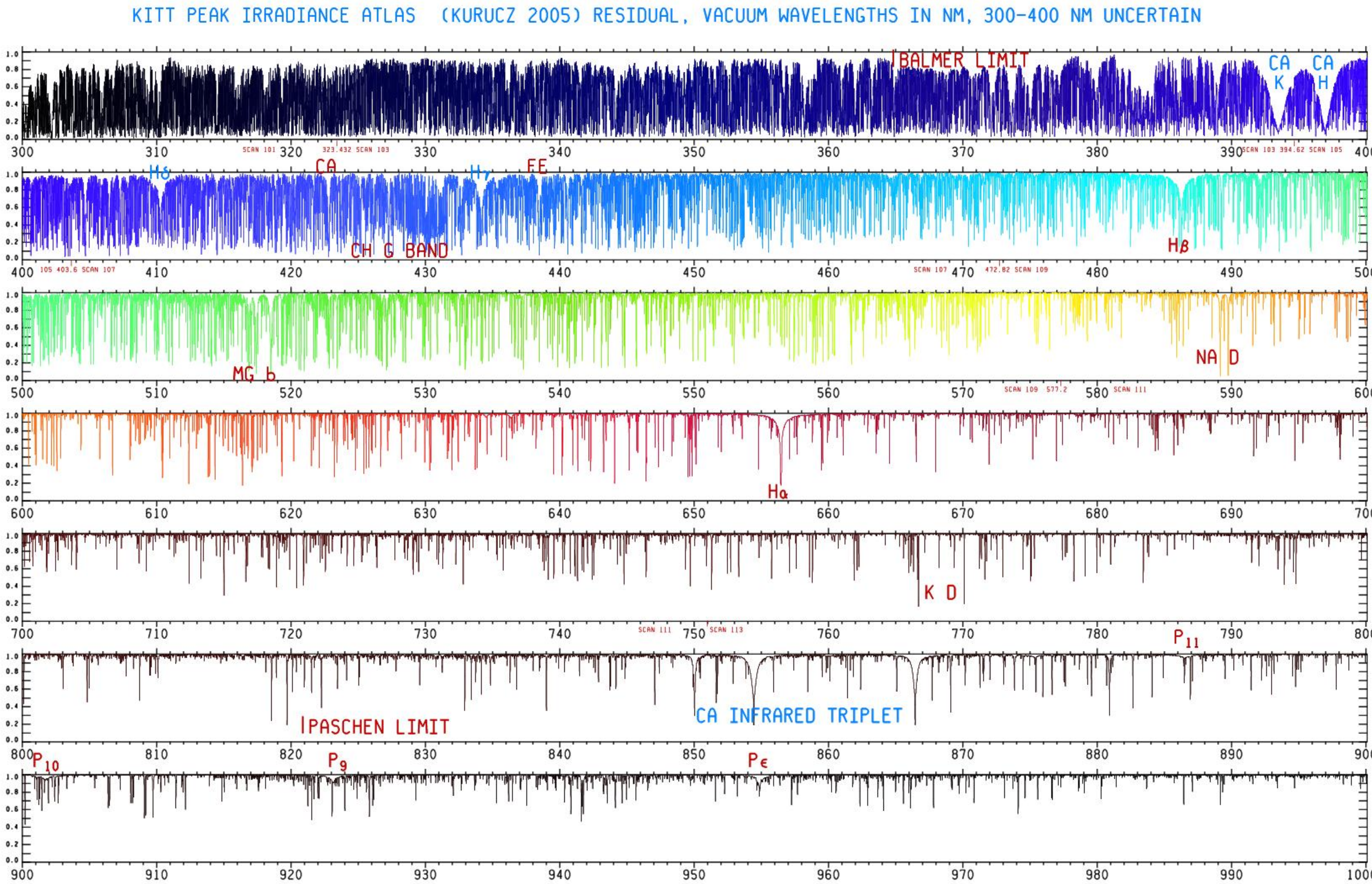
Tools and techniques for modeling stellar spectra in 1D LTE

ChETEC INFRA SNAQs **How to interpret stellar spectra?**
November 10, 2021

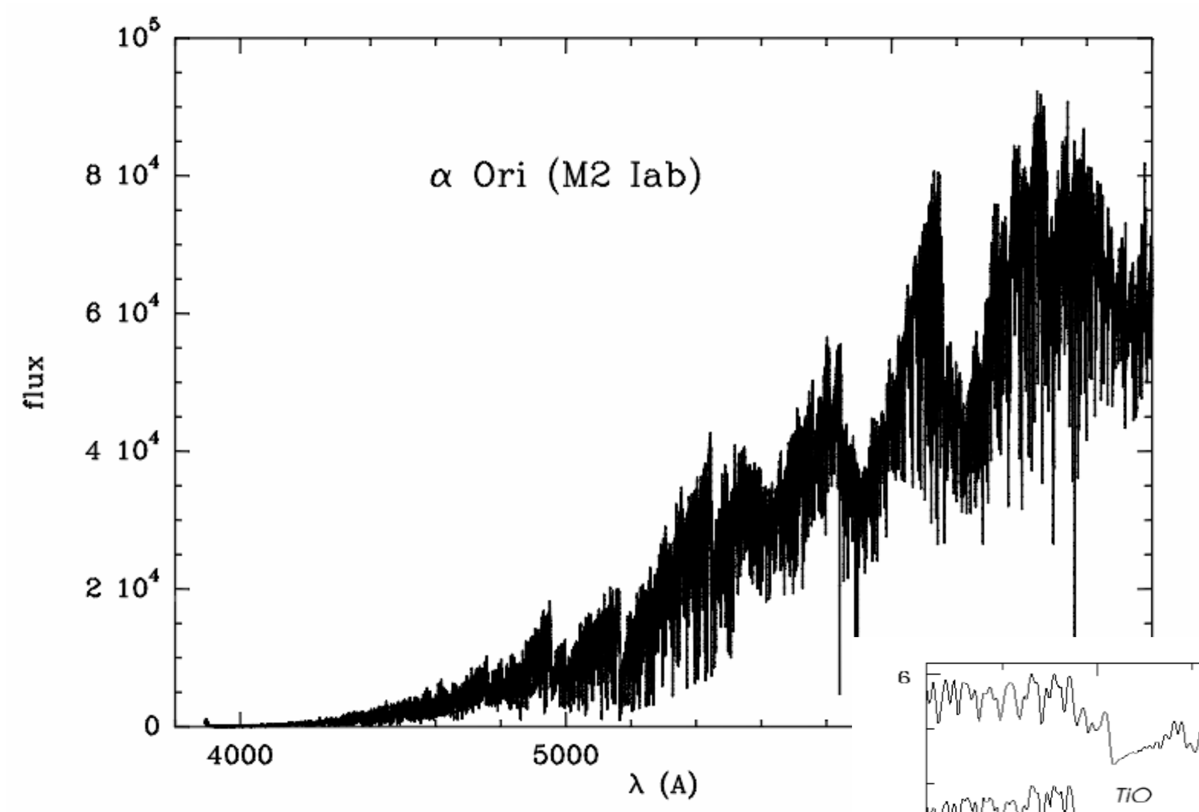
Bertrand PLEZ, Montpellier University, and CNRS, France

The solar spectrum (without telluric absorptions)



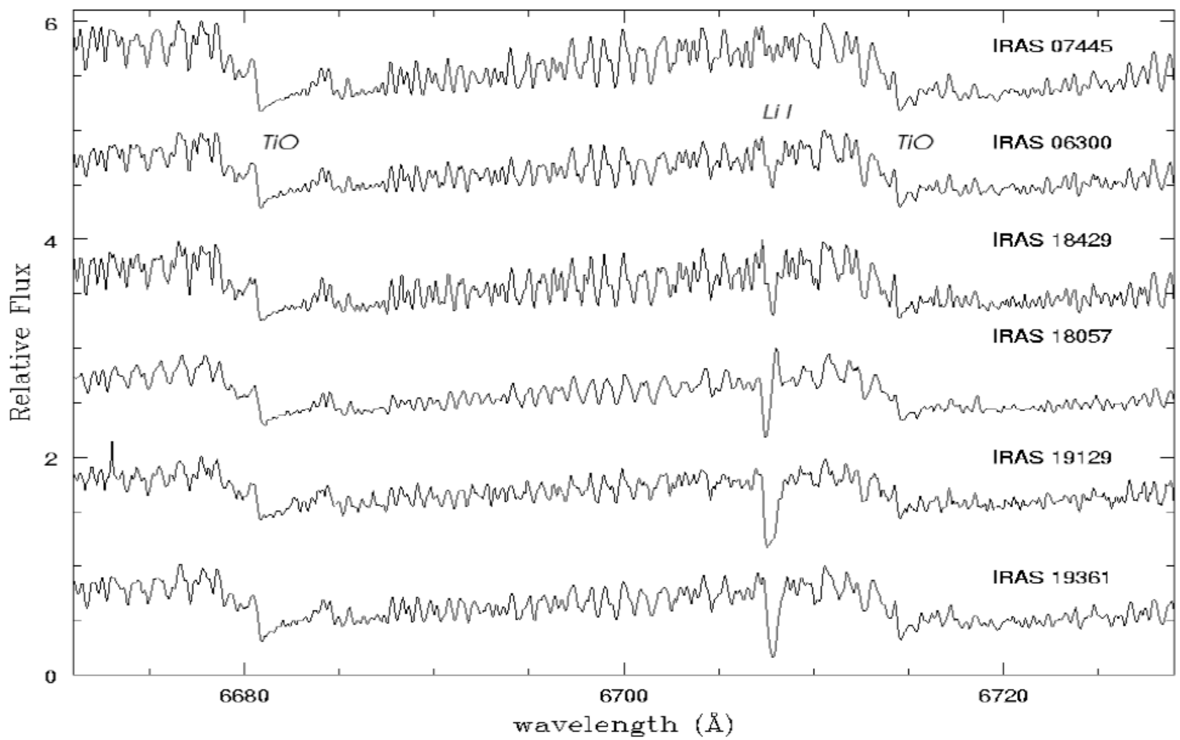
Many lines! => Large amount of data needed to correctly model this

Other spectacular examples



These are high S/N spectra.
All wiggles are lines!

spectra of red giant stars
in the 671nm Li I line region



Betelgeuse, a red Supergiant star.
Large absorption bands in the optical are mostly due to TiO

Deriving stellar parameters

How do we model these spectra, in order to derive stellar parameters, in particular chemical composition?

=> Compute a model atmosphere and compare the emergent spectrum with observations.

Atomic and molecular lines being ubiquitous in stellar spectra, we need lots of (good) data

Model atmospheres (1D)

Stellar atmosphere models: what for?

Stellar atmosphere models are needed for:

- computing line profiles / spectra / limb darkening …
- deriving stellar parameters / diagnostics from observations
- boundary condition for interior models or winds

T, P, v, **B**, … vs (x,y,z)

or more simply T(r), P(r)

A given model is defined by fundamental parameters :

at least T_{eff} , logg, abundances

+M, R, or L for a spherical model

In addition there may be parameters for convection (mixing-length, …)

Stellar atmosphere models: parameters

- Star of mass M, radius R, luminosity L (total emitted power) [W]
- gravity: $g = GM/R^2$
- Bolometric flux, $\mathcal{F}_{\mathrm{bol}}$ [W/m^2]: $L = 4\pi R^2 \mathcal{F}_{\mathrm{bol}}$

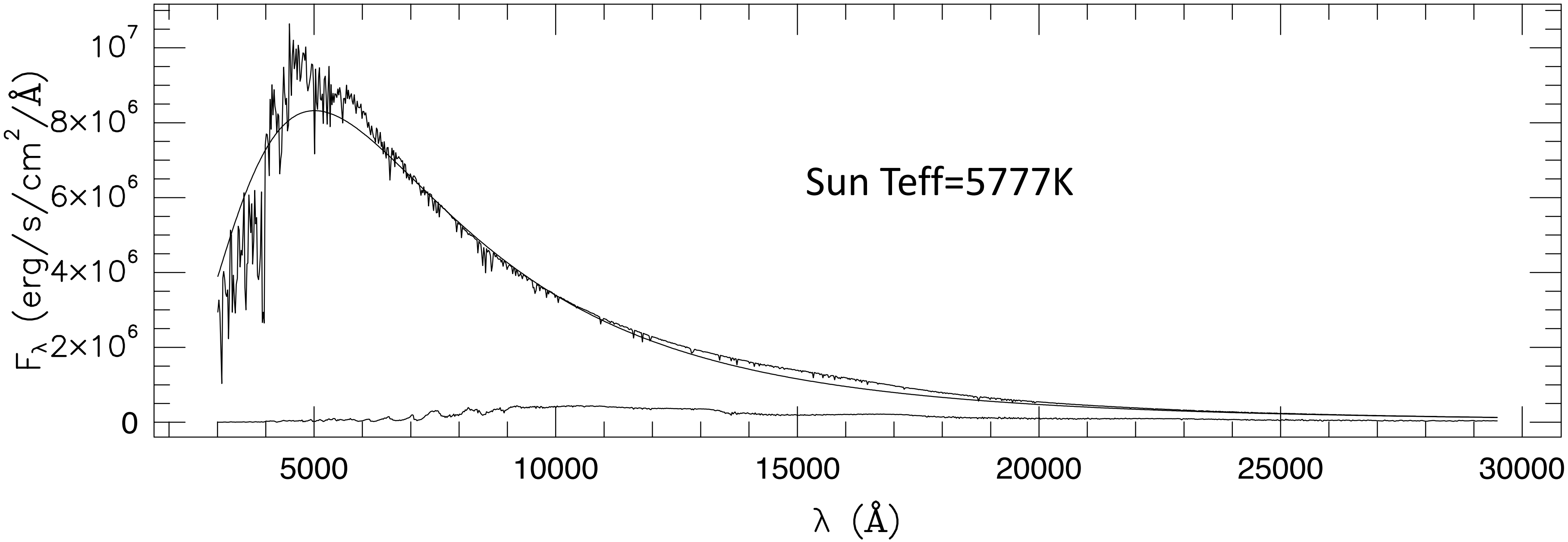
- $\mathcal{F}_{\mathrm{bol}} = \int \mathcal{F}_\lambda d\lambda$ $\mathcal{F}_\lambda$ = monochromatic flux, [W/m^3]

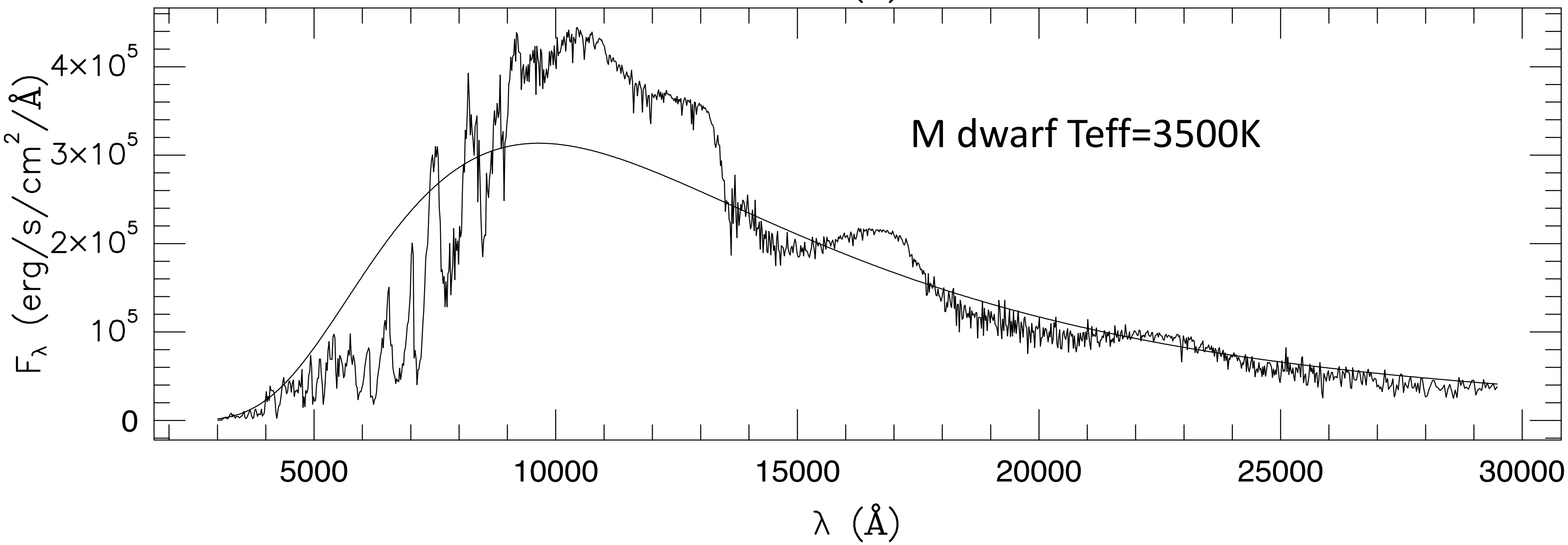
- Effective temperature: $\mathcal{F}_{\mathrm{bol}} = \sigma T_{\mathrm{eff}}^4$

  $\mathbf{T_{eff}}$ is the temperature of the black body emitting the same bolometric flux

  (reason for that convention obvious in next slide)

Stellar (model) spectra and black body emission at the same temperature





Ingredients for model atmospheres

- **Geometry**: 3D, 1D (PP or Sph)
- **Dynamics**: (magneto-)hydrodynamics / static
- **equation of state** : T, Pe, Pg with most/all atoms and many ions, up to hundreds of molecules, … solids
- **Radiative transfer** plays a central role: N/LTE, polarization, … coupling with hydrodynamics

Ingredients for model atmospheres

- **Geometry**: 3D, 1D (PP or Sph)
- **Dynamics**: (magneto-)hydrodynamics / static
- **equation of state** : T, Pe, Pg with most/all atoms and many ions, up to hundreds of molecules, … solids
- **Radiative transfer** plays a central role: N/LTE, polarization, … coupling with hydrodynamics

Requires great quantities of physical data:
e.g., partition functions, ionisation and dissociation energies, line positions, strengths, broadening, hfs, Landé factors, cross-sections for collisional excitation/ionisation, photoionisation

Ingredients for model atmospheres

- **Geometry**: 3D, 1D (PP or Sph)
- **Dynamics**: (magneto-)hydrodynamics / static
- **equation of state** : T, Pe, Pg with most/all atoms and many ions, up to hundreds of molecules, … solids
- **Radiative transfer** plays a central role: N/LTE, polarization, … coupling with hydrodynamics

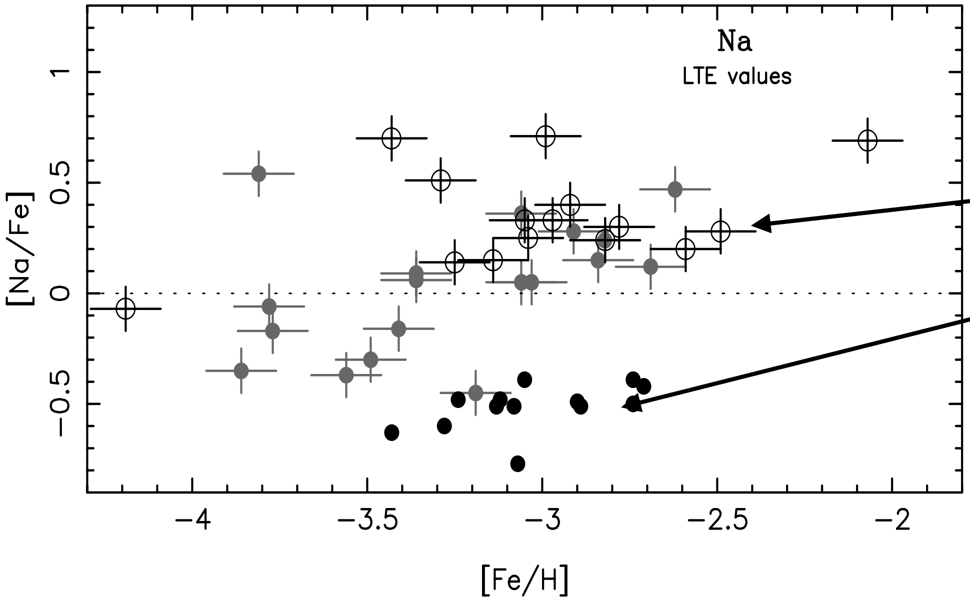
Requires great quantities of physical data:
e.g., partition functions, ionisation and dissociation energies, line positions, strengths, broadening, hfs, Landé factors, cross-sections for collisional excitation/ionisation, photoionisation

In 3D, calculations become tremendously expensive, esp. with NLTE.

