Stellar synthetic spectroscopy in the VO era

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Astronomical Spectroscopy and Virtual Observatory Workshop, ESAC 23/03-2007

Why synthetic spectra in VO ?

Synthetic spectra naturally provide absolute flux (or normalisation to continuum!) and can be computed for whatever stellar parameters (even rare or unobserved types...)!

- population synthesis
- preparation of instruments (GAIA, ...)
- predictions for extractions from surveys (eg. color-color diagrams)
- analysis of observed spectra (extraction of T_{eff}, logg, [Fe/H], etc)

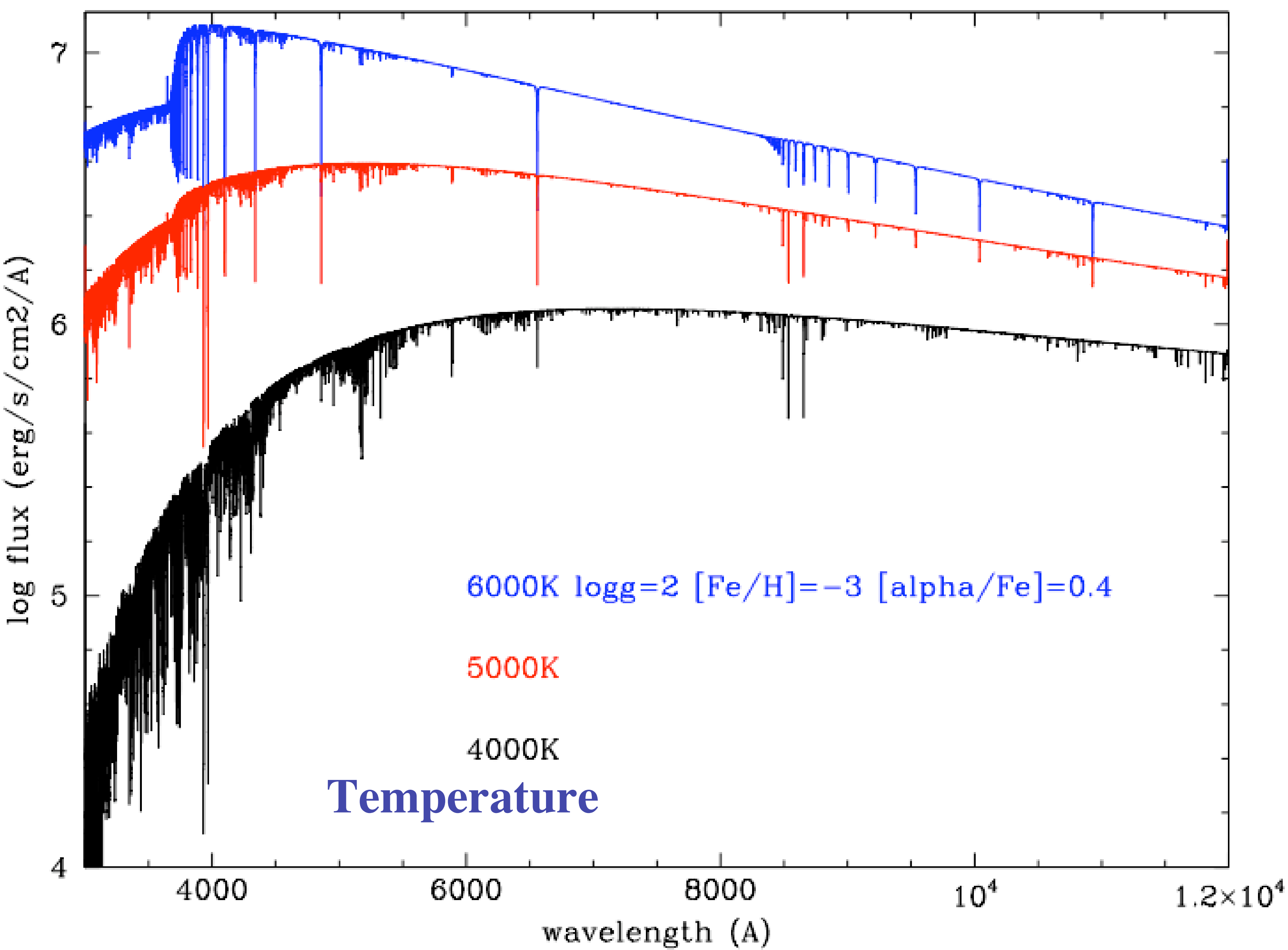
What kind of synthetic spectra?

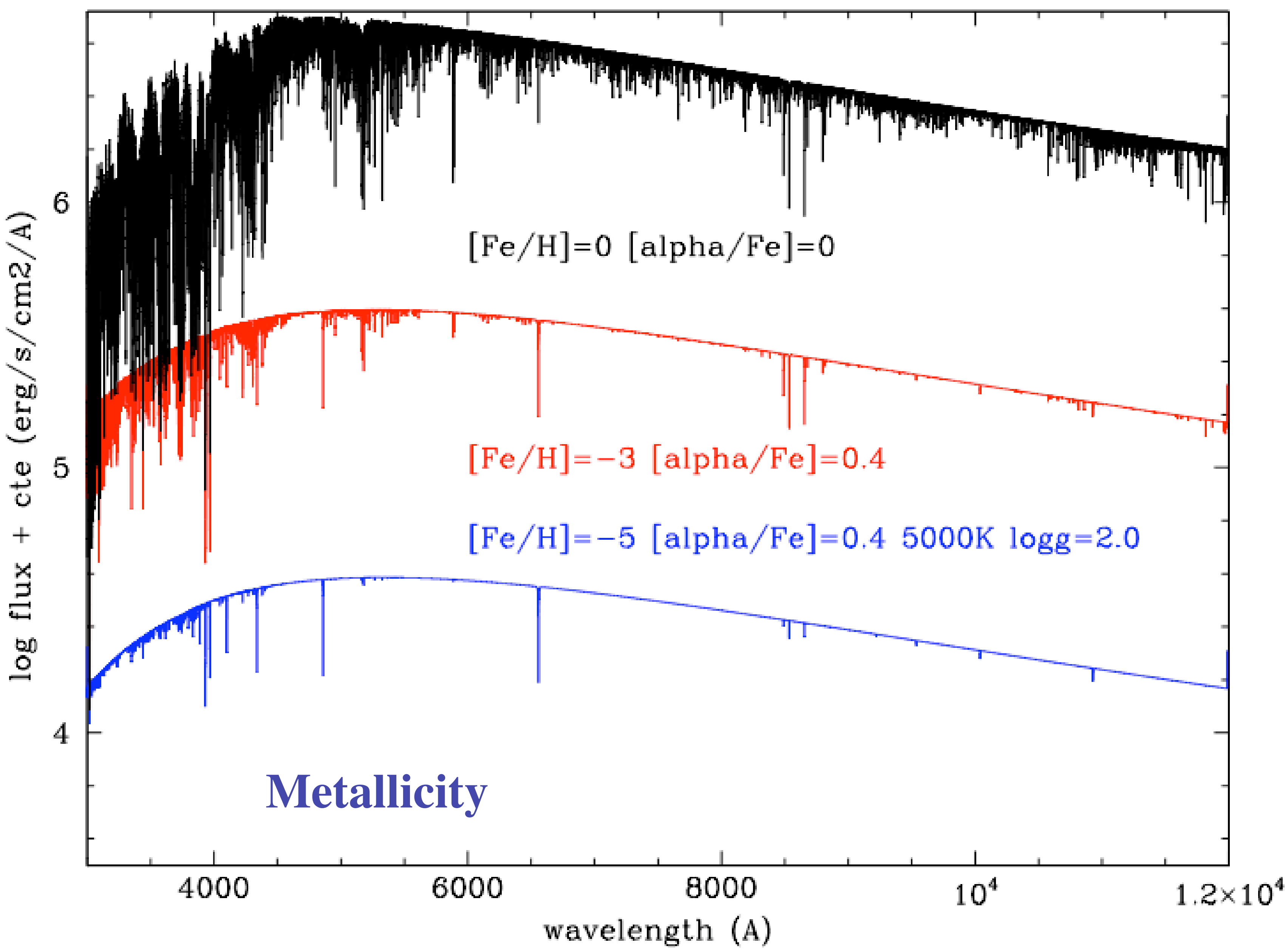
- low resolution, full spectral coverage: pop. synth.
  (... or high resolution, small coverage, e.g. in H band)
- high res. small coverage (e.g. GAIA CaII triplet)
- high res. long coverage (e.g. UVES, ...)
- in all cases: variation of many parameters: T_{eff}, logg, [Fe/H], alpha/Fe, CNO, $^{12}C/^{13}C$, ... etc

=> MANY spectra!!!

