NPA-X school, CERN, Switzerland & France (& Spain), 29/8-3/9 2022

Hands-on experience with stellar spectroscopy

I. Target selection

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gaia

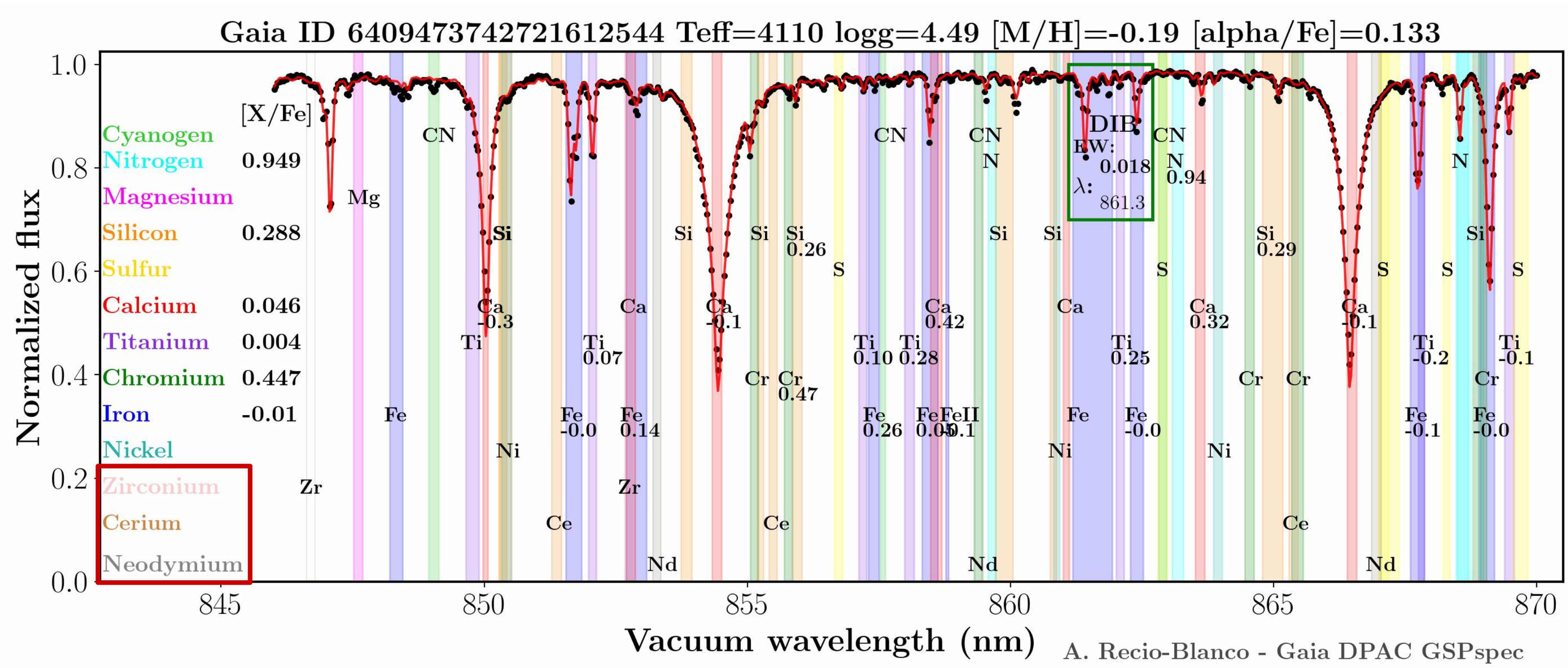
UPPSALA UNIVERSITET

CHETEC INFRA

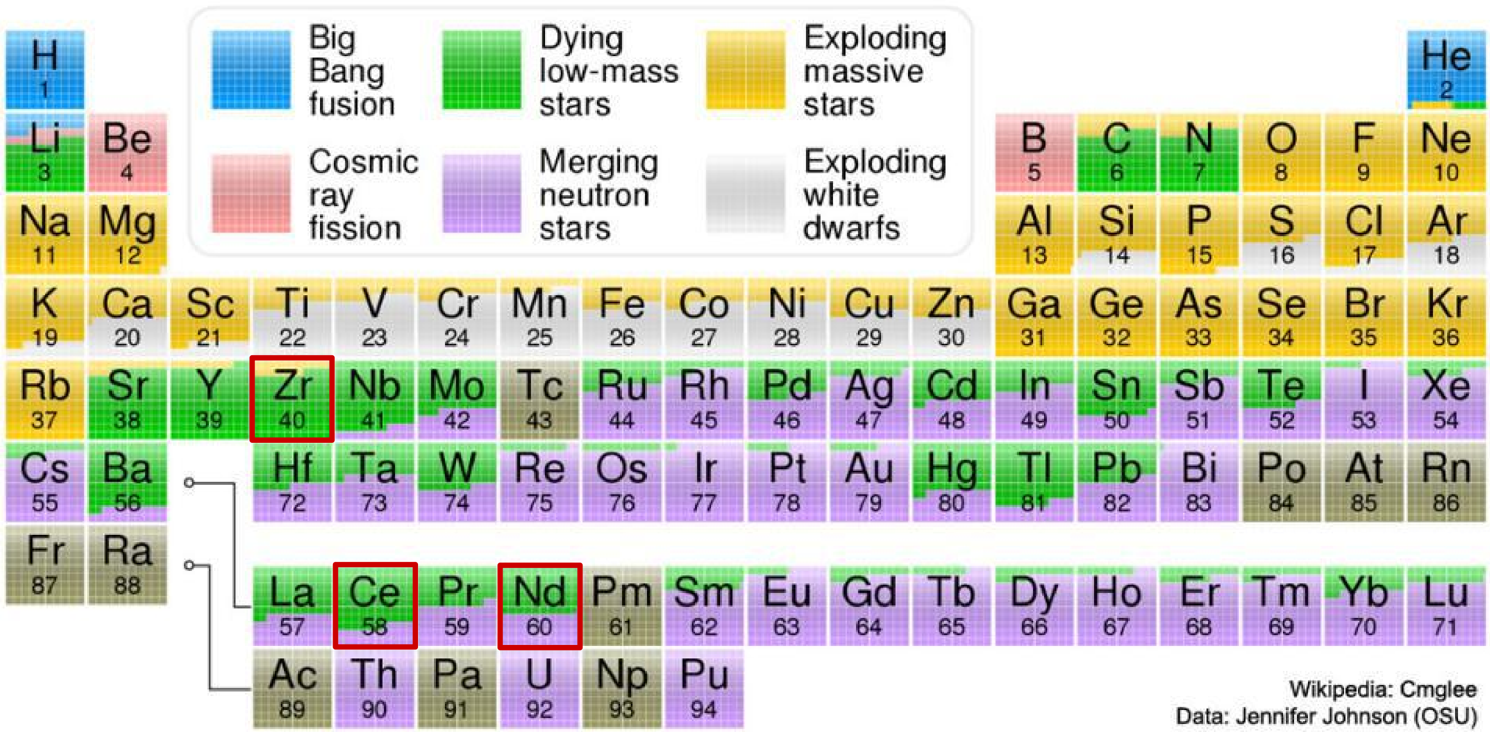
Science first

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!



Our NAP research focus



Of the three neutron-capture elements measured by Gaia,
Zr seems to have the clearest s-process origin. (Disputed.)

Let's look at Zr as one of the three Gaia n-capture elements!

Target selection 1

The run of [Zr/Fe] vs [Fe/H] depicted on the right seems to indicate the existence of mildly metal-poor Zr-rich stars. Are these real? What is the nature of these objects?

Can we preselect, observe and confirm such objects starting from Gaia data? What biases/limitations do we have?

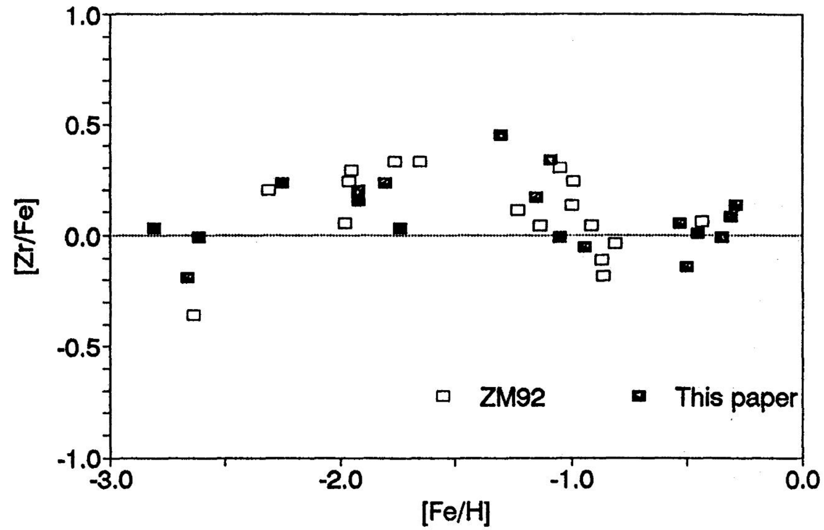


Fig. 5. Run of [Zr/Fe] with [Fe/H]

Gratton & Sneden (1994)

Target selection 2

Even more fundamental is the need to select stars which are visible (and meaningfully observable) when you have observing time (tonight!).

Important aspects:

* location on the sky (RA, DEC) and thus how high in the sky the star is ("airmass" = amount of water)
* apparent brightness (V, G) and achievable signal-to-noise ratio
* efficient observing strategy = minimized dead time at the telescope

Reasonable choices for NOT and our science case:

RA range: 24 ± 5 h or $360 \pm 75°$

DEC range: $> -15°$ (airmass < 1.4) Avoid getting too close to zenith.