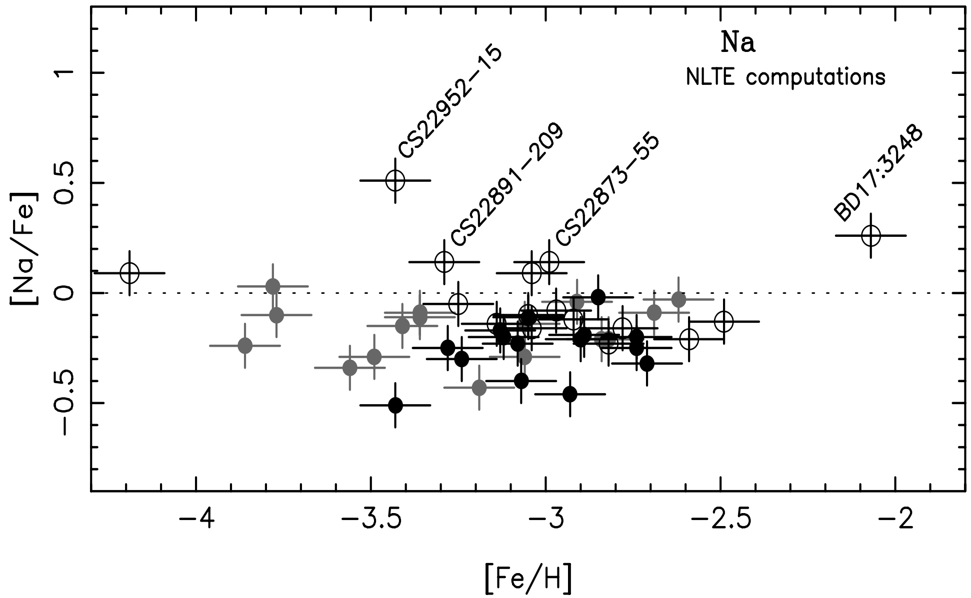
Next: a few examples to demonstrate this is worth the effort.

(note: not at all exhaustive, many such works through the years, I just picked a few. I apologise for those not represented here.)

Sodium in metal-poor stars



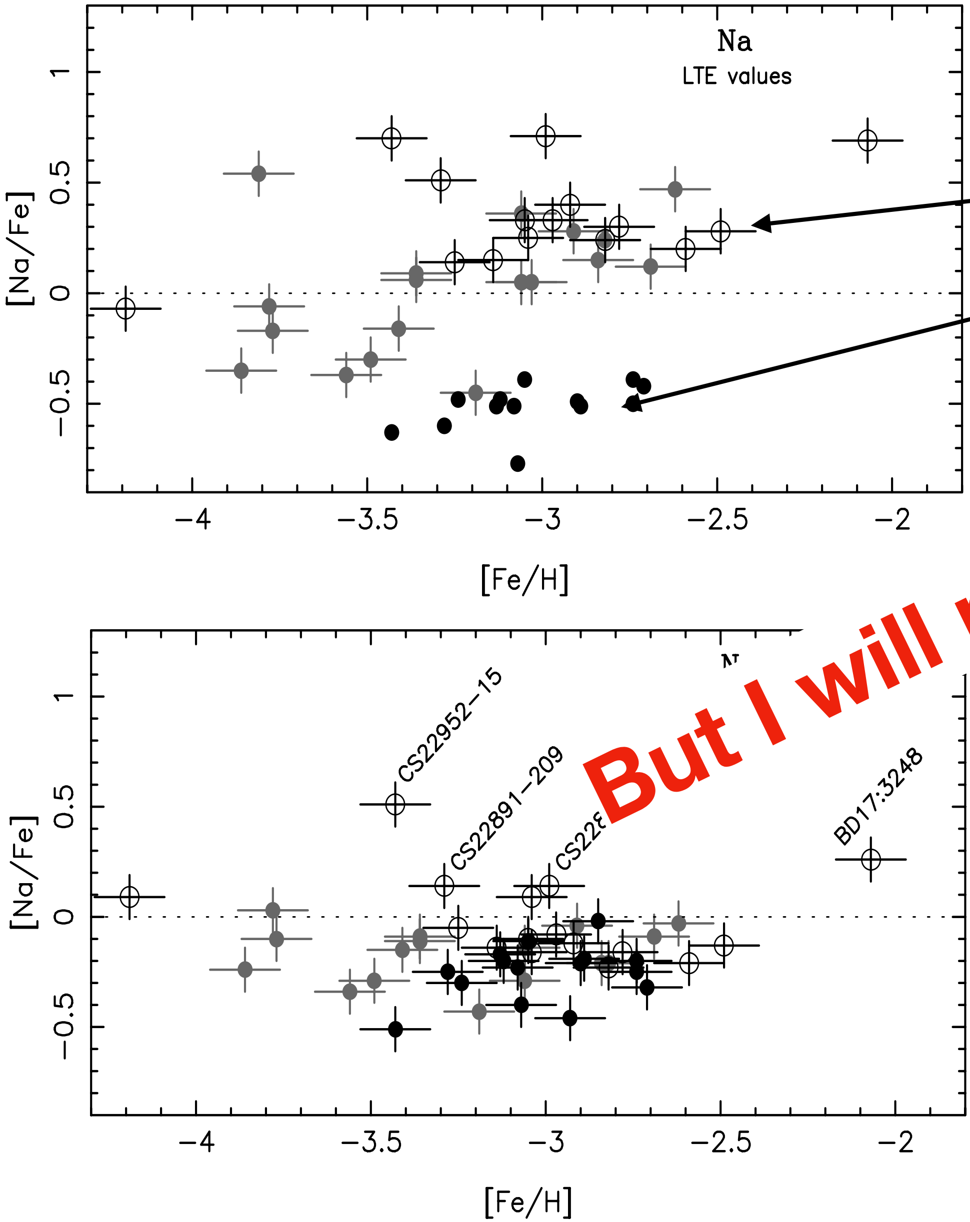
LTE Na abundances differ in dwarfs and giants



NLTE Na abundances are similar in dwarfs and giants

Andrievski et al. 2007, A&A 464, 1081

Sodium in metal-poor stars



LTE Na abundances differ in dwarfs and giants

But I will not discuss NLTE

NLTE Na abundances are similar in dwarfs and giants

Andrievski et al. 2007, A&A 464, 1081

Note that abundances are quoted like this:

$$A(X) = \log[n(X)/n(H)] + 12$$

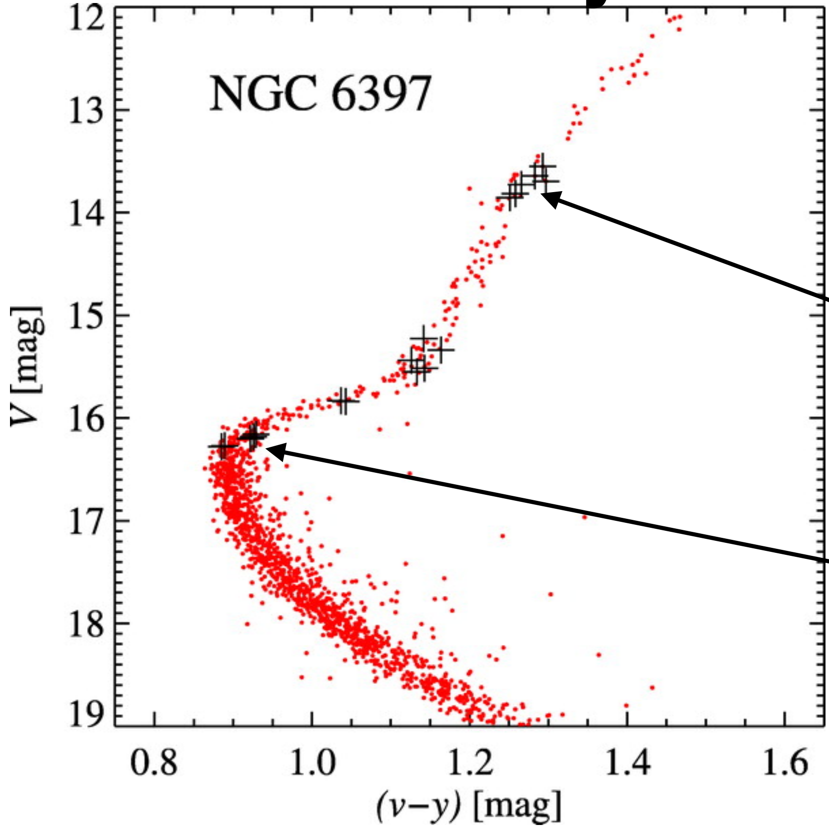
$$[X/H] = A(X) - A(X)_\odot$$

$$[X/H] = \log[n(X)/n(H)] - \log[n(X)/n(H)]_\odot$$

$[X/H] = -2$ means X/H is 1/100 solar X/H

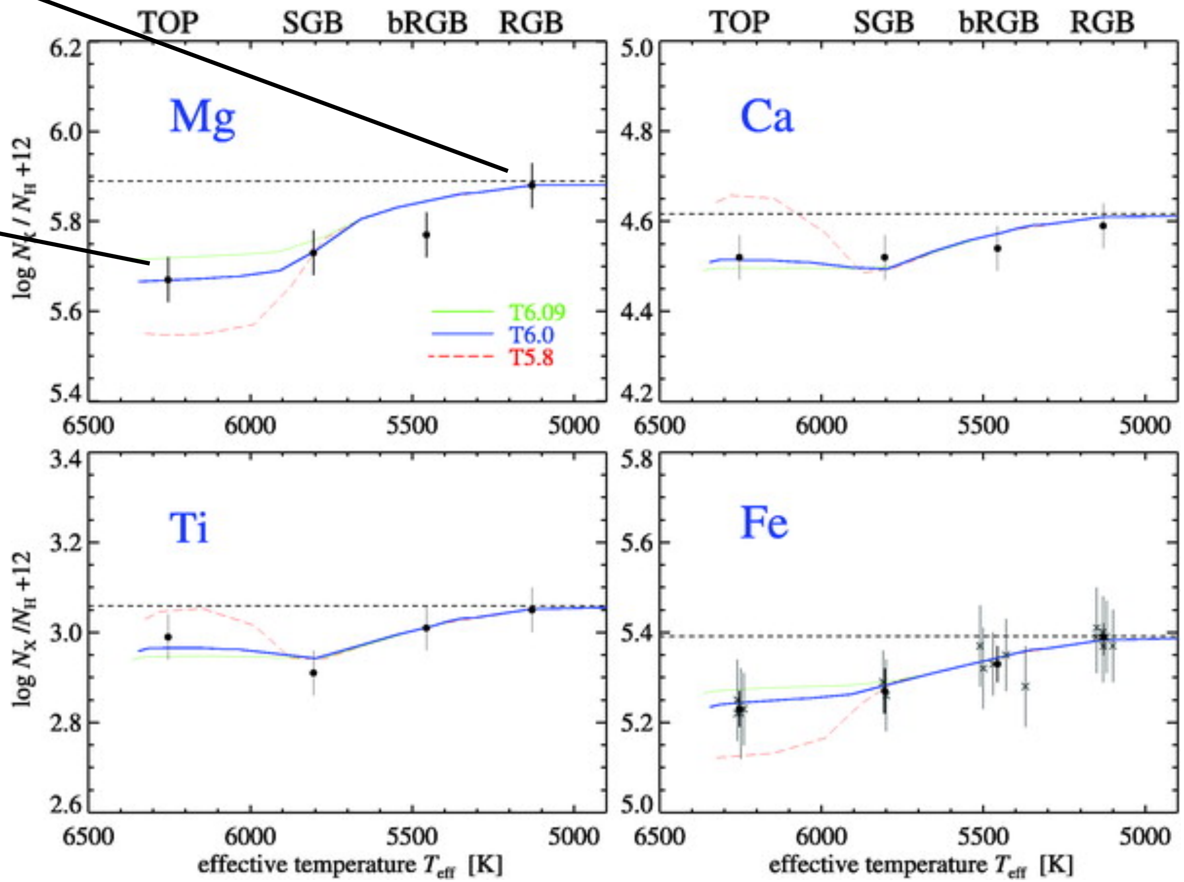
Most of the time in stellar spectroscopy

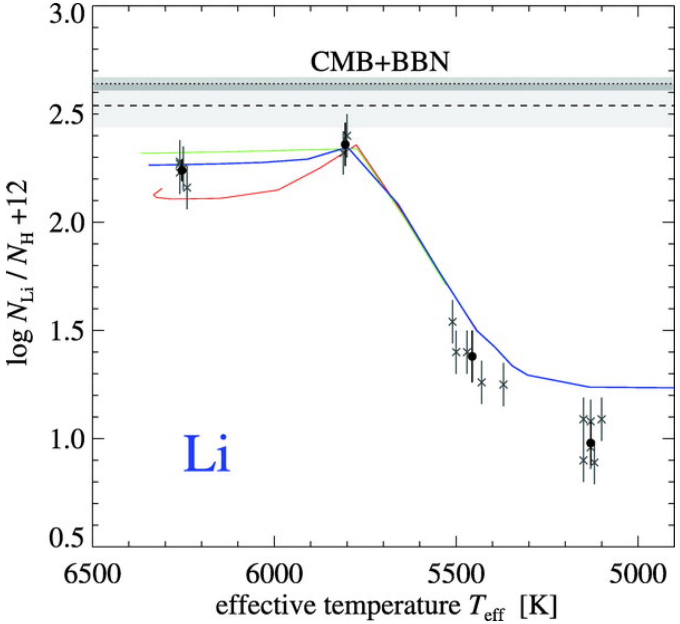
Why accurate abundances? one example



Atomic diffusion and the **primordial Li problem.**

very accurate abundances are necessary!

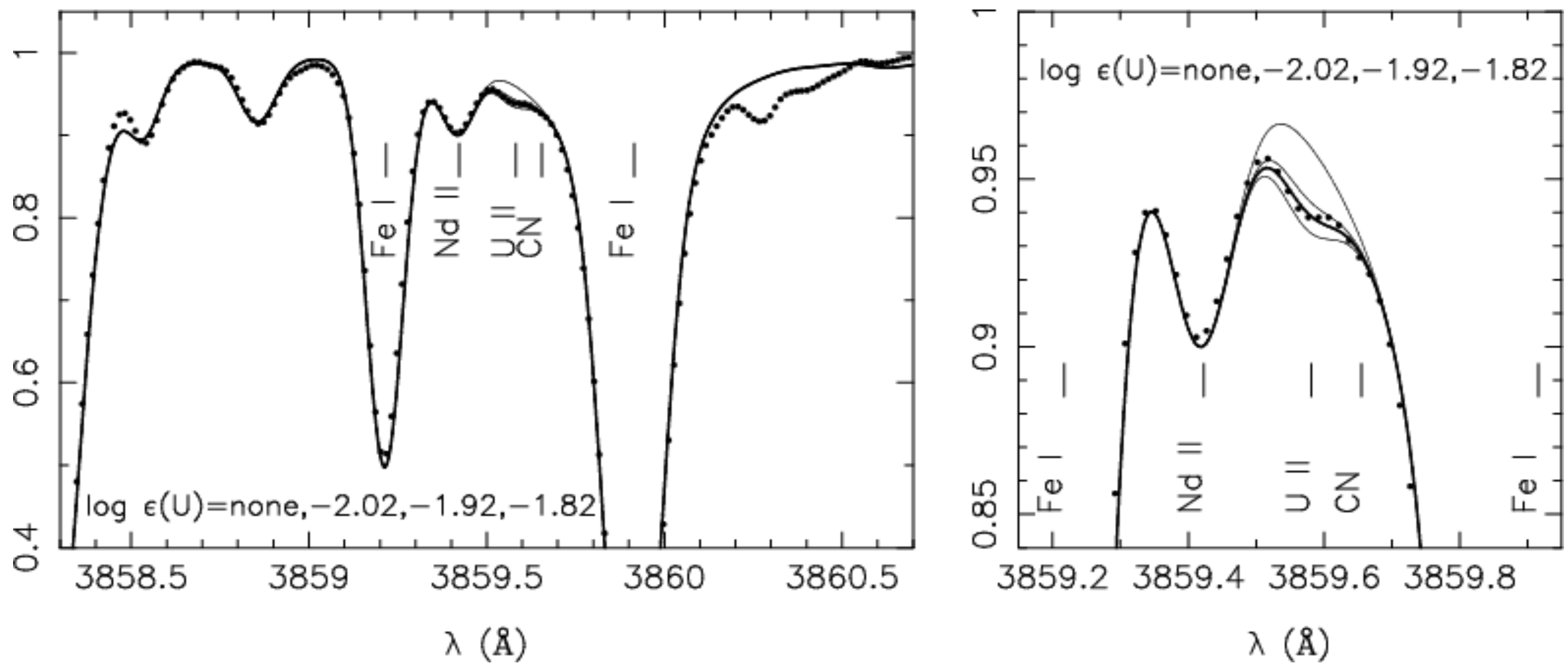




NB: required modelling Fe in NLTE, and carefully establishing the T_{eff} scale (based in particular on H line profiles)

Korn et al. 2007, ApJ 671, 402; Korn et al. 2006, Nature 442, 657

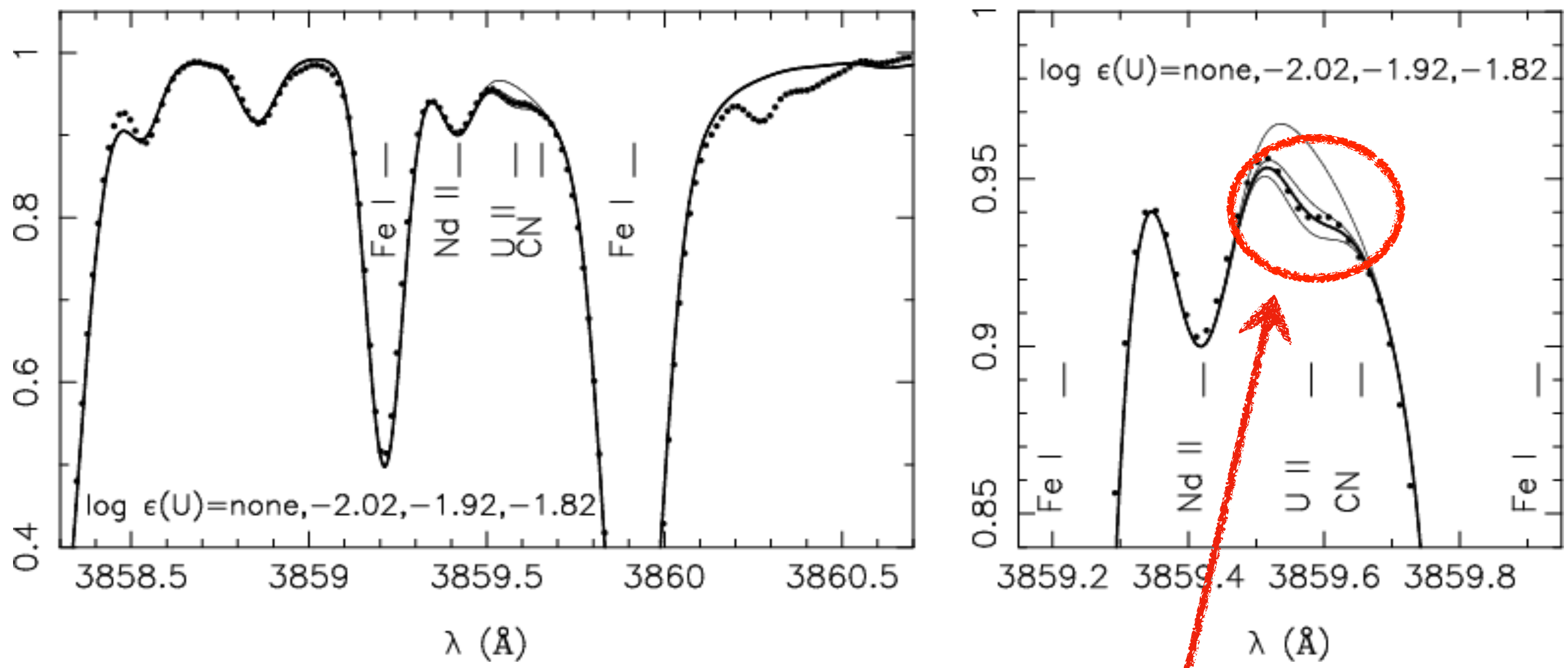
The art/science of deriving detailed abundances



Uranium abundance in CS31082-001:

Cayrel et al. 2001, Nature 409, 691

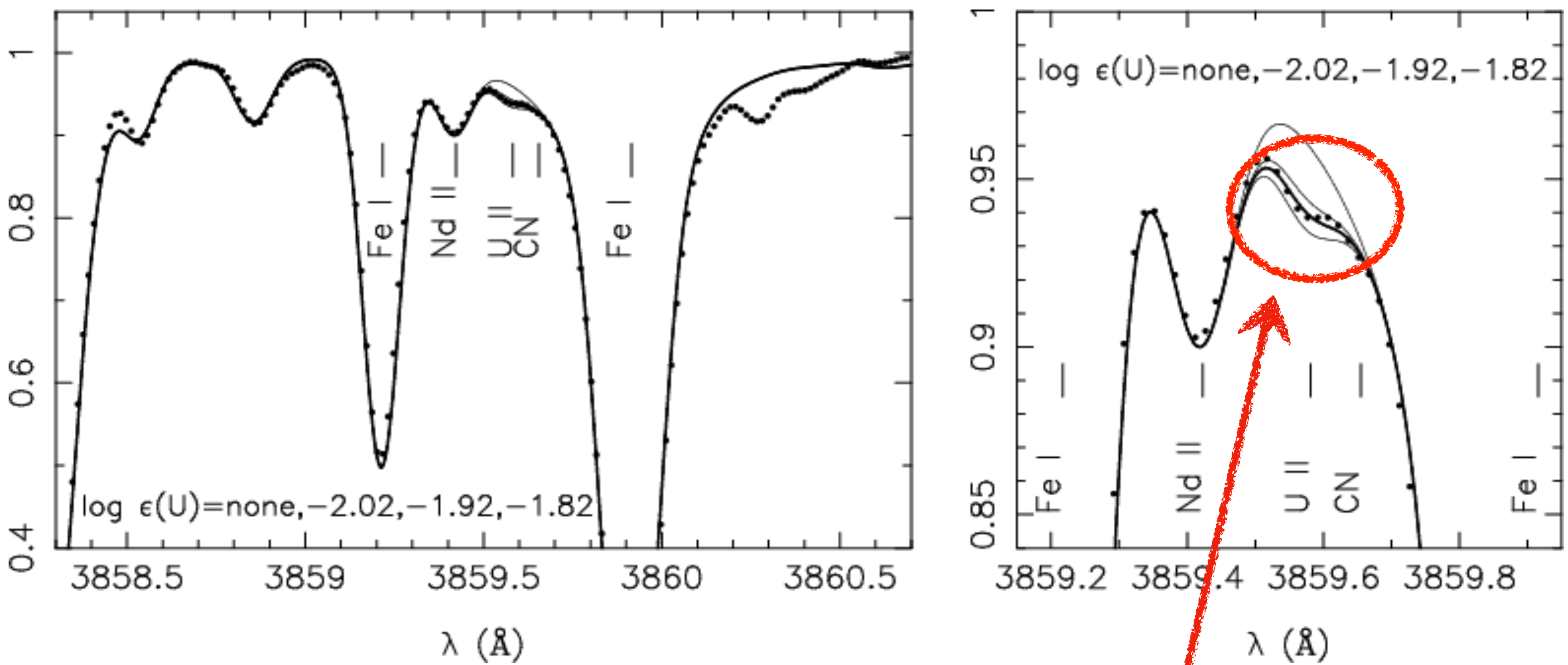
The art/science of deriving detailed abundances



Uranium abundance in CS31082-001:
0.1 dex difference in abundance corresponds to sub-percent variations of the flux level,
and *over 1 Gyr of uncertainty on the age*.