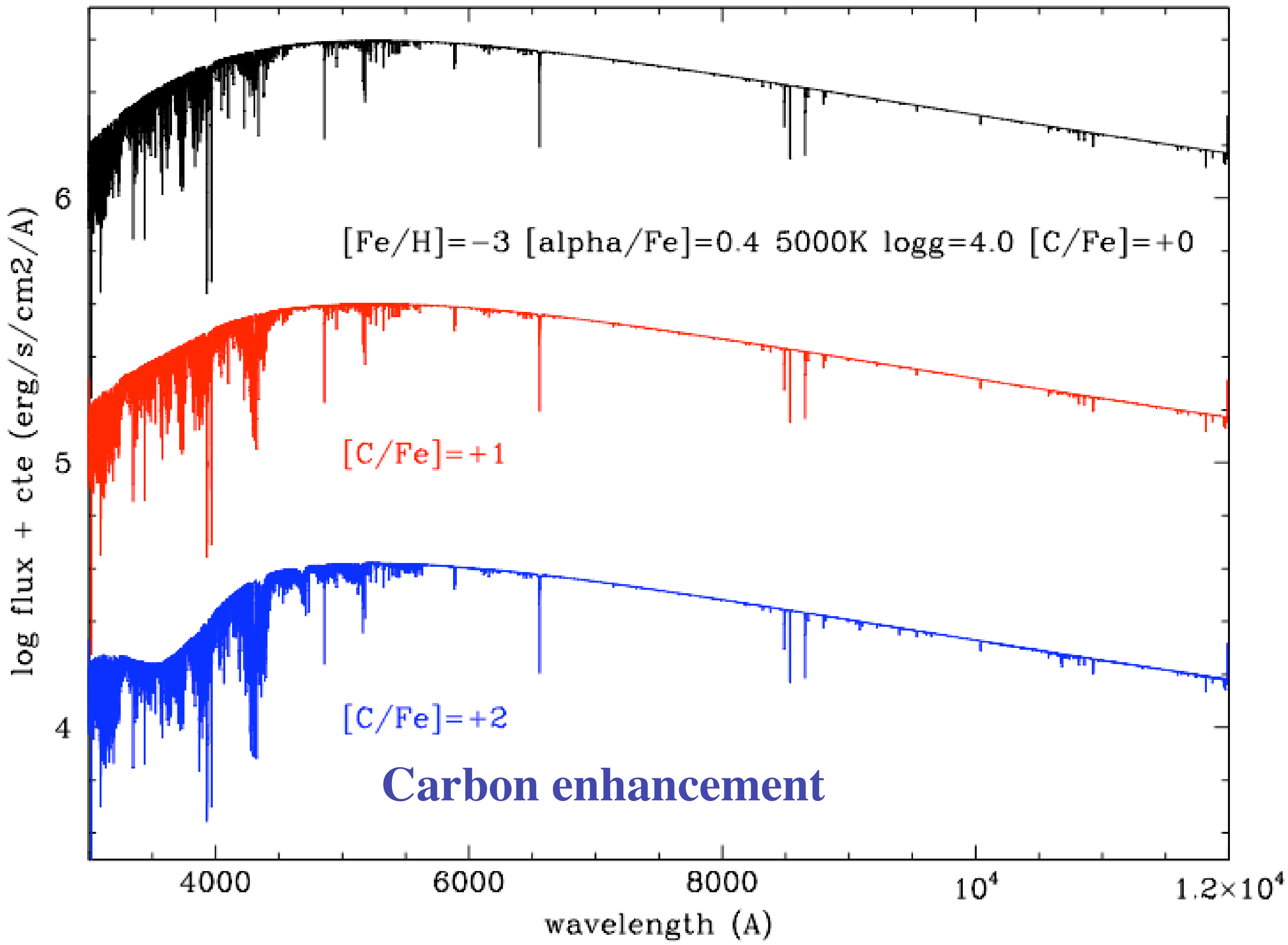
What can be done with synthetic spectra: four illustrations

- Check variation of spectrum with stellar parameters T_{eff}, Fe/H, C/Fe (here on rare CEMP stars, for SDSS-SEGUE calibration)
- interesting remarks on continuum vs. line variations (difficult to notice on continuum-normalized observed spectra)
- predictions of Balmer lines equivalent widths
- dereddening and parameters of red supergiant stars


6000K logg=2 [Fe/H]=−3 [alpha/Fe]=0.4
5000K
4000K
Temperature
log flux (erg/s/cm2/A)
wavelength (A)
7
6
5
4
4000
6000
8000
10^4
1.2×10^4

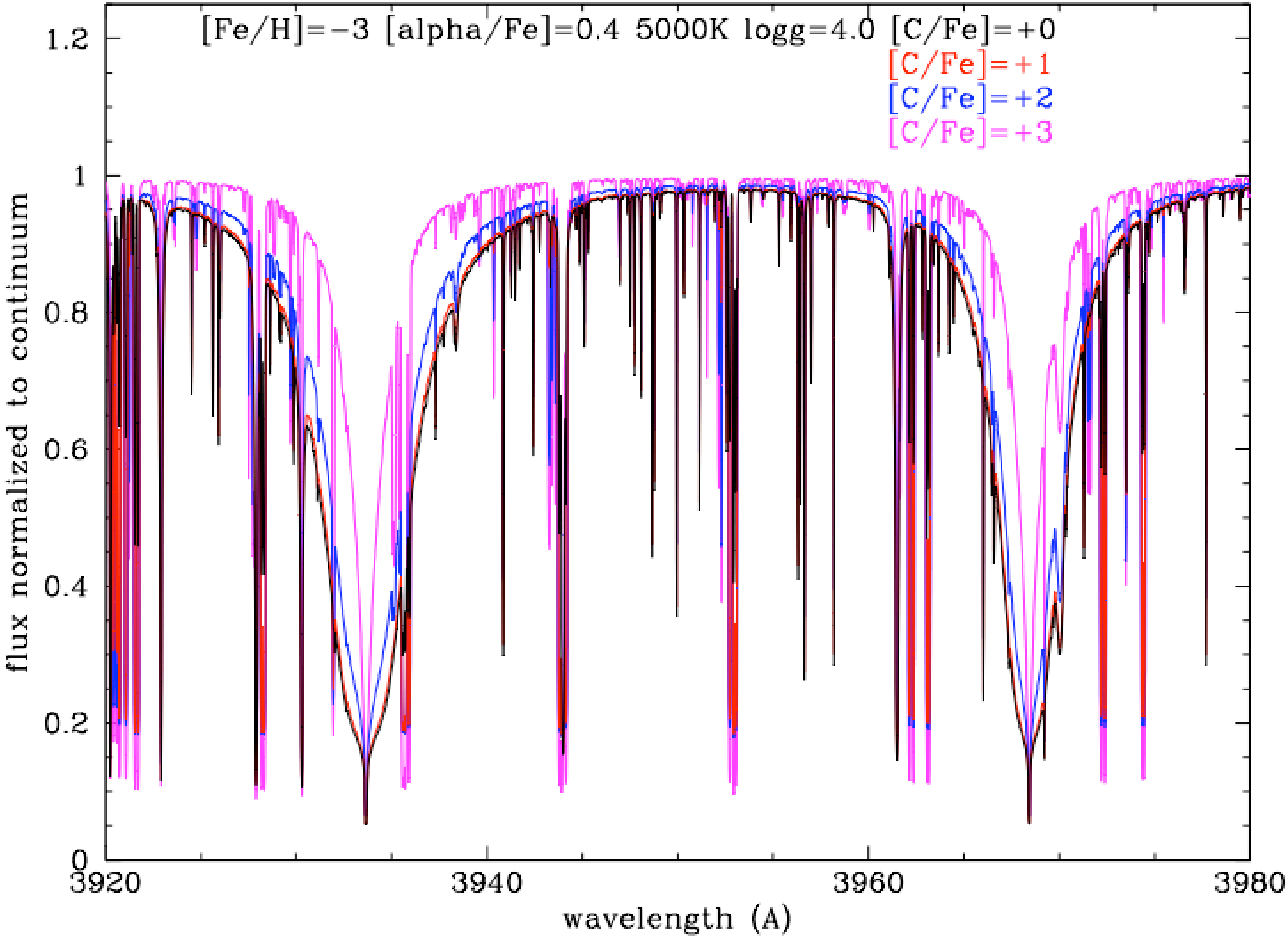


[Fe/H]=0 [alpha/Fe]=0
[Fe/H]=−3 [alpha/Fe]=0.4
[Fe/H]=−5 [alpha/Fe]=0.4 5000K logg=2.0
Metallicity
log flux + cte (erg/s/cm2/A)
wavelength (A)
4000
6000
8000
10⁴
1.2×10⁴
4
5
6