SNR: Can be estimated using an Exposure Time Calculator (ETC) for the instrument of your choice (FIES). $V/G < 10$ for SNR ≈ 65 around 450 nm in 1800 s, but even brighter stars will make your life as a spectrosopist a lot easier...

Target selection 3

Run the interactive Gaia archive query at

https://gea.esac.esa.int/archive/

The “Advanced (ADQL)” tab allows you to launch (smaller) jobs.

You will work in teams of 6 to select interesting targets. Given the many possible selection criteria one can apply, your queries will likely return (some) unique targets.

Be smart! **Read up!** Ask Alex and me!

A skeleton ADQL qyery:

SELECT top 100
gaiadr3.gaia_source.source_id,
gaiadr3.gaia_source.ra,
gaiadr3.gaia_source.dec,
gaiadr3.astrophysical_parameters.zrfe_gspspec,
… *(additional parameters of relevance for the selection and observations)*
FROM gaiadr3.gaia_source LEFT join
gaiadr3.astrophysical_parameters ON
gaiadr3.gaia_source.source_id =
gaiadr3.astrophysical_parameters.source_id
WHERE gaia_source.dec >= -15
AND gaia_source.rvs_spec_sig_to_noise >= 100
… *(additional conditions on observability and stellar physics)*
ORDER BY phot_g_mean_mag ASC

Archival parameters related to Zr

ZRFE_GSPSPEC : Abundance of zirconium [Zr/Fe] from GSP-Spec MatisseGauguin using RVS spectra and Monte Carlo realisations, applied to the individual N lines of the element, given in `zrfe_gspspec_nlines` (float, Abundances[dex])

Median abundance of zirconium (assuming source is a single star) from RVS spectra and Monte Carlo realisations derived using MatisseGauguin (Recio-Blanco and et al. 2022) atmospheric parameters and the Gauguin algorithm, applied to the individual N lines of the element, where the number of lines is given in `zrfe_gspspec_nlines`.