Cayrel et al. 2001, Nature 409, 691

The art/science of deriving detailed abundances

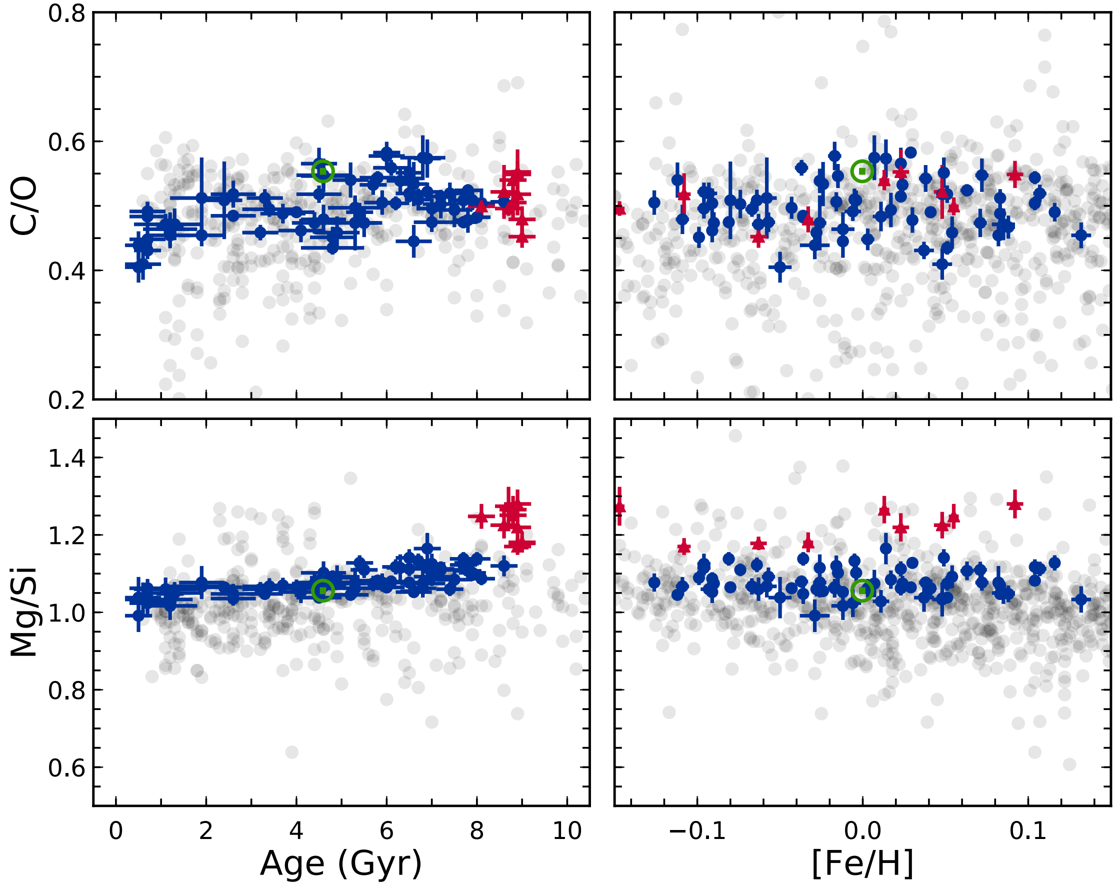


Uranium abundance in CS31082-001:
0.1 dex difference in abundance corresponds to sub-percent variations of the flux level,
and *over 1 Gyr of uncertainty on the age*.

=> Importance of completeness of line lists with **accurate line positions, gf-values, partition functions, broadening and line formation mechanism,** …
in addition to a good model atmosphere (i.e. T, P, (**v**) in the line forming region) !

Cayrel et al. 2001, Nature 409, 691

Is the Sun/solar system special?



Grey dots: Brewer & Fischer 2016, ApJ 831, 20

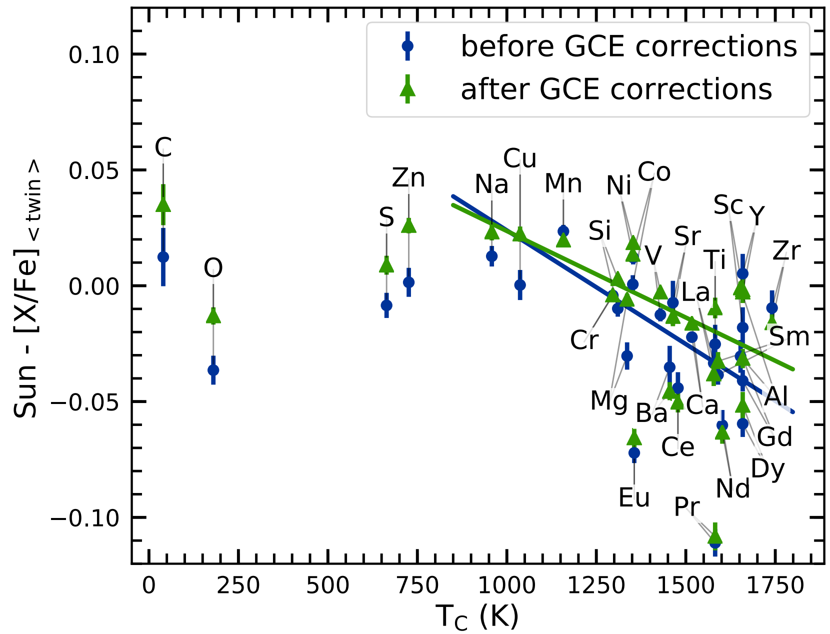
Blue dots: Bedell et al. 2018, ApJ 865, 68

Differential analysis of solar twins, i.e.: within 100K in Teff, 0.1 in logg, 0.1 in [Fe/H]
=> most sytematic, model-dependent errors cancel out.

Result: much less scatter in abundances, trend of Mg/Si vs. age

=> the Sun appears deficient in refractory elements, relative to 93% of the twins.

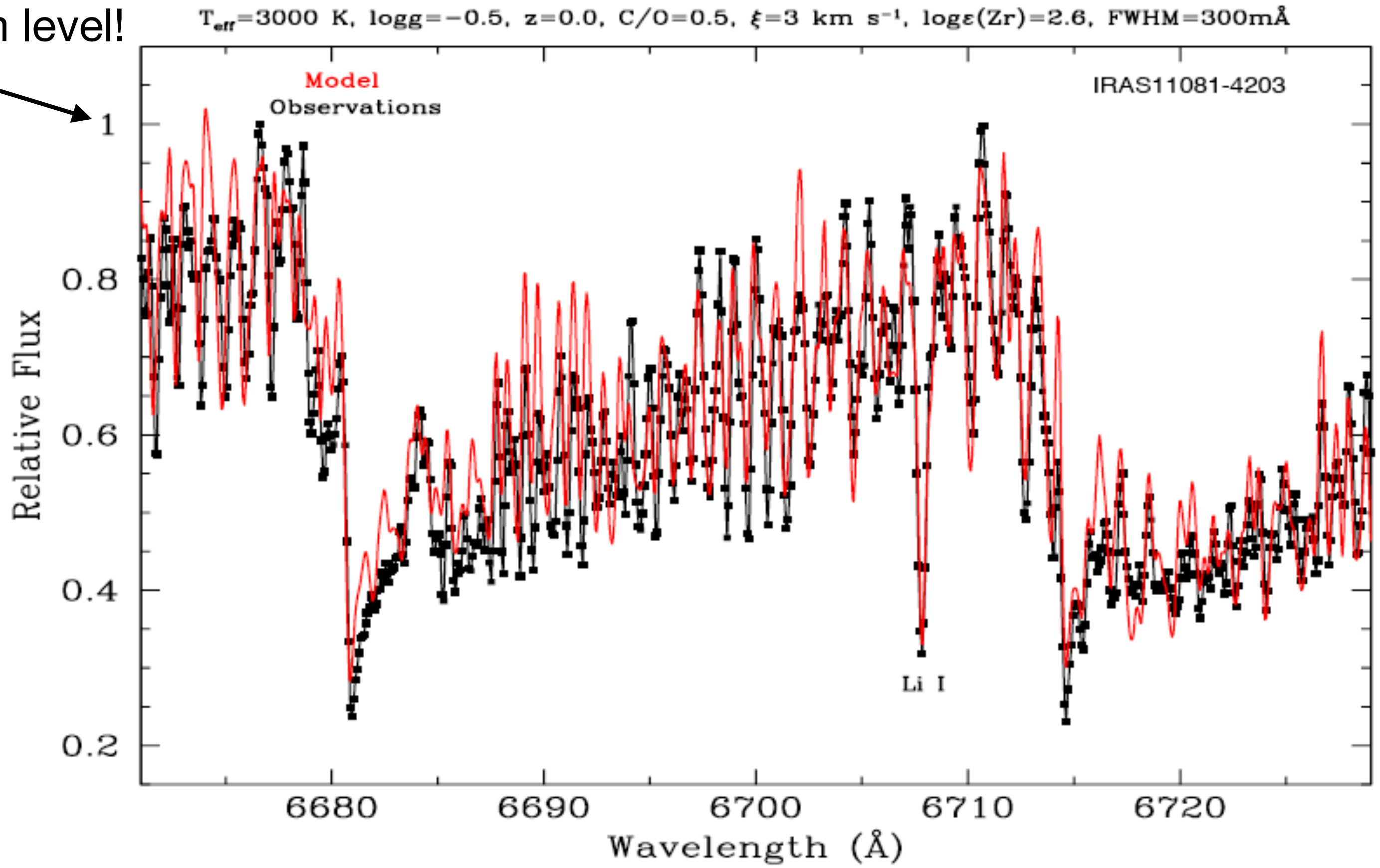
To extend such studies to non-twin stars, we need better models!



Fitting the Li line of a cool red giant

T_{eff} = 3000K
Absorption veil mostly due to TiO.
The Li line is far below the continuum!

This is **not** the continuum level!

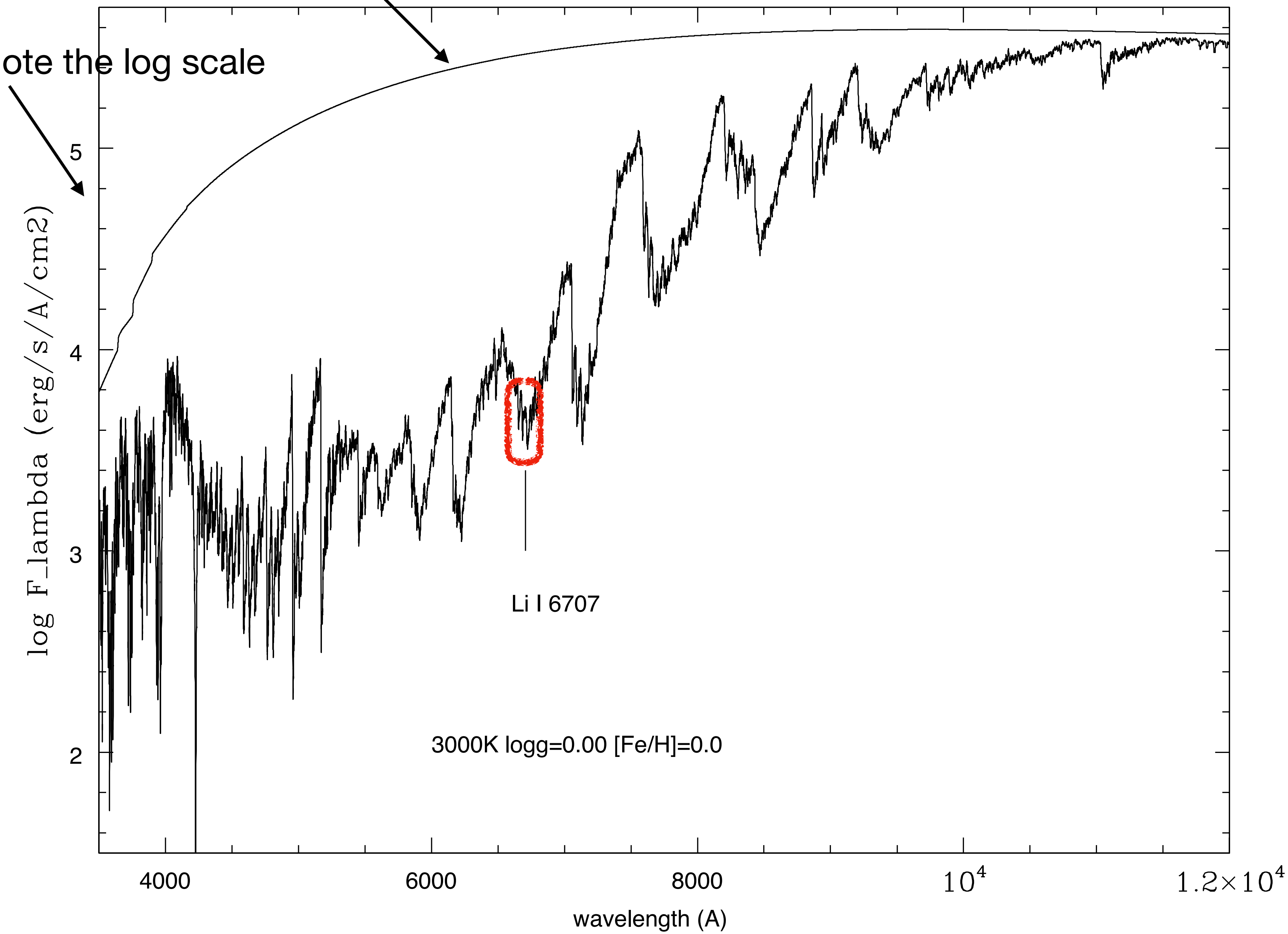


García-Hernández et al. 2007, A&A 462, 711

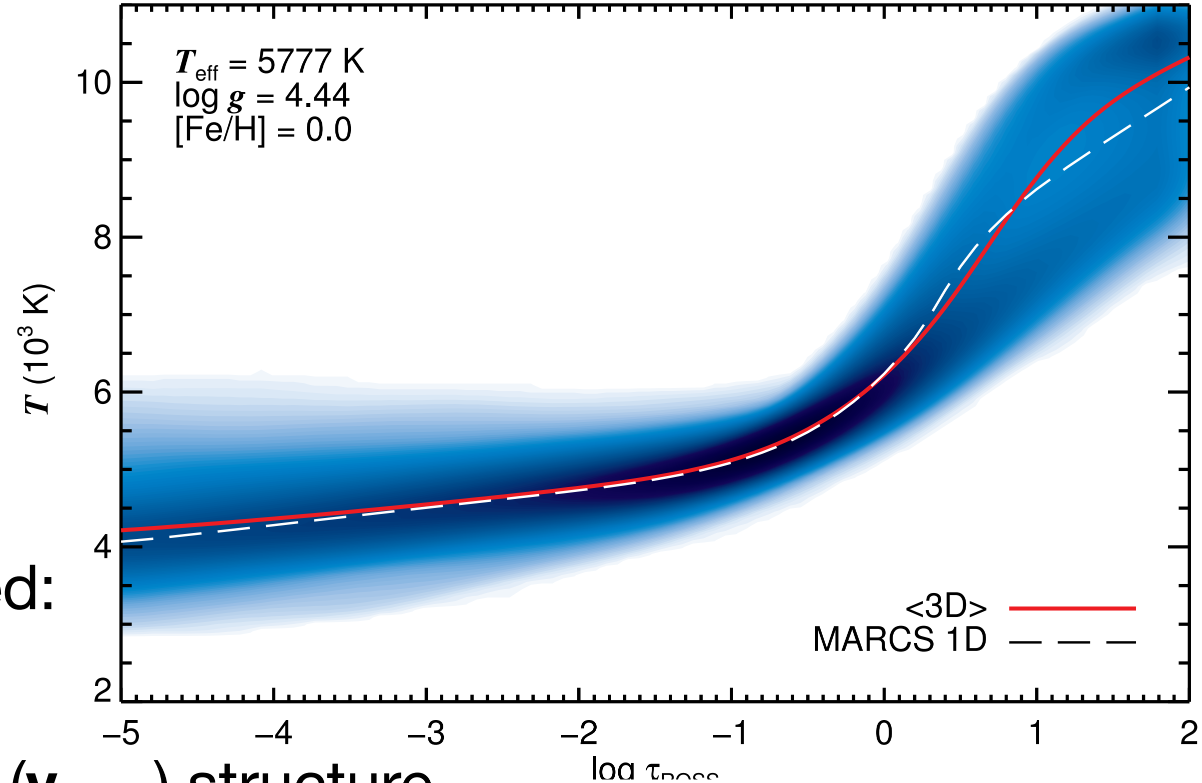
Li in red giants

This is the continuum!

Note the log scale



So, to model spectra, we need:



- **models** with a realistic T, P (**v**, …) structure
- **accurate physical data**, e.g., detailed line lists with accurate line positions, strengths, broadening parameters, partition functions, etc
- **methods and codes** to efficiently compute spectra at various approximation levels, e.g., 1D LTE or 3D NLTE
- and, be clever in **choosing the spectral domain**, which may not be possible when dealing with special lines (e.g. Li I , Pb I , U II, …). *The IR is a domain of choice* with new instruments coming-up and less line blending.

T and P stratification

- Pressure stratification is ruled by gravity

- Temperature stratification depends on energy flux at the base of atmosphere (T_{eff}), and how it is transported, i.e. opacities and convection

Opacities

Continuum and line opacities impact the thermal structure and the spectrum

=> For the thermal structure we need to include all sources, at least in a statistical way. Very accurate line positions are not necessary.

Opacities

Continuum and line opacities impact the thermal structure and the spectrum

=> For the thermal structure we need to include all sources, at least in a statistical way. Very accurate line positions are not necessary.

=> For the spectrum we need accurate line positions

In addition : line broadening (collisions with e, H, …), hfs, isotopic shifts, …

For cool stars : many molecules, possibly dust

Opacities

Continuum and line opacities impact the thermal structure and the spectrum

=> For the thermal structure we need to include all sources, at least in a statistical way. Very accurate line positions are not necessary.