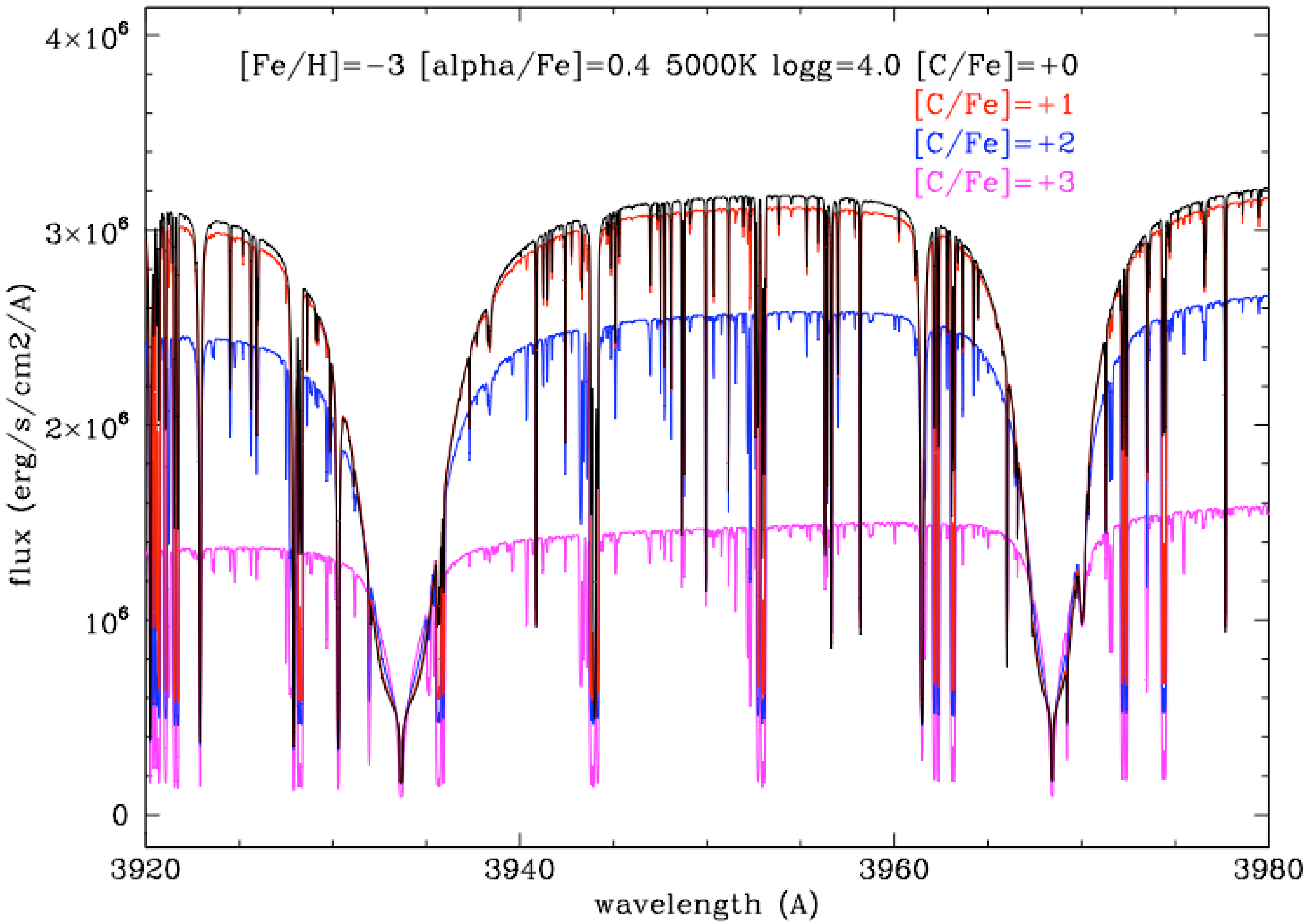


[Fe/H]=−3 [alpha/Fe]=0.4 5000K logg=4.0 [C/Fe]=+0
[C/Fe]=+1
[C/Fe]=+2
Carbon enhancement
log flux + cte (erg/s/cm2/A)
wavelength (A)
4
5
6
4000
6000
8000
10^4
1.2×10^4

Effect of carbon enhancement on Ca II H&K



Effect of carbon enhancement on Ca II H&K



Theoretical equivalent widths of Balmer lines as a function of T_{eff}

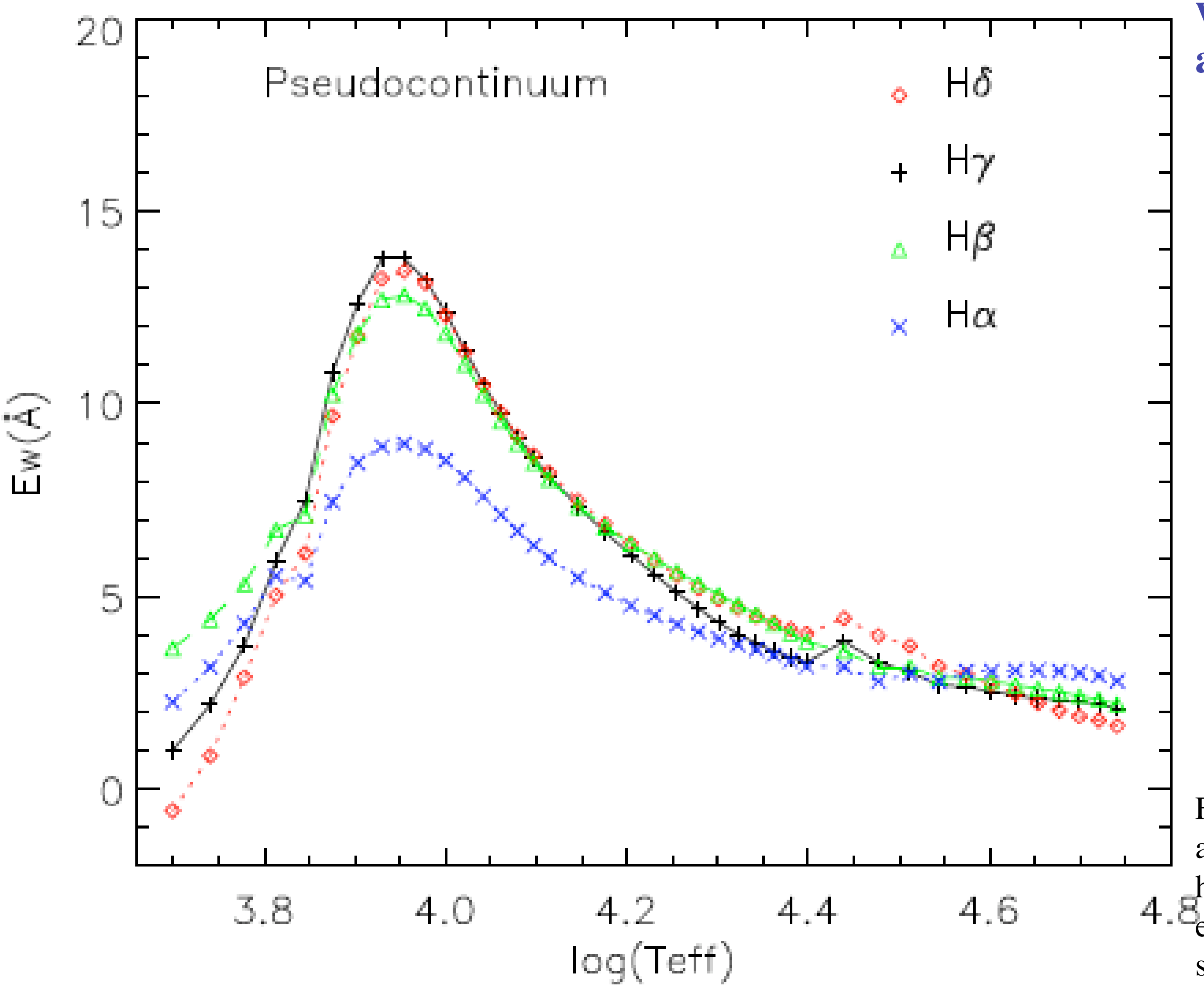
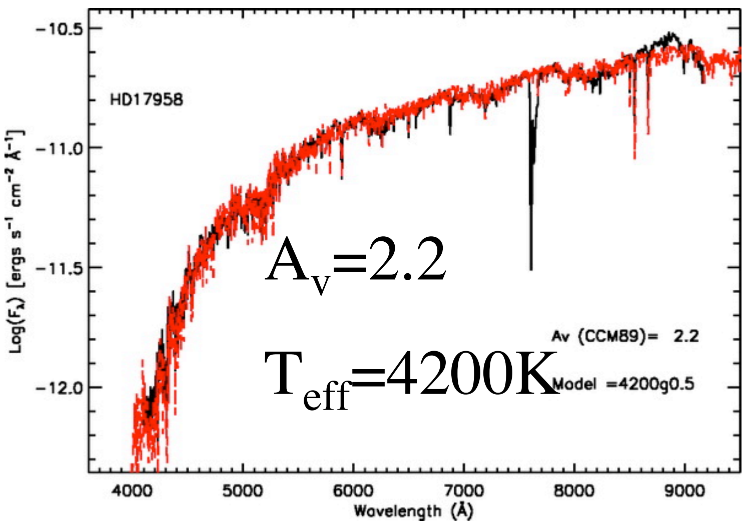
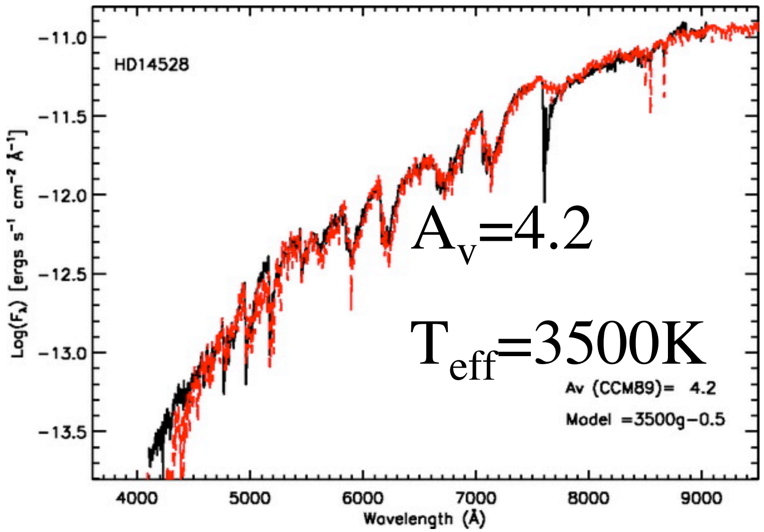
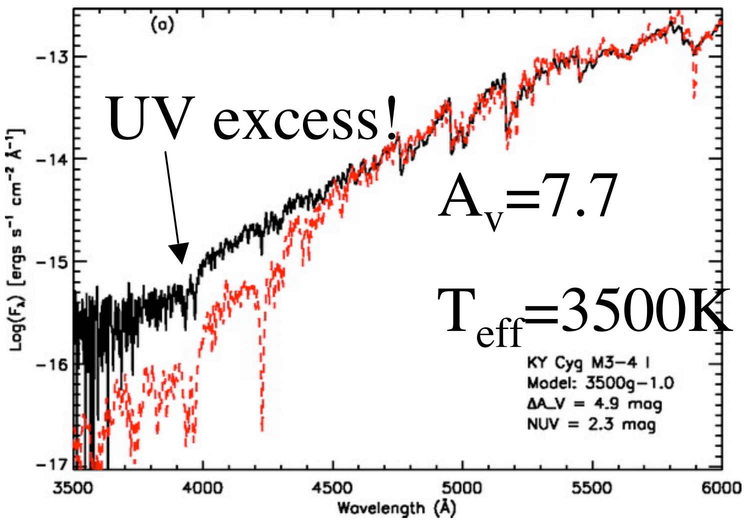