ZRFE_GSPSPEC_LOWER : 16th percentile of the abundance of zirconium [Zr/Fe] from GSP-Spec MatisseGauguin using RVS spectra and Monte Carlo realisations (float, Abundances[dex])

Lower confidence level (16%) of the median abundance of zirconium (assuming source is a single star) inferred by GSP-Spec MatisseGauguin (Recio-Blanco and et al. 2022) using RVS spectra. Lower and upper levels include 68% confidence interval.

ZRFE_GSPSPEC_UPPER : 84th percentile of the abundance of zirconium [Zr/Fe] from GSP-Spec MatisseGauguin using RVS spectra and Monte Carlo realisations (float, Abundances[dex])

Upper confidence level (84%) of the median abundance of zirconium (assuming source is a single star) inferred by GSP-Spec MatisseGauguin (Recio-Blanco and et al. 2022) using RVS spectra. Lower and upper levels include 68% confidence interval.

ZRFE_GSPSPEC_NLINES : Number of lines used for [Zr/Fe] abundance estimation (int)

Number of lines used to compute the [Zr/Fe] abundance. Lines with interquartile difference (84th quantile value - 16th quantile value) in the Monte Carlo line abundance distribution higher than 0.5 dex have been excluded.

ZRFE_GSPSPEC_LINESCATTER : Uncertainty estimation of [Zr/Fe] abundance using N lines of the element, given in `zrfe_gspspec_nlines` (float, Abundances[dex])

Standard deviation of the individual N lines (`zrfe_gspspec_nlines`) abundance results.

And similar for Ce and Nd. See
https://gea.esac.esa.int/archive/documentation/GDR3/Gaia_archive/chap_datamodel/sec_dm_astrophysical_parameter_tables/ssec_dm_astrophysical_parameters.html

Gaia's instruments 101

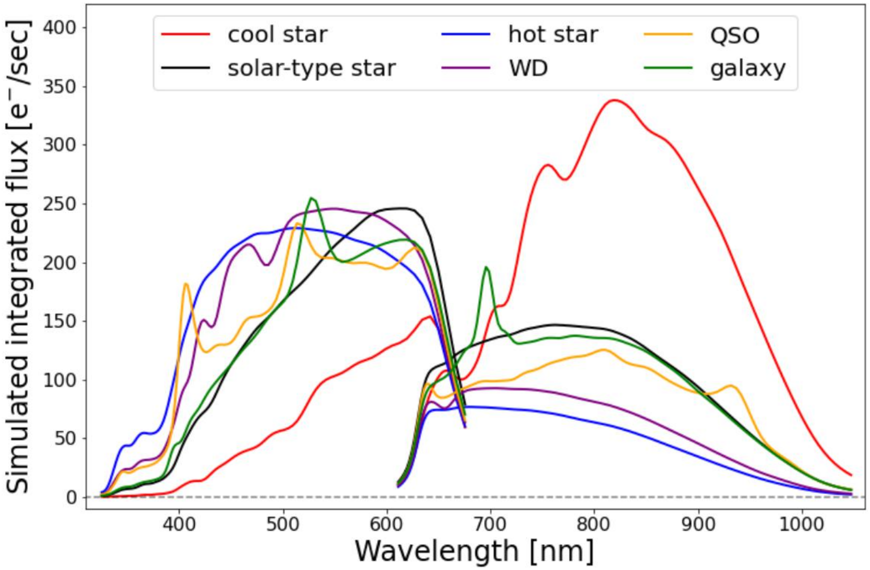
stars

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. — $2\ 10^9$

BPRP: two (spectro)photometers providing colour information (BP-RP, giving a rough estimate of stellar temperature) and resoved BPRP spectra. They can be used to derive $T_{\rm eff}$, interstellar reddening along the line of sight, metallicity, surface gravity etc. With significant degeneracies. See Andrae *et al.* (2022) — $2\ 10^9$ / $5\ 10^8$

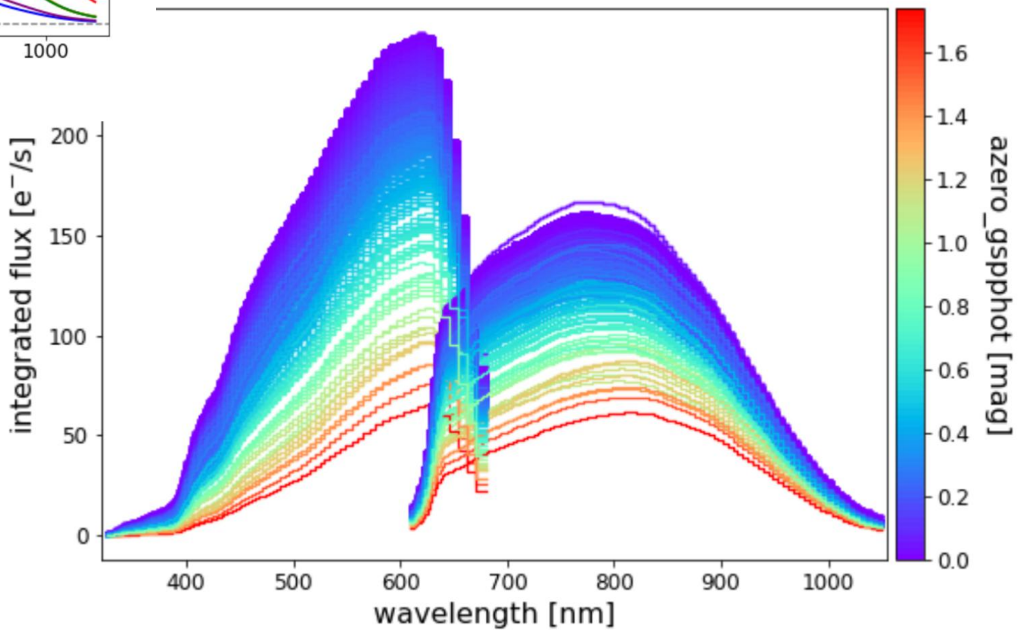
RVS: provides medium-resolution spectra (R = 11,500) in the near-infrared (847 - 870 nm). Mostly for radial velocities, but access to lines allows one to derive stellar parameters and individual chemical abundances for brighter stars. See Recio-*Blanco et al.* (2022) — $2\ 10^6$

