ChINOSchool, Ondřejov Observatory, Czech Republic (& Spain), July 24 - 28, 2023

Hands-on experience with stellar spectroscopy

I. Stellar parameters *a la carte*

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gaia

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CHETEC INFRA

Who am I

Studied in the 1990s in Marburg, Heidelberg and London (Master's in physics, Master's in astrophysics)

Got my PhD from the University of Munich (LMU) in 2002 with a thesis on “Cool-star gravities”

Did one year as a postdoc at the Max Planck Institute for Extraterrestrial Physics (MPE) in Garching

Moved to Uppsala on a German scholarship, received national funding for my research, joined Gaia in 2008 and have been a lecturer at Uppsala university since 2010

Nowadays, I mostly work on solar-type stars and stellar surveys (Gaia, Gaia-ESO, 4MOST), plus some work for ELT instruments like ANDES and MOSAIC

stars

10s

...

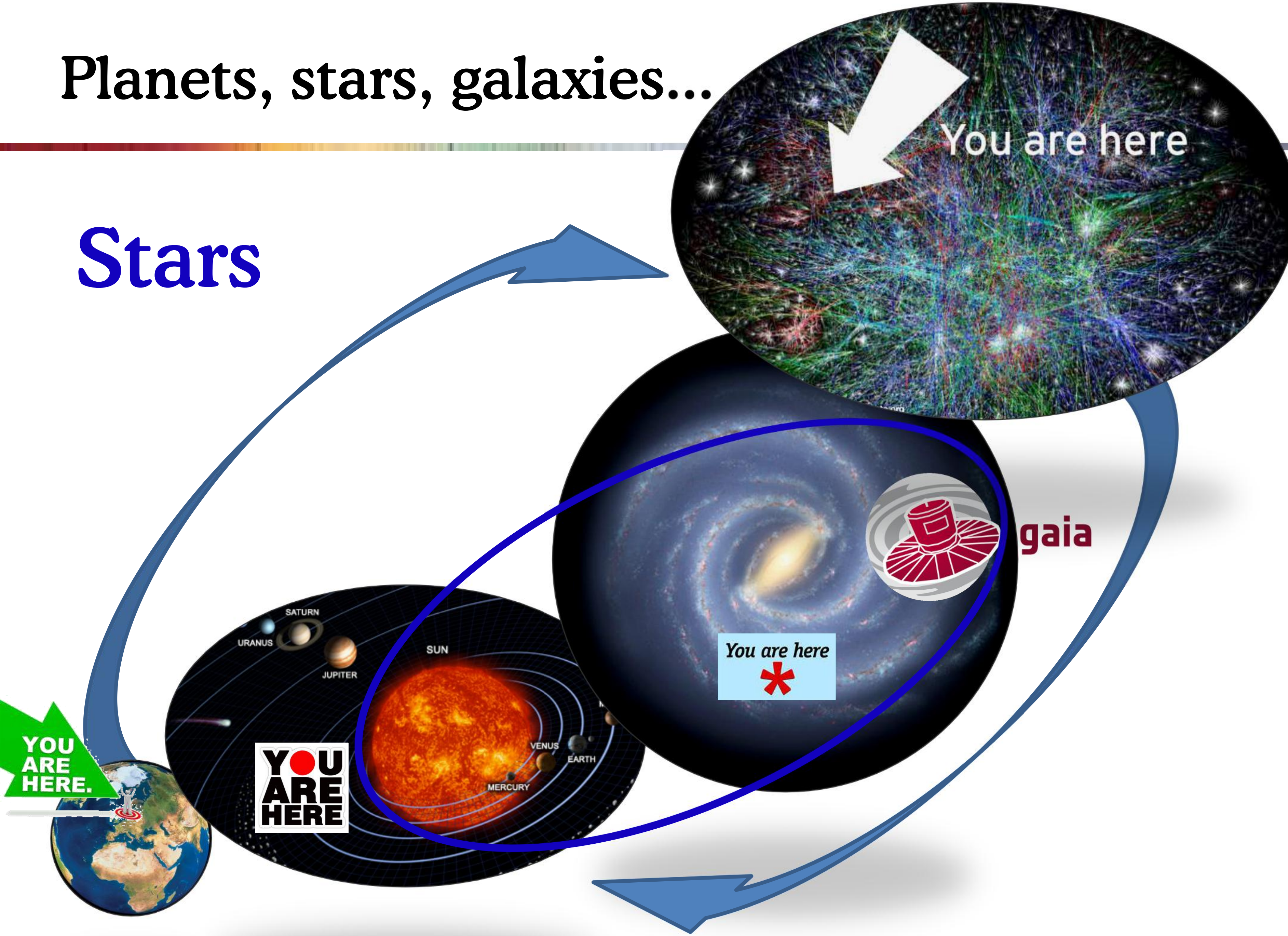
1000s

...

$5 \cdot 10^8$

Planets, stars, galaxies…

Stars



Stars: typical figures

The Sun

$M = 2 \times 10^{33}$ g $= M_\odot$

$R = 7 \times 10^{10}$ cm $= R_\odot$

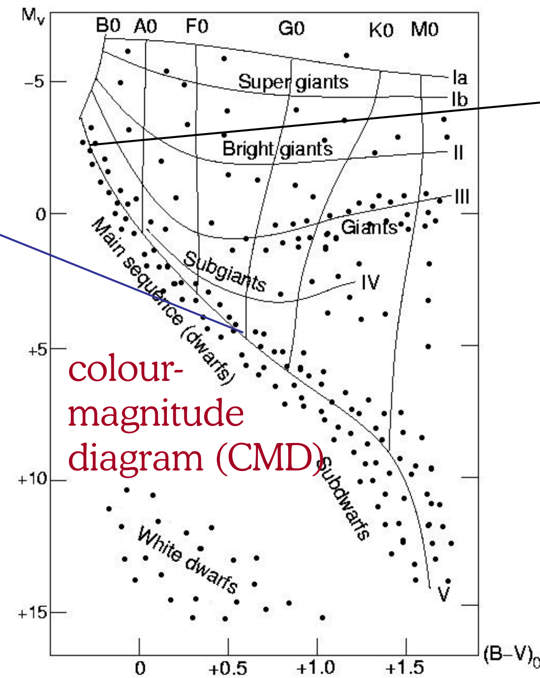
$L = 4 \times 10^{33}$ erg/s $= L_\odot$

photosphere:

$\Delta R \approx 200$ km $< 10^{-3} R_\odot$

$n \approx 10^{15}$ cm^{-3}

$T \approx 6000$ K



colour-magnitude diagram (CMD)

an O star

$M \approx 50\, M_\odot$

$R \approx 20\, R_\odot$

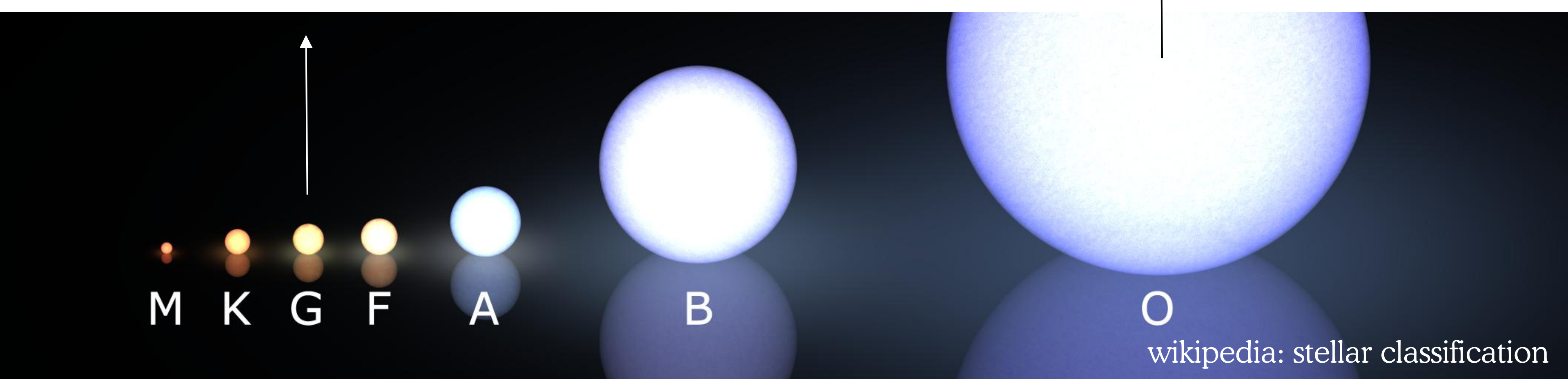
$L \approx 10^6\, L_\odot (\propto M^3)$

photosphere:

$\Delta R \approx 0.1\, R_\odot$

$n \approx 10^{14}$ cm^{-3}

$T \approx 40\,000$ K



wikipedia: stellar classification

Gaia's instruments 101

stars

ASTRO: the core of the mission = astrometry = positional astronomy in space and time (10+ years in total). Spatial positions as a function of time = space velocities. $2 \cdot 10^9$

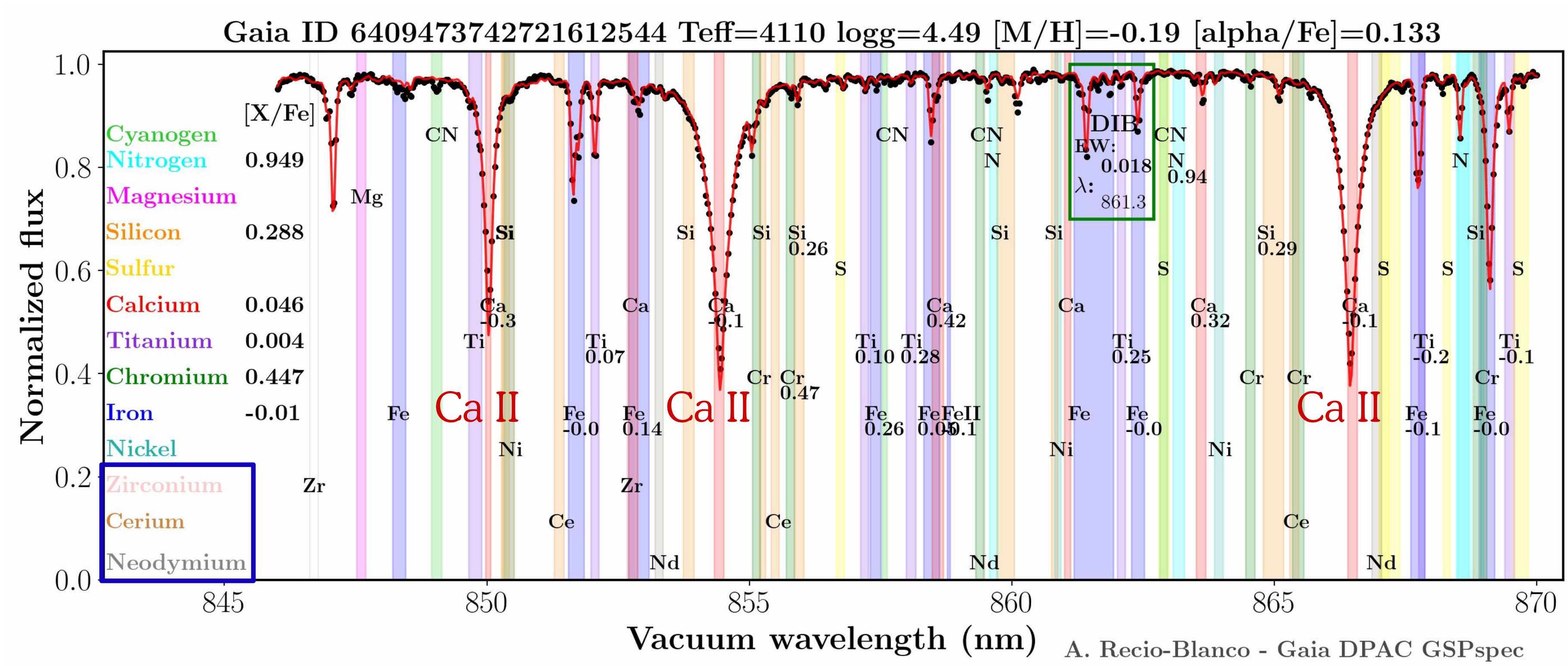
BPRP: two (spectro)photometers providing colour information (BP-RP, giving a rough estimate of stellar temperature) and $2 \cdot 10^9$ resoved XP spectra. They can be used to derive $T_{\rm eff}$, interstellar reddening along the line of sight, metallicity, $5 \cdot 10^8$ surface gravity etc. with some significant degeneracies.
See Andrae *et al.* (2023)

RVS: provides medium-resolution spectra (R = 11,500) in the $2 \cdot 10^6$ near-infrared (847 - 870 nm). Mostly for radial velocities, but access to lines allows one to derive stellar parameters and individual chemical abundances for brighter stars.
See Recio-Blanco *et al.* (2023)

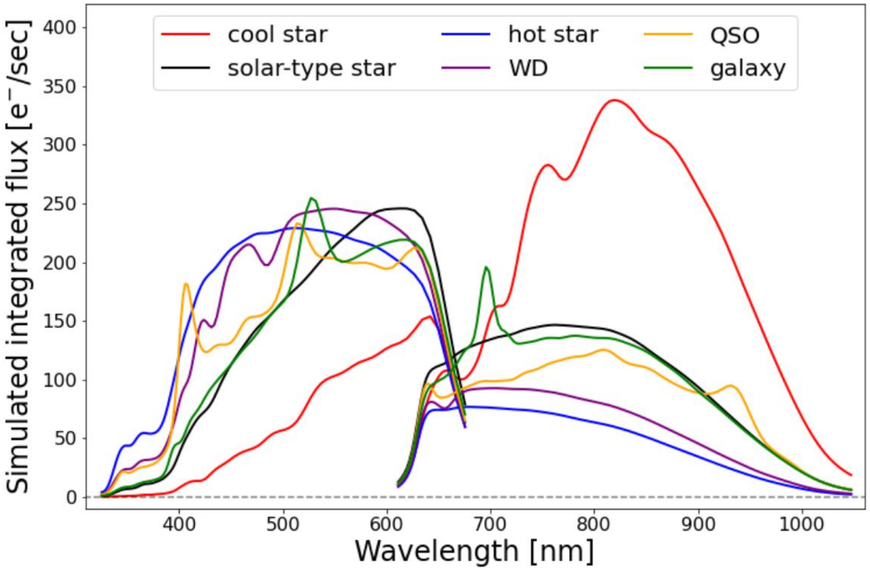
Science first

With Data Release 3 (June 2022), the Gaia archive contains individual chemical abundances for a few million stars. Up to a ~dozen elements are derived from the RVS spectra (R=11500, see below).

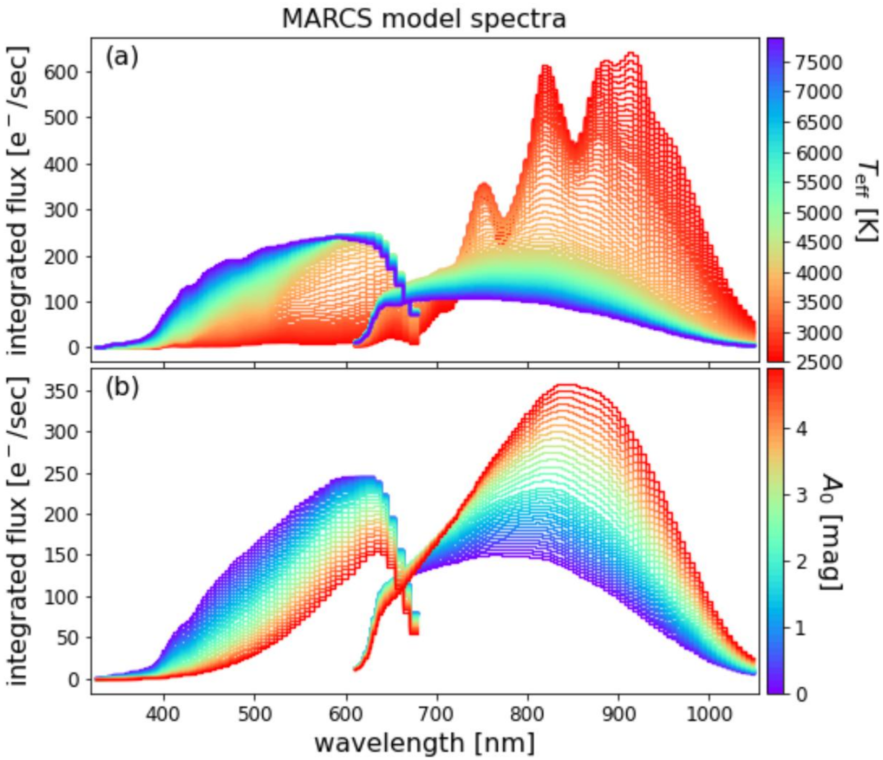
We would like to tap into this treasure trove of stellar abundances!