Figure adapted from Martins et al. 2005, MNRAS, 538, 49, a high resolution stellar library for evolutionary population synthesis

Red supergiants: getting the right reddening, and a diagnostic on circumstellar dust from simultaneous fitting of SED and reddening







Correlation UV excess & mass-loss -> extra extinction from large grains?

Levesque et al. 2005, ApJ 628, 973

What are ~~the~~ some challenges?

- Analyse huge amounts of spectra: GAIA, SDSS-SEGUE*, RAVE, multifibre spectrographs, ELT, ... (10^6-10^9 spectra).
- Synthesize stellar populations at high redshifts, in various wavelengths regions.

=>For that, we need huge grids of synthetic spectra, and fast, reliable, and accurate algorithms to do the job automatically.

* Sloan Extension for Galactic Understanding and Exploration

Approaches

- use large spectral libraries from VO to compare to observations with VO tools

or

- compute specific spectra for each observation
  - at home with own software and computer, using input data and other tools from VO

  or

  - with codes running on a server inside VO

Libraries of synthetic spectra

- SEDs are available for ATLAS, MARCS and PHOENIX models
- detailed high-resolution spectra only available for subsets. Too many to cite them all (see page below)
- there are more and more libraries on the web. See the rich page of David Montes Gutiérrez: http://www.ucm.es/info/Astrof/invest/actividad/spectra.html
- problem: include them in VO?

From the page by David Montes Gutiérrez

Synthetic spectra
Kurucz stellar atmosphere models

- Robert L. Kurucz home page (Harvard-Smithsonian CfA)
- Kurucz 1993 stellar atmosphere models -- models
- Kurucz Atomic Linelist data from Kurucz CD-ROM 23
- **New grids of ATLAS9 atmospheres**
- I: Influence of convection treatments on model structure and on observable quantities (Heiter, et al., 2002, A&A, 392, 619)
- II: Limb-darkening coefficients for the Str^mgren photometric system for A-F stars (Barban, et al., 2003, A&A, 405, 1095)
- New Grids of ATLAS9 Model Atmospheres (F. Castelli, R.L. Kurucz, 2004, IAU Symp. No 210)
- Grids of ATLAS9-ODFNEW models and fluxes
- **ATLAS12**
- ATLAS, WIDTH and SYNTHE GNU Linux port by L. Sbordone, P. Bonifacio and F. Castelli
- ATLAS 12 and Related codes Workshop (11-15 July 2005, Trieste, Italy)
- Source Codes for Linux
- **Kurucz ODFNEW /NOVER models**

- available throughout the Theoretical Models Web Server of the SVO (Spanish Virtual Observatory)

A grid of synthetic spectra for the determination of effective temperature, gravity and metallicity of F, G, and K stars.

- I - Description of the method. Cayrel R., Perrin M.-N., Barbury B., Buser R., 1991, A&A 247, 108
- II - Application to 41 stellar spectra taken in the Basel field of SA 141 Cayrel R. et al., 1991, A&A 247, 122

The calibration of MK spectral classes using spectral synthesis. 1: The effective temperature calibration of dwarf stars Gray R.O., Corbally C.J., 1994, AJ 107, 742

BaSeL (Basel Stellar Library) - An extensive and uniform grid of theoretical stellar energy distributions

- **A standard stellar library for evolutionary synthesis**.
- I. Calibration of theoretical spectra, (Lejeune Th., Cuisinier F., and Buser R.) (1997, A&AS 125, 229)
- II. The M dwarf extension., (Lejeune Th., Cuisinier F., and Buser R.) (1998, A&AS 130, 65)
- III. Metallicity calibration., (Westera P., Lejeune Th., Buser R., Cuisinier F., Bruzual G.A.) (2002, A&A 381, 524)
- Libraries of Stellar Spectra and Synthetic Photometry (Roland Buser, Pieter Westera, Erich Wenger)
- BLoIS 1.0 - The Basel Library of Integrated Spectra (Erich Wenger, Roland Buser, Pieter Westera)

An Atlas of high resolution synthetic spectra in the wavelength region 4850-5400≈.
(Chavez M., Malagnini M.L., Morossi C., 1997, A&AS 126, 267)
Synthetic spectra of H Balmer and HeI absorption lines. I: Stellar library
(R.M. Gonzalez Delgado, C. Leitherer,1999, ApJS 125, 479)
Synthetic Spectra of B Main-Sequence Stars from 3000 - 10000≈ (Gummersbach & Kauferi, Landessternwarte Heidelberg-K^nigstuhl)
SPECTRUM A Stellar Spectral Synthesis Program (R.O. Gray)

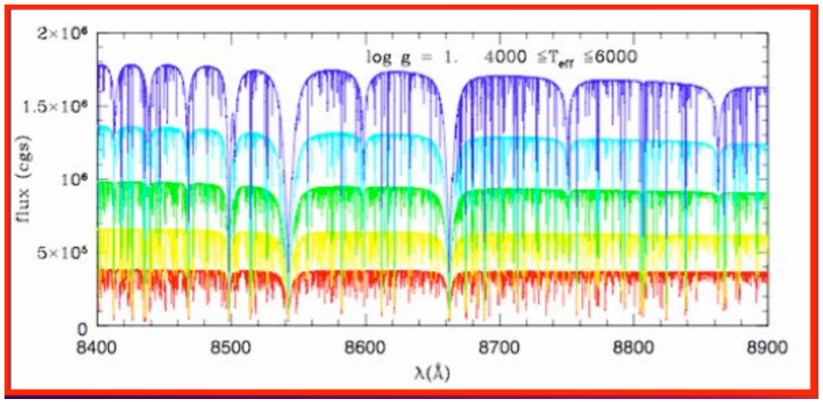
The physical basis of luminosity classification in the late A-, F-, and early G-type stars.