BPRP spectra: examples



Different astrophysical objects have very different BPRP spectra!

However, for a given object reddening matters a lot!



[Creevey *et al.* (2022a,b)]

Your first task today

Study how to query the Gaia archive.

Select stars that fulfill your science case: most likely related to Zr, Ce or Nd.

Make sure the targets are observable and determine a reasonable exposure time for them.

The team providing the target with the shortest, scientifically meaningful exposure time will go first tonight.

This will be a spectrum that all groups can download and work on while not doing observations themselves.

Otherwise, work on the example spectra.

Hands-on experience with stellar spectroscopy

II. NOT observations

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gaia

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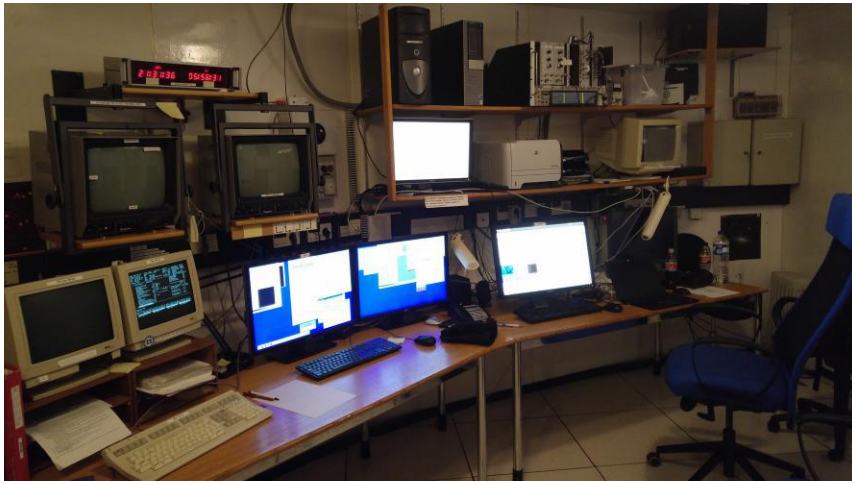
The telescope: NOT



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 1984 and is known for its reliability.

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

The spectrograph: FIES

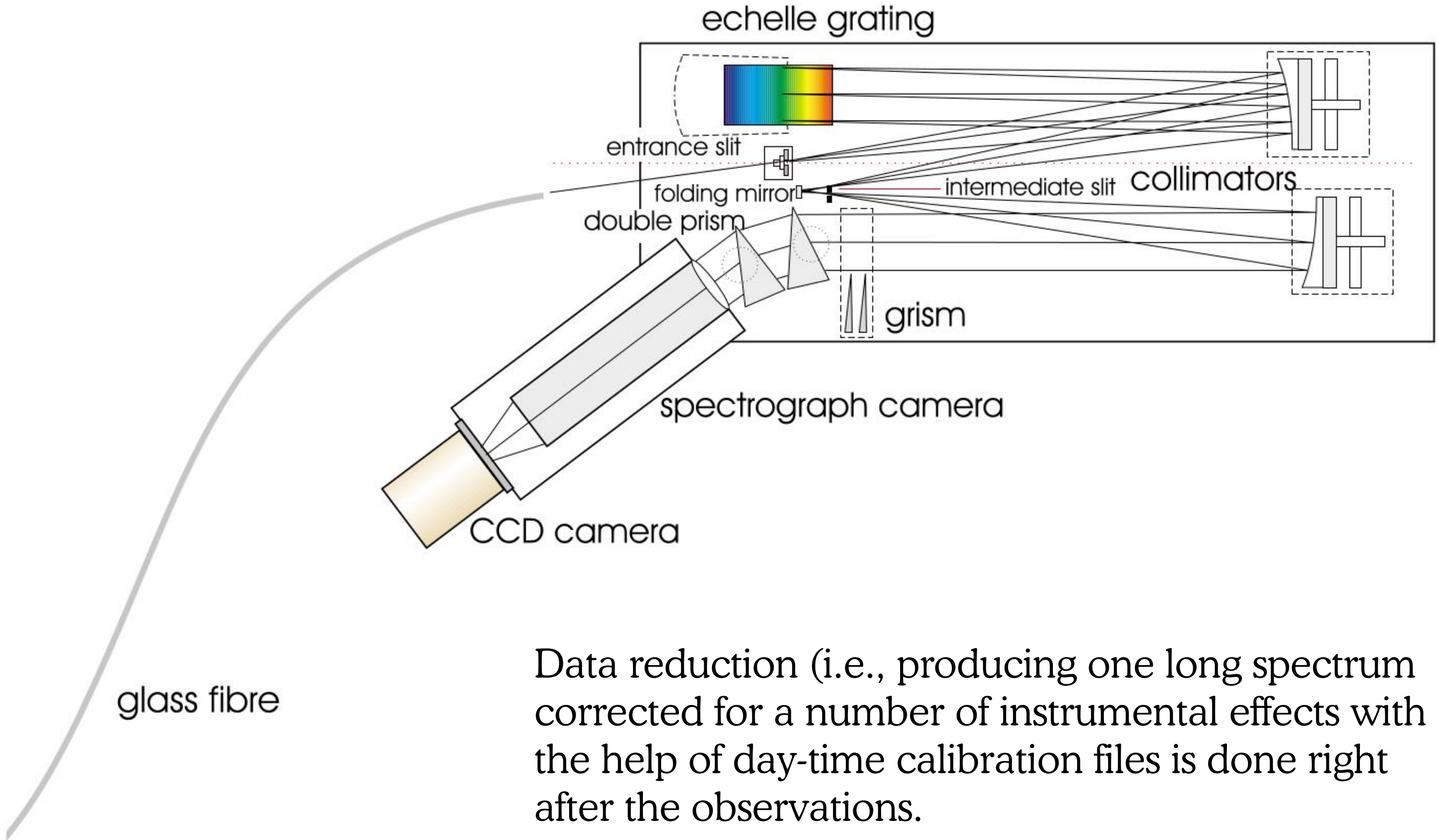
FIES is a modern high-resolution fibre-fed echelle spectrograph. Light enters the spectrograph through a fibre with a 1.3 arcsec diameter on the sky. This means that if the seeing at the telescope is 1.3”, roughly one third of the light gets lost.