XP spectra: examples

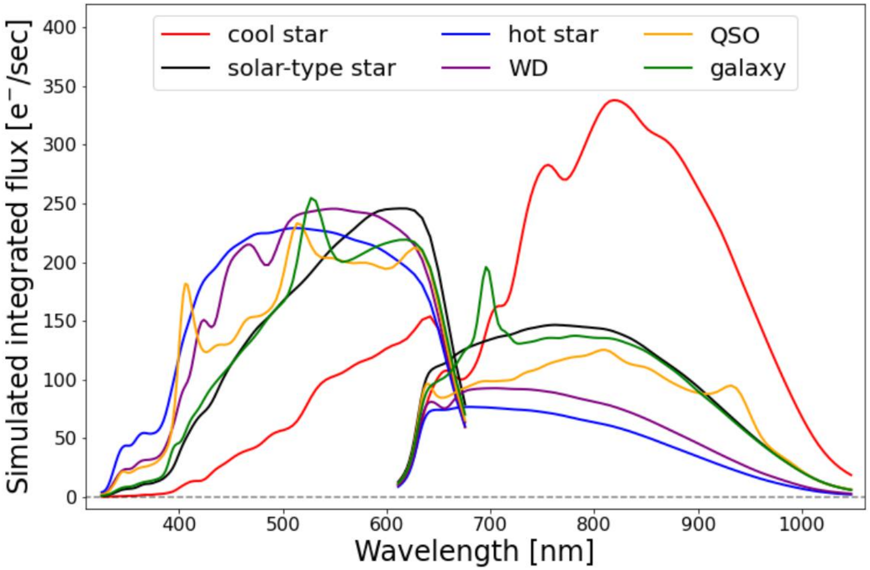


Different astrophysical objects have very different XP spectra!



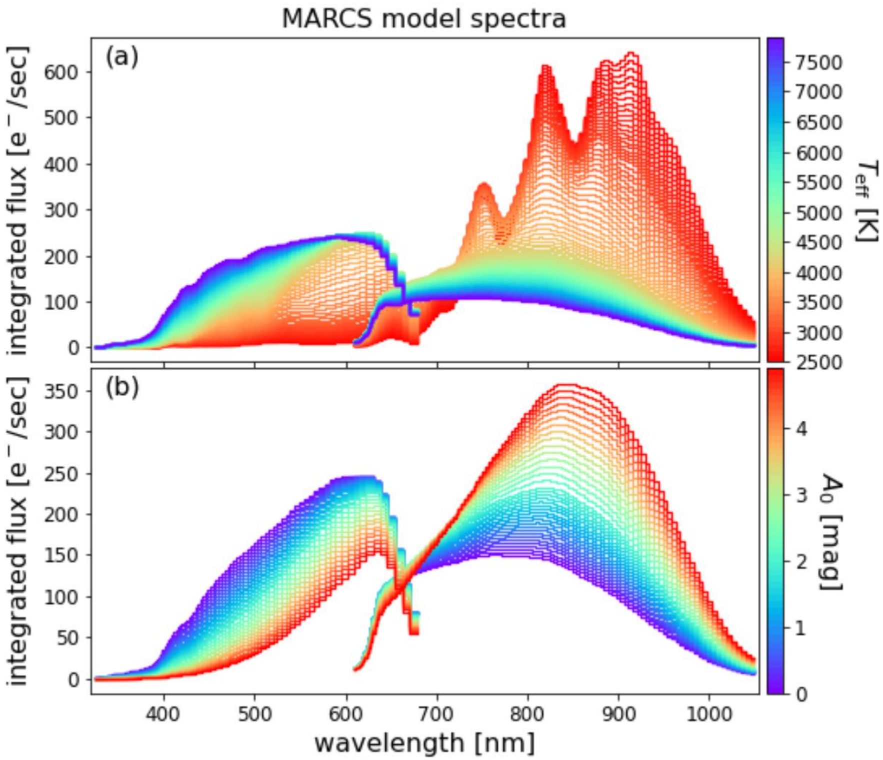
Creevey *et al.* (2023)

XP spectra: examples



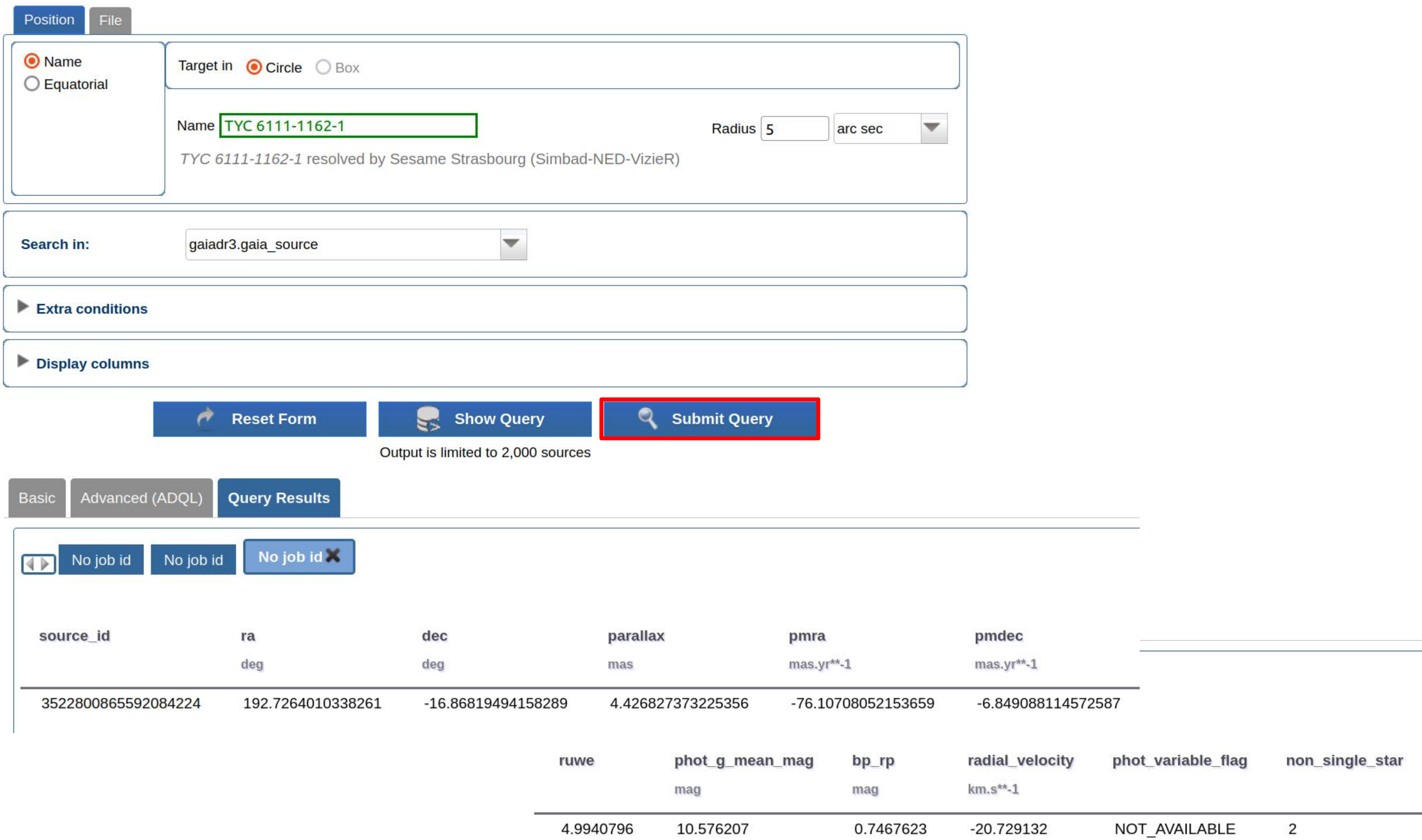
Different astrophysical objects have very different XP spectra!

However, space is not empty. Interstellar extinction can matter a lot! This leads to parameter degeneracies.

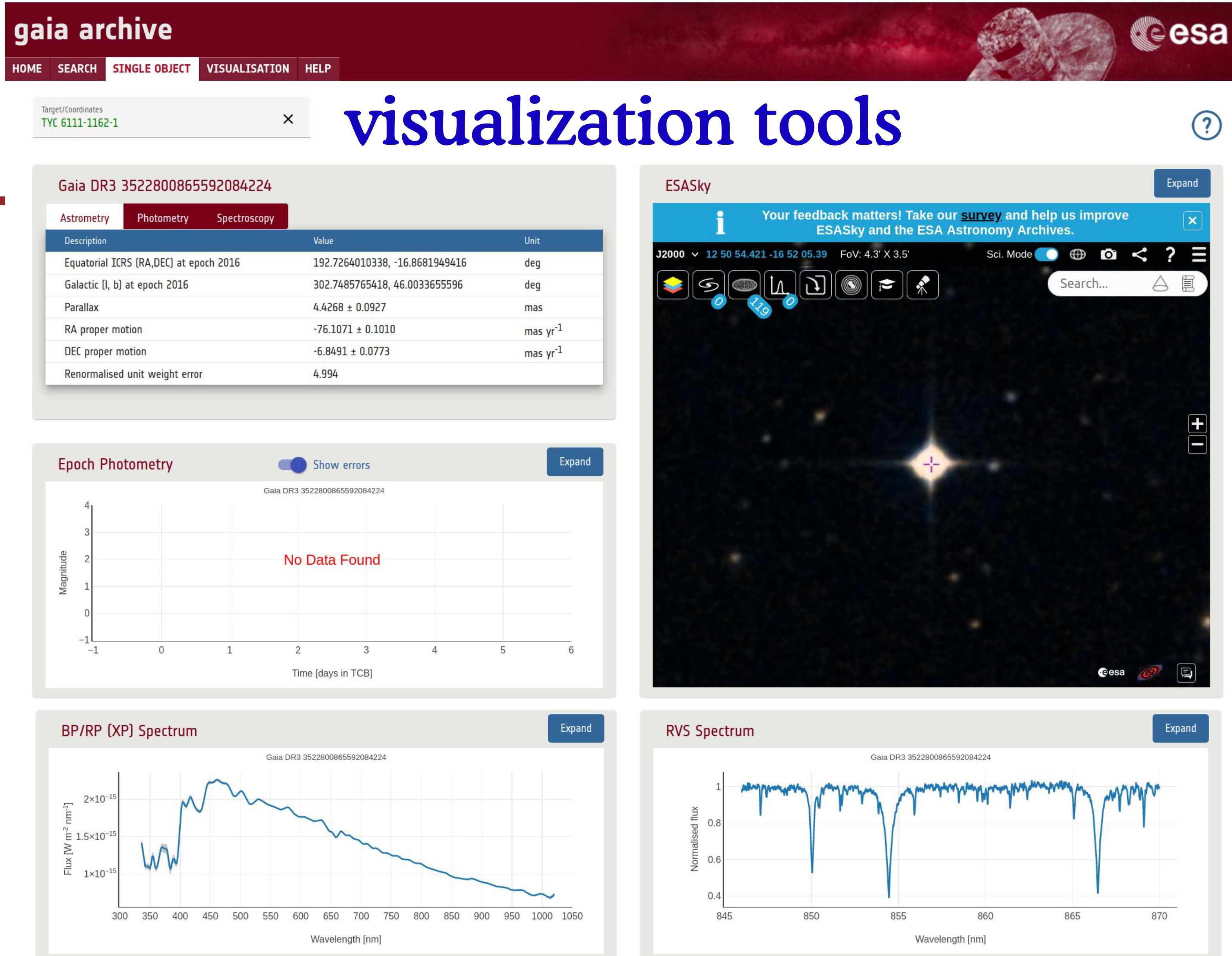


Creevey *et al.* (2023)

To-go starting point: the Gaia archive



visualization tools



How would Gaia see the Sun? Query e.g. “18 Sco”, a classical solar-twin star.

Can't find parameters? Derive 'em!

For FGK stars, there are several spectroscopic techniques to derive stellar parameters. We will mostly use:

Hα (6563 Å): The line shape in the wings is sensitive to T_{eff}.

Mg Ib: The wings of these three strong lines around 5160 Å are pressure-sensitive = **log g**-dependent.

Numerous Fe II lines: for what we call the stellar **metallicity**. Better than Fe I lines, as the latter are subject to stronger 3D/NLTE effects. But Fe II lines are fewer and weaker.

There are some auxiliary parameters we also need to derive, in particular the **microturbulence** (ξ), a fudge parameter for convective motions on small scales. Stronger lines are affected by ξ. A finite ξ (0-2 km/s) is needed to harmonize abundances from weak and strong lines.
To simply things, we will e.g. use scaling relations from the literature.

Hands-on experience with stellar spectroscopy

II. NOT observations

P

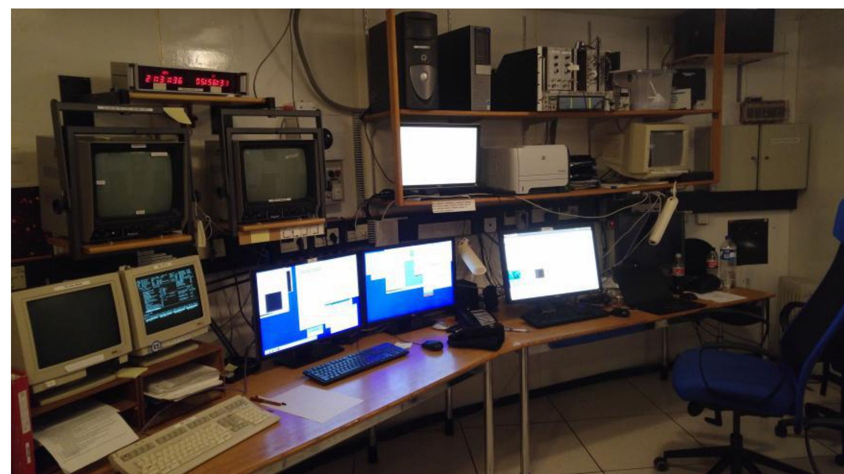
Marcin Rosadziński

The telescope: NOT

A 2.56m Nordic Optical Telescope (presently run by Arhus University, DK & University of Turku, FI) at the best site in Europe: Roque de los Muchachos, La Palma, Canary Islands, Spain.

The telescope has been operated since 1989 and is known for its reliability.

It has a modern spectrograph, FIES, which is the sole instrument we will use this week.



The spectrograph: FIES

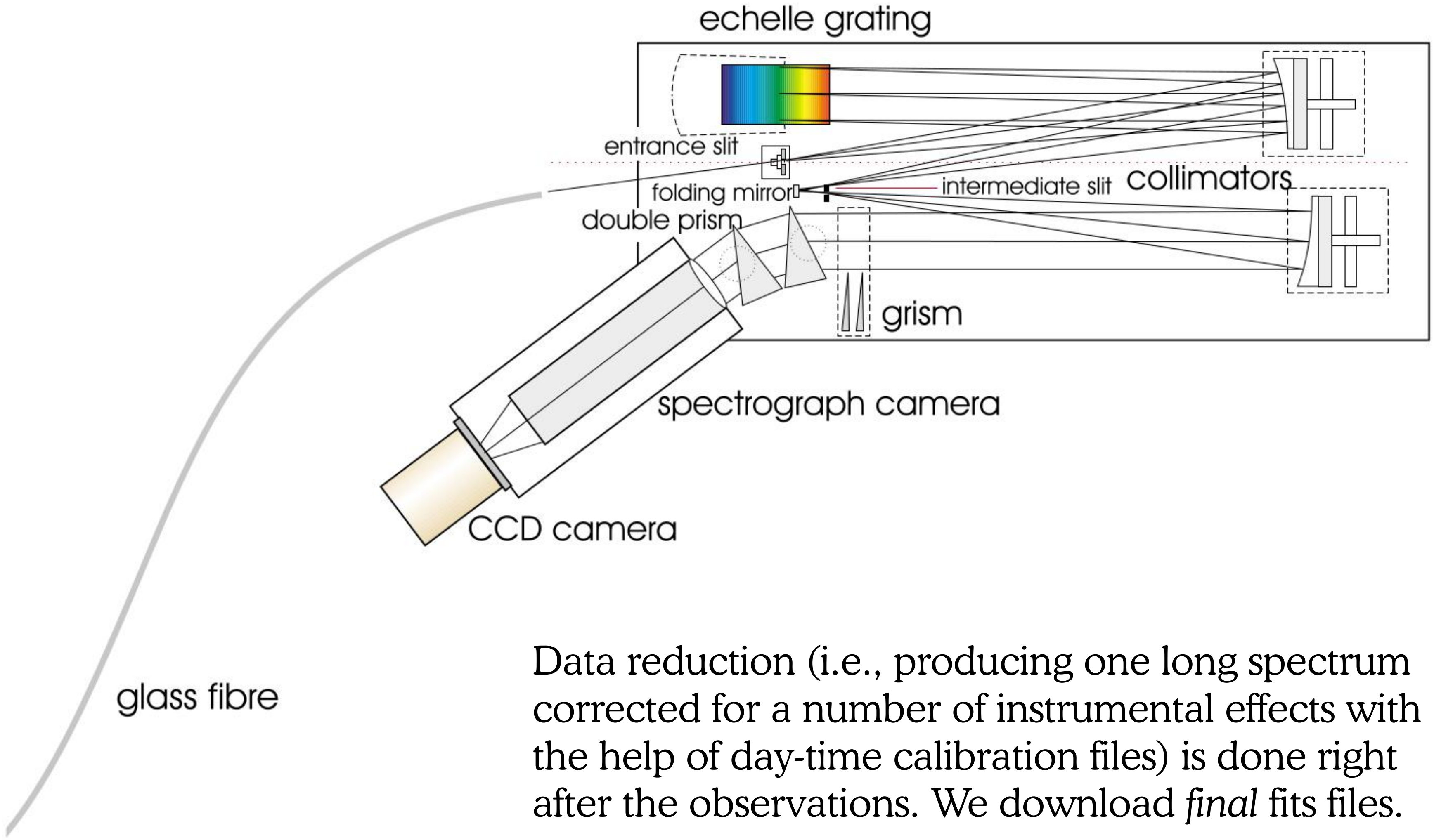
FIES is a modern high-resolution fibre-fed echelle spectrograph. Light enters the spectrograph through a fibre with a 1.3 arcsec diameter on the sky. This means that if the seeing at the telescope is 1.3”, roughly one third of the light gets lost.