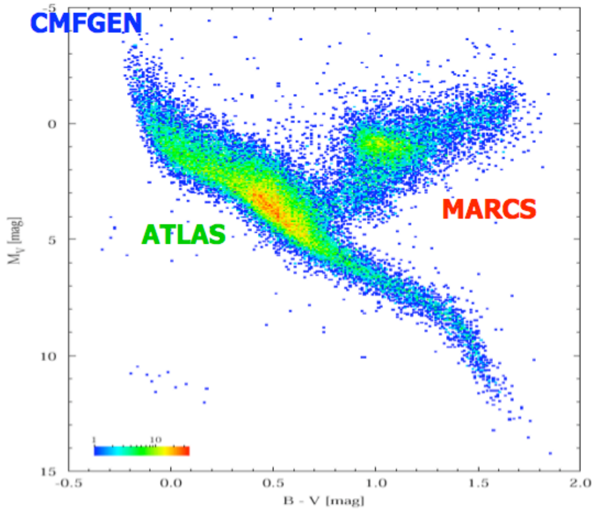
- I. Precise spectral types for 372 stars (R.O. Gray, et al., 2001, AJ 121, 2148)
- II. Basic parameters of program stars and the role of microturbulence (R.O. Gray, et al., 2001, AJ 121, 2159)

Spectral classification of stars using synthetic model atmospheres (Bertone E., Buzzoni A., 2001, 1st COROT-MONS Ground-Support Observations Workshop)
A critical appraisal of ATLAS9 and NextGen 5 model atmospheres
(Bertone E., et al. 2001,"New Quests in Stellar Astrophysics: The link between Stars and Cosmology")
ATLAS vs. NextGen model atmospheres: a combined analysis of synthetic spectral energy distributions
(Bertone E., et al.,2004, AJ, 128, 829)
Simulated quantitative stellar classification at different spectral resolutions (V. Malyuto, R. Lazauskaite and T. Shvelidze, 2001, New Astronomy, Vol. 6 (6) pp. 381)
Kurucz model energy distributions: a comparison with real stars. II. Metal-deficient stars (V. Straizys, R. Lazauskaite, G. Valiauga, 2002, Baltic Astronomy journal vol.11, in press)
A grid of synthetic spectra and indices Fe5270, Fe5335, Mgb and Mg2 as a function of stellar parameters and [a/Fe] (Barbuy et al., 2003, A&A 404, 661)
An extensive library of synthetic spectra covering the far red, RAVE and GAIA wavelength ranges (Zwitter T., Castelli F., Munari U., 2004, A&A, 417, 1055)
A library of high resolution Kurucz spectra in the wavelength range 3000–10000 A (Murphy T., Meiksin A., 2004, MNRAS, 351, 1430)
A High-Resolution Stellar Library for Evolutionary Population Synthesis (Martins, et al., 2005, MNRAS, 358, 49)
An extensive library of 2500-10500 ≈ synthetic spectra (Munari, et al., 2005, A&A, 442, 1127)
A Phoenix Modelatmosphere Grid For GAIA (Brott & Hauschildt, 2005, Proc. of "The Three Dimensional Universe With Gaia")
UVBLUE: a new high-resolution theoretical library of ultraviolet stellar spectra (Rodriguez-Merino et al., 2005, ApJ 626, 411)
A library of high resolution synthetic stellar spectra from 300nm to 1.8 micron with solar and alpha-enhanced composition
(P. Coelho, B. Barbuy, J. Melendez, R. Schiavon, B. Castilho, 2005, A&A 443, 735)
- available throughout the Theoretical Models Web Server of the SVO (Spanish Virtual Observatory)

The POLLUX database

- Database of high resolution theoretical spectra and SEDs (and later observed high-res. spectra)
- See poster by A. Palacios et al.
- 300-1200nm, R=150000
- Will be integrated in VO from start or almost...
- cover HR diagram (from O to M-S-C stars, all metallicities)
- 3 model brands: MARCS, ATLAS, CMFGEN with overlap and coherence check
- regular update
- opening soon



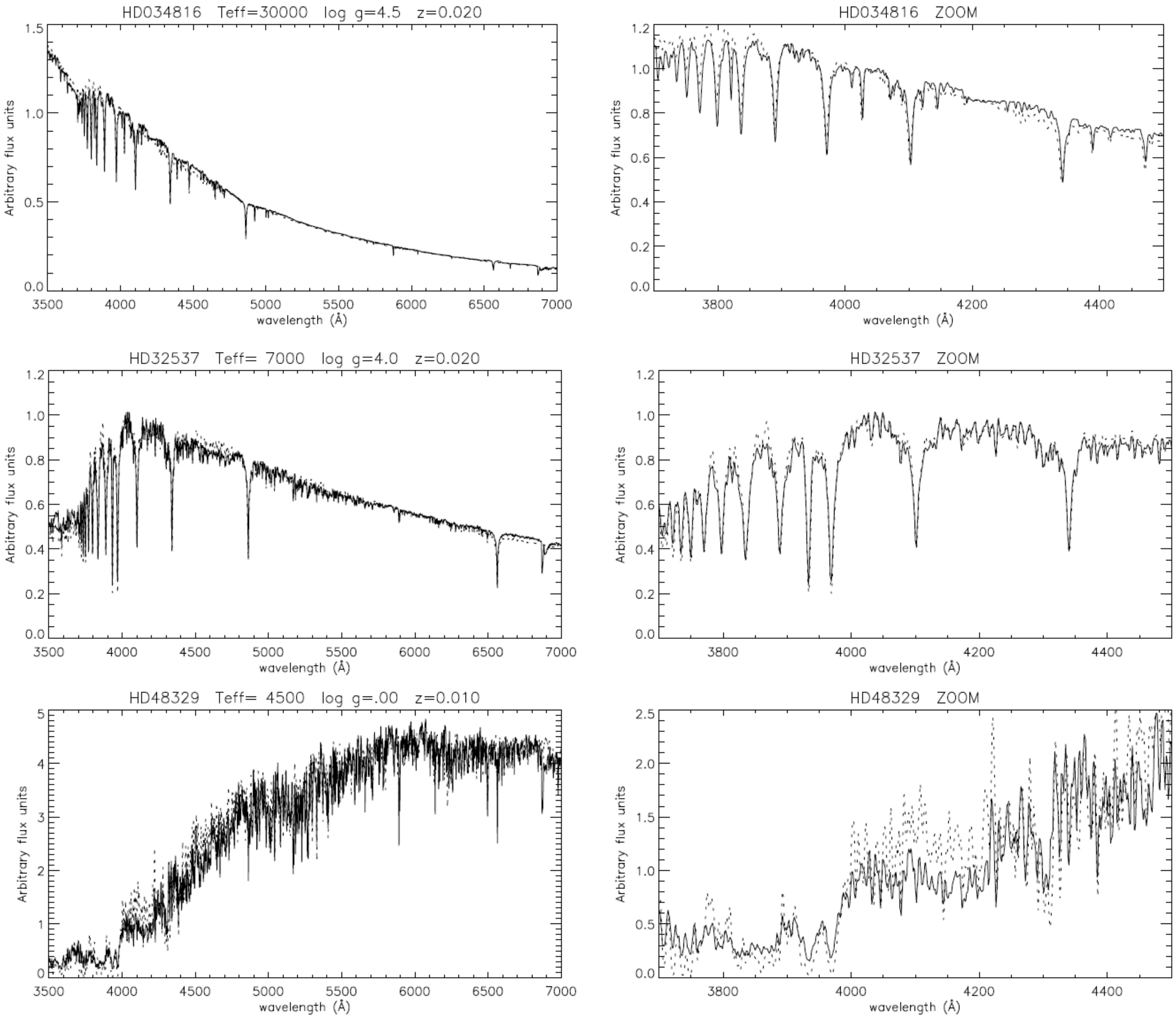


Benefits of providing grids

- large public grids of spectra are a good way of getting models tested (because they get used!)
- users must remember that they may be flawed, because of
  - inappropriate physics (e.g. LTE O-B star models, 1D static models for convective 3D atmospheres, ...)
  - inaccurate input data (e.g. line positions and strengths)
  - missing data (e.g. cool stars without TiO)
- It may be hard to tell if differences between observed and synthetic spectra are due to models or to observations...

One WARNING!