=> For the spectrum we need accurate line positions

In addition : line broadening (collisions with e, H, …), hfs, isotopic shifts, …

For cool stars : many molecules, possibly dust

And now … a few illustrations of the **importance of securing the best and most complete opacities**

Effect of lines on the thermal structure (line blanketing)

Radiative energy balance requires:

$$q = \int \kappa_\lambda (J_\lambda - B_\lambda) d\lambda = 0$$

at every level in atmosphere

J_λ : radiation from (hotter) deeper layers

B_λ : local (cooler) radiation field

Effect of lines on the thermal structure (line blanketing)

Radiative energy balance requires:

$$q = \int \kappa_\lambda (J_\lambda - B_\lambda) d\lambda = 0$$

at every level in atmosphere

J_λ : radiation from (hotter) deeper layers

B_λ : local (cooler) radiation field

- In the blue $J_\lambda - B_\lambda > 0$ and in the red $J_\lambda - B_\lambda < 0$

=> if an opacity is efficient in upper atmospheric layers:

heating (e.g. TiO in optical) or cooling (e.g. H_2O, C_2H_2 in IR).

- and backwarming deeper, because the flux is blocked.

Model atmospheres

Illustration with *classical models:*

- 1D
- homogeneous
- hydrostatic
- Local Thermodynamic Equilibrium (LTE)
- convection: mixing-length theory
- **detailed radiative transfer with > 10^5 wavelengths**

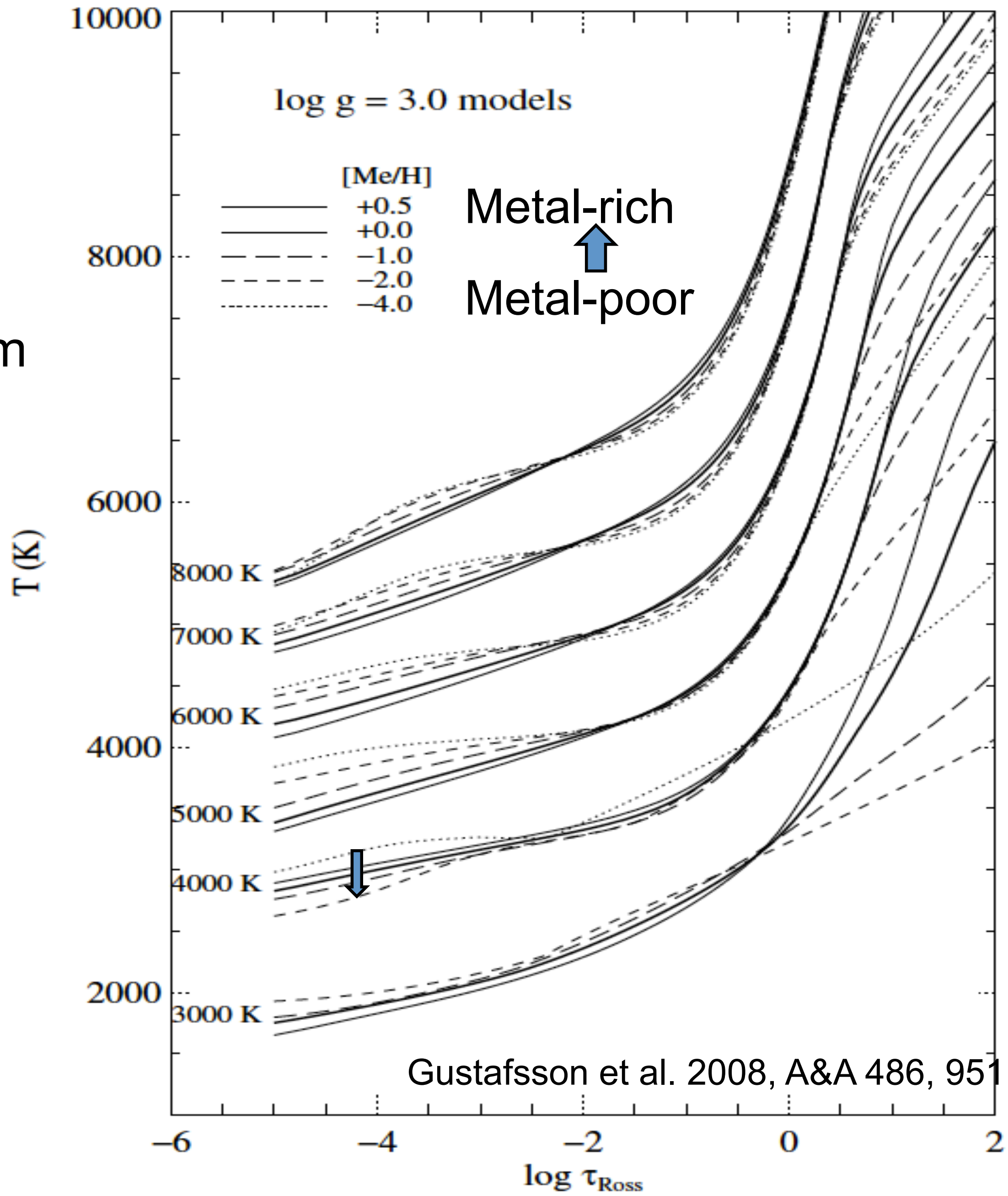


Fig. 2. The temperature structures for a set of model atmospheres with different $T_{\rm eff}$, $\log g = 3$ and different metallicities.

Model atmospheres

Illustration with *classical models:*

- 1D
- homogeneous
- hydrostatic
- Local Thermodynamic Equilibrium (LTE)
- convection: mixing-length theory
- **detailed radiative transfer with > 10^5 wavelengths**

opacities affect the thermal structure (line blanketing)

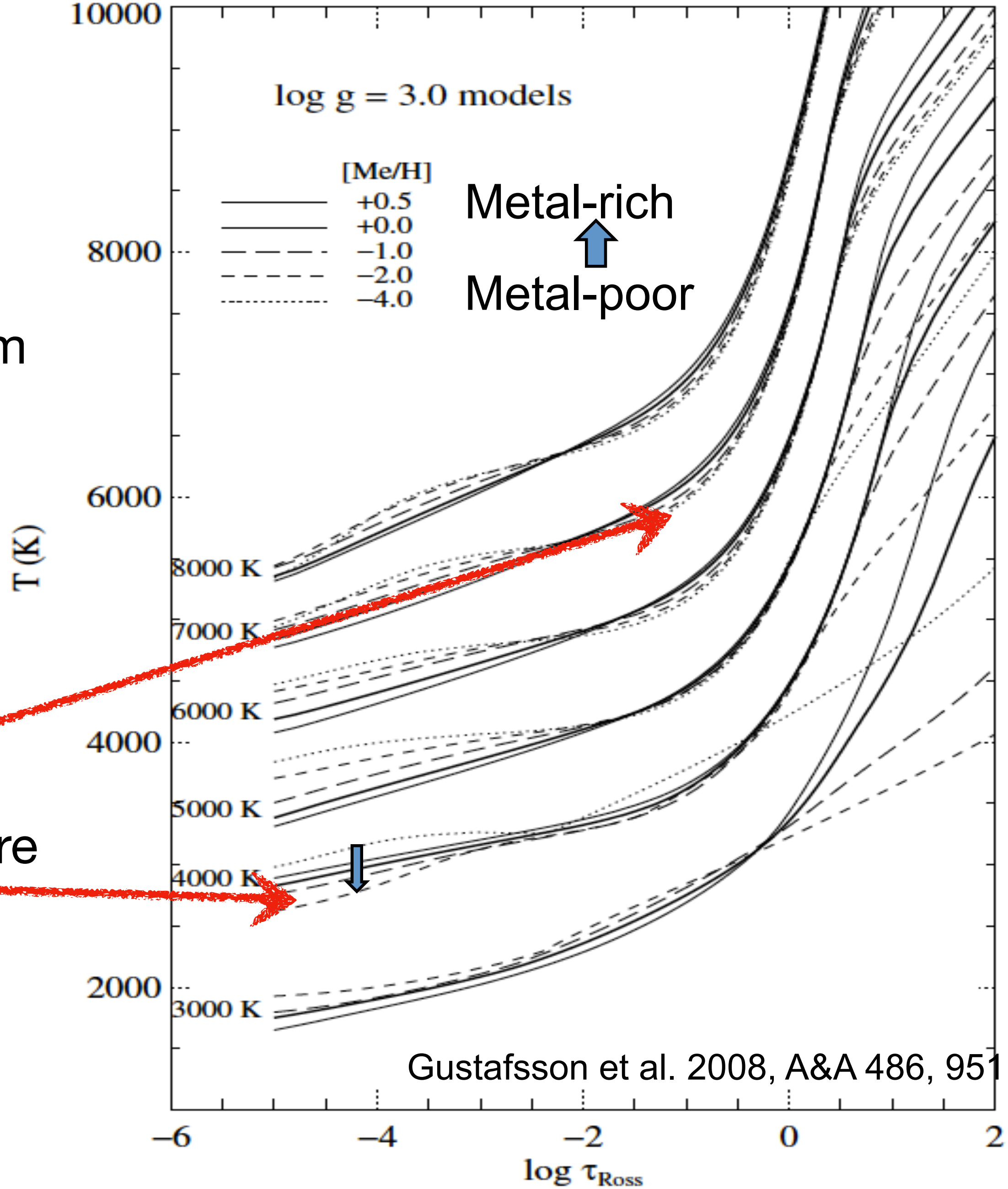


Fig. 2. The temperature structures for a set of model atmospheres with different $T_{\rm eff}$, $\log g = 3$ and different metallicities.

Model atmospheres

Illustration with *classical models:*

- 1D
- homogeneous
- hydrostatic
- Local Thermodynamic Equilibrium (LTE)
- convection: mixing-length theory
- **detailed radiative transfer with > 10^5 wavelengths**

opacities affect the thermal structure (line blanketing)

1D models include the **description of opacities in great detail**. This is their major advantage, … and they are quick to compute!

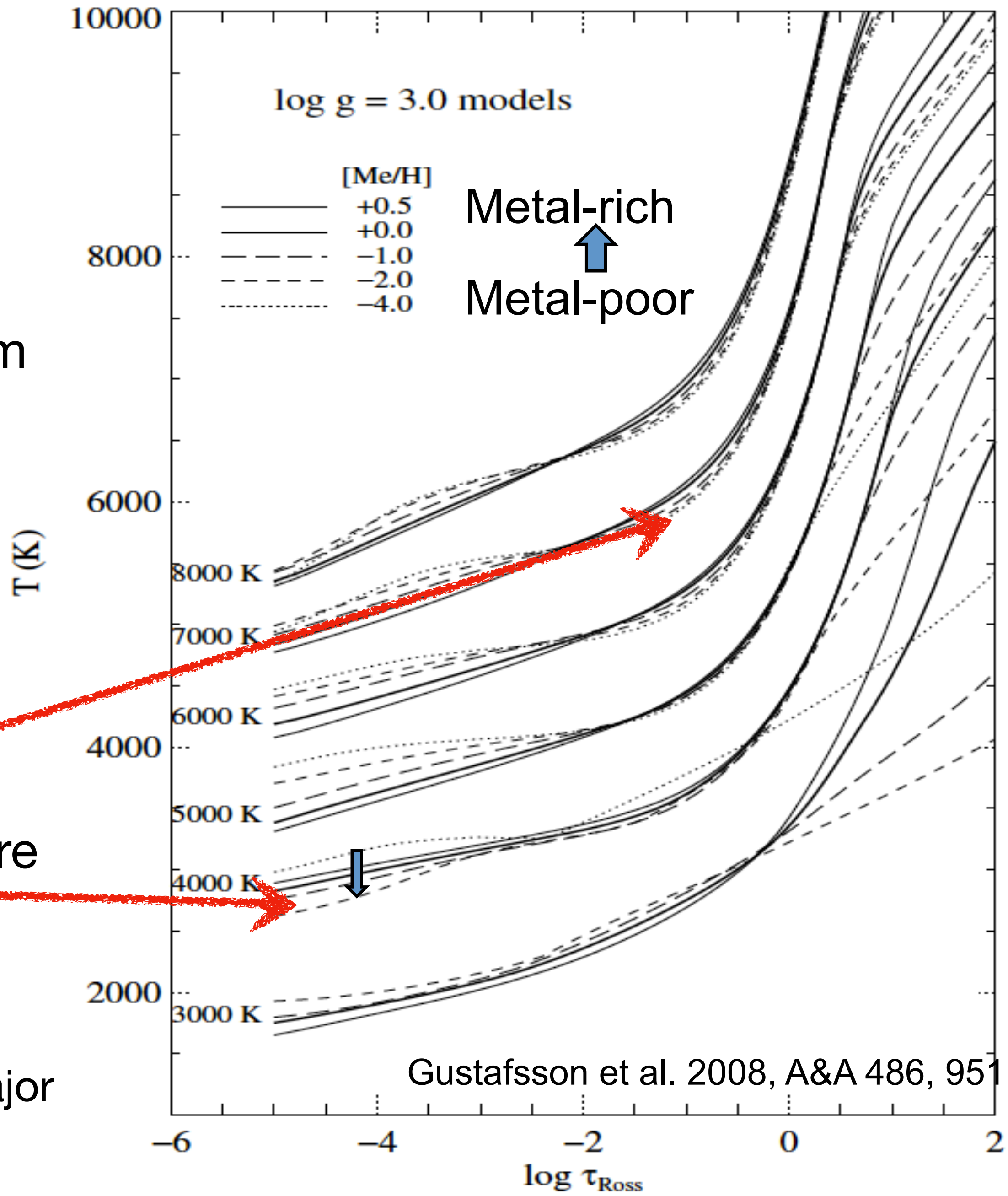
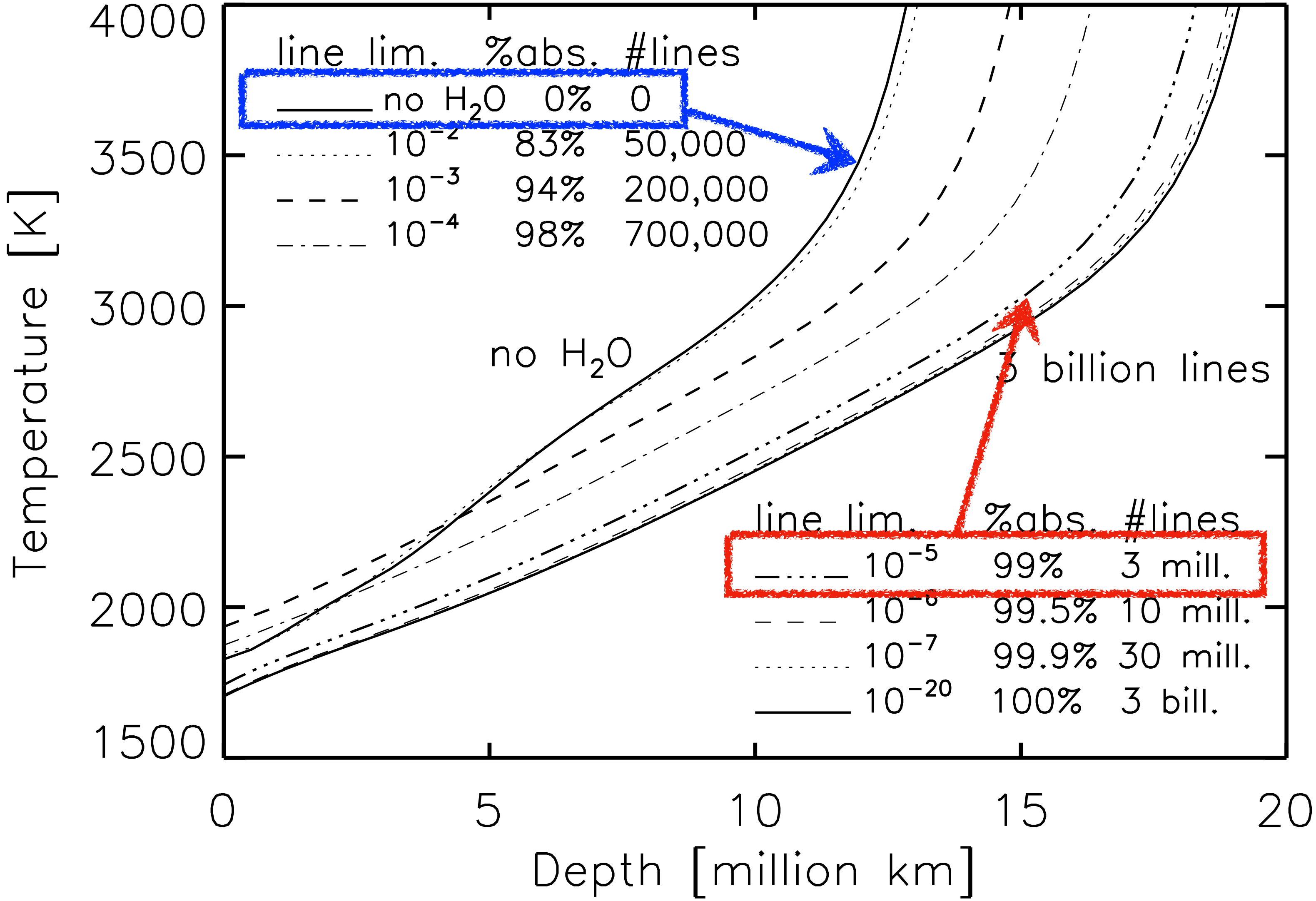


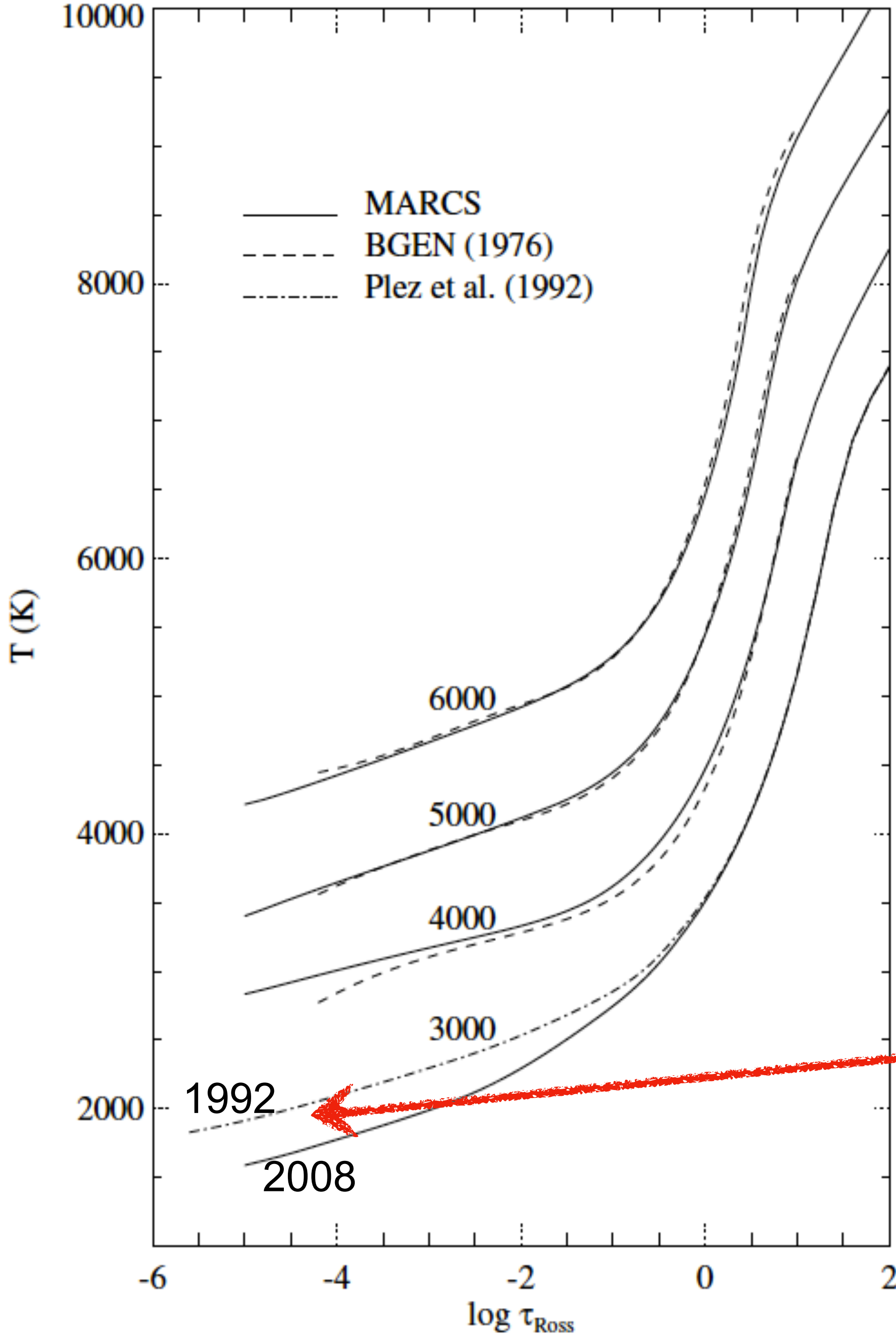
Fig. 2. The temperature structures for a set of model atmospheres with different T_{eff}, $\log g = 3$ and different metallicities.