The dispersive element is an echelle grating. Cross-dispersion is provided by yet another grating. The spectral orders are recorded on a CCD. Data reduction is done on-the-fly, i.e. we receive a fits file with the reduced (w/o radial-velocity correction and normalization) spectrum right after the observations.

FIES has several modes with different resolving powers. Since we are dealing with cool stars with intrinsically sharp lines, we go for the highest-*R* setting (67,000). Full optical coverage.

See http://www.not.iac.es/instruments/fies/ and http://www.not.iac.es/instruments/fies/devel/telting2014FIES.pdf

Schematic of an echelle spectrograph



Data reduction (i.e., producing one long spectrum corrected for a number of instrumental effects with the help of day-time calibration files) is done right after the observations. We download *final* fits files.

Hands-on experience with stellar spectroscopy

III. Abundance analysis

DIY

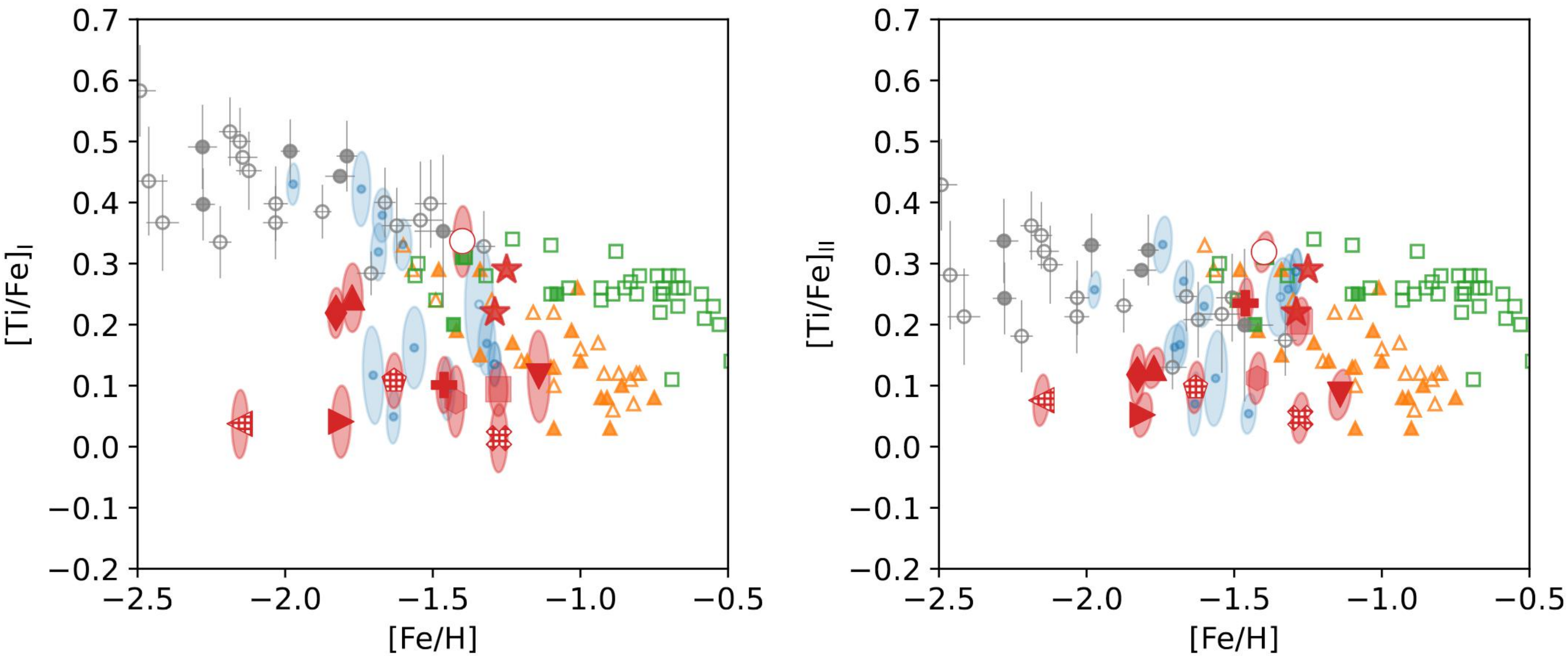
ChETEC

ChETEC

Chemical Elements as Tracers
of the Evolution of the Cosmos

ChETEC

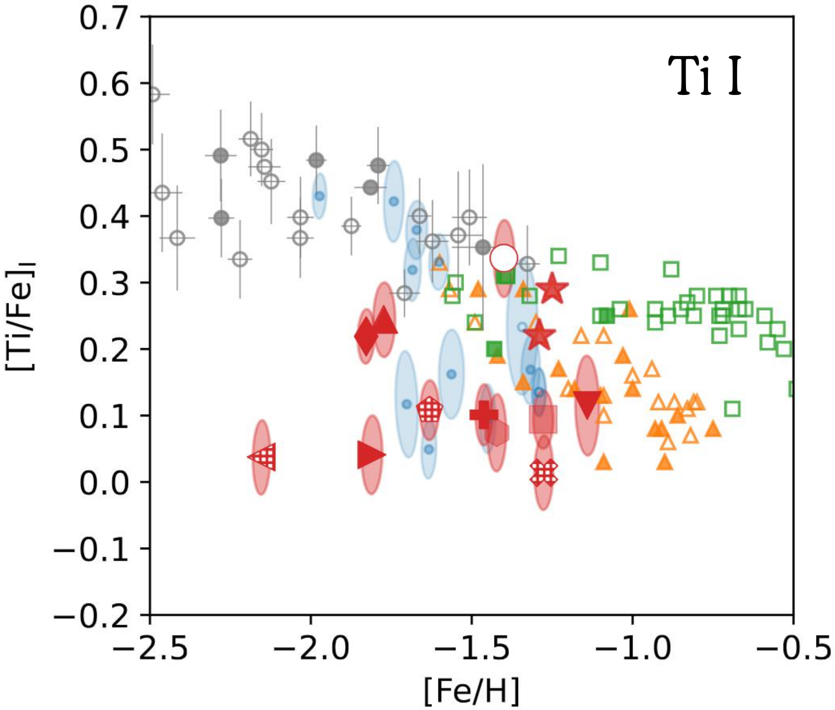
Chemical Elements as Tracers
of the Evolution of the Cosmos

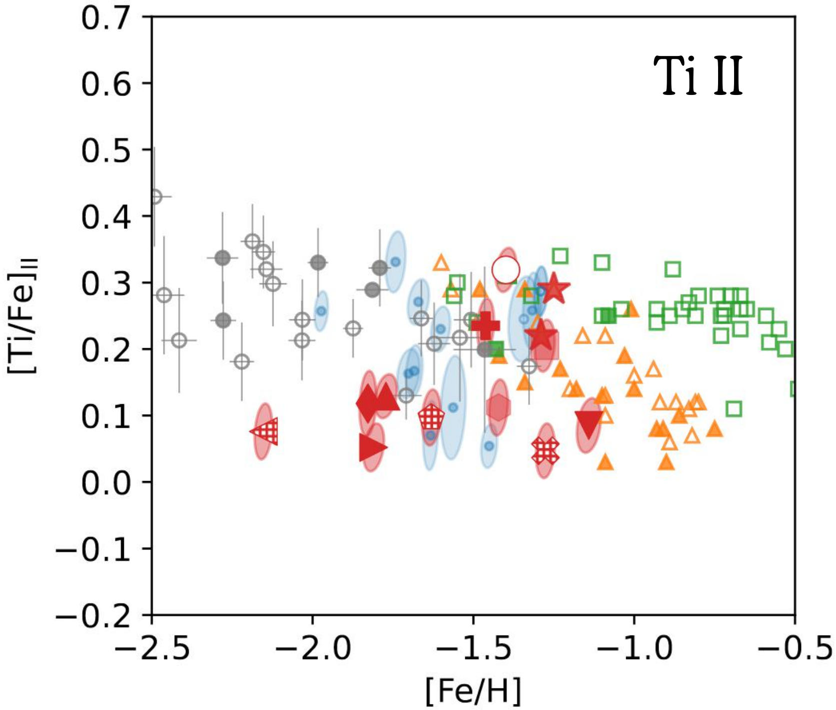


Matsuno *et al.* (2022)

ChETEC

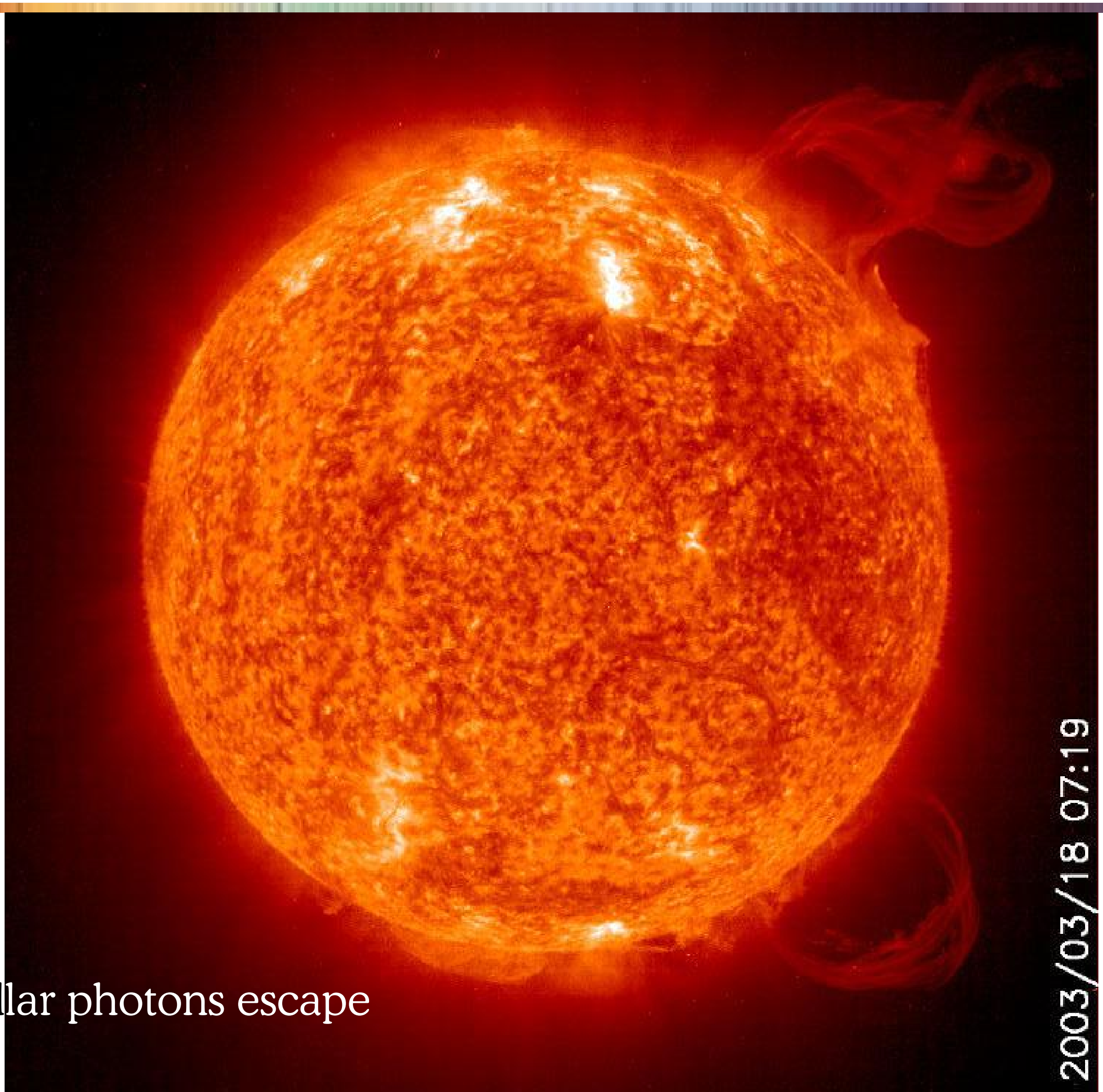
Chemical Elements as Tracers of the Evolution of the Cosmos





More sophisticated 3D and NLTE models will align the Ti I abundances with Ti II.

Stellar atmospheres…



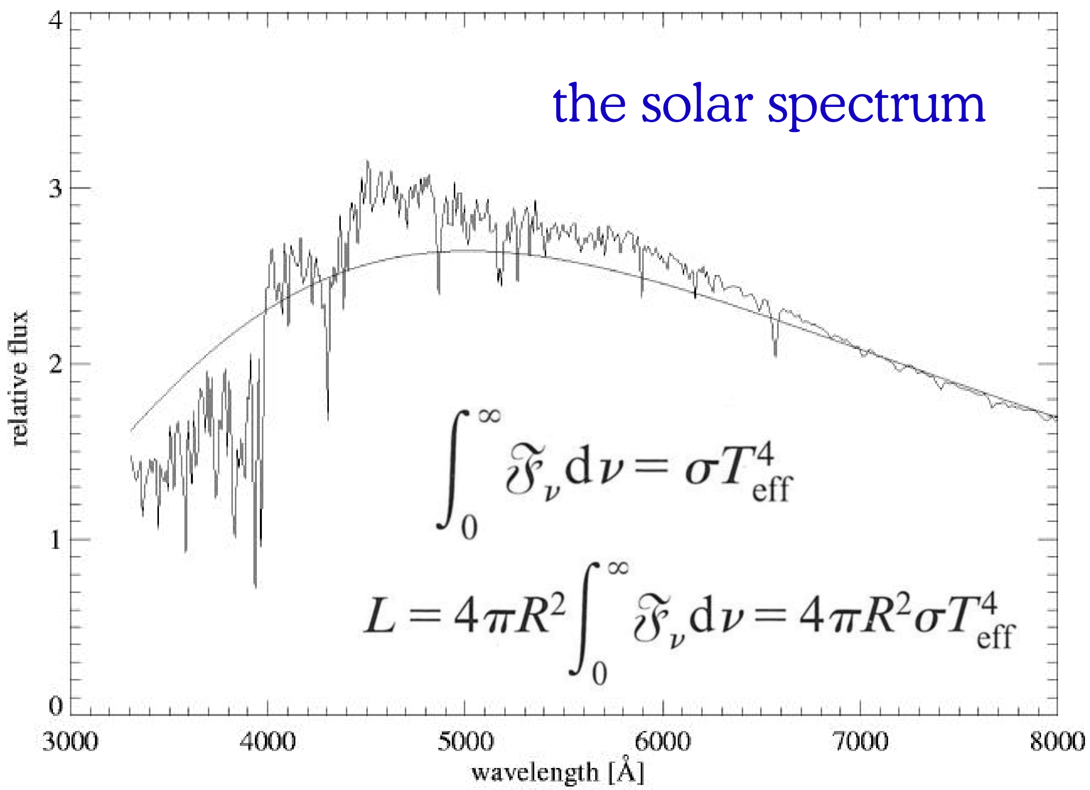
… where stellar photons escape

The spectra of stars

Luckily, stars (and other celestial bodies) are not in thermodynamic equilibrium (TE) and do not shine like blackbodies.

(Astronomy would be the dullest of all sciences!)

In constrast to B_ν, I_ν depends on plasma properties and the viewing angle. One cannot use TE to describe starlight.