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.

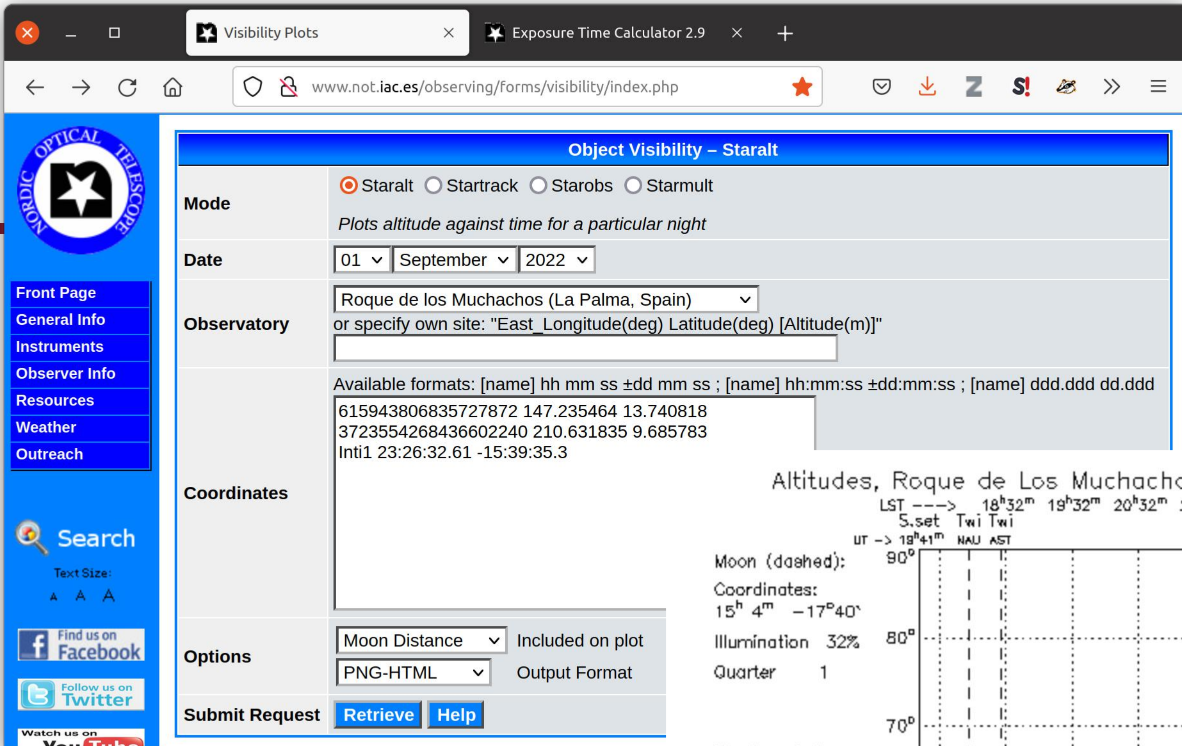
See http://www.not.iac.es/instruments/fies/ and http://www.not.iac.es/instruments/fies/devel/telting2014FIES.pdf