Importance of using sufficiently complete line lists when computing stellar atmospheres



NB: line limit is in km/mol @ 3500K

Jørgensen et al. 2001, A&A 372, 249

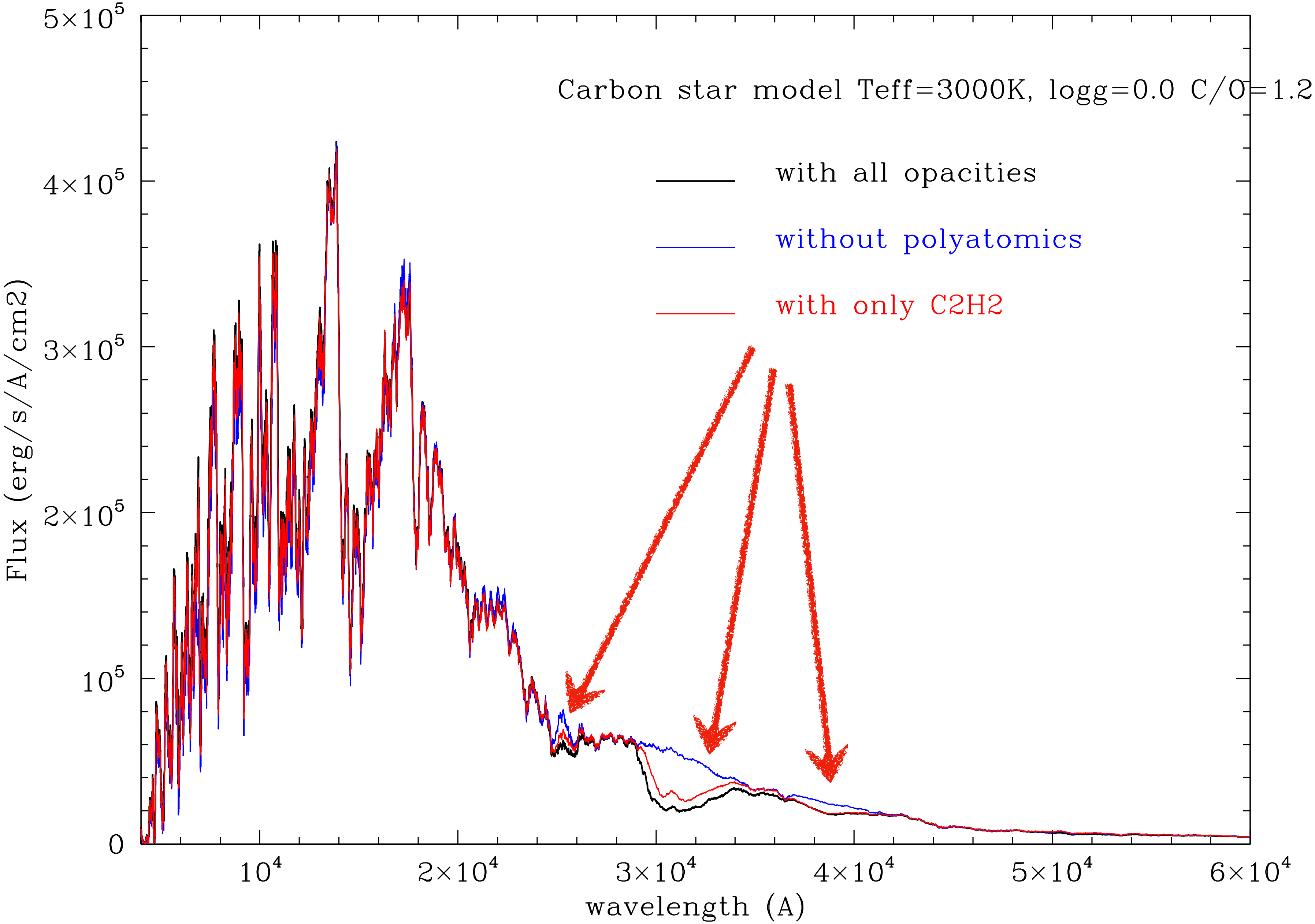


Importance of using sufficiently complete line lists when computing stellar atmospheres

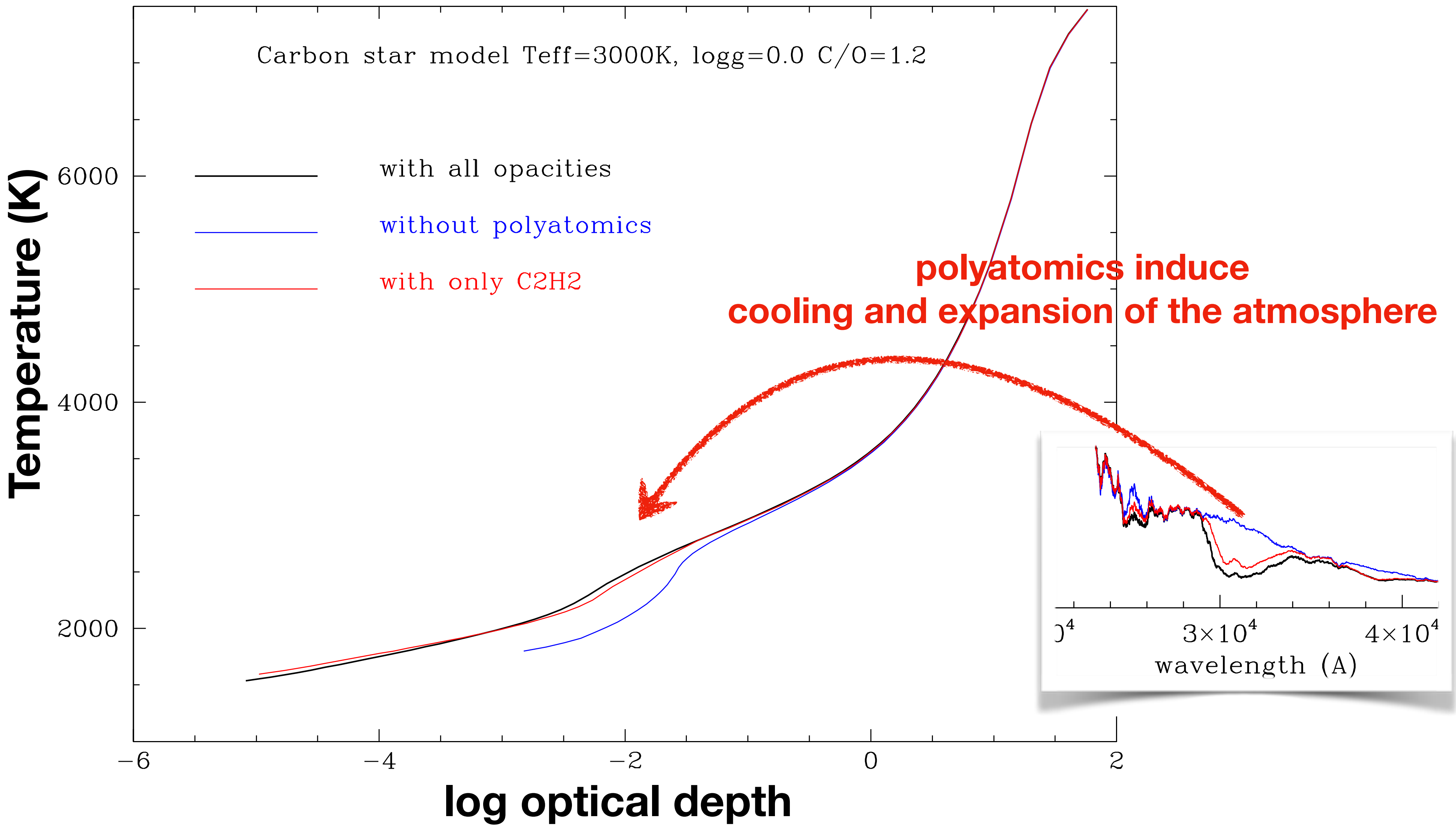
In 1992 MARCS models, H_2O opacity was *underestimated*, resulting in *hotter* surface layers (300K).

Gustafsson et al. 2008

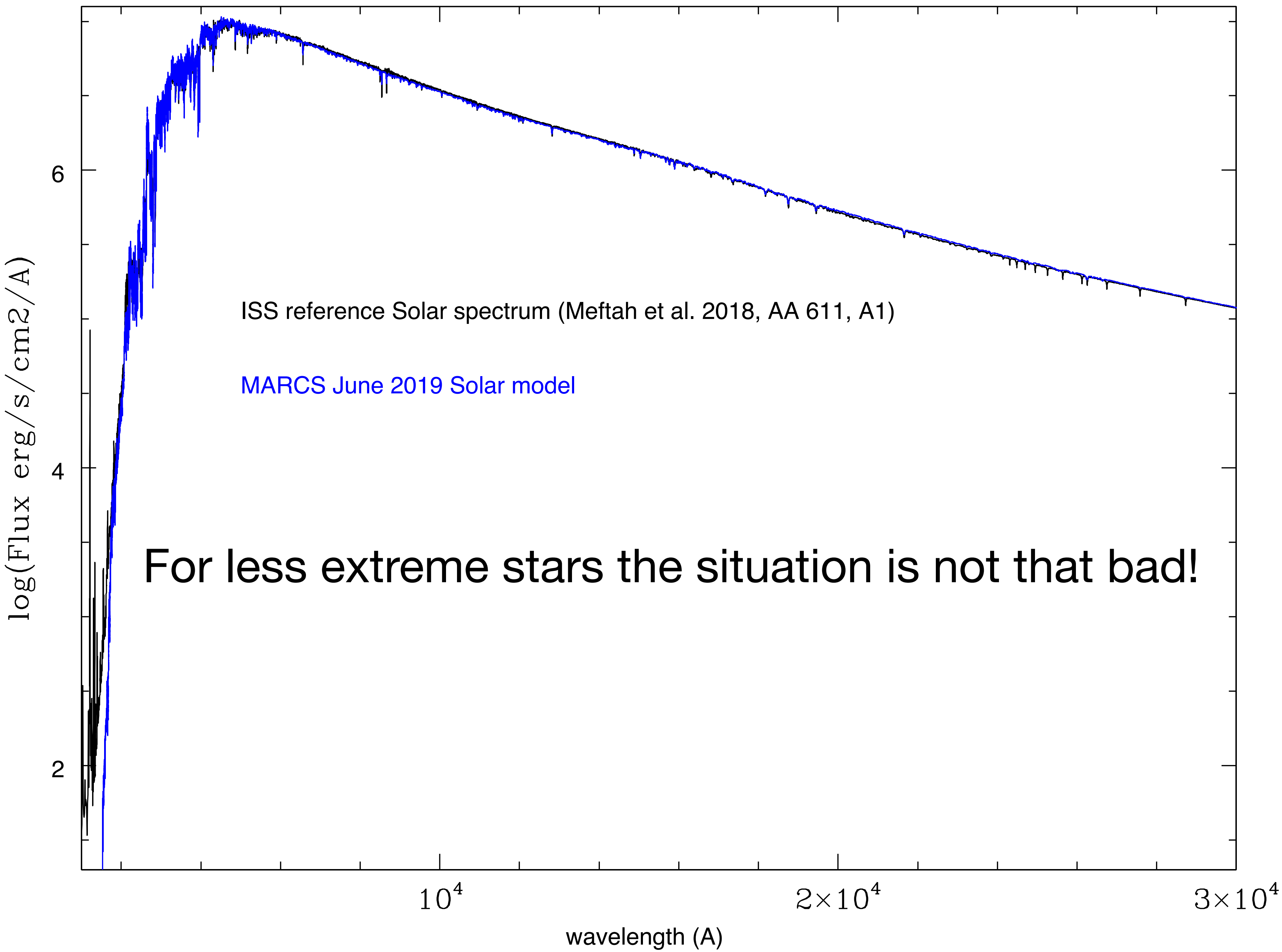
Importance of including all contributing species when calculating spectra