Quantitative stellar spectroscopy

observation vs. theory

NOT

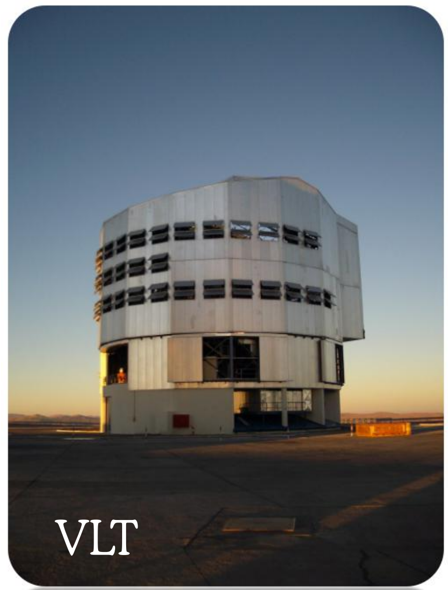
telescope

FIES

spectrograph

E2V 42-40

CCD



$$\frac{\mathrm{d}I_\nu}{\mathrm{d}\tau_\nu} = -I_\nu + S_\nu$$

concepts

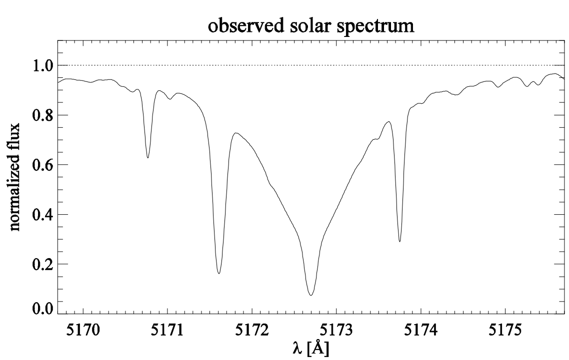
$$\frac{\mathrm{d}}{\mathrm{d}x}\mathcal{F} = 0$$

LTE

approximations

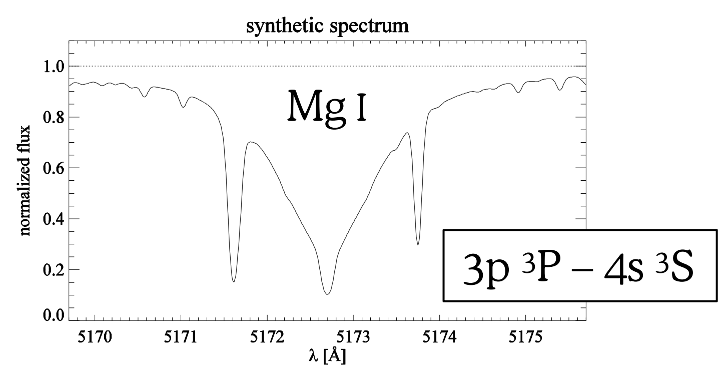
MLT

numerical model



comparison

to constrain
thermodynamic variables
and abundances



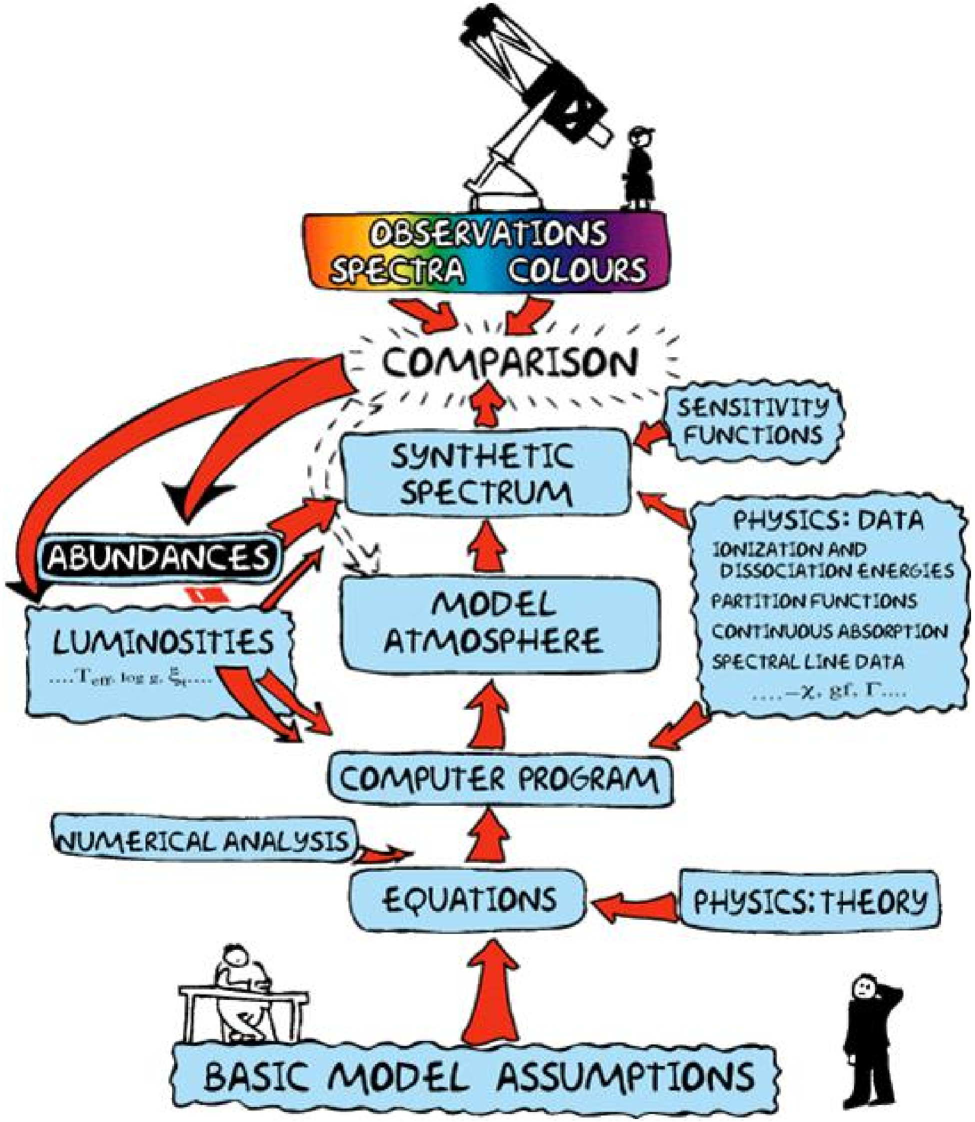
Modelling stellar spectra

For practical reasons, the task of computing stellar spectra is divided up into two subtasks:

* the computation of an appropriate model atmosphere

and

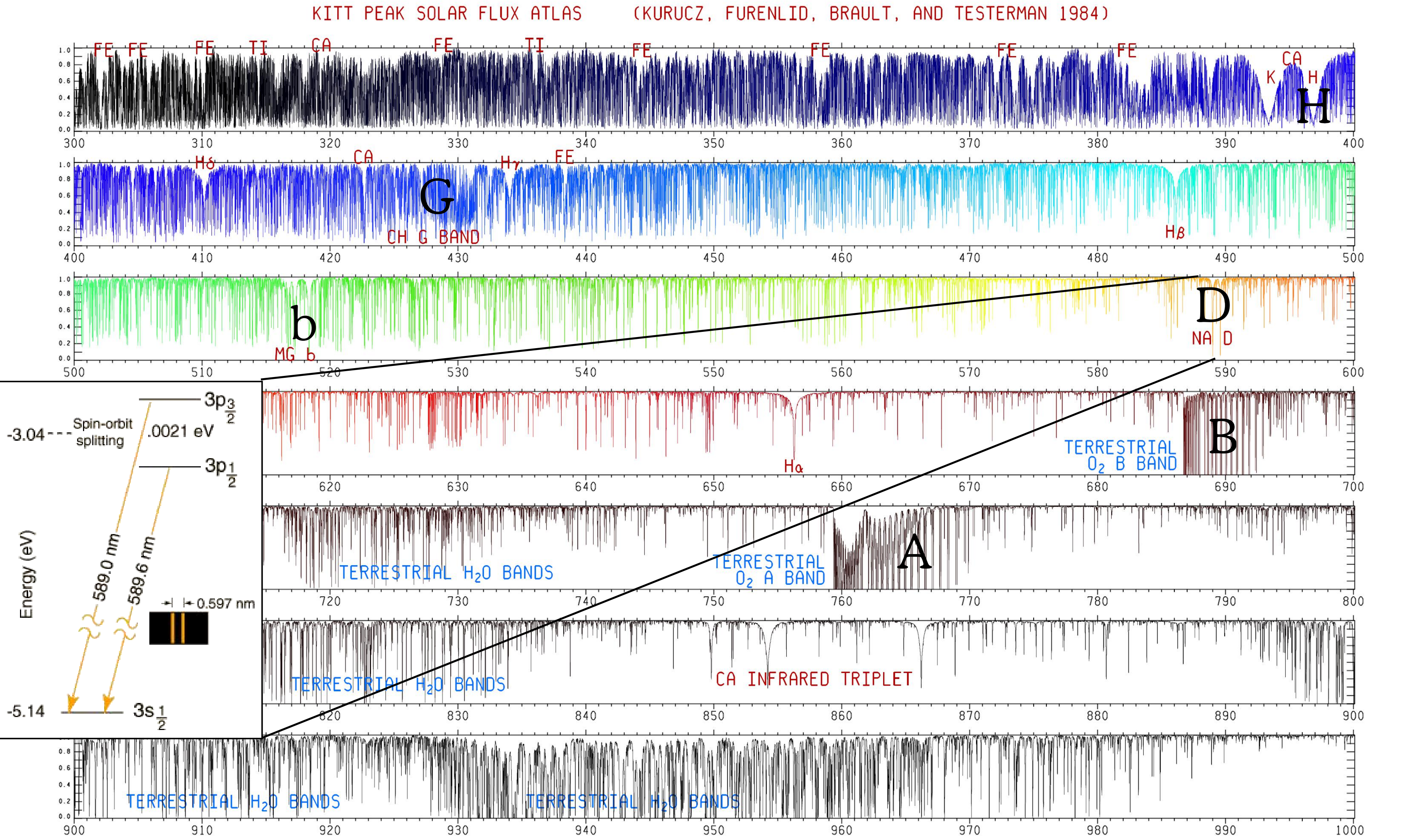
* the computation of a synthetic stellar spectrum.



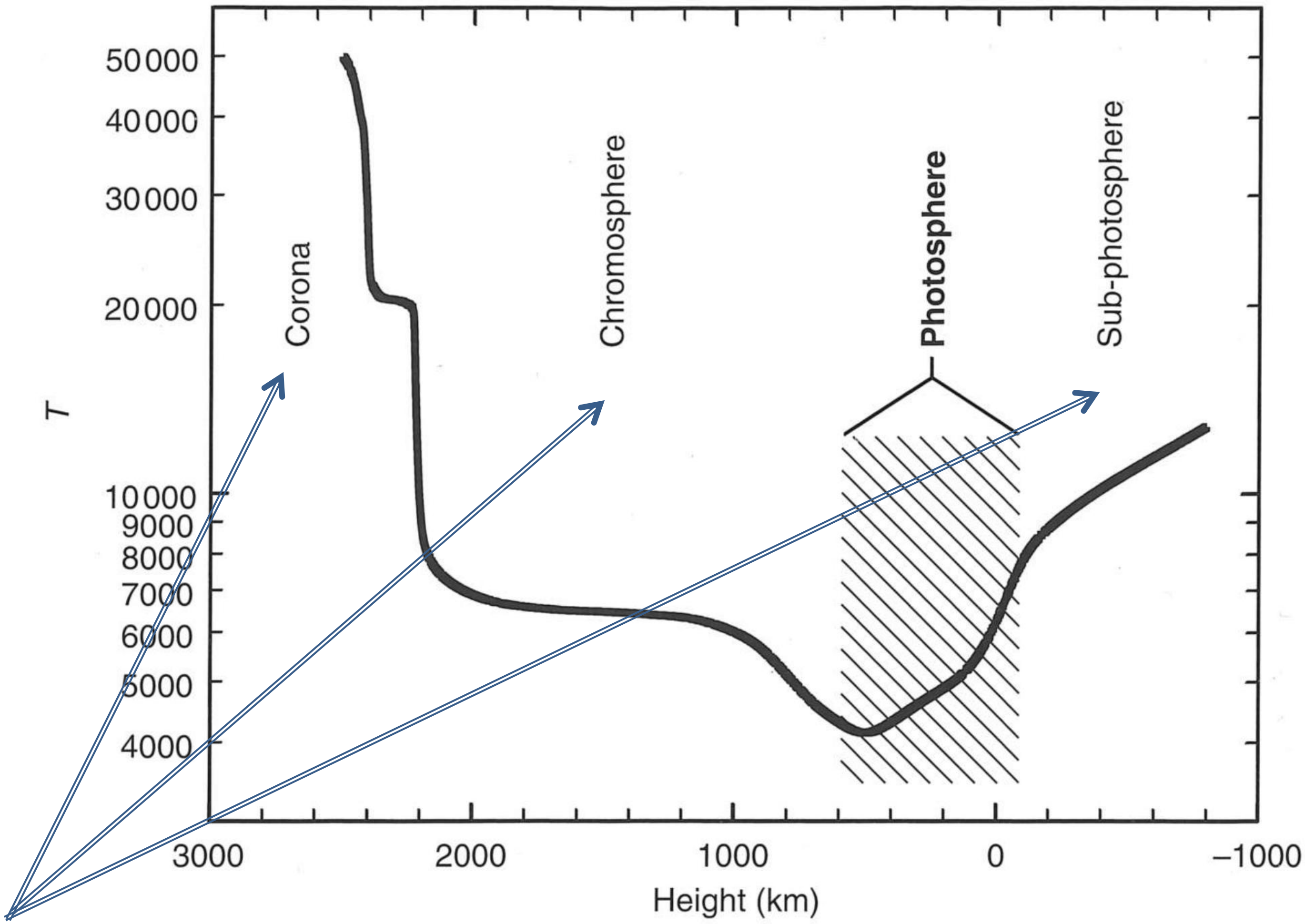
https://www.wikiwand.com/en/Model_photosphere

Bengt Gustafsson

The solar spectrum



Why only model the photosphere?



Why can't we see these hotter sub-photospheric and outer layers?

Model atmospheres 101

The cool tenuous layer of stars we call stellar atmospheres absorb and emit photons. We model this by solving the **radiative transfer equation**:

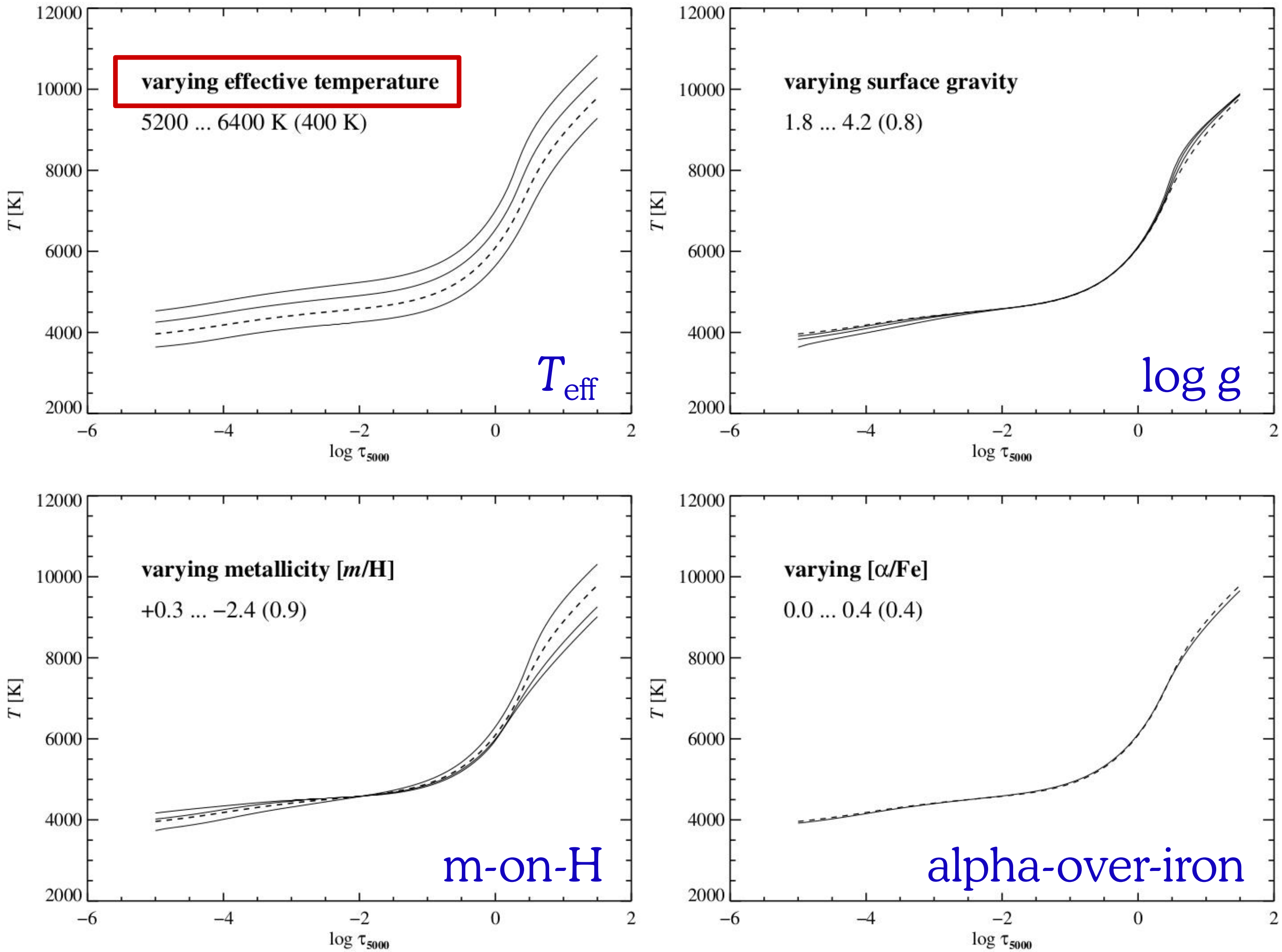
$$\frac{\mathrm{d}I_\nu}{\mathrm{d}\tau_\nu} = -I_\nu + S_\nu$$

A central goal is to find the temperature gradient that establishes itself in order to conserve the total flux (flux-constancy models).

A model atmosphere tabulates two or more thermodynamic variables as a function of (optical) depth. It is one of the main inputs to calculations of synthetic stellar spectra.