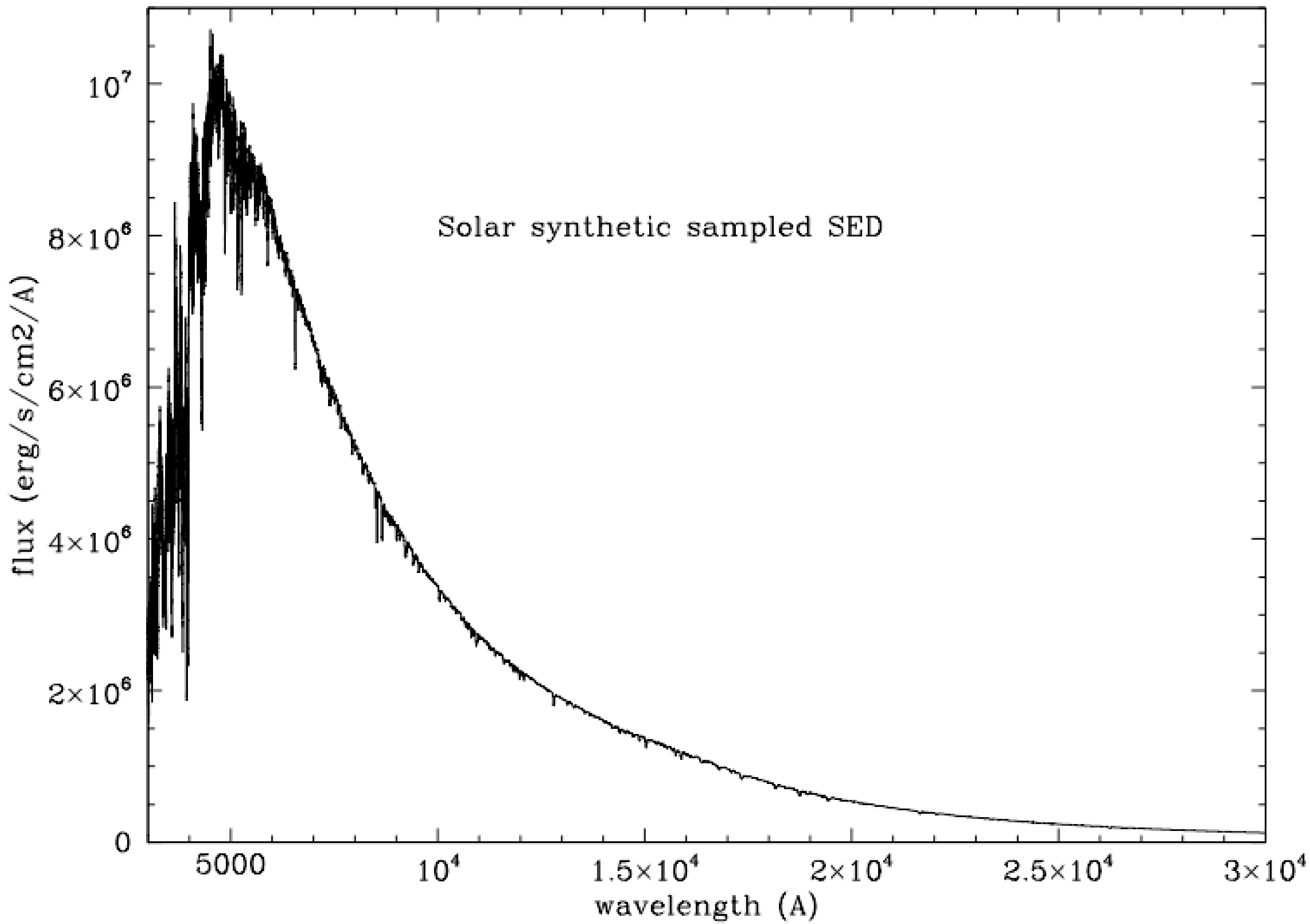
Synthetic spectra may not be perfect... But the same applies to observations!



21. Comparison between representative from the STELIB library (solid line) and synthetic spectra having similar stellar
otted line). Left panels: full wavelength range; right panels: zoomed view of the region around the 4000 Å break.

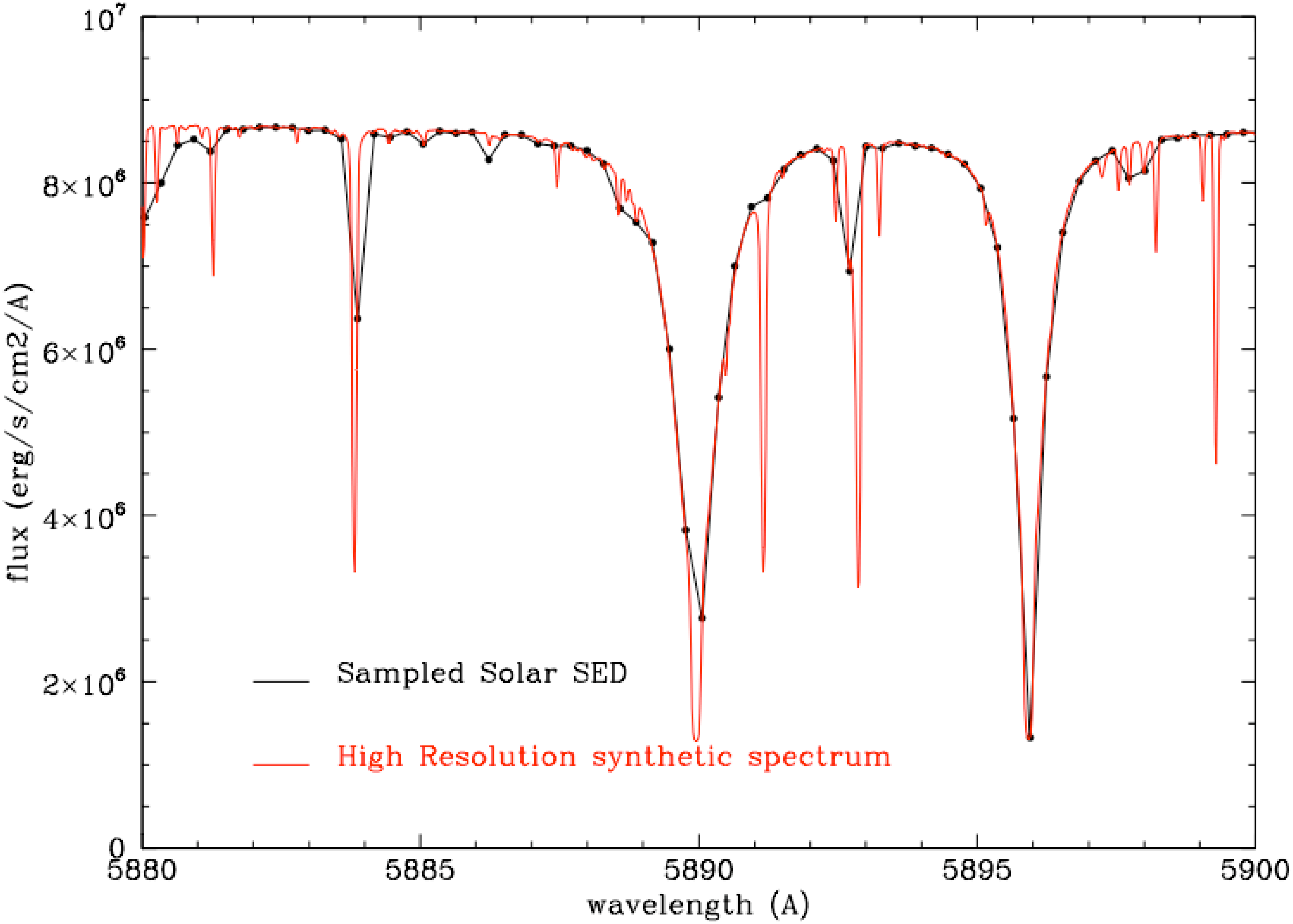
Figure adapted from Martins et al. 2005, MNRAS, 538, 49, a high resolution stellar library for evolutionary population synthesis

Another WARNING! calculated spectra are **sampled**, and should be used with caution!



Another WARNING! calculated spectra are **sampled**, and should be used with caution!