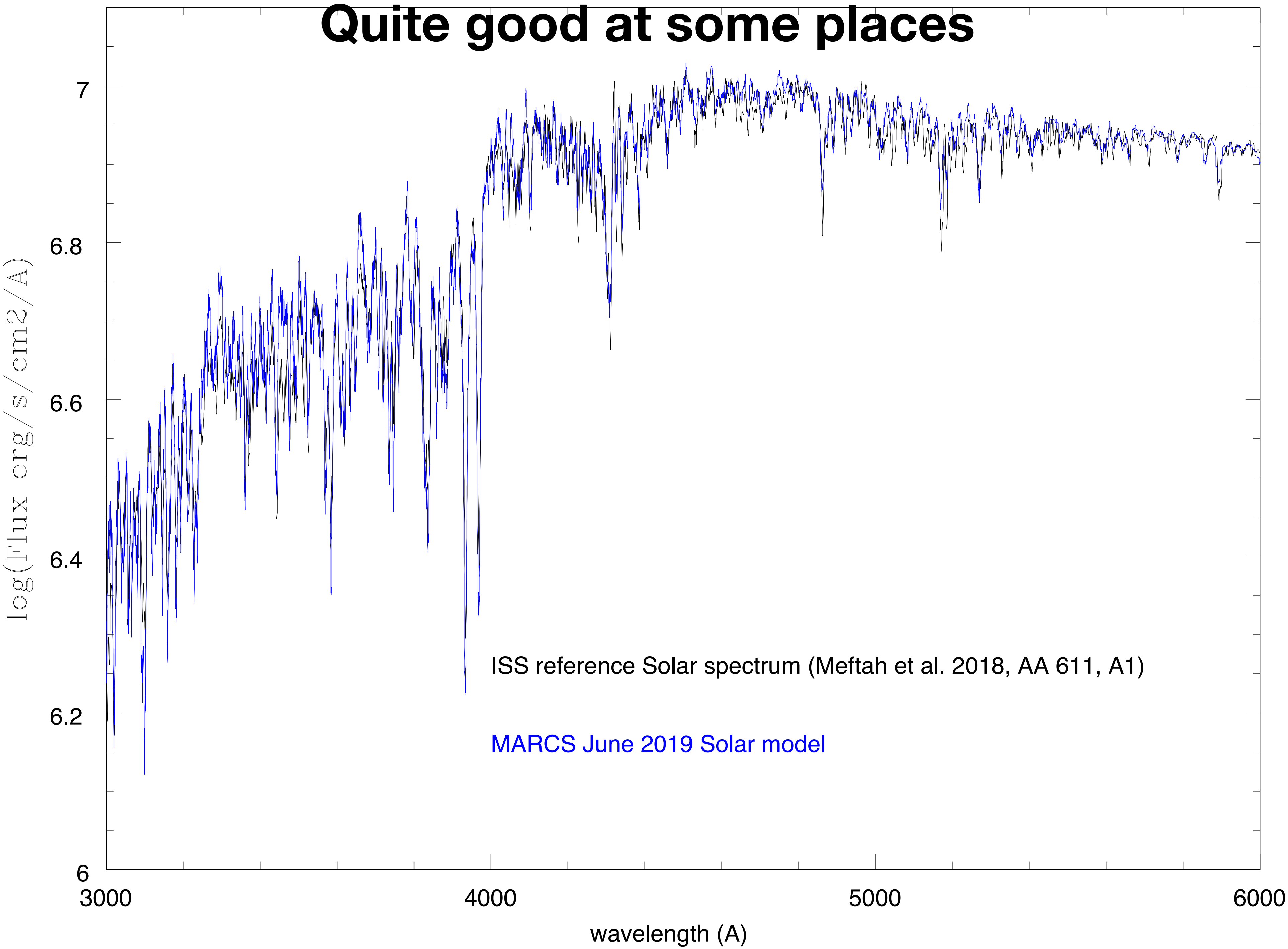
Impact on the model structure



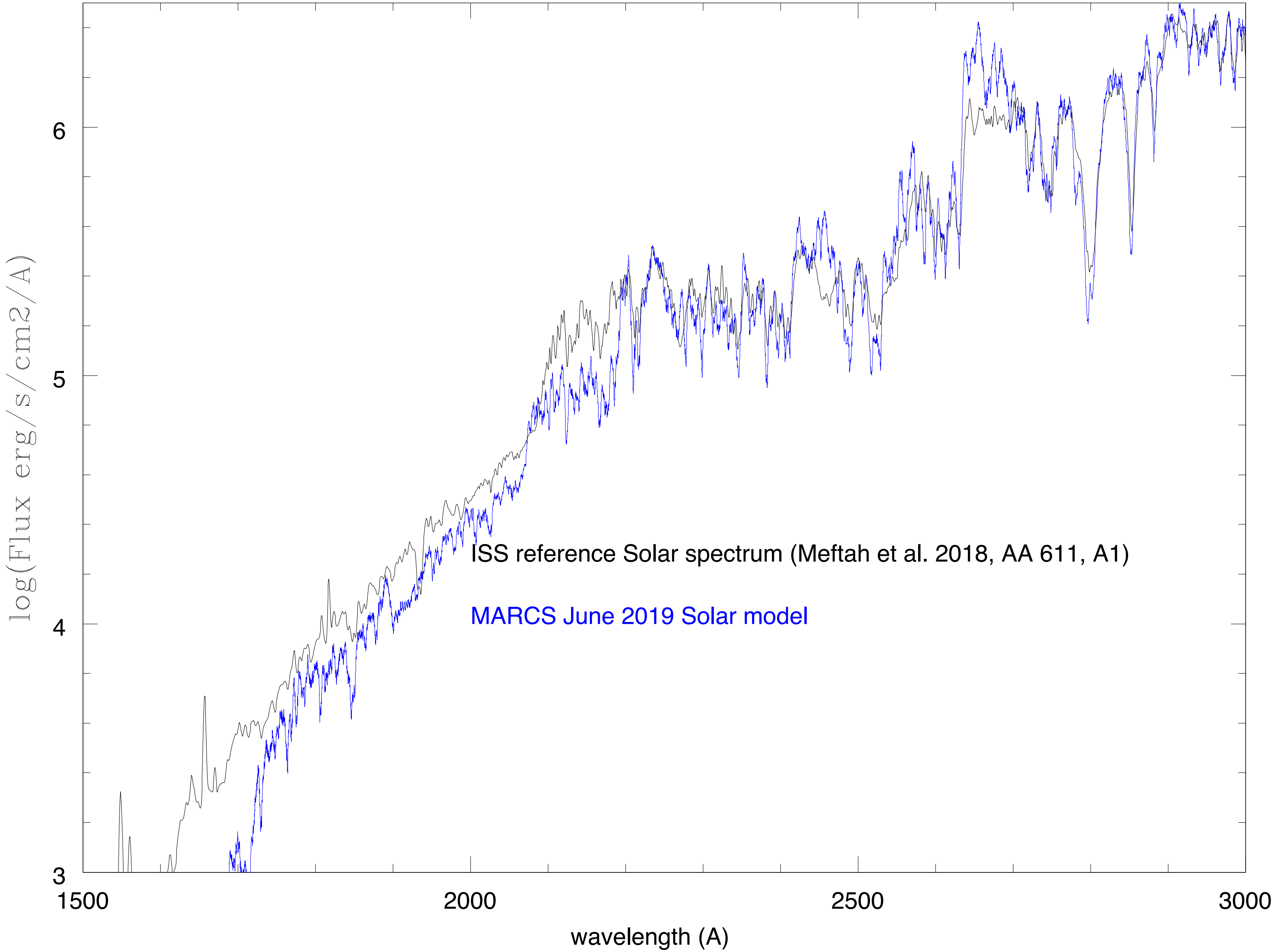
MARCS model of the solar spectrum



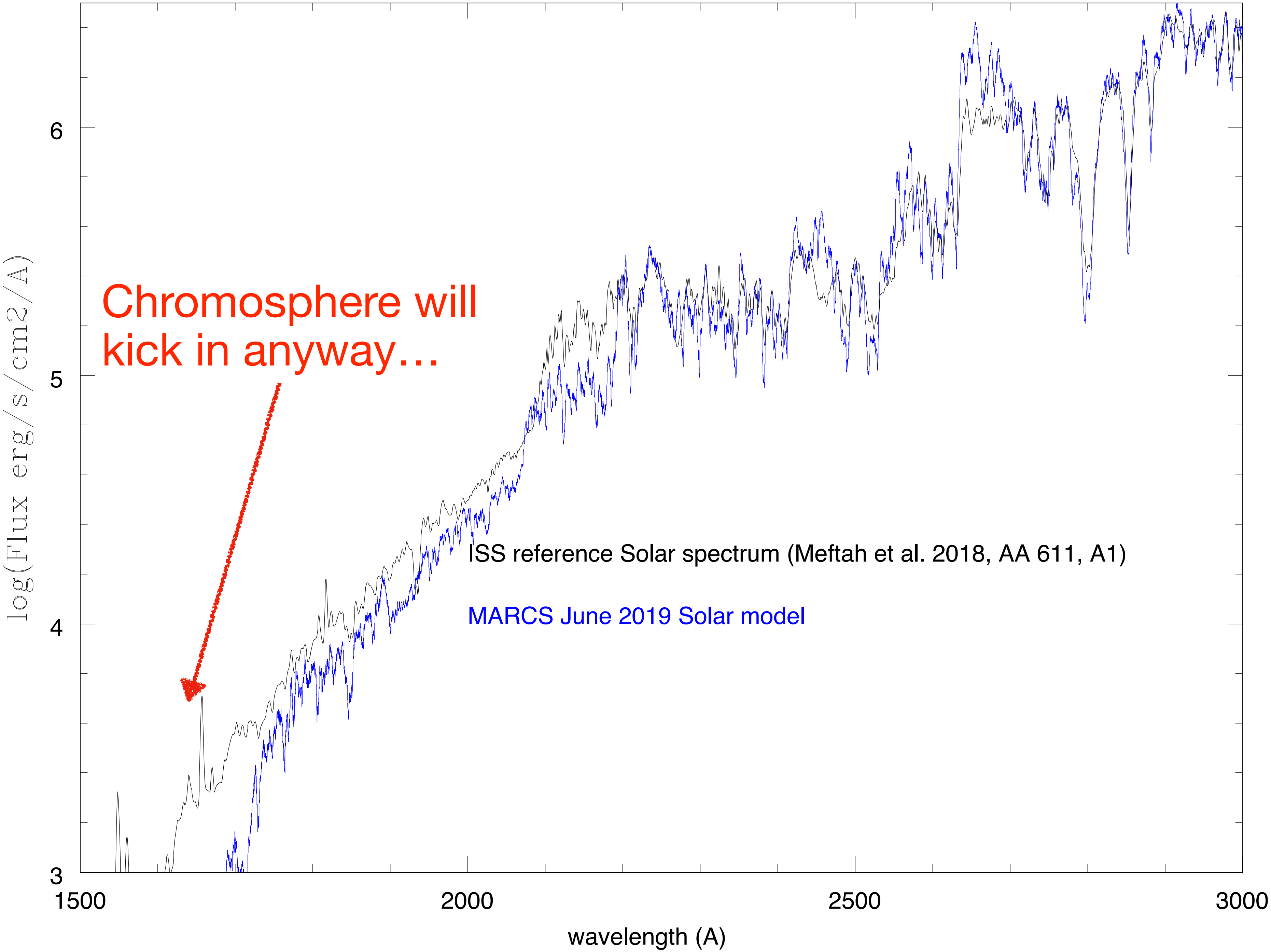
Quite good at some places



In need of improvement at some other places



In need of improvement at some other places

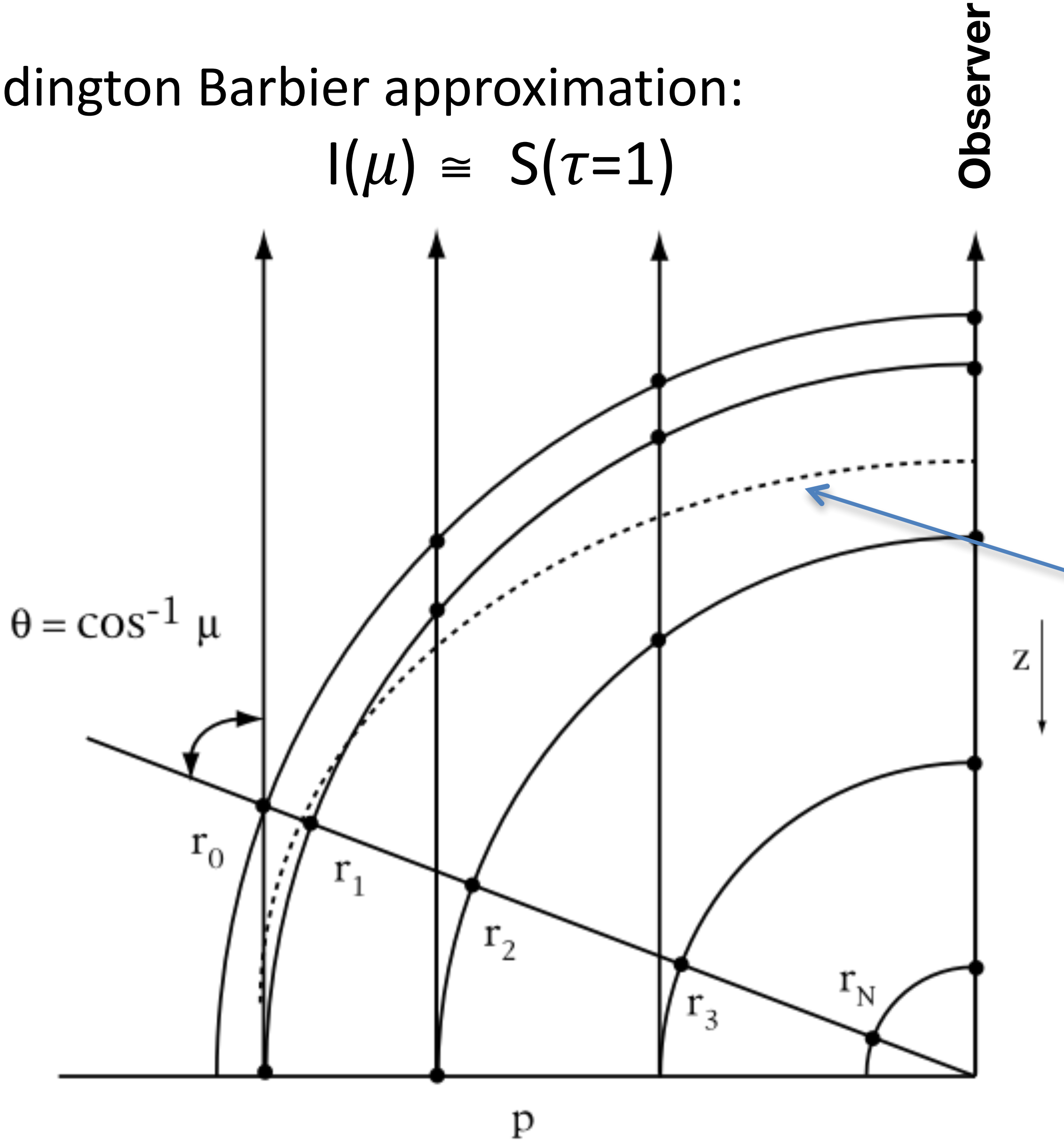


Limb darkening

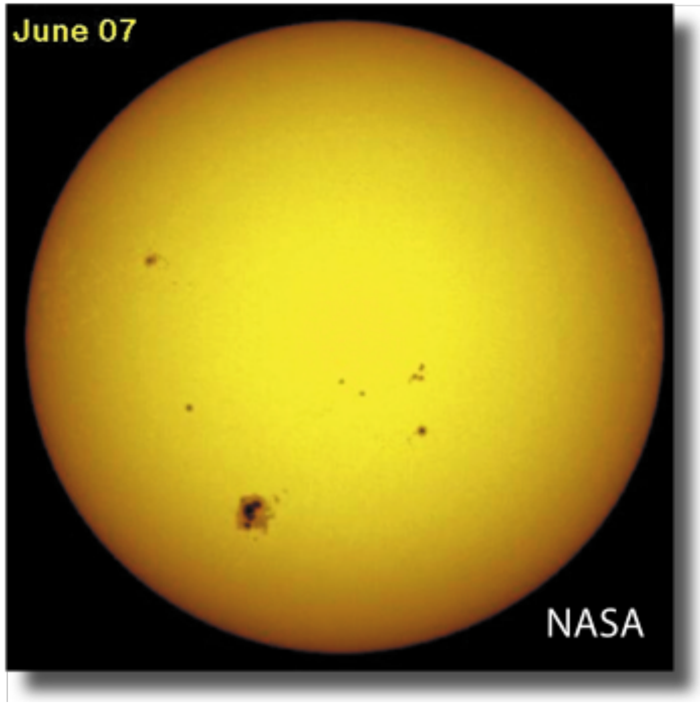
A stringent test of models

Eddington Barbier approximation:

$$I(\mu) \cong S(\tau=1)$$

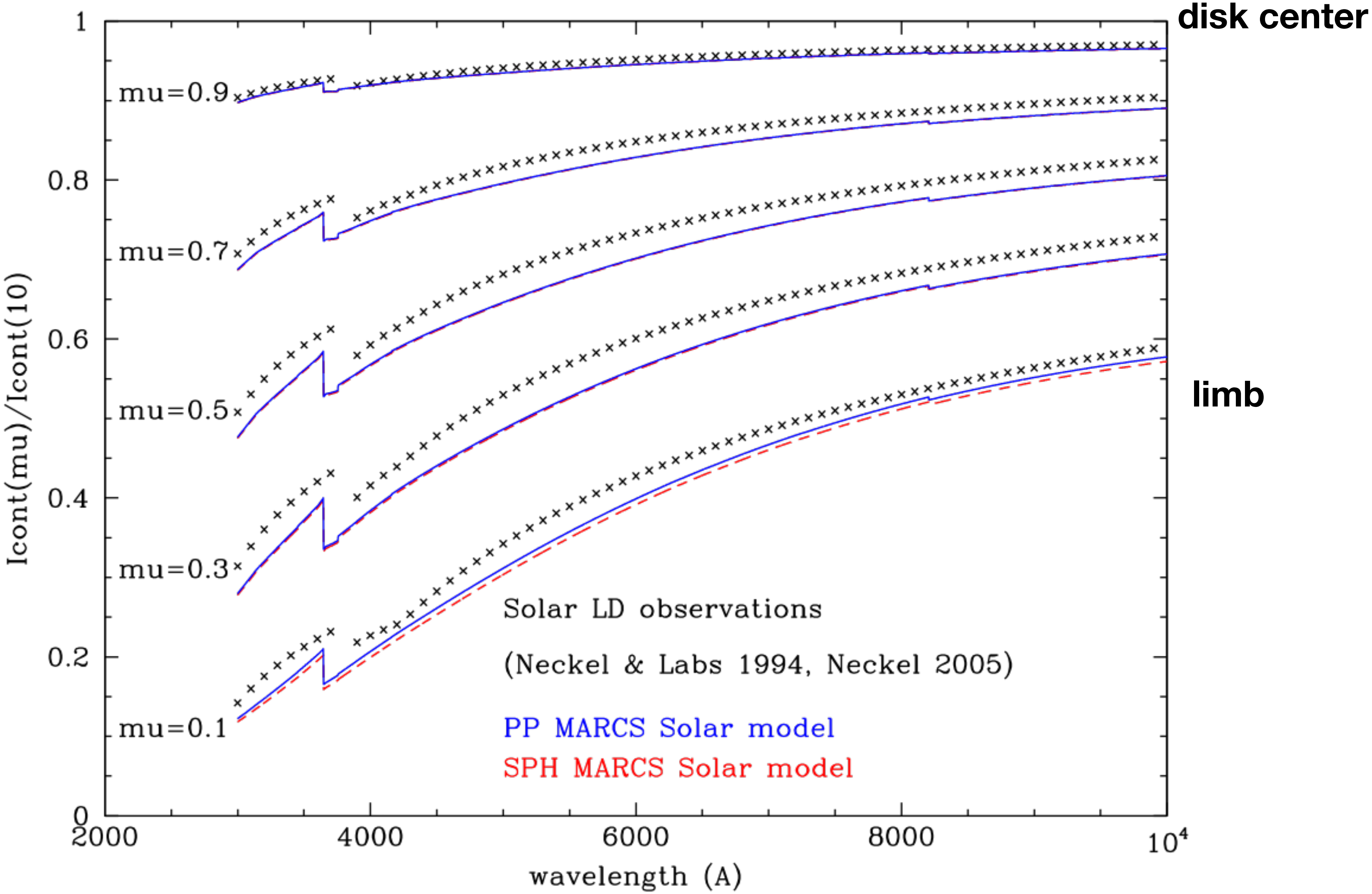


τ=1 surface for observer



Solar continuum limb darkening: 1D models

1D models do not reproduce the solar limb darkening.
Their thermal gradient is too steep



1D LTE model atmosphere codes and grids

MARCS (Gustafsson et al. 2008 A&A 486, 951) FGKMSC stars, ongoing update to include A-type + improve line and continuum opacities.

grids: https://marcs.astro.uu.se

https://marcs.oreme.org (unlimited download)

ATLAS (Kurucz 2005, MSAIt suppl 8, 189) all types (but hot models should be NLTE, and some molecules missing in coolest)

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

PHOENIX (Hauschilldt 1992, JQSRT 47, 433; 1993, JQSRT 50, 101) Also for NLTE, expanding envelopes etc.

grids for hydrostatic models, including brown dwarfs

https://lydu.ens-lyon.fr/phoenix/

Lines

Huge progress in the past decades concerning the knowledge of spectral lines

However:

Heiter et al. (2015) find problems when comparing calculated spectra with Gaia-ESO survey spectra.

- master line list built from databases (VALD) + molecules
- specific laboratory work for some lines
- careful selection of gf-values (lab or calculated), collisional broadening, with quality flags

=> still unidentified lines in the optical spectrum of FGK stars!

Heiter et al. 2015
3 iron lines with different quality flags :
Y = yes
U = undecided
N = no

Black line is observation
red and blue calculations

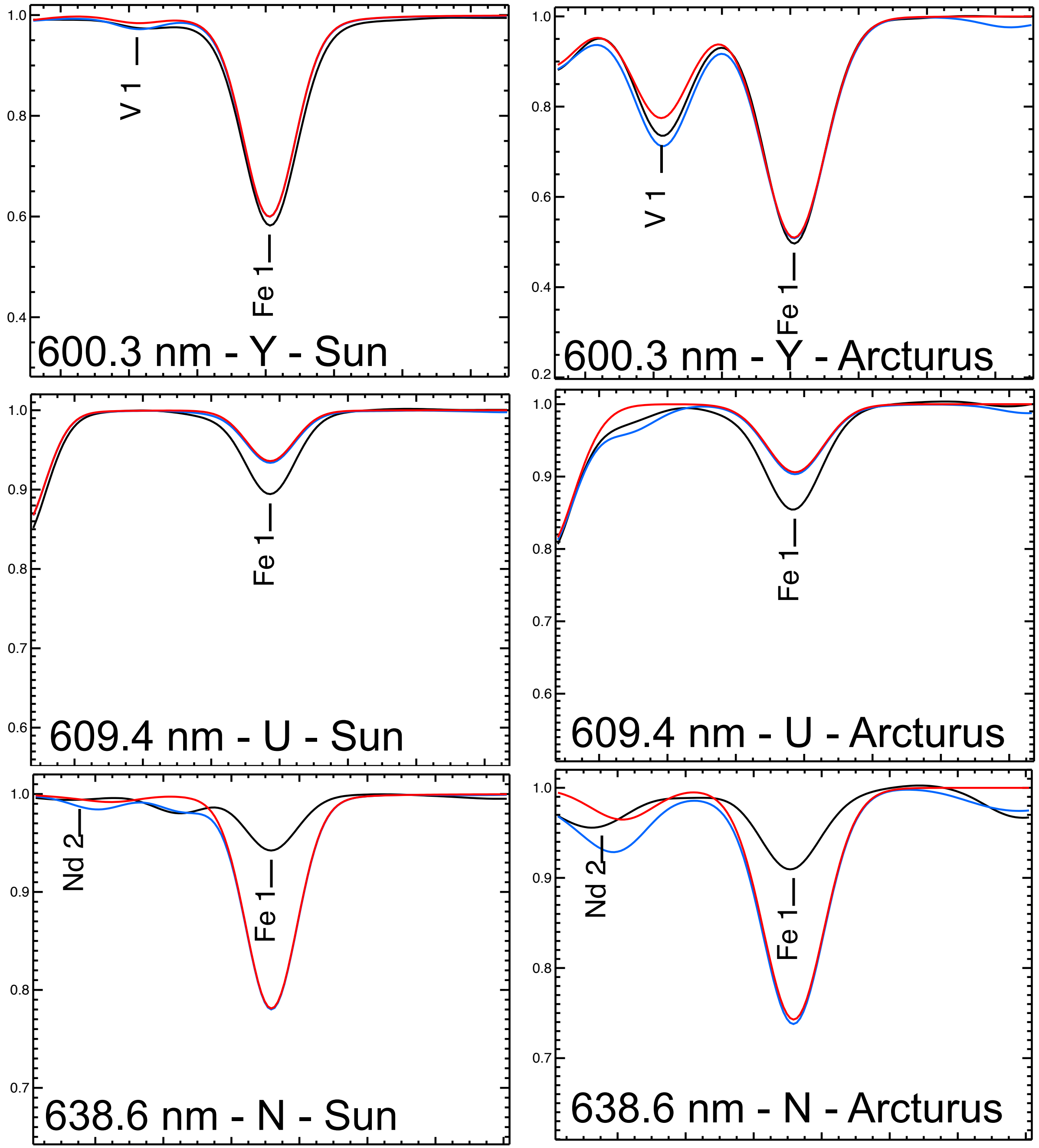


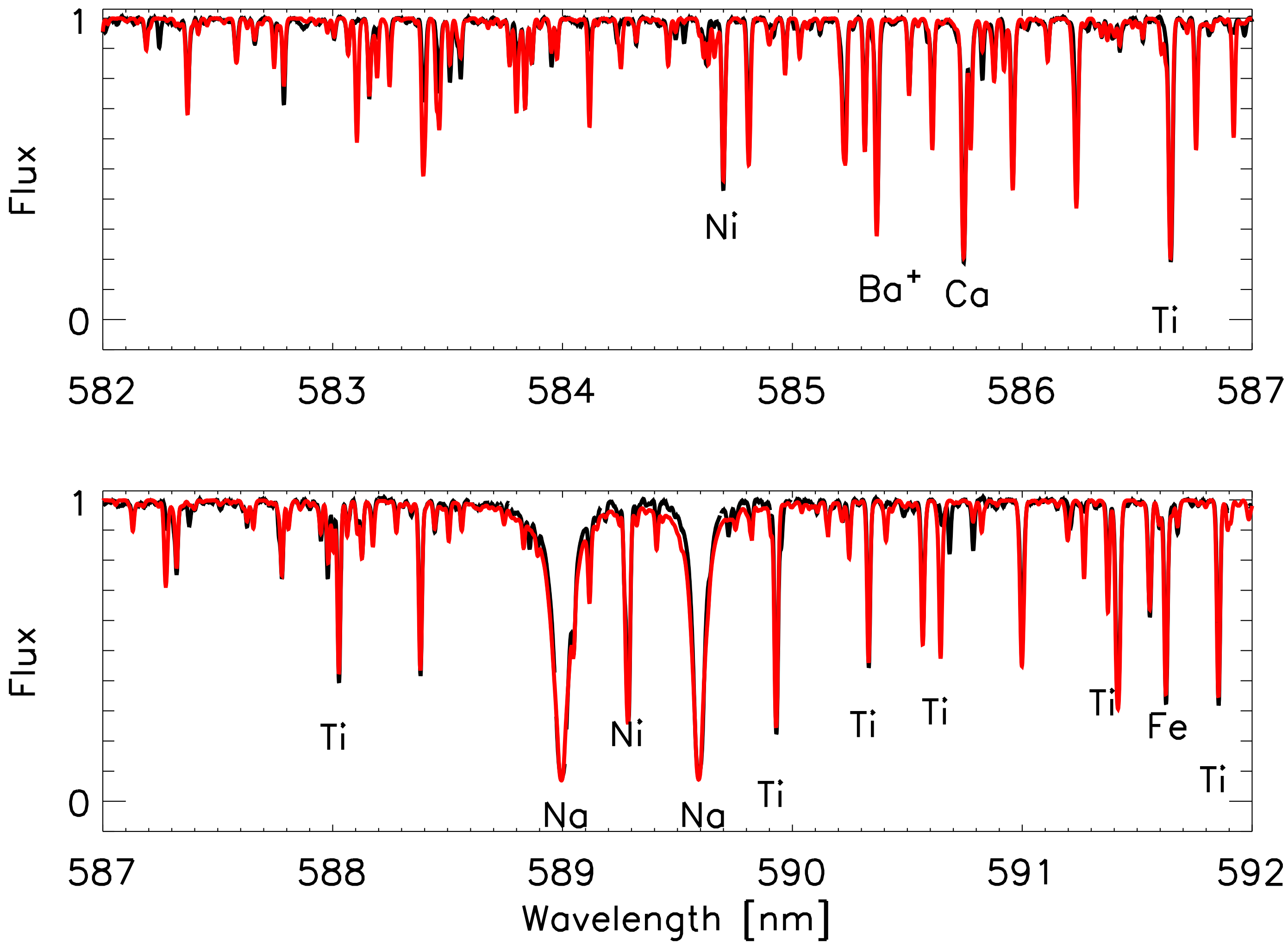
Figure 3. Comparison of observed and synthetic spectra around three Fe lines with different flags (Y for *Yes*, U for *Undecided*, N for *No*) for the Sun (left) and Arcturus (right). Black lines: observations, red lines: calculations including preselected spectral lines only, blue lines: calculations including blends.

see also the BRASS effort: talk by Alex Lobel and poster by Mike Laverick

Completeness of line data

A number of lines are still missing, or have insufficiently accurate data, even for FGK stars!

observed and calculated spectrum of Arcturus



Heiter et al. 2015, Phys. Scr 90, 054010

Figure 4. Observed (black) and calculated (red) spectra for Arcturus around the Na doublet lines at 589 nm. The calculations include the full Gaia-ESO line list.