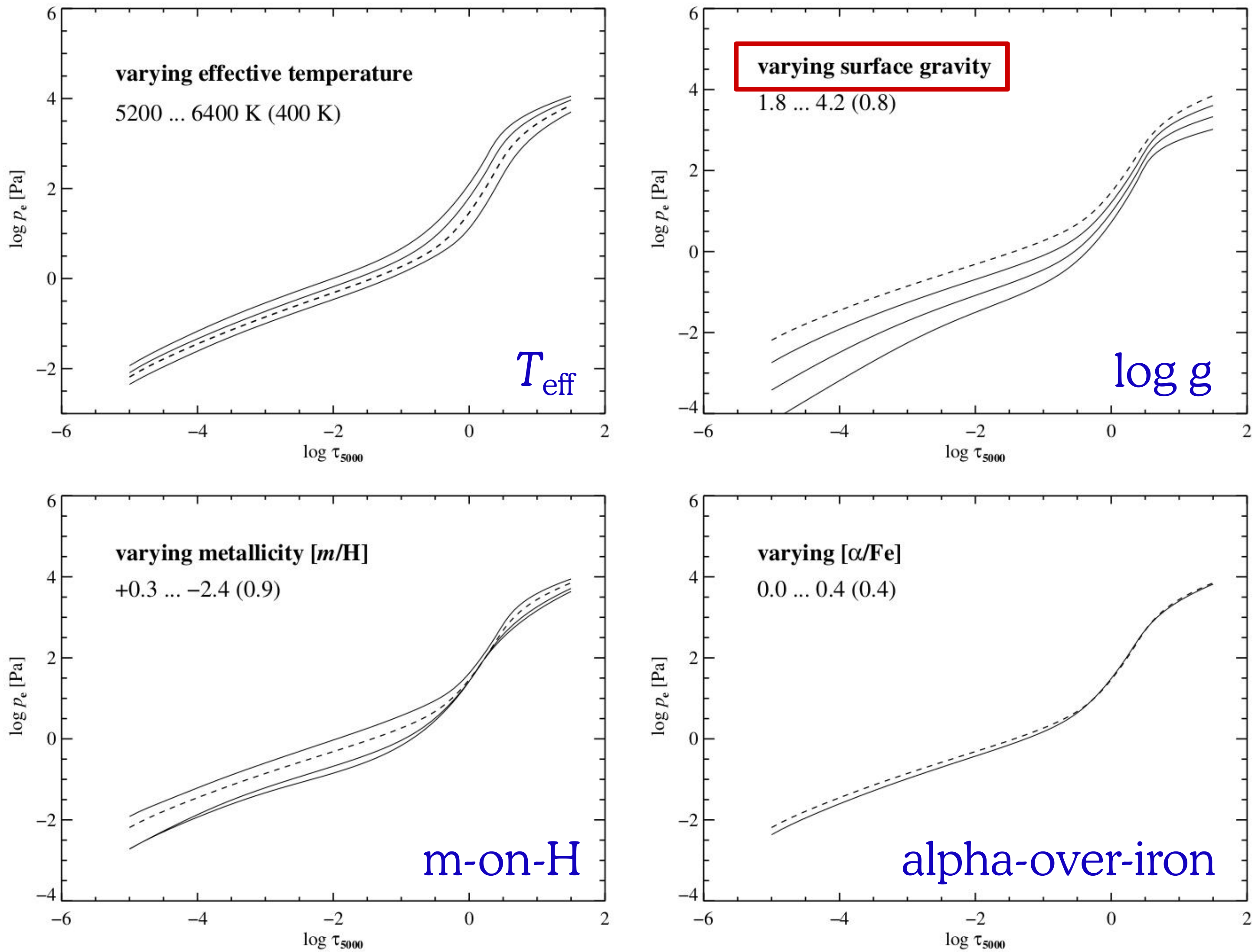
In order to derive reasonably realistic models, one needs to consider 100s of 1000s of opacity sources from atoms and molecules. See e.g. Gustafsson *et al.* (2008) for one set of models ("MARCS").

Grids of model atmospheres: T vs τ



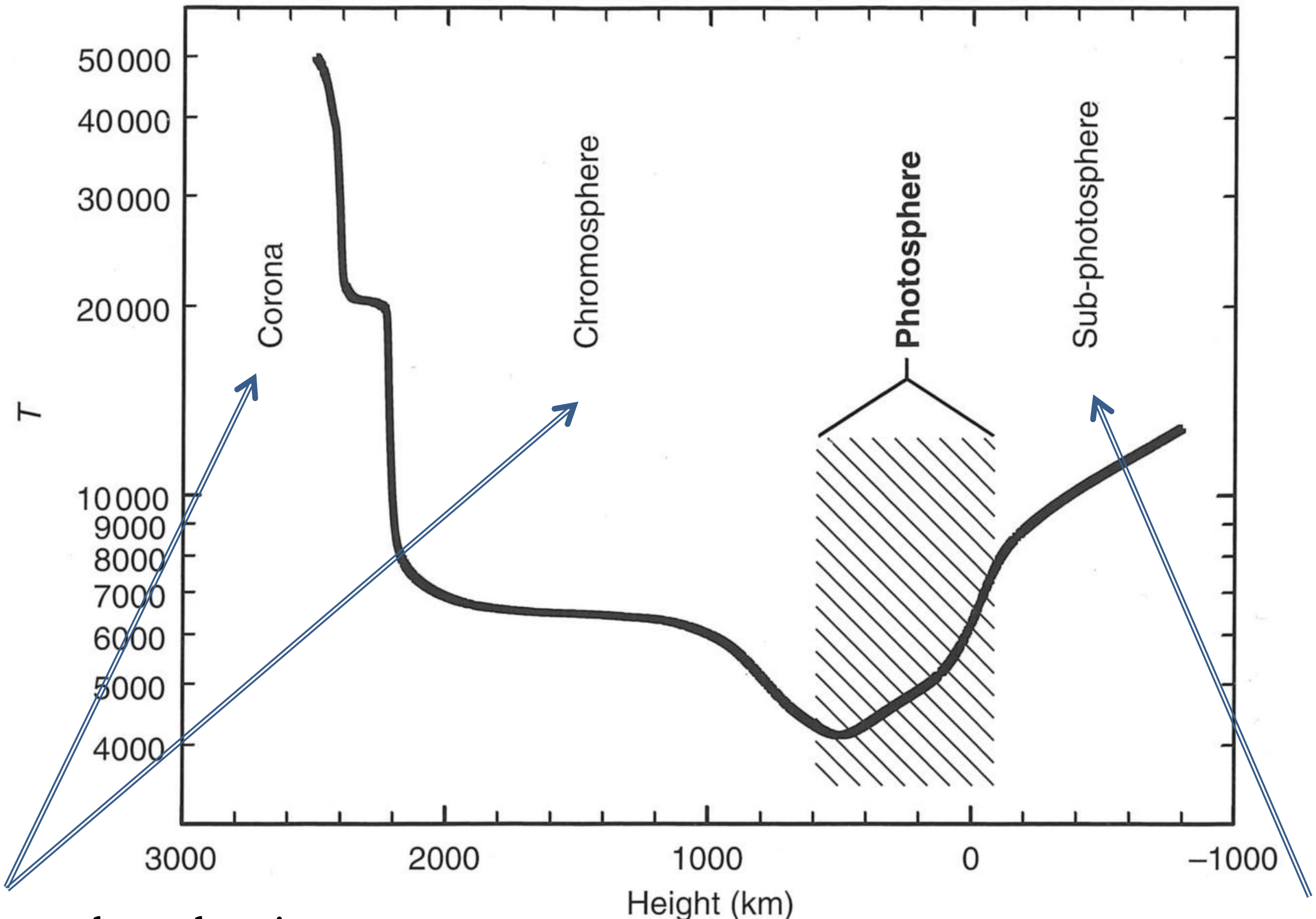
⇦ towards surface towards interior ⇨

Pressure stratification: here P_e



⇦ towards surface towards interior ⇨

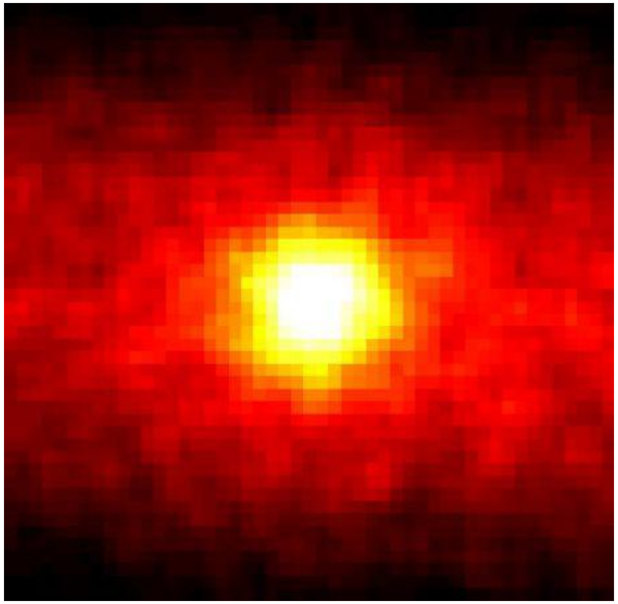
Why only model the photosphere?



Hot, but very low density
⇨ transparent in the optical

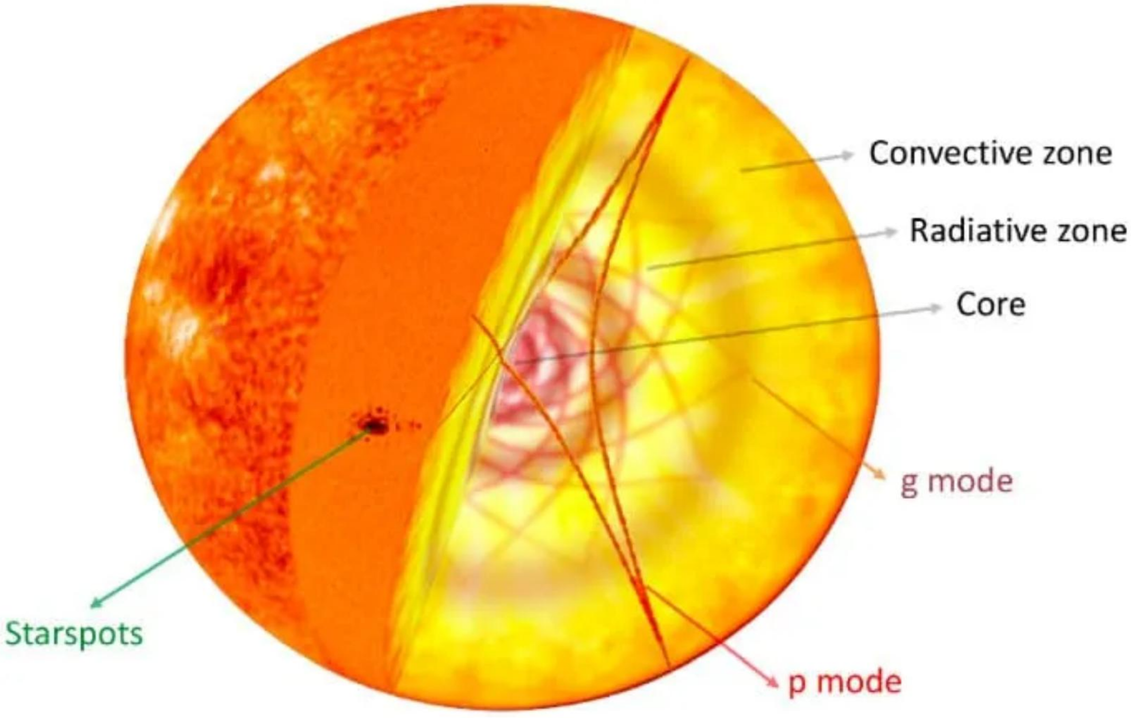
Hot and dense
⇨ opaque at all λ

The interior of the Sun



Neutrinos from the fusion reactions in the Sun's core as seen by Superkamiokande (Japan) looking right through Earth!

Probing acoustic waves through helioseismology also lets us study the Sun's interior structure. These are excited by near-surface convection.



Asteroseismology of solar-type stars. Image by link.springer.com

This week

We will not look into the complexities of how model atmospheres are constructed.

Instead we will simply assume that grids of such models exist and can be interpolated in to simulate the stars we are interested in. We will use the MARCS grid (Gustafsson *et al*. 2008).

For Gaia, several such grids were specifically computed during the past 15 years (MARCS, PHOENIX etc.). You can thus find more than one set of stellar parameters in the Gaia archive.

For RVS, only MARCS models were used.

Line formation 101

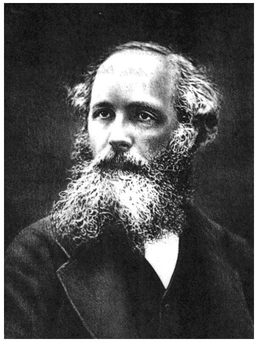
The flux coming from subphotospheric layers (where the mean free path of photons is small) is Planckian, i.e. a blackbody.

Based on the run of temperature and pressure as a function of (optical) depth, you can study how the electronic transitions in atoms and molecules lead to absorption lines at characteristic wavelengths.

The strength of a spectral line is proportional to the ratio of the line vs the continuous absorption coefficient. It also depends on the gradient of the source function throughout the depths of line formation.

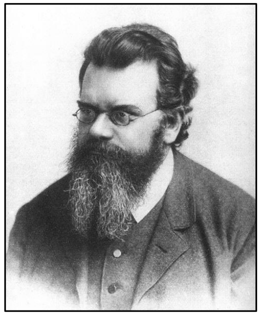
In the classical LTE approximation, the formation of every lines is taken as an isolated process following equilibrium (Saha-Boltzmann) statistics.

TE statistics



Particle velocities are assumed to be Maxwellian:

$$\frac{n(v)}{n_{\rm tot}}\mathrm{d}v = (\frac{m}{2\pi kT})^{\frac{3}{2}} e^{-\frac{mv^2}{2kT}} \mathrm{d}v \, \frac{,^2}{T} \, \mathrm{d}v$$



Excitation follows the Boltzmann distribution:

$$\frac{n_u}{n_{\rm tot}} = \frac{g_u}{u(T)} e^{-\frac{\chi_u}{kT}}$$

χ: excitation energy

Ionization can be computed via the Saha equation:

$$\frac{n_{\rm II}}{n_{\rm I}} P_e = \frac{(2\pi m_e)^{3/2} kT^{5/2}}{h^3} \frac{2u_{\rm II}(T)}{u_{\rm I}(T)} e^{-\frac{I}{kT}}$$

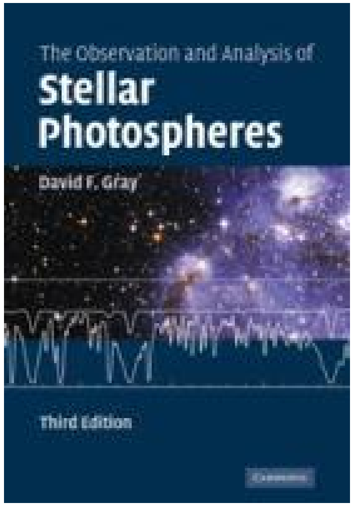
I: ionization energy

In **local thermodynamic equilibrium** (LTE), these are applied ***locally***.

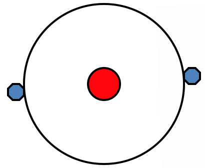
Line strength dependencies

$$\frac{\mathfrak{F}_c - \mathfrak{F}_\nu}{\mathfrak{F}_c} \approx \tau_1 \frac{d \ln S_\nu}{d\tau_c}\bigg|_{\tau_1} \frac{\ell_\nu}{\kappa_\nu}$$

The left-hand side of the above equation is a measure of the line flux (subscript nu) eaten out of the continuum (subscript c). Integrate this and you get the line strength. The right-hand side shows important dependencies:
* gradient of the source function with optical depth and
* the ratio of line to continuous absorption coefficient.
With this, one can basically understand how different lines (transitions) behave. See Gray.



Opacities



Continuous opacity

Caused by *bf* or *ff* transitions

In the optical and near-IR of cool stars, H^- (I = 0.75 eV) dominates:

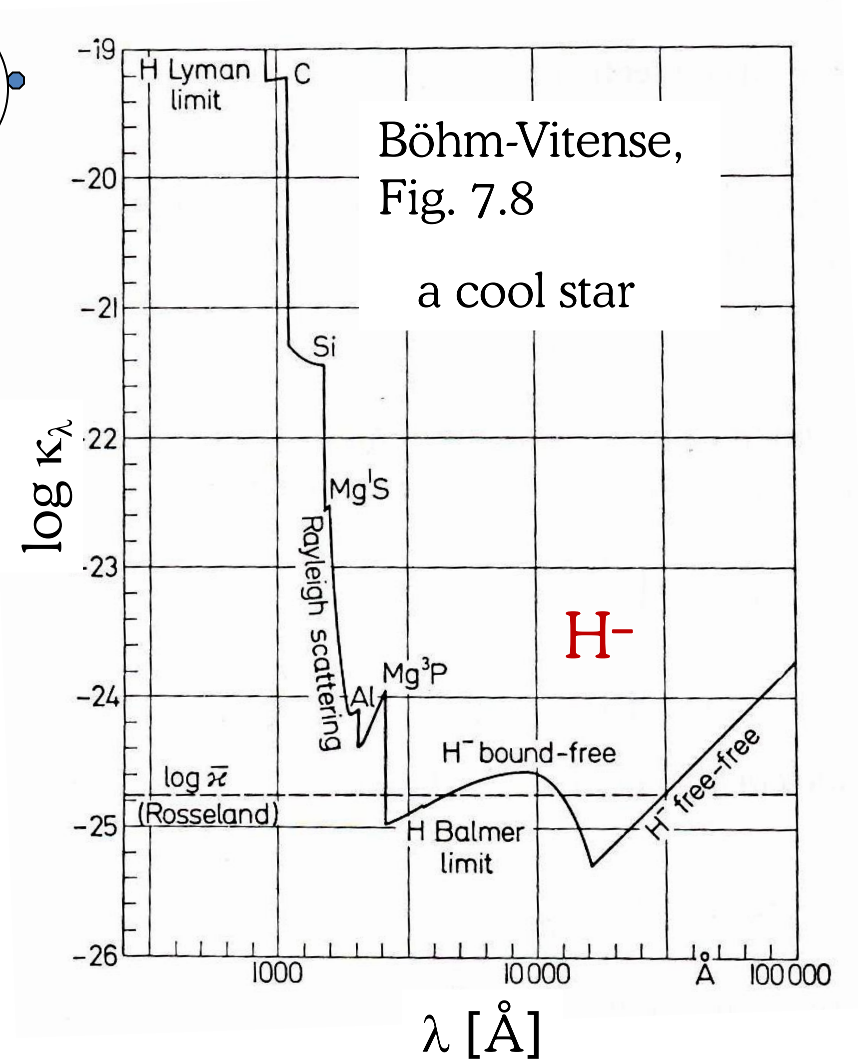
$\kappa_\nu(H^-_{bf})$ = const. $T^{-5/2} P_e \exp(0.75/kT)$

NB: There is only 1 H^- per 10^8 H atoms in the Solar photosphere.

