], Cr [+0.2], Mn [+1.5], Y [+1.2], Hg [+2.7], and He, C, N, O, Al, Mg, Si, S, Cl, Sc, V, Co, Ni, and Sr underabundant. With initial guidance from Johansson, Castelli analyzed the Fe II lines and has determined 126 new 4d, 5d, 6d, and 4f energy levels (Castelli, Johansson, and Hubrig 2008; Castelli, Kurucz, and Hubrig 2009; Castelli and Kurucz 2010). These levels produce more than 18000 lines throughout the spectrum from ultraviolet to infrared. Fig. 1 shows the improvement between Fe II computed with the 2008 Kurucz linelist and the current linelist. Fig. 2 shows the improvement in the spectrum including all the lines. Note that many lines are still missing and remain to be identified.

In stars these Fe lines are seen in absorption and the Boltzmann factor for the lower level determines the line strength. Laboratory sources in emission have to populate the upper level. These lines appear in more “normal” stars as well but are smeared out and blended by rotation velocities 10 to 100 times higher.

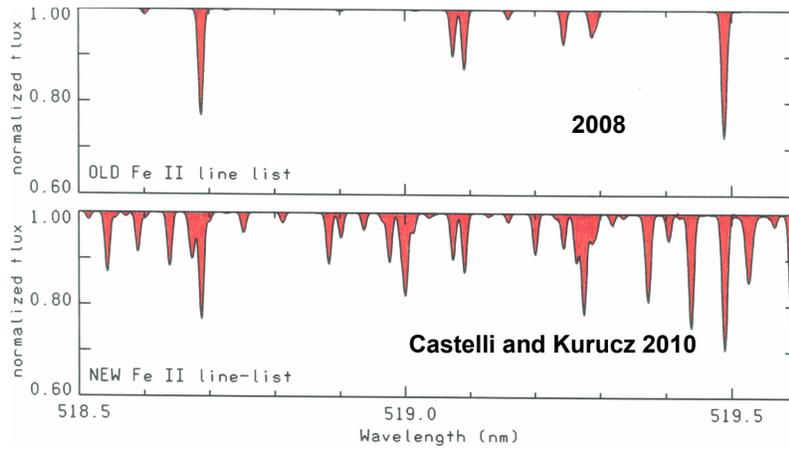


Fig. 1 The upper panel shows the Fe II spectrum computed for HR6000 ($T_{\text{eff}}=13450\text{K}$, $\log g=4.3$, $v_{\text{t}}=1.5\text{ km s}^{-1}$, $\text{Fe}=[+0.9]$) using Kurucz data as of 2008. The lower panel is the same calculation using the current Kurucz Fe II line list.

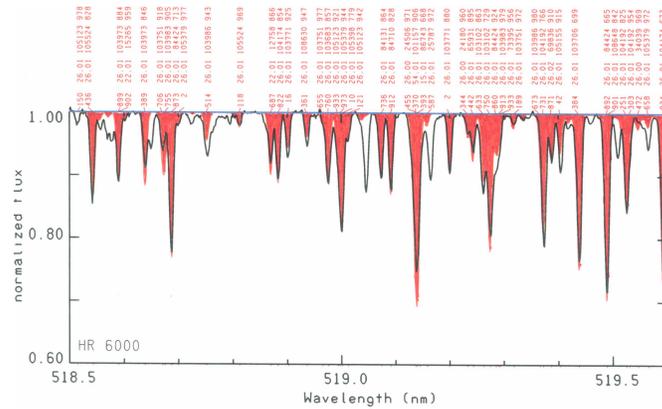


Fig. 2 The synthetic spectrum (in red) computed with a line list including the new Fe II lines compared to the observed spectrum of HR6000 (in black). Note that many lines are missing and remain to be identified. The line identifications can be decoded as follows: for the first line, 150 = last 3 digits of the wavelength 518.5150; 26 = atomic number of Fe; .01 = charge/100, i.e. 26.01 identifies the line as Fe II; 105123 is the energy of the lower level in cm^{-1} ; 970 is the residual central intensity in per mil.

Considerable telescope time should be allocated to making high-resolution, high-signal-to-noise atlases in the UV, visible, and IR of selected CP stars. These would be used as tools for extending laboratory spectrum analyses to higher energy levels for as many elements as possible.

Of course, high quality solar atlases have been used to extend laboratory analyses for as long as they have existed (cf. Geller 1992; Colin and Bernath 2010).

6 Conclusion

Inclusion of heavier elements, higher stages of ionization, additional molecules, and higher energy levels will increase the opacity in stellar atmosphere, pulsation, stellar interior, asteroseismology, nova, supernova, and other radiation hydrodynamics calculations. Detailed and more complete linelists will allow more accurate interpretation of features in spectra and the more accurate determination of stellar properties at any level from elementary 1D approximations to the most sophisticated 3D time-dependent treatments.

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