example below for MARCS SED



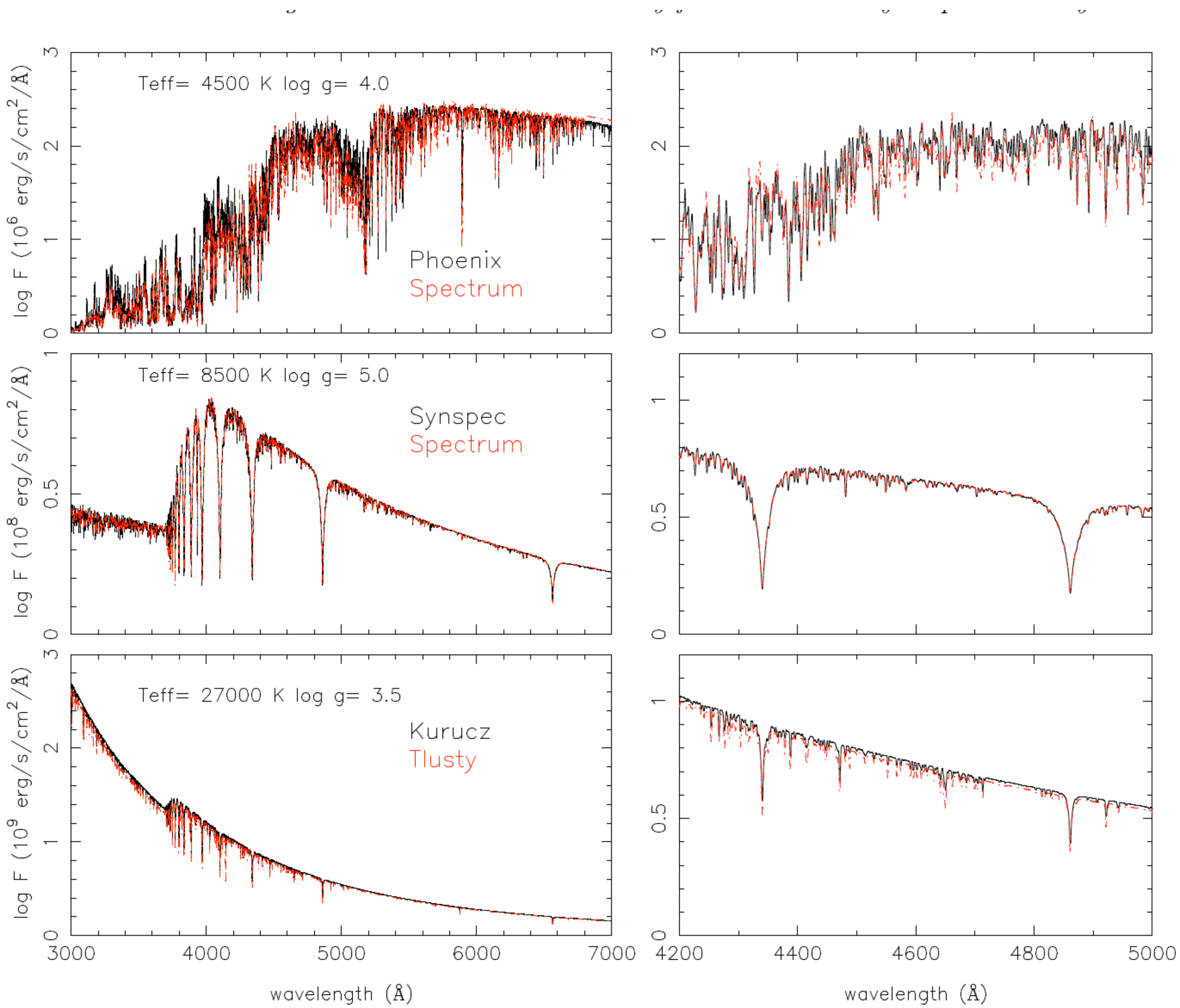


Figure 6. Comparison between the spectra obtained with different codes. Botton: Teff= 27000 K obtained with Kurucz+Synspec (full black line) and Tlusty+Synspec (dotted red line) stellar atmosphere models. Middle: Teff= 8500 K obtained with Kurucz+Synspec (full black line) and Kurucz+Spectrum (dotted red line). Top: Teff= 4500 K obtained with Phoenix (full black line) and Kurucz+Spectrum (dotted red line). Solar abundance for all models.

Synthetic spectra from different codes do not always agree

Differences are larger for extreme spectral types (note log Flux scale).

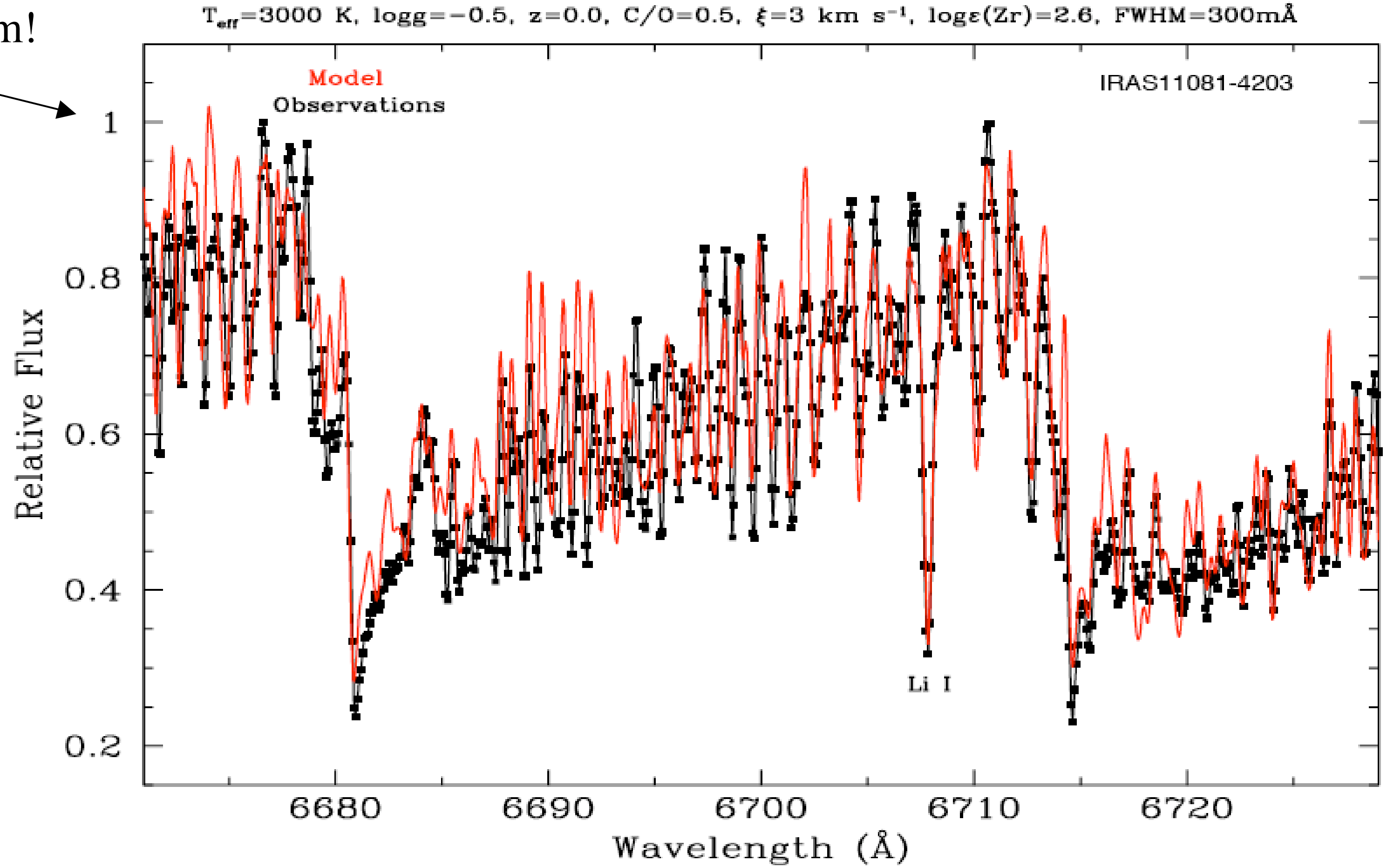
=> progress must be made on carbon stars and very cool dwarfs

Figure adapted from Martins et al. 2005, MNRAS, 538, 49, a high resolution stellar library for evolutionary population synthesis

But we do a good job in many instances.

Fit of a very cool, very obscured AGB star spectrum :

this is not continuum!



From García-Hernández et al. 2007, A&A 462, 711

Spectra on Demand from VO

compute on the fly/on demand (SOD = spectra on demand ;-)

- that is expensive! what will be the demand? a new spectrum for just the variation of a single small parameter (e.g. U abundance...)?
- the detailed analysis of a single spectrum (several dozen individual abundances), demands many tens of spectra to be computed!
- **rather** : large grids of full spectra with few parameters varied, to feed automatic analysis codes providing first estimates (T_{eff}, logg, Fe/H), followed by home work, with own codes ?