Line opacity *(all the lines you see!)*

Caused by *bb* transitions

Need to know log *gf*, damping and assume an abundance



Abundance nomenclature

Mass fractions: let X, Y, Z denote the mass-weighted abundances of H, He and all other elements ("metals"), respectively, normalized to unity ($X + Y + Z = 1$).

example: $X = 0.744$, $Y = 0.242$, $Z = 0.014$ for the present Sun

The 12 scale: $\log \varepsilon(\mathrm{X}) = \log (n_\mathrm{X} / n_\mathrm{H}) + 12$

example: $\log \varepsilon(\mathrm{O})_\odot \approx 8.7$ dex, i.e., oxygen, the most abundant metal, is 2000 times less abundant than H in the Sun (the exact value is still debated!) ($\log \varepsilon(\mathrm{H}) \equiv 12$)

Square-bracket scale: $[\mathrm{X/H}] = \log (n_\mathrm{X} / n_\mathrm{H})_\star - \log (n_\mathrm{X} / n_\mathrm{H})_\odot$

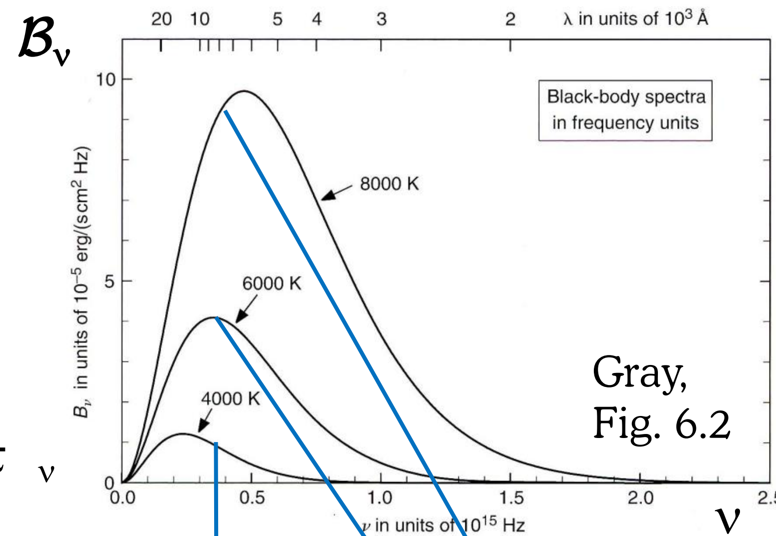
example: $[\mathrm{Fe/H}]_{\mathrm{HE0107-5240}} = -5.3$ dex, i.e., this star has an iron abundance (metallicity) a factor of 200 000 below the Sun (Christlieb *et al.* 2002) ($[\mathrm{X/H}]_\odot \equiv 0$)

How spectral lines originate

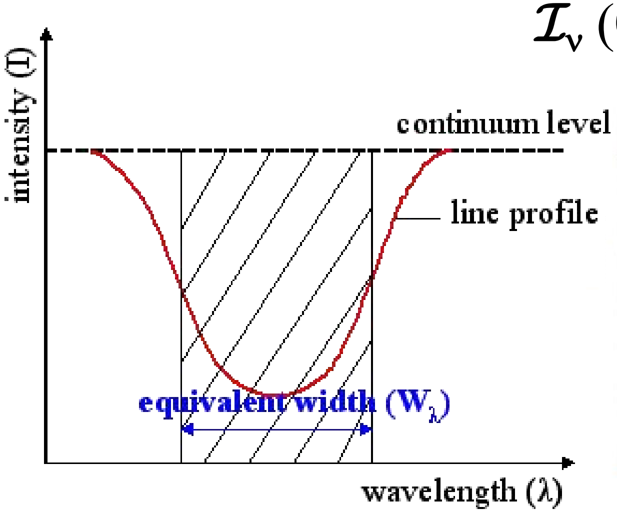
The formation of absorption lines can be qualitatively understood by studying how

$\mathcal{S}_\nu$ changes with depth.

$$W_\lambda \propto d \ln \mathcal{S}_\nu / d\tau_\nu$$



Gray, Fig. 6.2



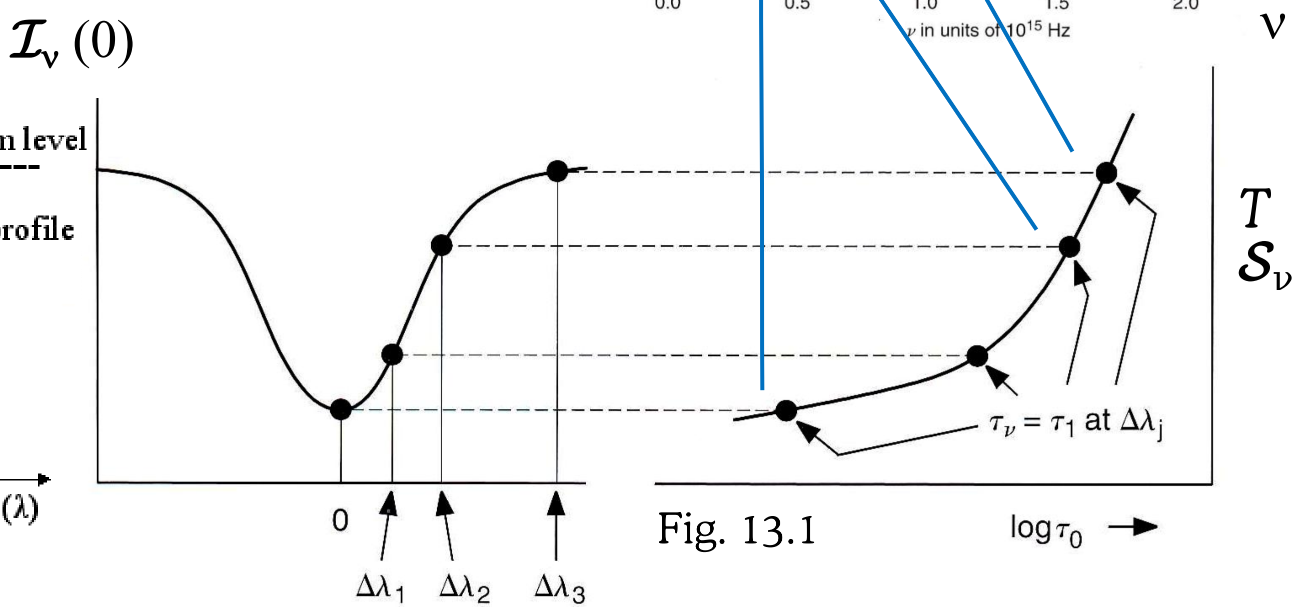


Fig. 13.1

Spectral lines as a function of T_{eff}

The **strength of a weak line** is **proportional to** the ratio of line to continuous absorption coefficients, l_ν / κ_ν . Evaluation of this ratio can tell us about the T_{eff} sensitivity of spectral lines:

$R = l_\nu / \kappa_\nu = \text{const. } T^{5/2} / P_e \exp-(\chi + 0.75) / kT$

for a neutral line of an element that is mostly ionized.

Fractional change with T: $1/R \, dR/dT = (\chi + 0.75 - I) / kT^2$

⇨ depending on χ **neutral lines decrease with T_{eff}** by between 10 and 30% per 100 K (typically 0.07 dex per 100 K). Lines of different χ can be used to constrain T_{eff} (**excitation equilibrium** condition).

For **ionized lines** of mainly ionized elements, one finds low sensitivities to T_{eff}, except those **with a large χ**. These **become stronger with T_{eff}** by up to 20% per 100 K.

Spectral lines as a function of abundance

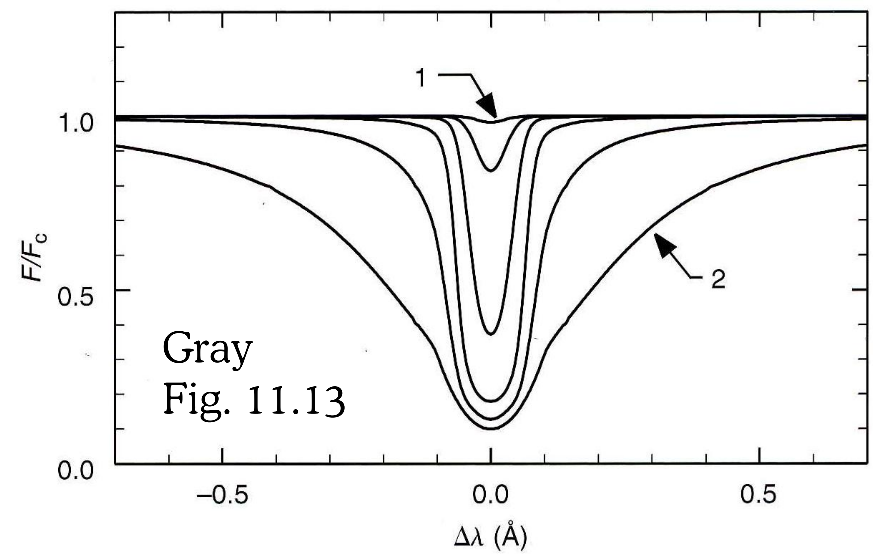
Starting from low log ε (low log *gf*), the line strength is directly proportional to *f* and n_X:

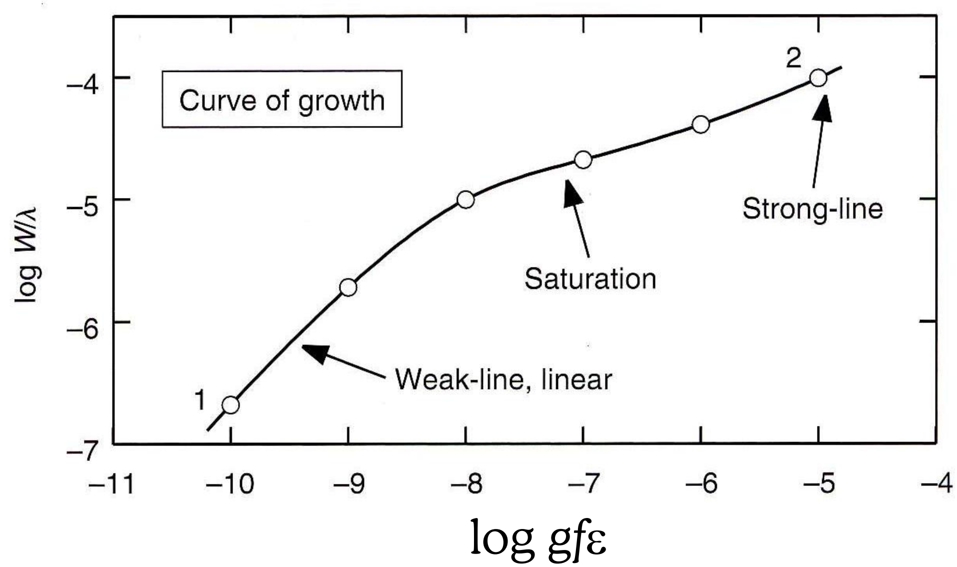
$$W_\lambda \propto gf\, n_X$$

When the line centre becomes optically thick, the line begins to saturate. The dependence on abundance lessens. Only when damping wings develop, the line can grow again in a more rapid fashion:

$$W_\lambda \propto \mathrm{sqrt}(\, gf\, n_X\,)$$

Weak lines are thus best suited to derive the elemental composition of a star, given that they are well-observed (high SNR, little or known blending)





Spectral lines as a function of log g

The T_{eff} sensitivity of spectral lines may be surpassed by sensitivities with respect to other stellar parameters.

Dependence on log g in cool stars, e.g. of Fe I and II lines?

Fe I: (weak) neutral line of an element that is mainly ionized

W_λ is proportional to the ratio of line to continuous absorption coefficients, l_ν / κ_ν .

$n_{r+1} / n_r = \Phi(T) / P_e \quad \Leftrightarrow \quad n_r \approx \text{const.}\, P_e$

$\Rightarrow l_\nu / \kappa_\nu \neq f(P_e)$ neutral lines do not depend on log g

Fe II: (weak) ionized line of an element that is mainly ionized

(**universal**) log g sensitivity via the continuous opacity of H^-

But how to we tell apart a log g sensitivity from an abundance sensitivity?

Spectral lines as a function of log g

The $T_{\rm eff}$ sensitivity of spectral lines may be surpassed by sensitivities with respect to other stellar parameters.

Dependence on log g in cool stars, e.g. of Fe I and II lines?

Fe I: (weak) neutral line of an element that is mainly ionized

W_λ is proportional to the ratio of line to continuous absorption coefficients, l_ν / κ_ν .

$n_{r+1} / n_r = \Phi(T) / P_e$ ⇔ $n_r \approx$ const. P_e

⇨ $l_\nu / \kappa_\nu \neq$ f(P_e) neutral lines do not depend on log g

Fe II: (weak) ionized line of an element that is mainly ionized

(**universal**) log g sensitivity via the continuous opacity of H^-

combining Fe I + II: iron **ionization equilibrium** condition

NB: for strong lines, a damping-related log g sensitivity comes into play.

Broadening of spectral lines

There are numerous broadening mechanisms which influence the strength and apparent shape of spectral lines:

microscopic

1. natural broadening
(reflecting $\Delta E\ \Delta t \geq h/2\pi$)

2. thermal broadening

3. microturbulence ξ_{micro}
(treated like extra thermal br.)

(4. isotopic shift, *hfs*, Zeeman effect)

5. collisions (H: γ_6, log C_6; e^-: γ_4)
(important for strong lines)

macro

6. macroturbulence $\Xi_{r\text{-}t}$

7. rotation

(8. instrumental broadening)

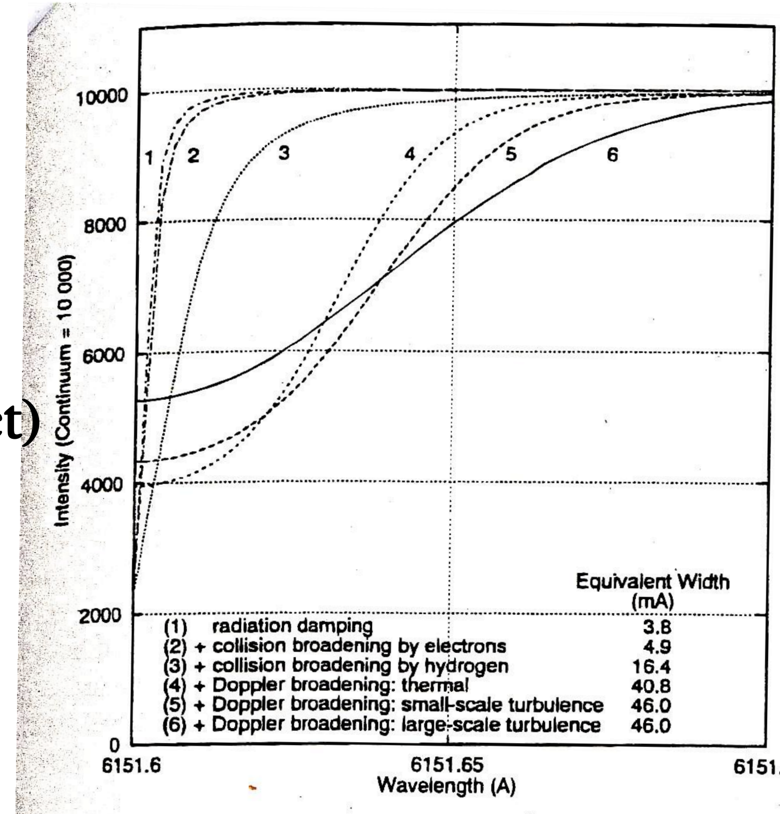


Fig. 3. Synthetic (half-)profiles of Fe I 6151.6 Å (Mult. 62, E.P. = 2.2 eV) showing the cumulative effect of various broadening mechanisms.

Holweger (1996)

Microturbulence and damping

If lines of intermediate or high strength return too high abundances, then the microturbulence or the damping constants are (both) underestimated (the *gf* values can also be systematically off).

Use an element with lines of all strengths to determine ξ.
In most cases, this will be an iron-group element.

3D models treating convection properly do away with the need for micro/macro-turbulence.

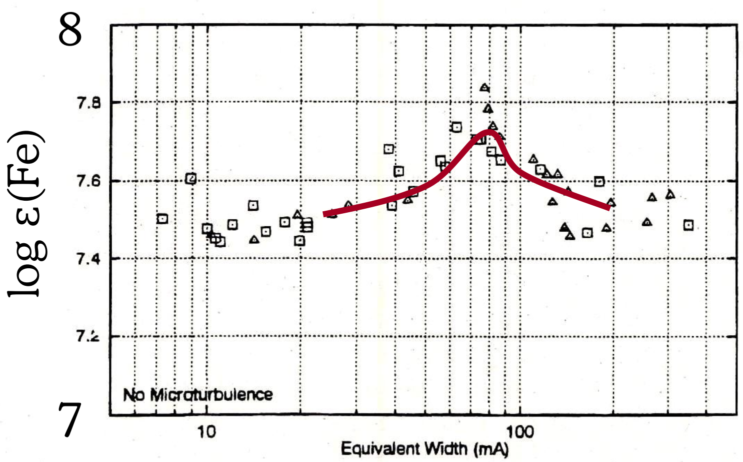


Fig. 7. Same as Fig. 6, but neglecting microturbulence.