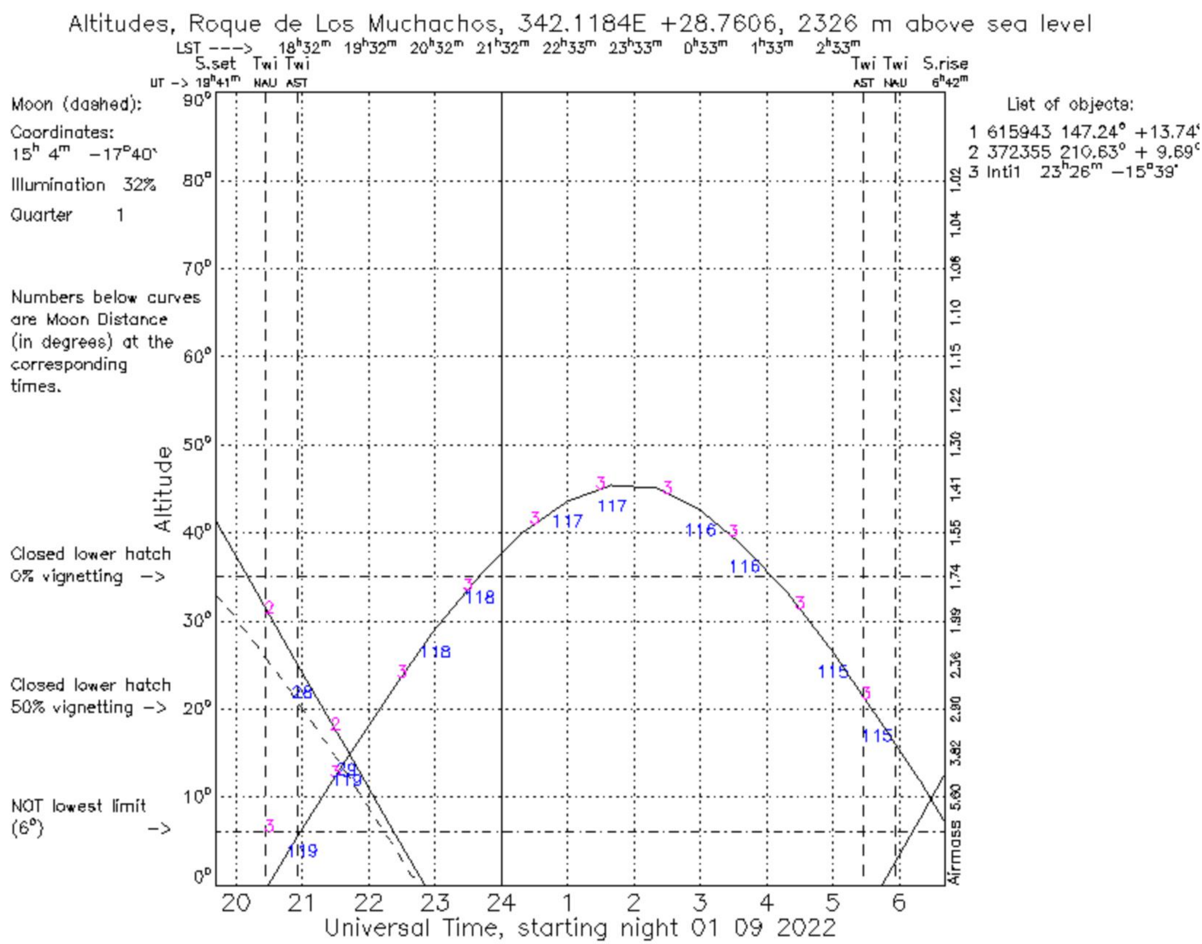
Schematic of an echelle spectrograph



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.