Huge progress in the past decades concerning the knowledge of spectral lines

However:

Heiter et al. (2015) find problems when comparing calculated spectra with Gaia-ESO survey spectra.

- master line list built from databases (VALD) + molecules
- specific laboratory work for some lines
- careful selection of gf-values (lab or calculated), collisional broadening, with quality flags

=> still unidentified lines in the optical spectrum of FGK stars!

Need laboratory work, and calculations.

And use stellar spectra, where higher levels may get excited:

E.g. Peterson and Kurucz (2015): identification of high-lying FeI energy levels using stellar spectra.

See also Masseron et al. (2014): same thing for CH.

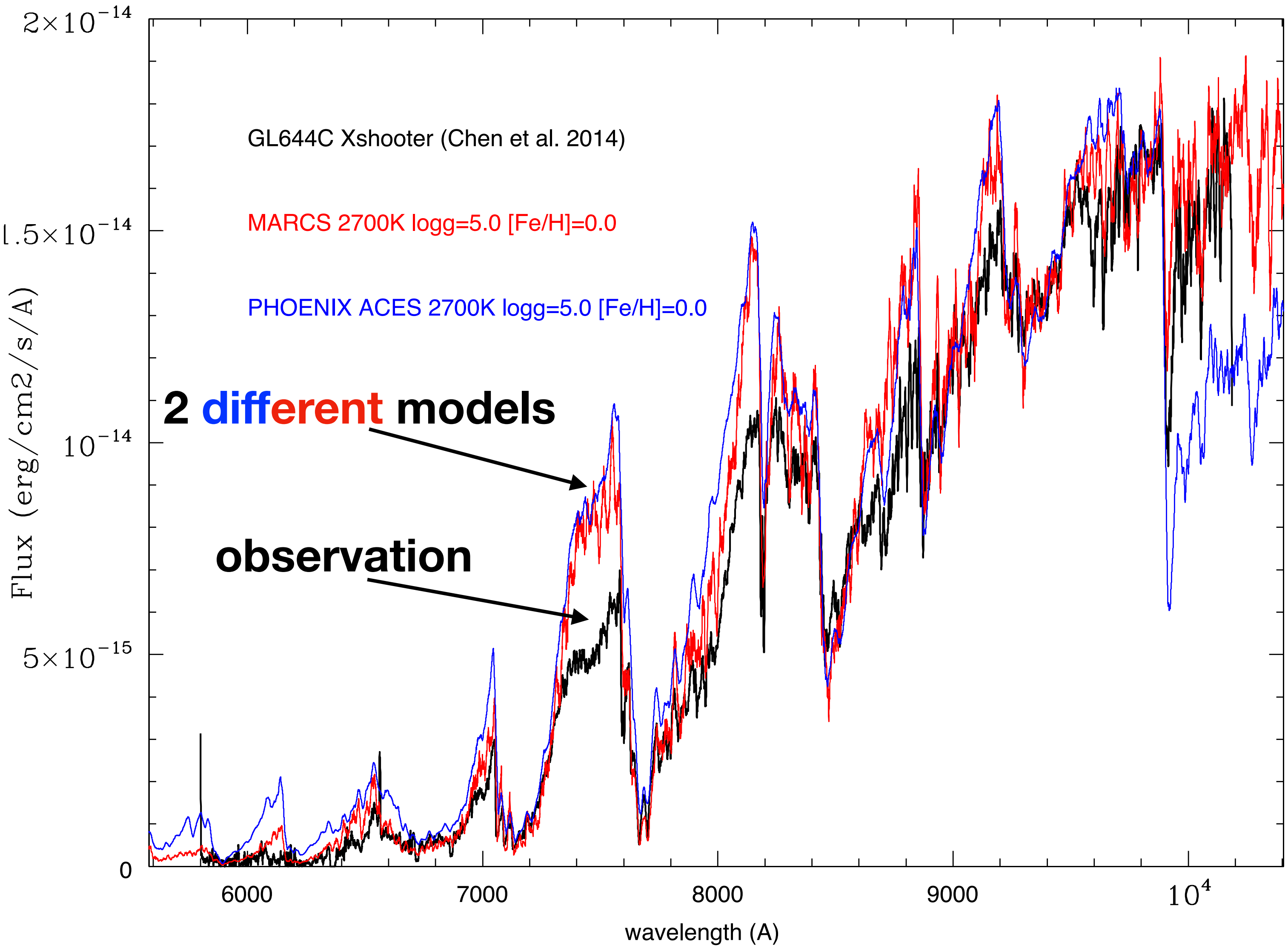
Table 2

New Fe I Levels and Energies

Expanded Label	Label	J	E (cm^{-1})	σ (cm^{-1})
23 Even Levels:				
3d6 4s(6D)4d e7F	4s6D4d e7F	0	51143.92	0.03
3d7(4F)4d 5D	(4F)4d 5D	0	54304.21	0.02
3d6 4s(6D)4d 5D	4s6D4d 5D	0	58428.17	0.03
3d6 4s(4D)4d 5P	4s4D4d 5P	1	58628.41	0.03
3d7(4P)5s 3P	(4P)5s 3P	1	59300.54	0.03
3d6 4s(4D)4d 3D	4s4D4d 3D	2	58779.59	0.02

Another example: cool M dwarf

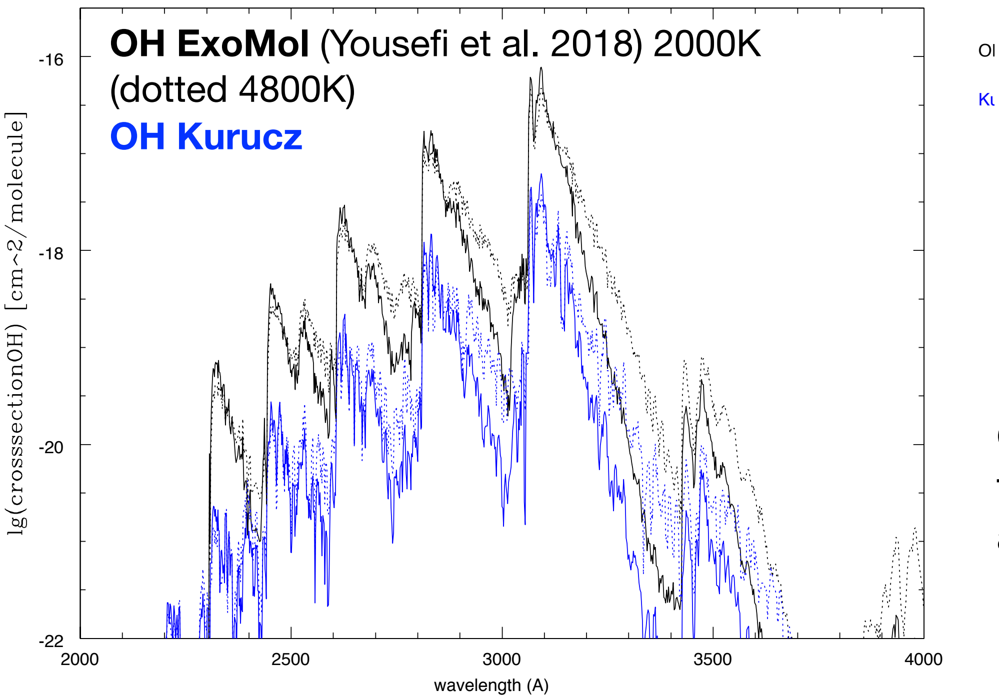
Improvements needed in terms of line list completeness and line strengths

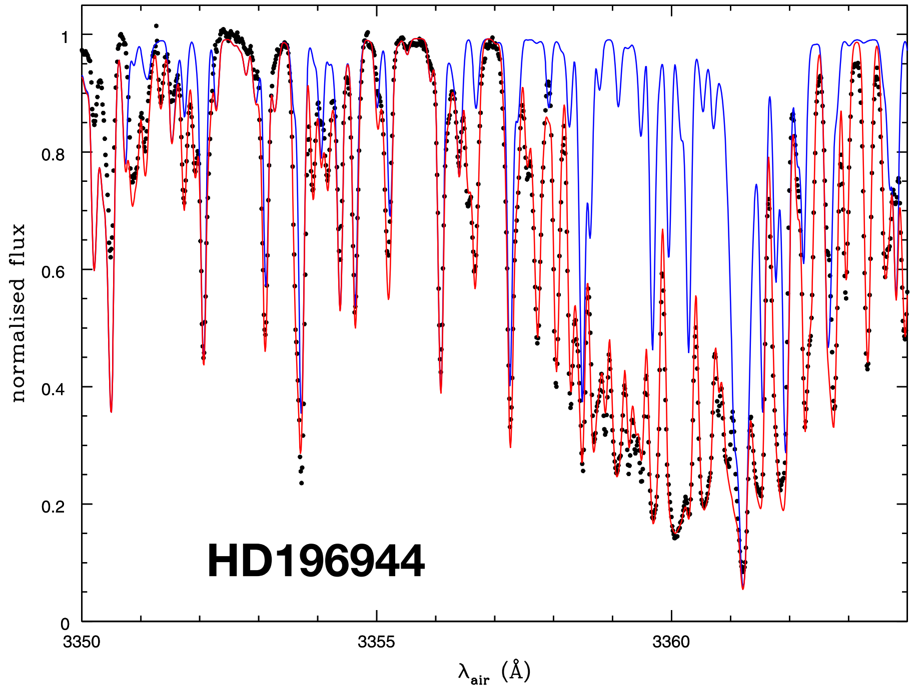


Molecules

Large scale efforts, esp. **ExoMol** (J. Tennyson et al.): calculations and compilations of **line lists for many molecular species**

- targeted towards planets and (very) cool stars
- mostly for opacities, i.e. aiming at completeness in terms of levels and transitions
- not always accurate for spectroscopy.





NH: improved line list in red
(Bernath 2020, JQSRT 240, 106687)

Other theoretical and experimental efforts going on, thanks to a number of dedicated groups in atomic and molecular physics

Molecules

Search molecules: Search by formula

Exomol 2021 Nov 8

metal hydrides

- MgH
- NaH
- NiH
- AlH
- CrH
- CaH
- BeH
- TiH
- FeH
- LiH
- ScH

other diatomics

- PN
- KCl
- NaCl
- LiCl
- CN
- C_2
- H_2

other hydrides

- NH
- CH
- OH
- HCl
- SiH
- SH
- HF
- PH

ions

- LiH^+
- H_2^+
- HeH^+
- H_3^+
- OH^+
- H_3O^+

metal oxides

- VO
- AlO
- YO
- MgO
- TiO
- SiO
- CaO

larger molecules

- CH_4
- NH_3
- HNO_3
- H_2O_2
- H_2CO
- SO_3
- SiH_4
- CH_3F
- CH_3Cl
- C_2H_4
- C_2H_2

other oxides

- CO
- NO
- PO
- O_2

triatomic molecules

- H_2O
- CO_2
- SO_2
- HCN
- N_2O
- H_2S
- OCS
- KOH
- NaOH
- SiH_2
- SiO_2

- CS
- CP
- PS
- NS
- SiS
- NaF
- AlCl
- AlF
- KF
- LiF
- CaF
- MgF
- N_2

- AsH_3
- PF_3
- PH_3
- CH_3
- cis-P_2H_2
- trans-P_2H_2

ExoMol is funded by the ERC under the Advanced Investigator Projects 267219 and 883830

BRASS: Belgian Repository of Fundamental Atomic Data and Stellar Spectra

=> removing all systematic errors in atomic input data required for quantitative stellar spectroscopy.

The project thoroughly assesses the quality of fundamental atomic data available in the largest repositories by comparing very high-quality observed stellar spectra with state-of-the-art theoretical spectra.

PI: A. Lobel & P. Royer

Resources for line data

R.L. Kurucz home page: enormous ressource, but not always well documented, e.g., input data used to construct line lists.

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

VALD database: atomic lines + some molecules. Compilation of many sources, with quality flags : vald.astro.uu.se

BRASS database: Belgium, very careful quality assessment

http://brass.sdf.org

Molecular data scattered on many sites, but main resource is:

Exomol at University College London : https://www.exomol.com

Bernath group: http://bernath.uwaterloo.ca/molecularlists.php

see also, for **Turbospectrum**,

https://nextcloud.lupm.in2p3.fr/s/r8pXijD39YLzw5T

LTE codes for spectrum synthesis

Input = model atmosphere + line list

computes atomic and molecular equilibrium + level populations

computes continuum and line absorption + scattering

solves radiative transfer equation along rays

Output = intensities, flux spectrum, equivalent widths, …

Difficulties you may run into

Code without documentation

=> Risk of error when providing input to, or when interpreting output from the code

=> Some limits of the code (temperature, ionisation stages, species, ...) may not be known

=> Some options may remain hidden to the user. Only the developer knows

=> Risk of dangerous options or setup -> erroneous output with no obvious warning

=> look at the source code, but it will probably be intricate !

Code WITH documentation

=> Still risk that it is not read... ;-) … so, read it!

=> Something may have been forgotten (it is time-consuming 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.

1D spectrum synthesis codes (LTE)

•**SYNTHE** (R.L. Kurucz) : PP, companion to ATLAS models code.
https://github.com/dobos/kurucz-synthe

•**Turbospectrum** (B. Plez) No “cookbook”. PP or Sph, F-MSC stars, 600 molecules, fast with many lines, line broadening from Barklem et al., no plotting interface. Companion to MARCS models.
https://github.com/bertrandplez/Turbospectrum2019
NLTE departure tables version in development.

•**MOOG** (C. Sneden) available on the web, PP, older version pure LTE (S=B), F-K stars, with documentation
https://en.wikipedia.org/wiki/Moog_(code)

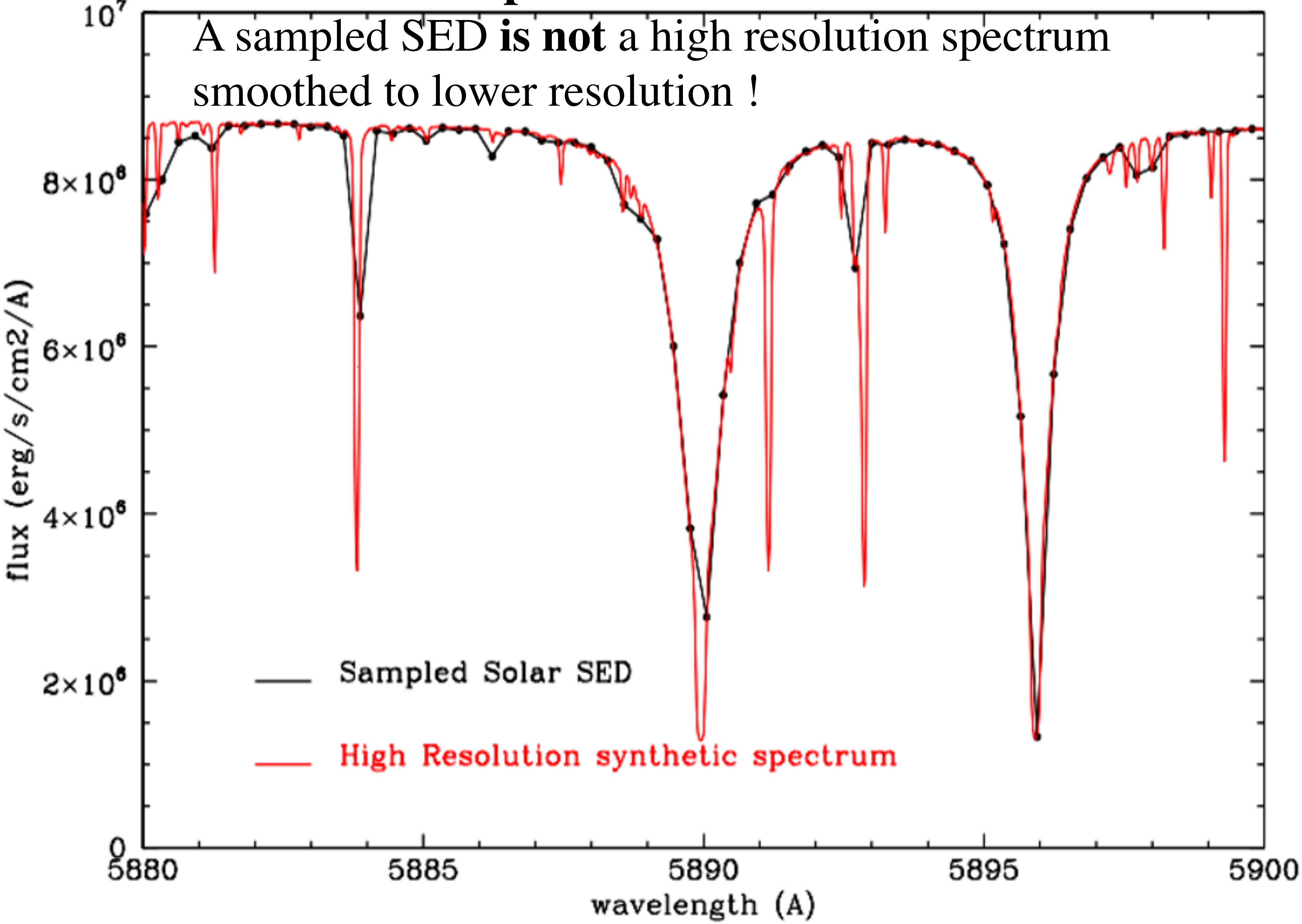
•**SME** (J. Valenti & N. Piskunov) : abundance stratification, automatic determination of stellar parameters and abundances, NLTE departure tables
https://www.stsci.edu/~valenti/sme.html
PySME: **http://sme.astro.uu.se/poster.html**

•**SPECTRUM** (Gray), documented, includes a few molecules, PP
https://www.appstate.edu/~grayro/spectrum/spectrum.html

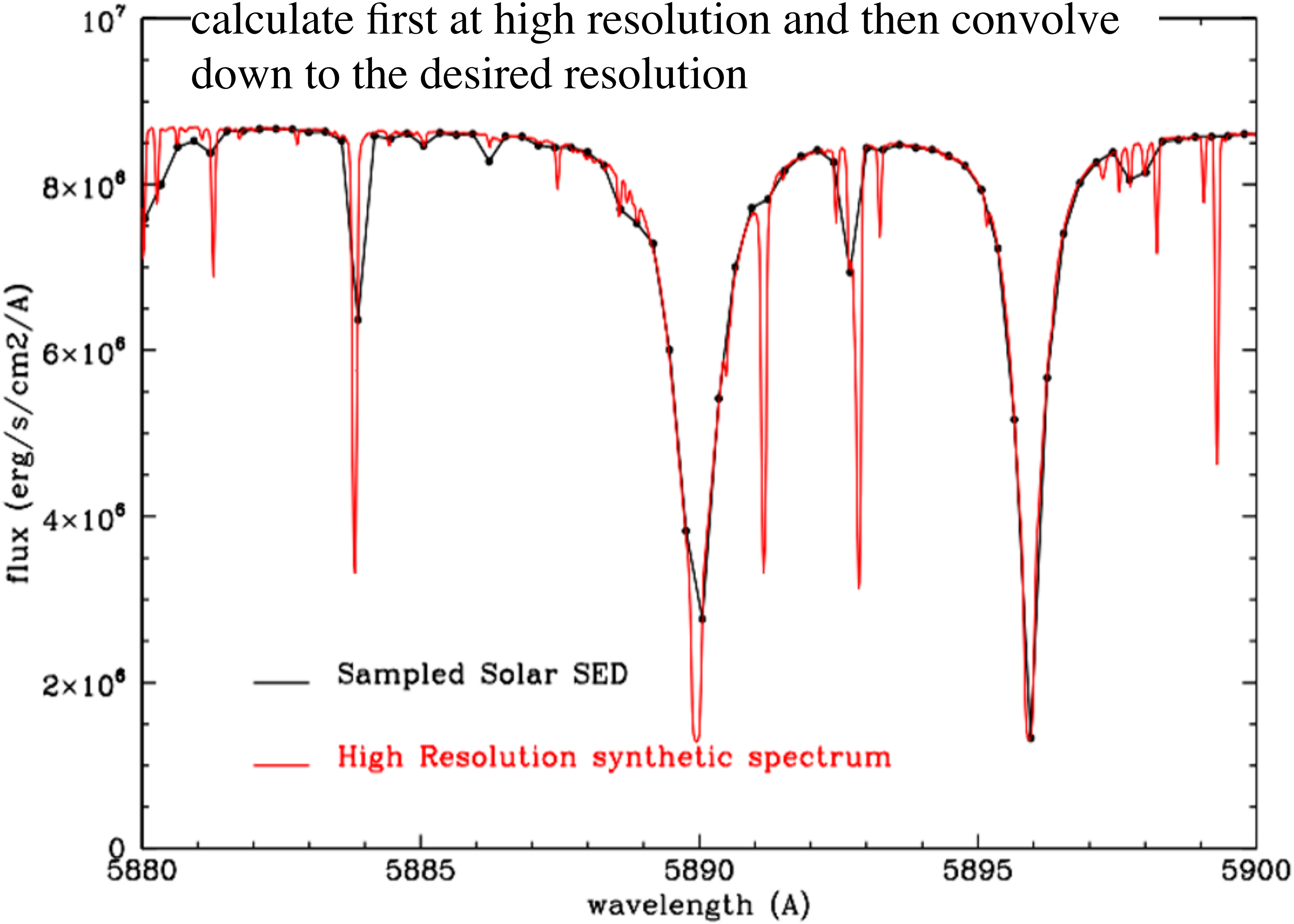
Words of caution

Spectral resolution

A sampled SED **is not** a high resolution spectrum smoothed to lower resolution !