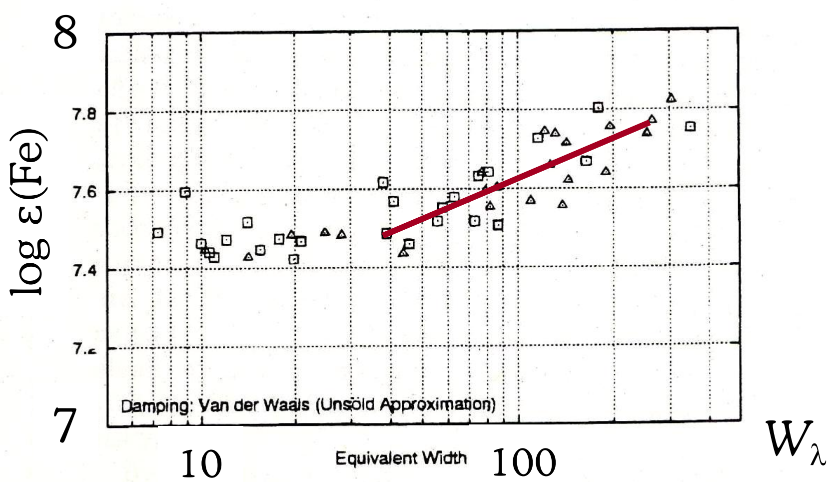


Fig. 5. Iron abundances derived from individual solar Fe I lines and Hannover *gf*-values. The two samples shown are from [4] (squares) and [18] (triangles). The deviation of the stronger lines indicates that the adopted damping constants are too small.

Line lists

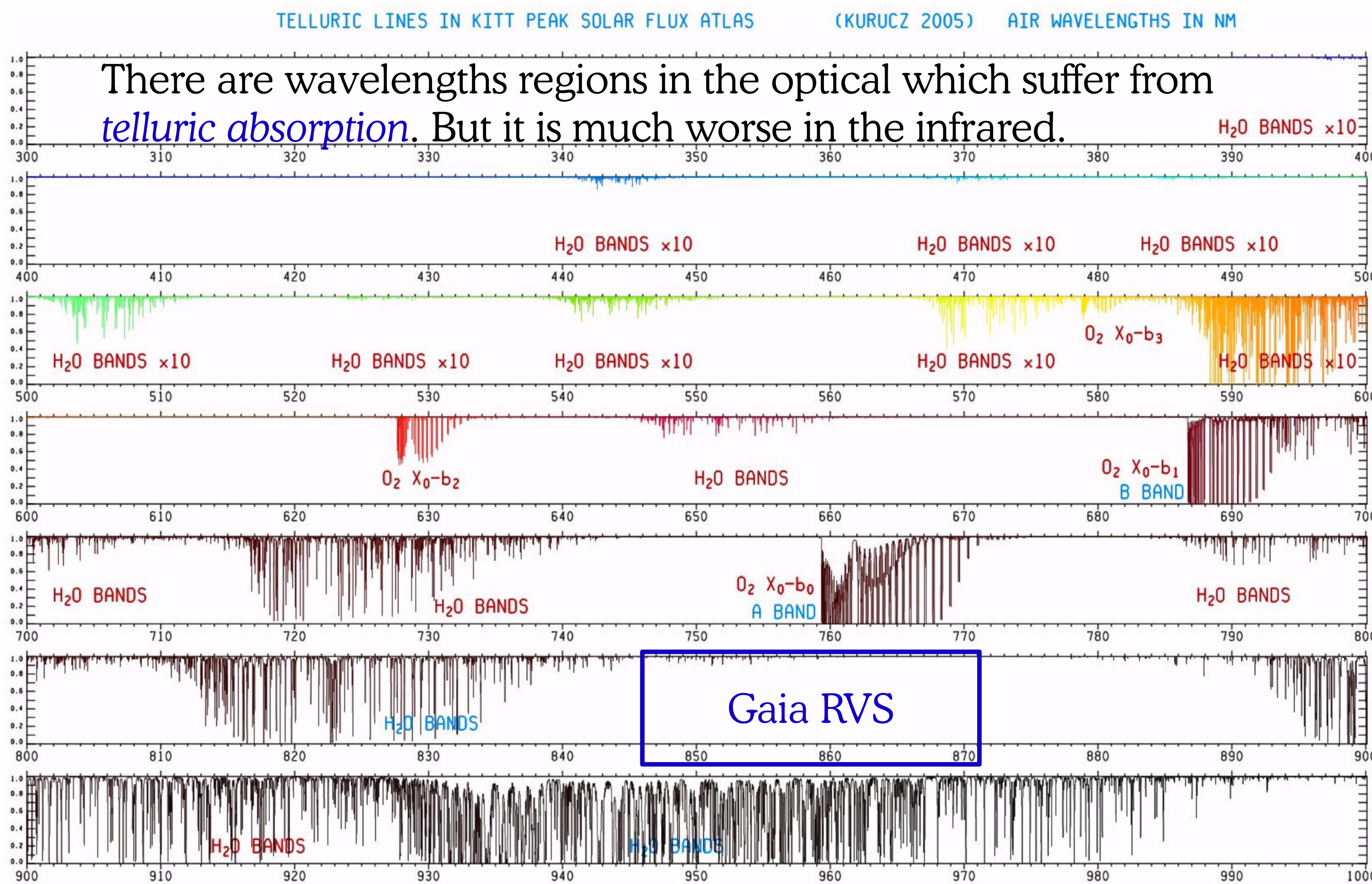
Much of the complexity and the ability to realistically model stellar spectra is encoded in atomic and molecular line lists. These tabulate, among other parameters, the **central wavelengths**, excitation energies and **transition probabilities** of known transitions.

The idea that you can observe an isolated spectral line is an oversimplification. Except at rather low metallicities (or in hot stars), lines tend to be blended with other lines.

Molecules produce molecular bands (from vibrational or rotational-vibrational transitions) and the Earth's atmosphere produces so-called telluric lines.

We peek through Earth's atmosphere

There are wavelengths regions in the optical which suffer from *telluric absorption*. But it is much worse in the infrared.



Example line list

Excerpt from GESv5_atom_nohfs_noiso.420_920nm.tsv, a line list produced for the Gaia-ESO Survey, which you may use this week:

element	wave_A	wave_nm	**loggf**	lower_state_eV	lower_state_cm1	lower_j	upper_state_eV	upper_state_cm1	upper_j	upper_g	…
Zr 2	5112.270	511.2270	**−0.850**	1.6650	13429.130	1.5	4.0900	32988.076	1.5	4.0	…

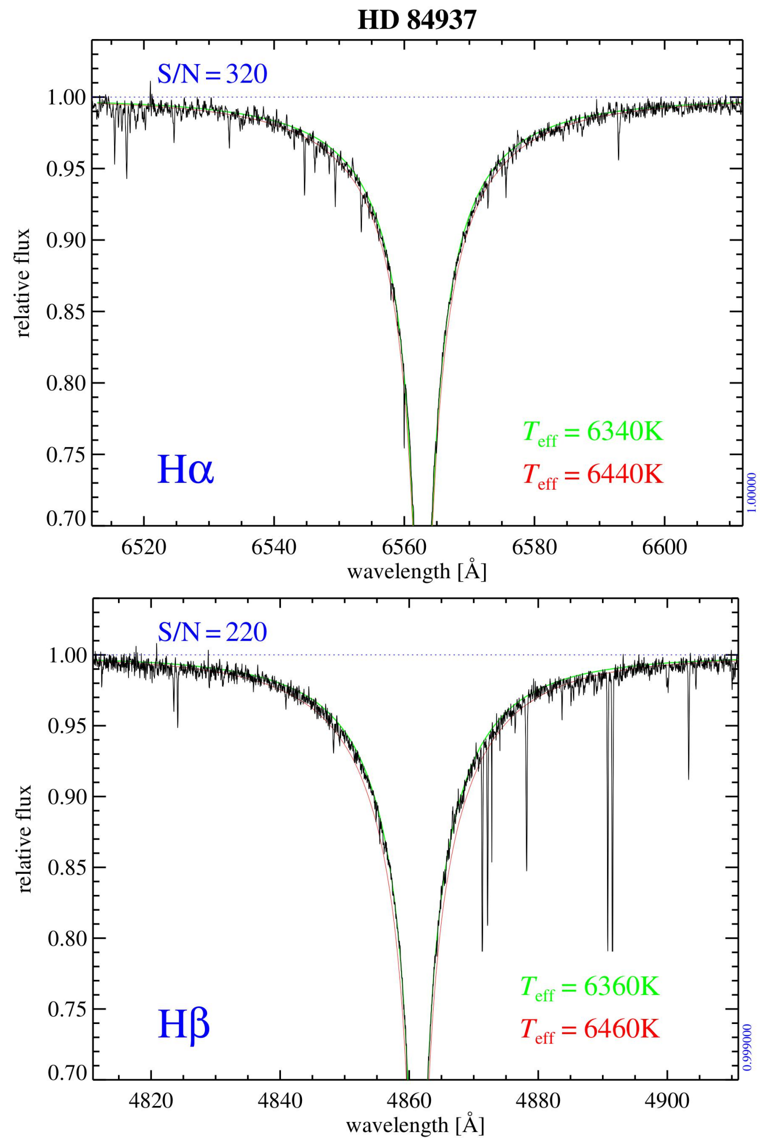
You are always determining $\log gf\,\varepsilon(X)$, i.e. the logarithmic product of the transition probability and the elemental abundance. A bias in one lead to the same-size opposite bias in the other. This is important to remember when comparing to literature results using different transition probabilities.

Spectroscopic T_{eff} indicators: H lines

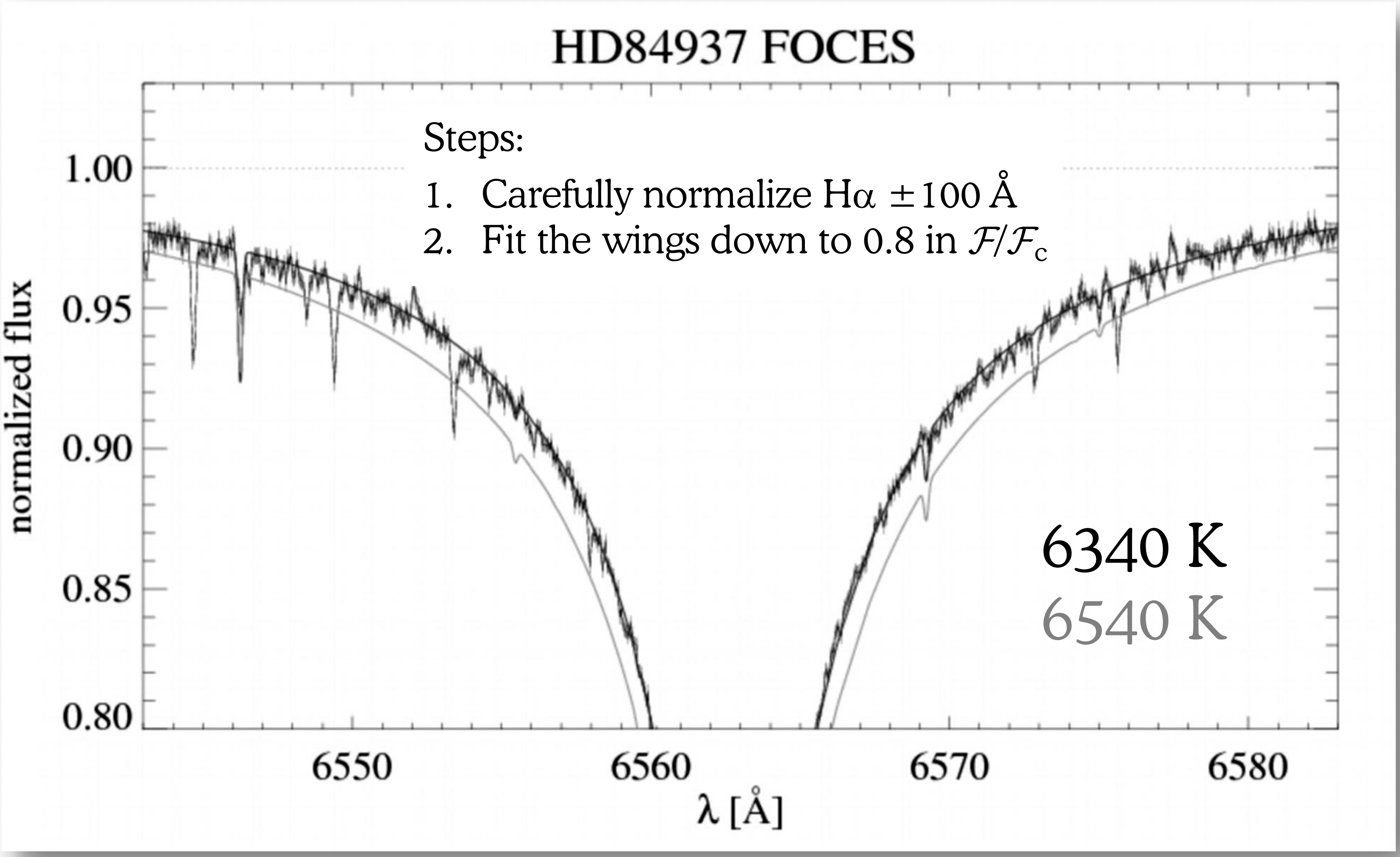
Above 5000 K, the **wings of Balmer lines** are a sensitive T_{eff} indicator, **broadened by H + H collisions** (mainly Hα) **and the linear Stark effect** (H + e⁻).

In cool stars, the log g sensitivity is low (line and continuous opacity both depend on P_e), as is the metallicity dependence. There is some dependence on the mixing-length parameter (Hβ and higher).

Main **challenge** (apart from the surprisingly complex broadening): **recovering the intrinsic line profiles** from (echelle) observations (see Korn 2001).



Hα as a function of $T_{\rm eff}$



Gravity sensitivity of ionized lines

Recall that ionized lines of an element that is mainly ionized have a P_e^{-1} sensitivity via the continuous opacity of H^-.

Integrating the hydrostatic equation, we find

$$P_g \propto g^{2/3}$$

and together with $P_e \propto \mathrm{sqrt}(P_g)$

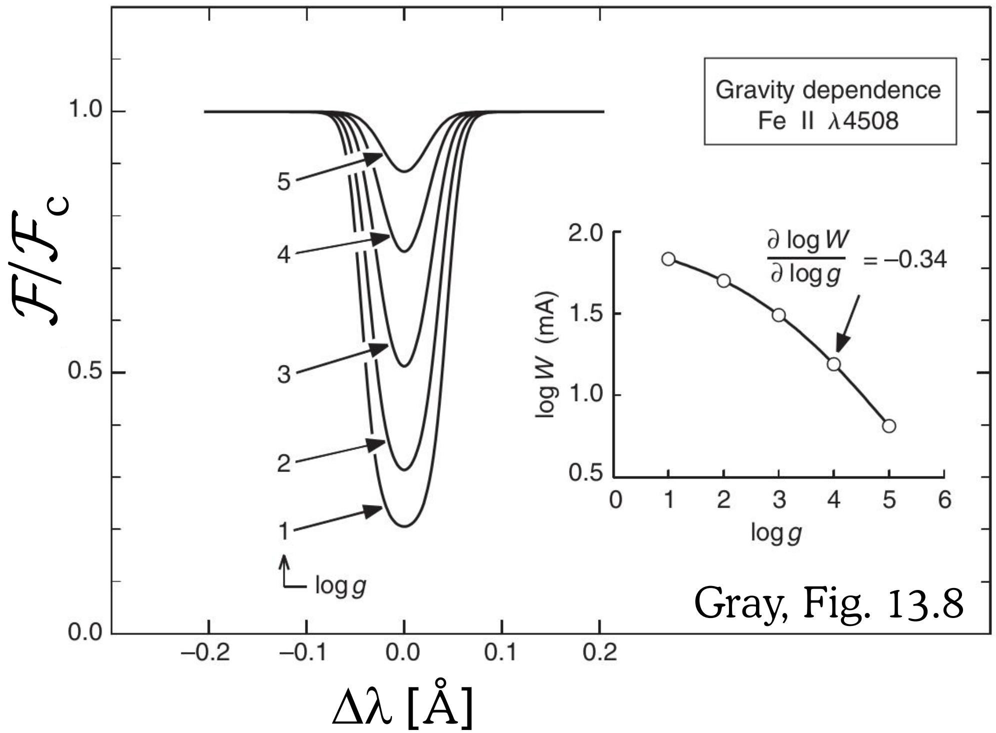
we expect

$$\boldsymbol{l_\nu / \kappa_\nu \propto g^{-1/3}}.$$

This is borne out by actual calculations (see rhs plot) .