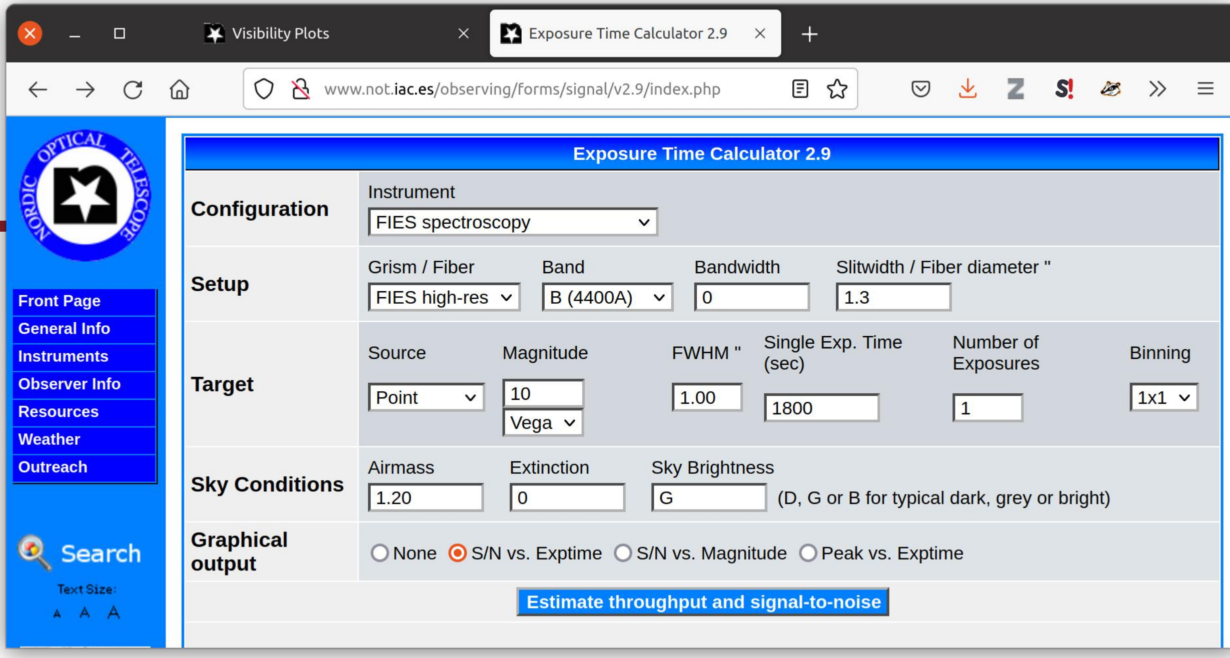
Visibility tool

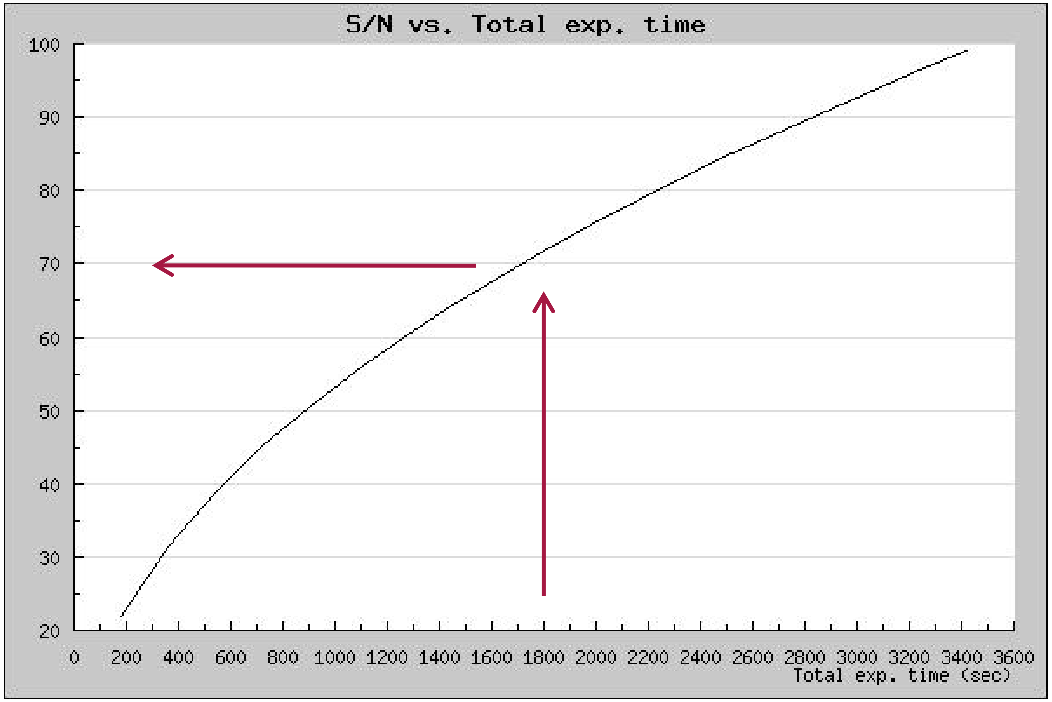




http://www.not.iac.es/observing/forms/visibility/index.php

ETC



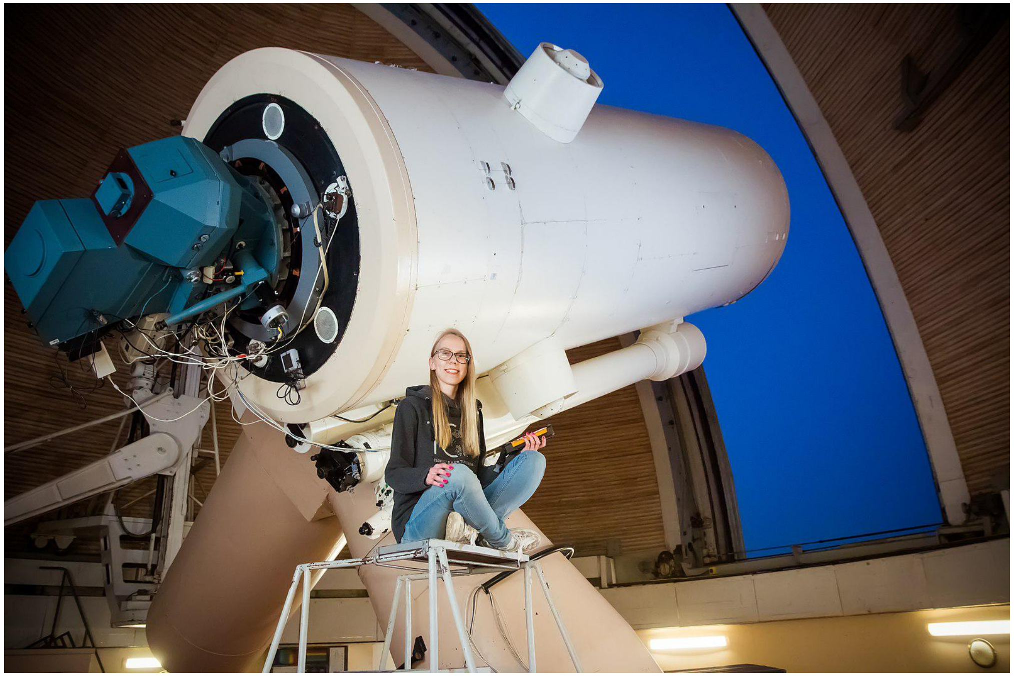


http://www.not.iac.es/observing/forms/signal/v2.9/index.php

Preparing each observing sequence

As we do not know our targets yet, our night assistant **Anni Kasikov** will help us with this. Luckily, for spectroscopy it is not much more difficult than knowing the target's coordinates and having decided on an appropriate exposure time.

We may also go to bed at some point and let Anni take care of remaining exposures.



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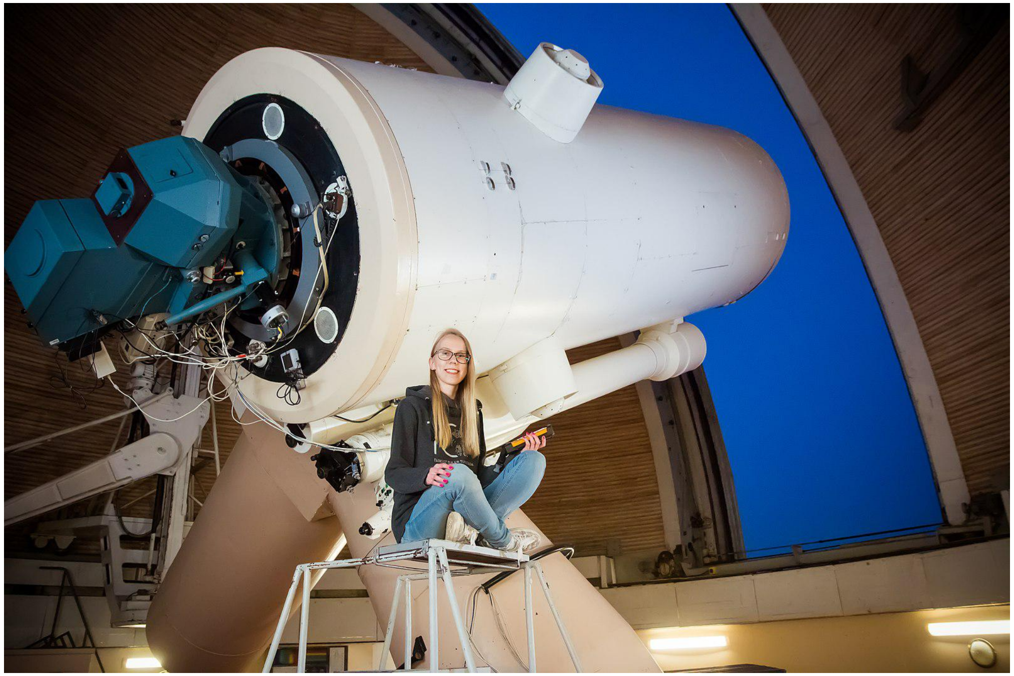