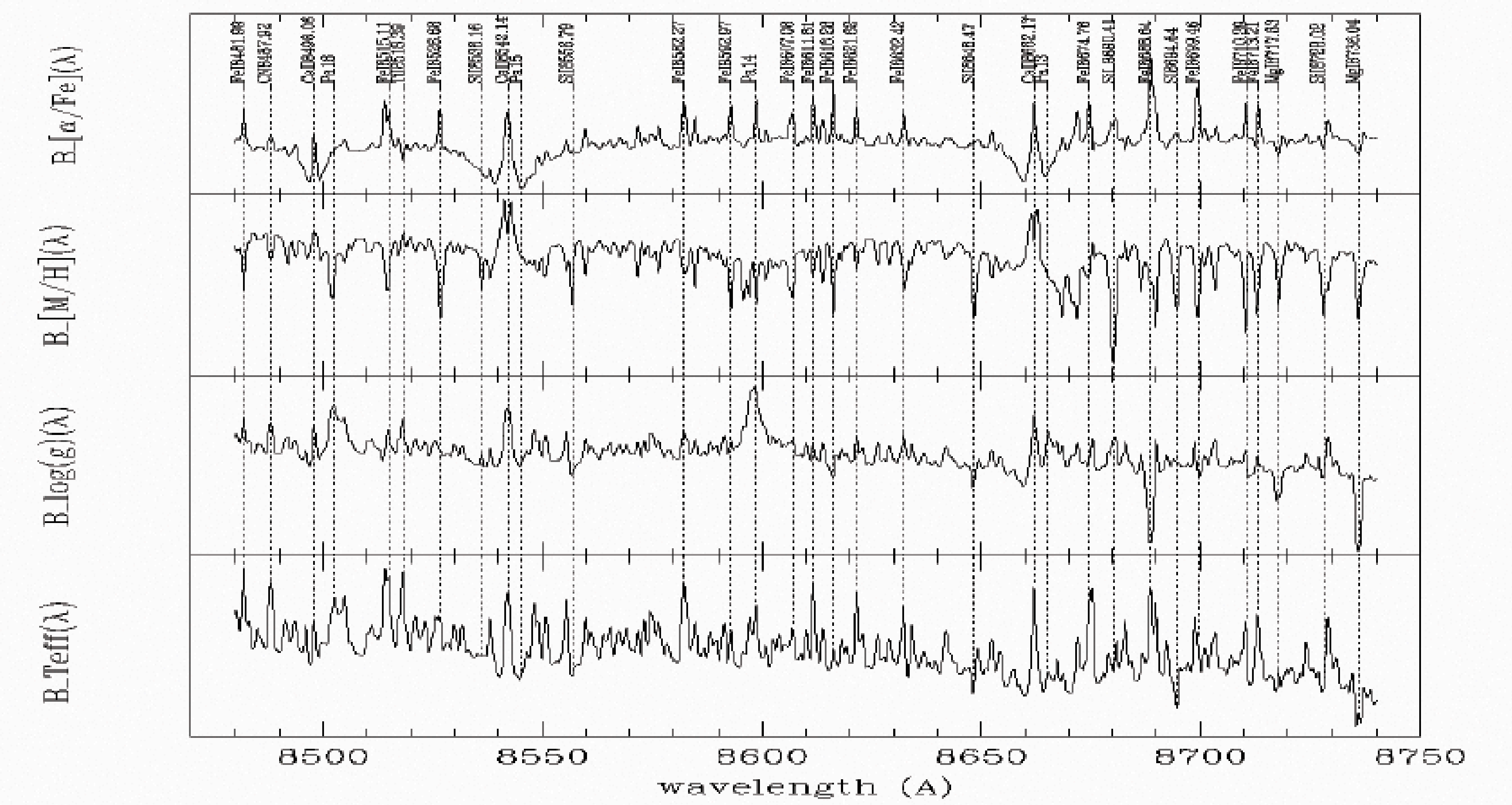
A few words on automatic determination of stellar parameters

- minimum distance. e.g: TGMet (Soubiran et al.), limited to few parameters (Fe/H, T_{eff}, logg), not whole HR diagram
- neural networks: learning difficult?
- new methods: e.g. MATISSE (Recio-Blanco et al. 2006) seems very powerful: fast and efficient. Must be tested on whole HR diagram. One of the solutions foreseen for GAIA (10^9 spectra!)

Algorithme MATISSE : MATrix Inversion for Spectral SynthEsis

$$\boxed{\theta = a \sum B(\lambda)\, R(\lambda)}$$

Spectre observé



Synthetic spectroscopy at home

- not possible to have SOD on line running on other machines?
- better ? locally installed and efficient (fortran) codes, fetching data from VO : models, line lists, (observed spectra)?
  - problem: must be user-friendly, ergonomic (graphical output), no black-box, which is a major difficulty!! e.g. molecular equilibrium: what's in or not, what lines to include at each T_{eff}, what hypotheses (LTE/NLTE, spherical/PP, ...), well documented, easily installed (download and "click"), ...

  ⇒lot's of work (i.e. no incentive for people writing codes?)

  ⇒Idea: the "ergonomic" layer could be part of VO?
- if many objects (>100), need automatic tools, at least as first iteration: use of parameter determination codes using on line large synthetic spectra grids (cf. previous slides).

LTE synthetic spectra codes

- SYNTHE (R.L. Kurucz) : available on the web. PP. Documentation on line : http://wwwuser.oat.ts.astro.it/atmos/Documentation.html
- Turbospectrum (B. Plez) available on demand. No "cookbook". PP or Sph, F-MSC stars, 600 molecules, fast with many lines, line broadening from Barklem et al., no plotting interface
- MOOG (C. Sneden) available on the web, PP, older version pure LTE (S=B), F-K stars, with documentation http://verdi.as.utexas.edu/moog.html
- SME (see N. Piskunov's talk) : abundance stratification, automatic determination of stellar parameters and abundances, available upon request.
- SPECTRUM (Gray), documented, includes a few molecules, PP

synthetic spectra codes (cont'd)

- I do not detail NLTE codes. There are a number of them : KIEL, MULTI (M. Carlsson), Synspec (/Tlusty) (I. Hubeny & T. Lanz)
- There are also multi-D codes, or including magnetic field, polarization, etc... Not freely available usually.

Notes on documentation

Code with no documentation

- risk of error when providing input to, or when interpreting output from the code
- Some options may remain hidden to the user. Only the developer knows
- Some limits of the code (temperature, ionisation stages, species, ...) are not known

If additionally the code was not intended for a broad distribution

- Risk of dangerous options or setup -> erroneous output with no obvious warning
- A solution may be to look at the source code, but it will probably be intricate !

Code with documentation

- There is still the risk that it is not read... ;-)
- Something may have been forgotten
- It is actually very painful to write a doc.
- Ideally, in all cases there should be continued contact between users and providers of codes: helps improve/correct/debug/document

Note that usually the very latest version(s) is not distributed.

Cautionary words from C. Sneden Valid for all codes!

A more general cautionary note really needs to be taken to heart by all MOOG users. This code, like all others of its type, makes opening assumptions about the kinds of stellar atmosphere situations that it will face. It has certain internally-stored atomic and molecular data that have been culled from various literature sources. And it includes, for example, representations of the typical major opacity sources that are easily coded, and such representations have proven to be adequate for most tasks. **HOWEVER**, it is the user's responsibility at all times to think about the computations! Tests need to be carried out to verify the applicability of the MOOG calculations to particular spectroscopic problems. Corrections to MOOG will be cheerfully carried out whenever they are brought to my attention. But those who blindly use this code, publishing whatever numbers MOOG spits out, will have only themselves to blame if abundances deduced with MOOG turn out to be fundamentally flawed.

(in writemoog.ps)

line databases

See also following talks (Piskunov, Roueff)

(Too?) Many databases on line.

Also lists of databases, but not complete. e.g.:

- http://www.cfa.harvard.edu/amdata/ampdata/amdata.shtml
- Kurucz home page, with all the programs and data of the Kurucz suite. Enormous ressource, but not always well documented (e.g. what input data was used to construct line lists?).

  http://kurucz.harvard.edu/

  http://kurucz.harvard.edu/linelists.html

More line databases

- http://ams.astro.univie.ac.at/vald/ VALD database (atomic lines) Cf talk by Piskunov
- Molecular line lists scattered on various sites: NASA-Ames (Partrige, Schwenke, et al. H2O, TiO), University College London (Barber, Tennyson et al. H2O, HCN, ...), etc...
- (see also following talks)

How do we pay the people doing the hard work?

- code development and testing is time-consuming. It deserves credit. Writing documentation is tedious and gives little credit (although probably a broader use of code)
- Once code is on line in VO, who gets the credit?
  - illustration: line data included in VALD sometimes cited only as "VALD", instead of its real source.
- Credit is needed to get jobs and money...
- if not, lack of incentive to create new tools, or add data.
- it seems we have an answer: info in metadata, and action towards journal editors and referees

Tools to implement in VO

Interaction with synthetic spectra needs:

- query them! (no position on sky, but abundances...)
- vizualization with rescaling, doppler shifting, overplot (also with observed spectra) simple eqw integration ...
- convolution with rotation, macroturbulence, intrumental profiles
- calculation of correlation profiles (see e.g. correlation masks used for planet detection)

Summary

- setup of large homogeneous synthetic spectra libraries quite straightforward for population synthesis
- large libraries will also allow analysis of huge surveys.
- challenge: automatic determination of parameters
- document and secure online codes
- tools: correlation, convolution, ...
- questions:
  - setup synthetic spectra code interfaces in VO or only allow queries from pre-calculated grids?
  - credit to developers?
  - how do we learn to sort out the tremendous amount of data (line data, spectra, ...)?

Maybe the greatest challenge!

- learn to use the large amount of data in an educated way!