Hydrostatic equilibrium

$$dP/d\tau_\nu = g / \kappa_\nu$$



Gray, Fig. 13.8

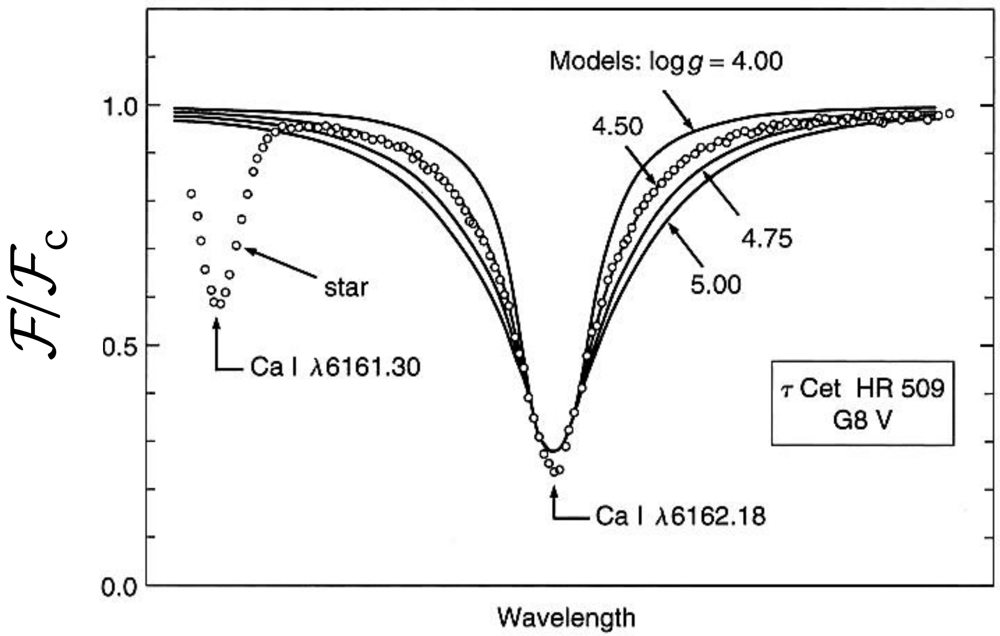
The strong-line method

Gray, Fig. 15.4

Damped (neutral) lines show a strong gravity sensitivity, because

$$l_\nu \propto \gamma_6 \propto P_g \propto g^{2/3}$$

Like with ionization equilibria, log ε needs to be known. This is to be obtained from weak lines of the same ionization stage, preferably originating from the same lower state (small differential NLTE effects).



Examples: Ca I 6162 (see above), Fe I 4383, Mg I 5183, Ca I 4226.

Below [Fe/H] ≈ −2, there are no optical lines strong enough to serve as a surface-gravity indicator.

Spectroscopy of the Solar neighbourhood

Aim

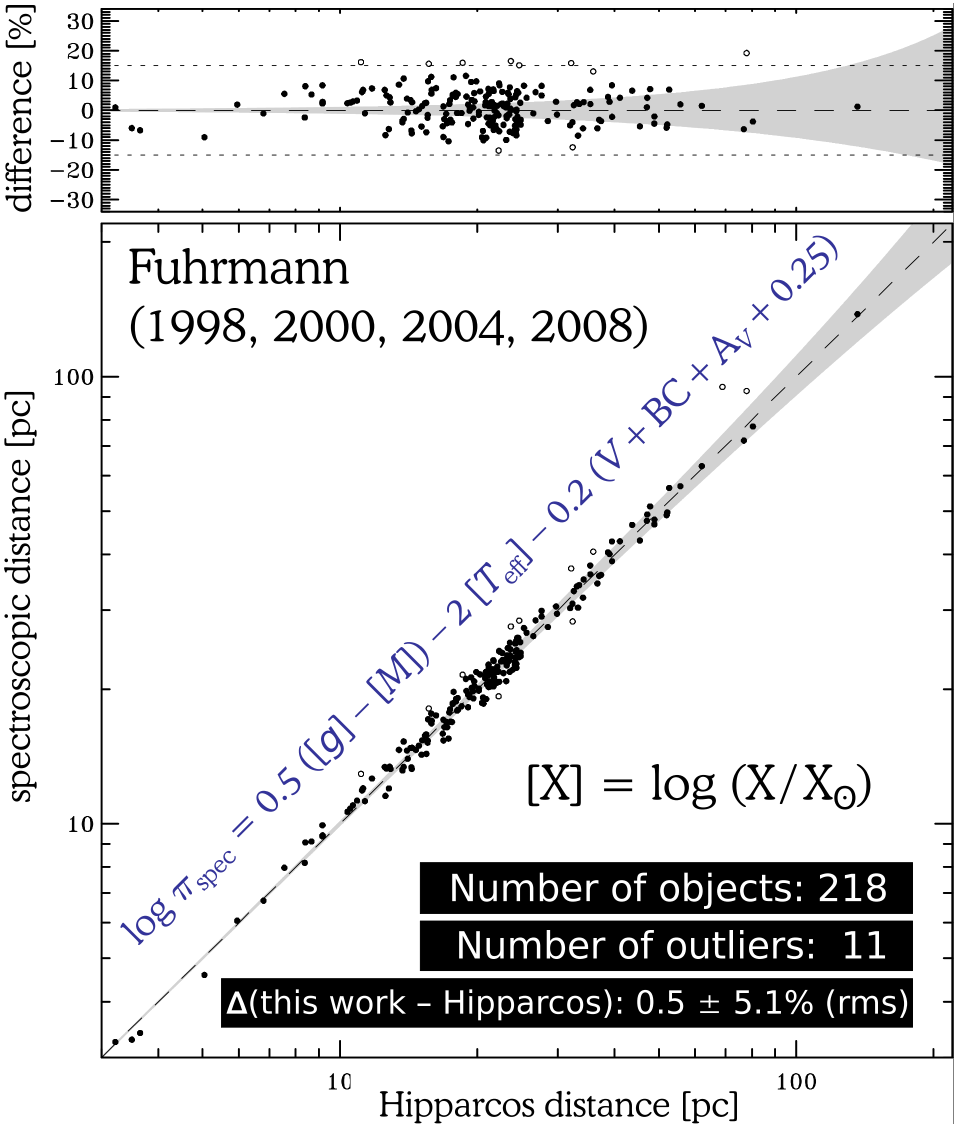
Derive precise stellar parameters and chemical abundances of FGK stars within $d = 25$ pc

Example

The strong-line method as a surface-gravity indicator for not too metal-poor, not-too-evolved stars
coupled with T_{eff} values from Balmer lines
and differential to the Sun.

Benchmark (then)

ESA's Hipparcos mission

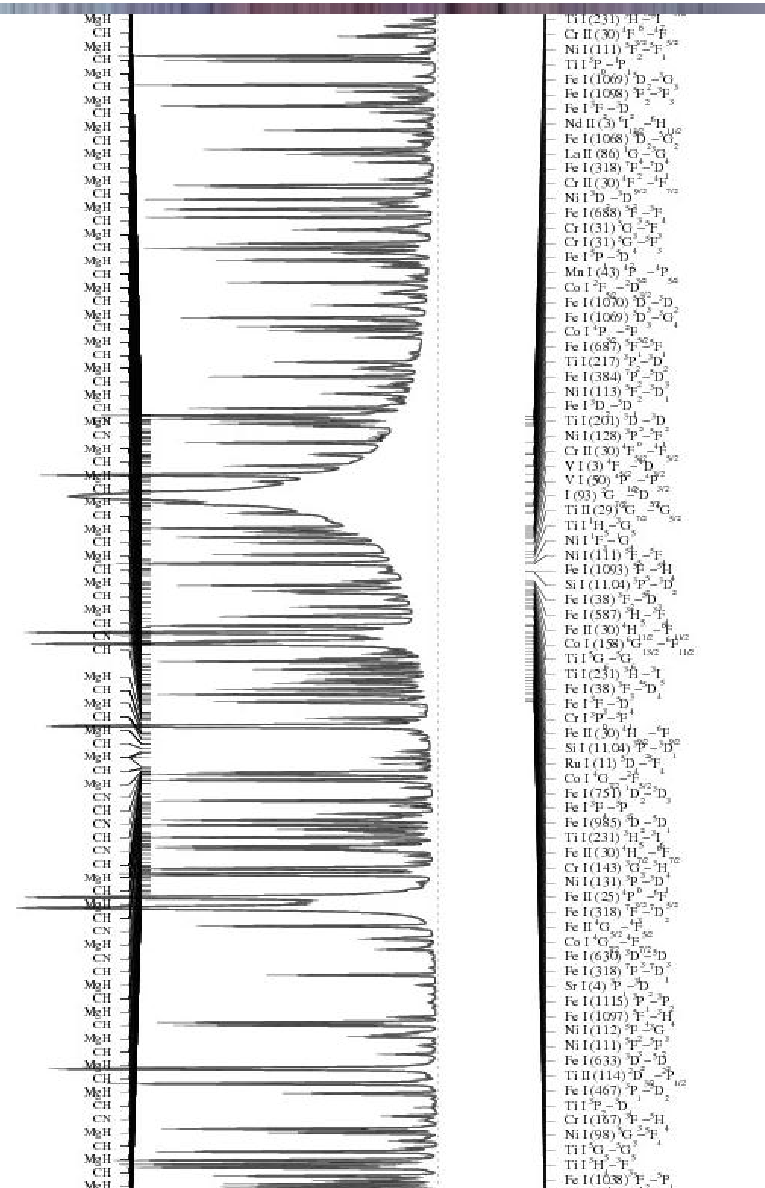


Abundances from H to U

Once you have *good* stellar parameters, it is relatively easy to determine chemical abundances for your favourite element(s).

Caveats

- some elements are not visible, e.g. noble gases in cool stars
- lines may lack or have inaccurate atomic data
- lines can be blended leading to overestimated abundances
- lines can be subject to effect you are unaware of, e.g. 3D and NLTE effects, hfs, isotopic and Zeeman splitting
- …



Important (questionable) approximations

Classical models rest on a number of assumptions that for certain classes of stars have been shown to be problematic for quantitative results:

1. Plane-parallel atmospheres

2. Hydrostatic equilibrium with a local theory for convective energy transport

3. Line formation in Local Thermodynamic Equilibrium (LTE)

   see Andy's lecture!

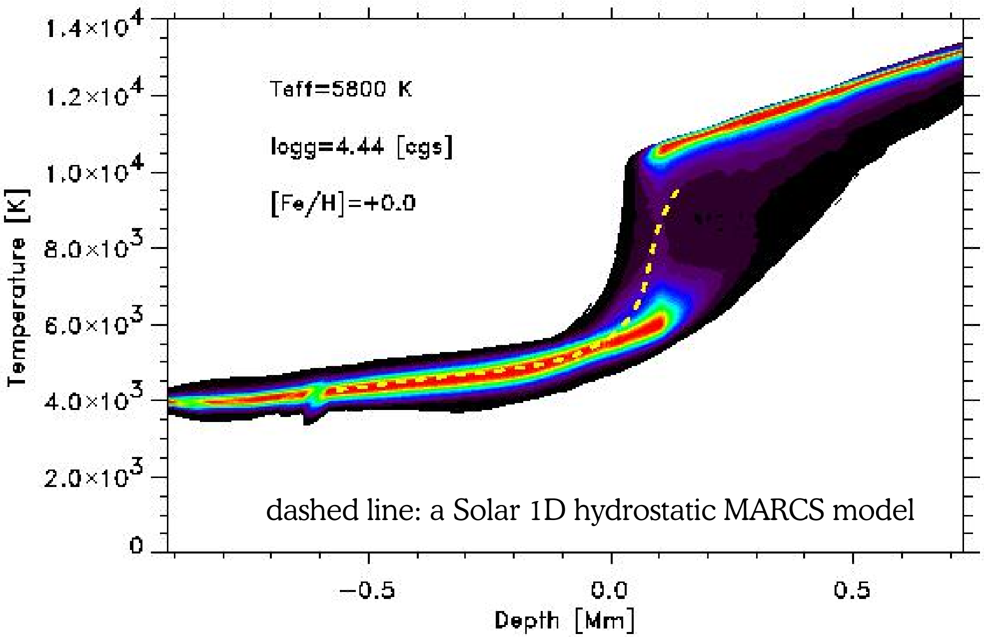
4. Well-mixed atmospheres

5. No chromospheres, no coronae, no magnetic fields, no mass loss

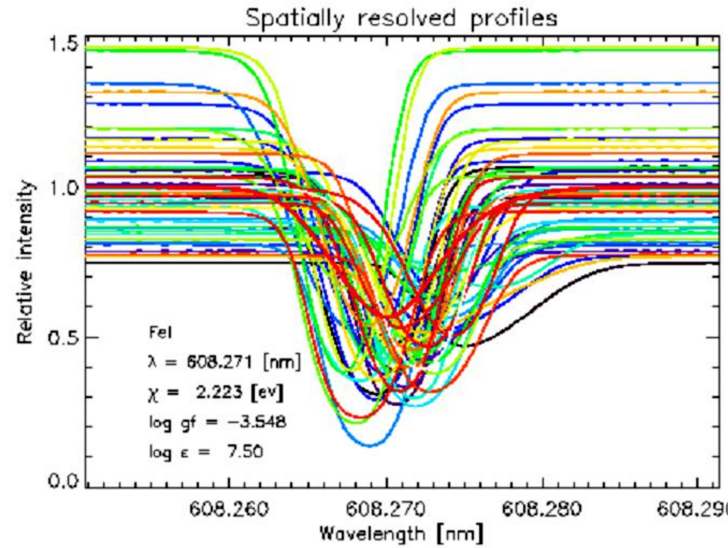
6. *Can you think of other approximations?*

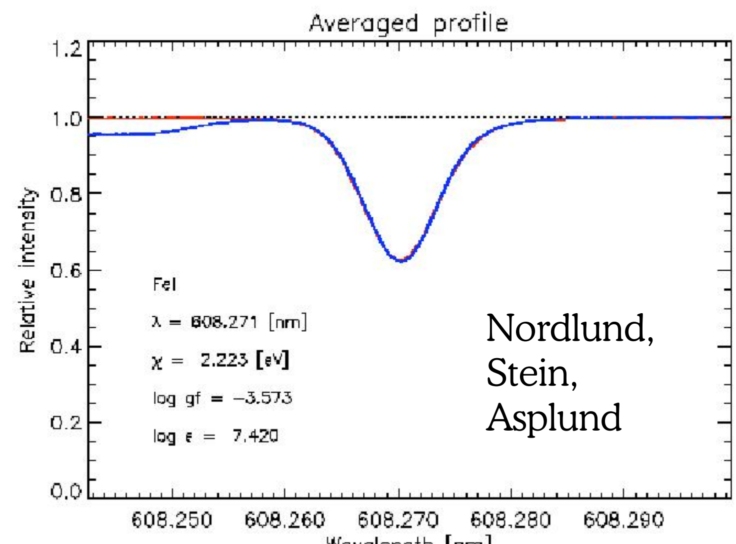
Beyond classical models

... all of the above in 3D hydrodynamic models!



Collet, PhD thesis, UU (2006)





Nordlund, Stein, Asplund

3D $T(\tau)$ relations are significantly cooler at small τ, especially at low metallicity.

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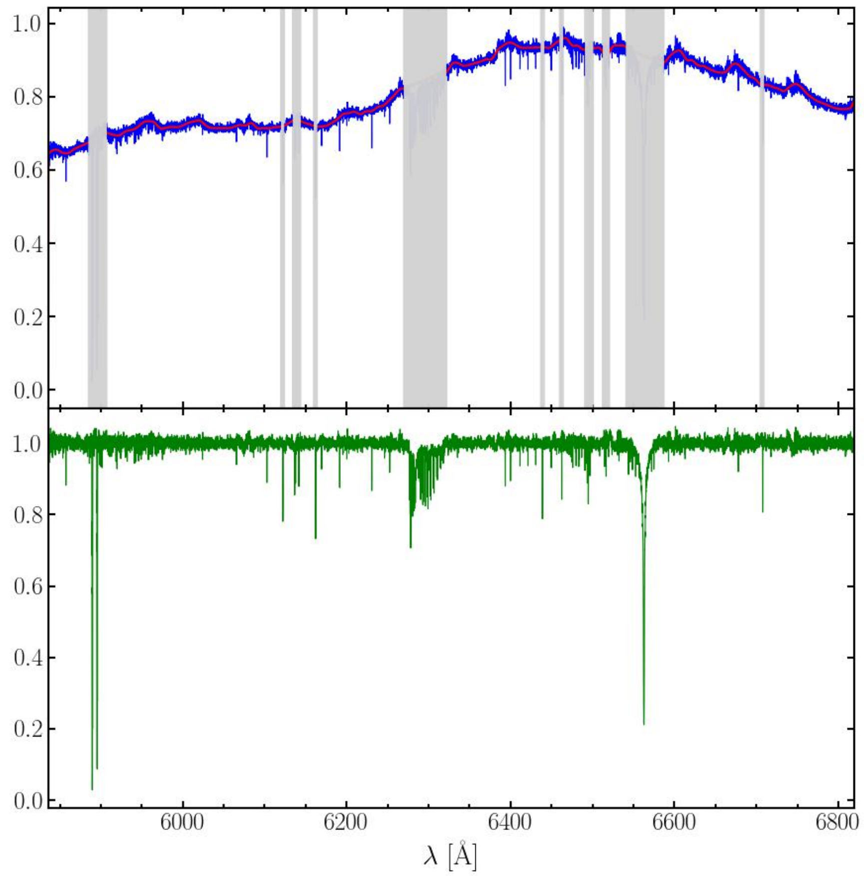
Suggested student groups

Group 1	Group 2	Group 3
Margarita	Thanh	Shilpa
Majid	Annika	Stefan
Laurie	Lapo	Barkha
Pavol	Susmita	Marcel
	Oskar	Raphaela

A small helper: normalizer

We need to provide webSME will a normalized spectrum, i.e. continuum = 1.
Does not have to be perfect, as it will be refined by SME.

To this end, a normalization tool by ChETEC-INFRA postdoc Johannes Puschnig (UU) is provided:
https://github.com/astrojohannes/normalizer
Check it out!



Backup science cases

TYC 6111: Can you retrace the stellar-parameter analysis of Zackrisson *et al*. (2018)? Hα, Mg Ib, Fe I/II…
What do you learn about our ability to constrain distances via spectroscopy? What does Gaia DR3 say?

NGC6397: Can you confirm abundance trends between the groups of stars in this globular cluster (Korn *et al*. 2007)? What do these mean? What other elements would you like to study and why? See Hannes' masterclass!

BD −15 779 and other metal-poor field stars (Hansen *et al*. 2020): Pick a stars and an element and try to confirm the derived line-by-line abundances. See zip file.