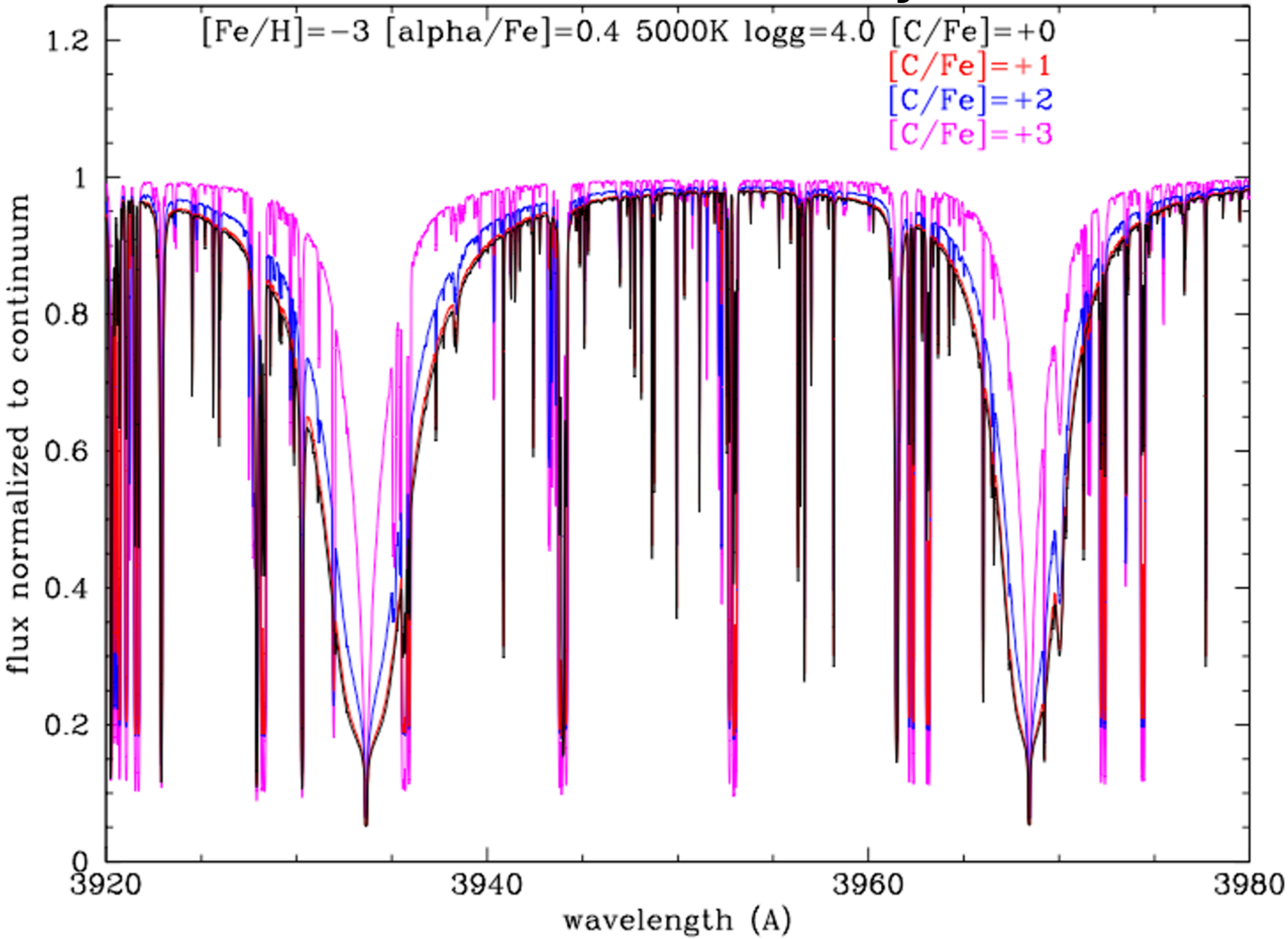
If you need a low resolution spectrum, calculate first at high resolution and then convolve down to the desired resolution



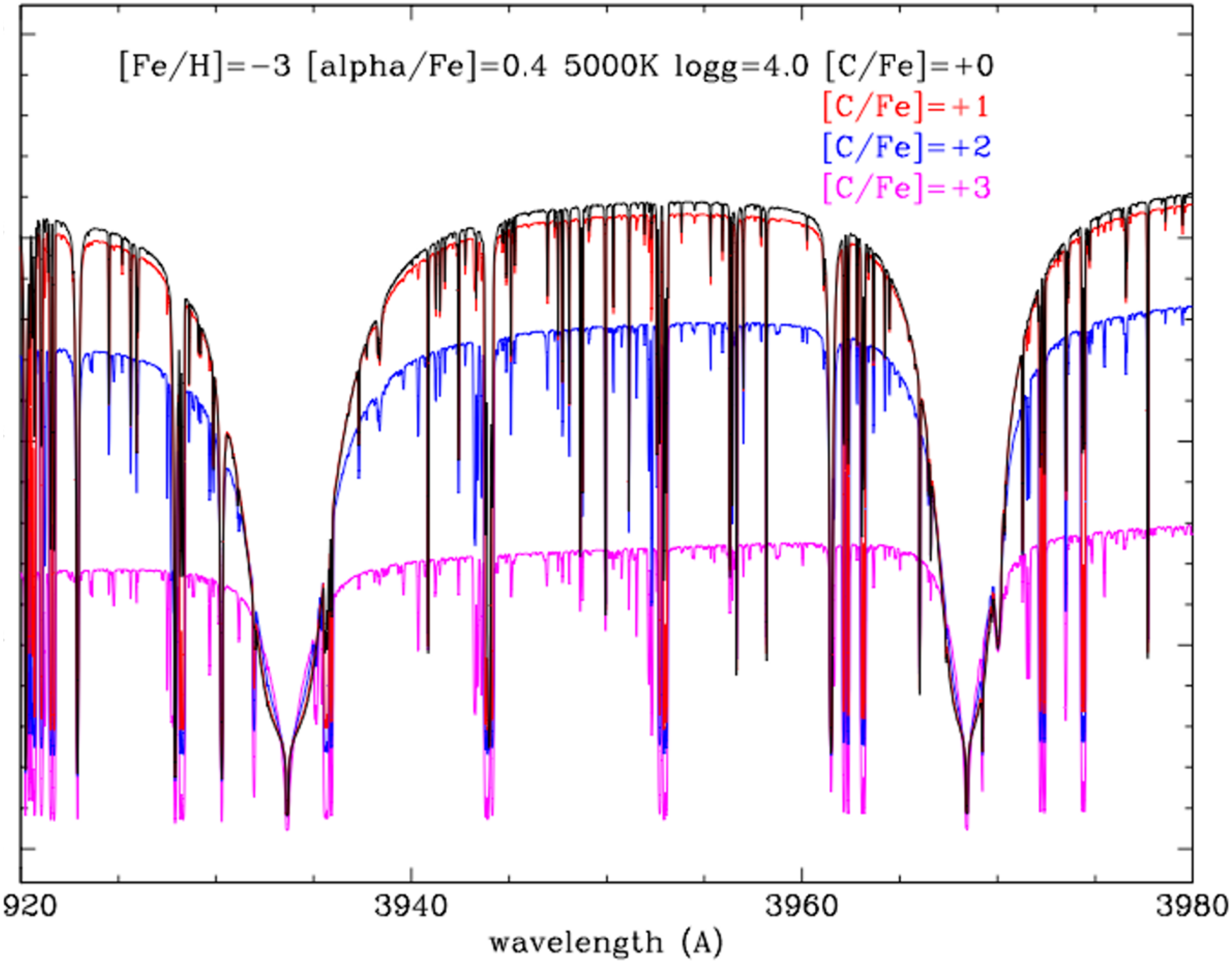
Surprising results

Effect of carbon enhancement on Ca II H&K

Looks like Ca becomes fainter. **Why is that???**

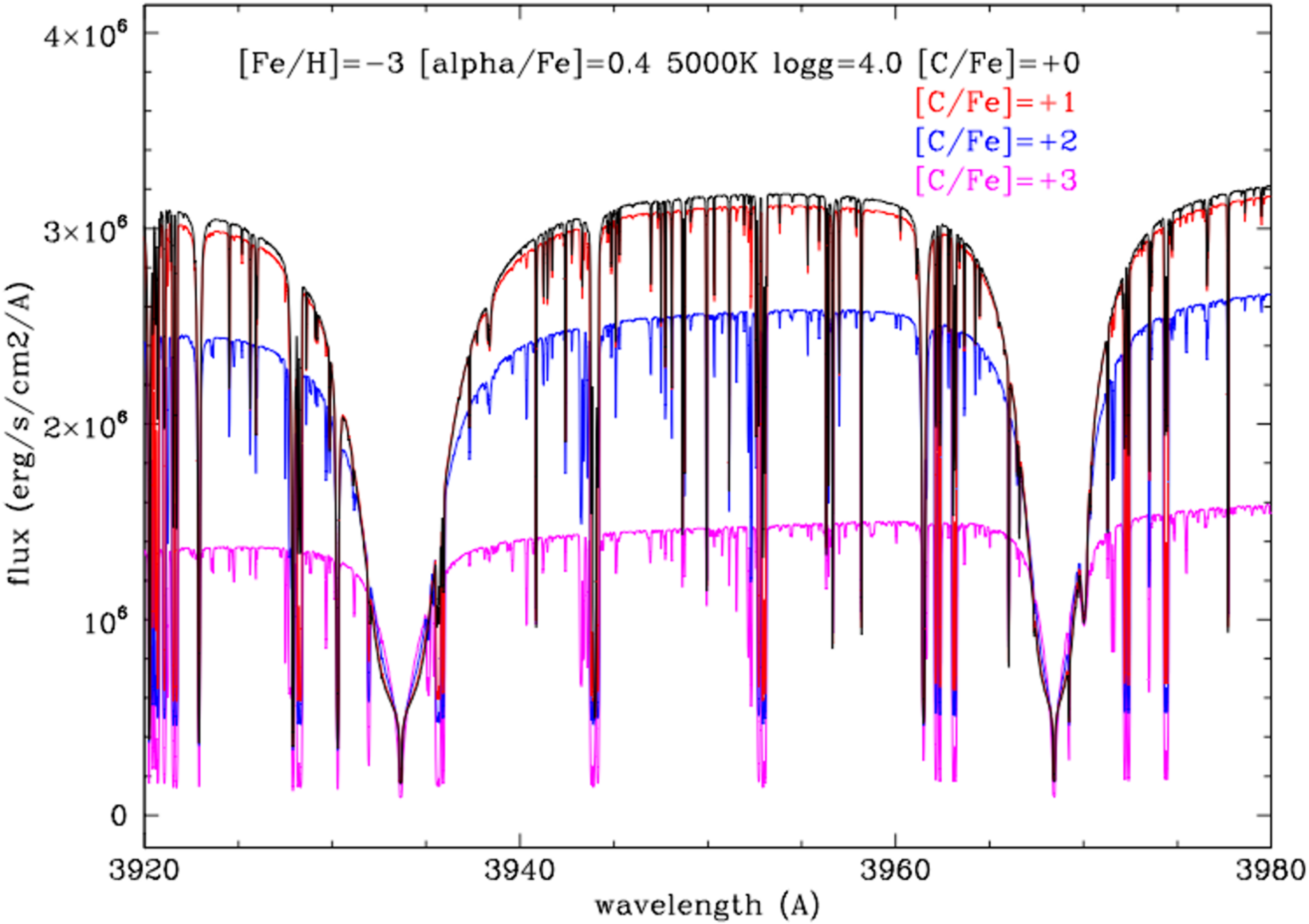


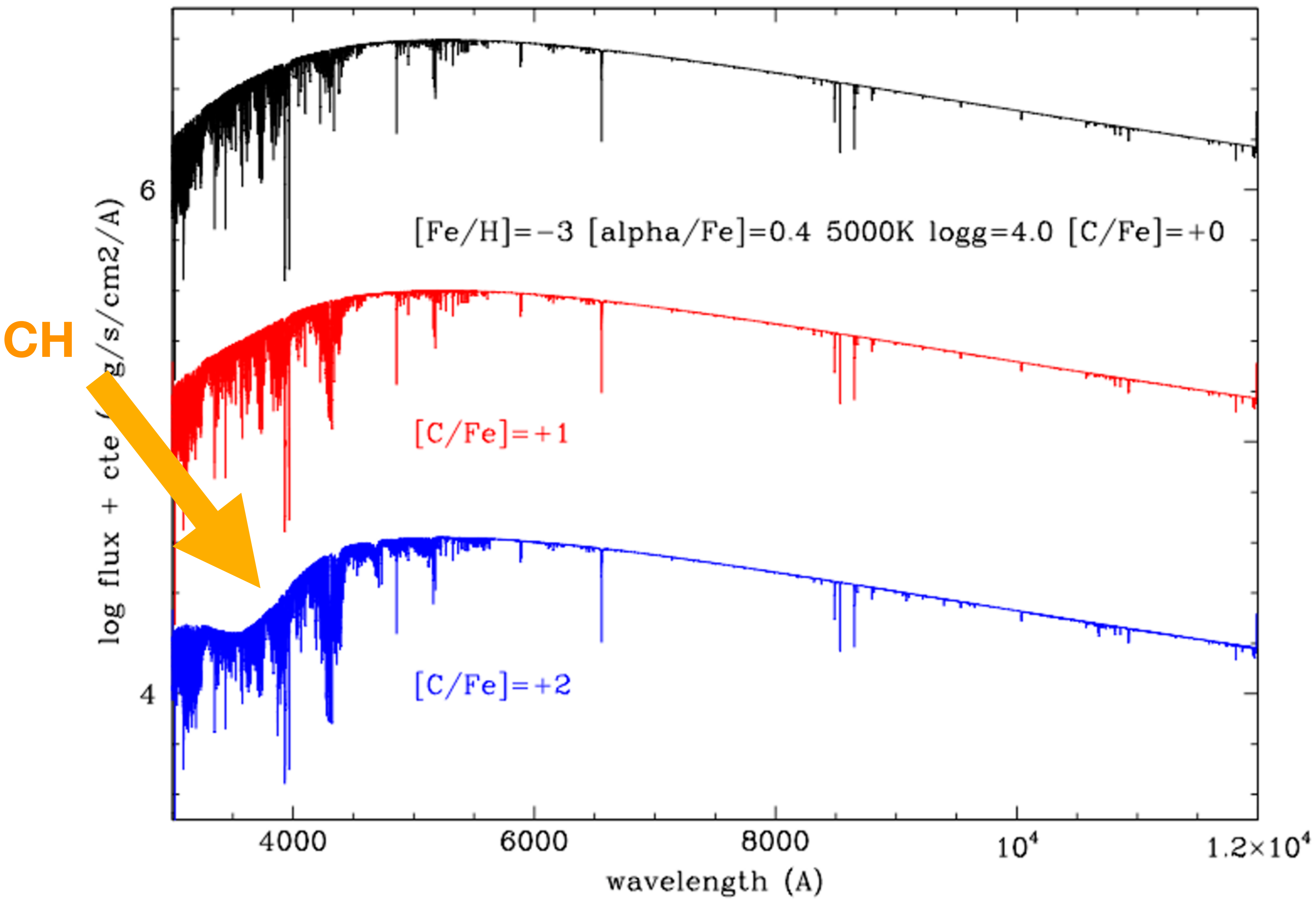
Plot differently !



Plot differently !

=> Absolute flux instead of continuum normalised…
and it becomes obvious : continuum change is the answer!





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

Words of caution

Always try to understand what you get !

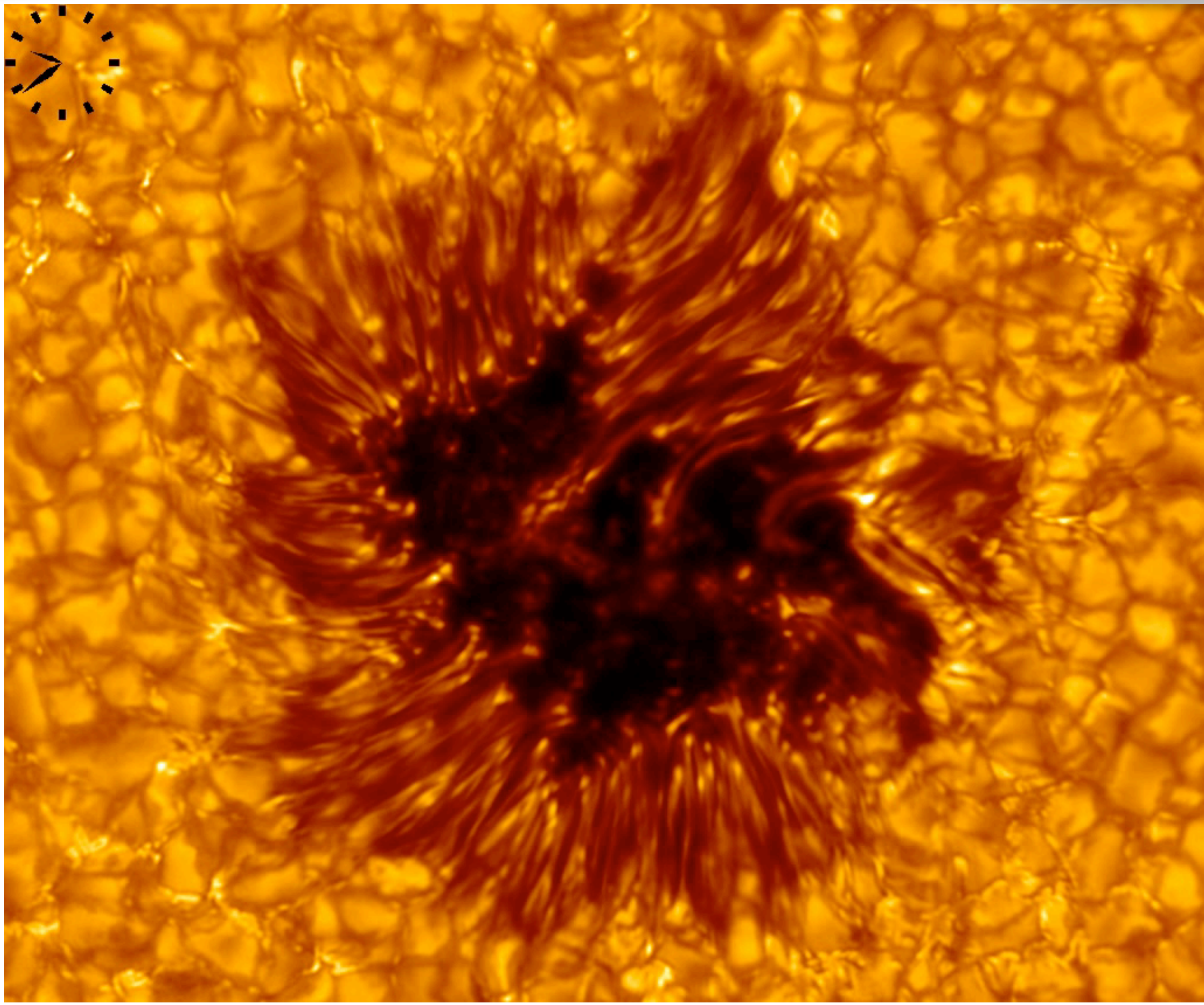
- ☑ scrutinize, plot differently
- ☑ understand the underlying physics and mechanisms
- ☑ make sure it is not a bug in your code or some bad setup of the input data

- ☑ Beware of black box codes
- ☑ Contact the developers

- ☑ A result is never better than the underlying model.

Finally: A real stellar atmosphere is NOT LTE 1D hydrostatic!
…even if the approximation might work sometimes

See Andy Gallagher's talk!



Credit: L.R. van der Voort (Swedish Solar Telescope)

No conclusions here,
the messages are scattered in
the green boxes.

Thank you !
… awaiting your questions and
comments

Something else I learned through the years

- **Be open:** make your codes and data public (once you got it officially published. This is the best way to get it used by others, get credit for it, and get feedback for improvement.

- **Be contructive :** Send feedback to the developers of the codes and data you use. They will just be happy about it, and try to improve the situation.