Clear skies!!!

Your task

Familiarize yourself with the Visibility tool and the ETC in order to select targets you can observe tonight.

Ideally, find targets for the whole night.

Come up with a priority list for your targets.

A side note: If you pick high-Zr,Ce,Nd stars from the Gaia catalogue and (dis)cornfirm their n-capture abundances, then you are strictly speaking not done. You should study the distribution of Zr,Ce,Nd abundances for a certain class of stars (dwarfs/giants in a certain [Fe/H] bin) to confirm the ensemble properties (min/max, scatter etc.).

Hands-on experience with stellar spectroscopy

III. Abundance analysis

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gaia

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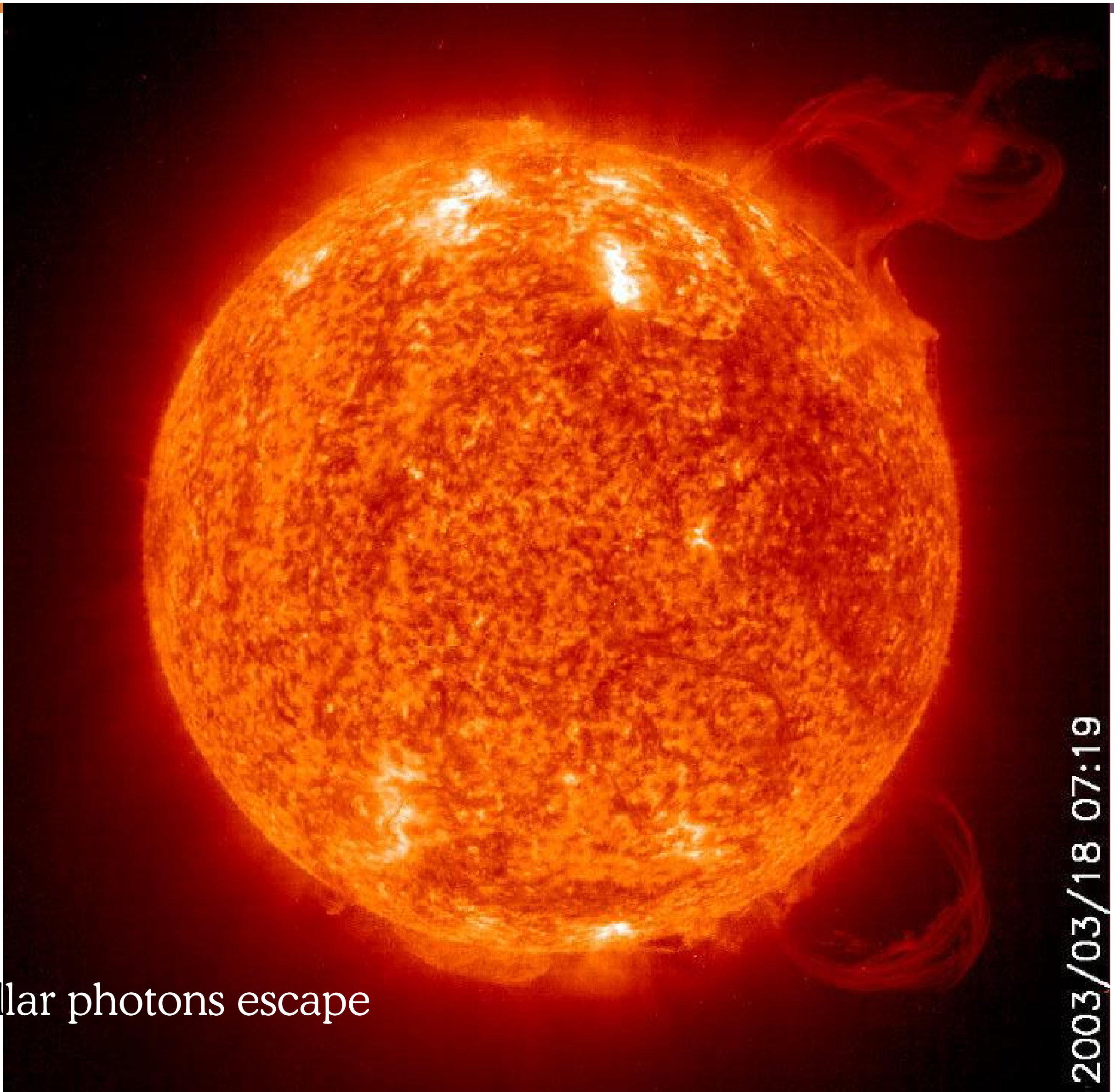
Stellar atmospheres…



… where stellar photons escape

Quantitative stellar spectroscopy

observation vs. theory

NOT

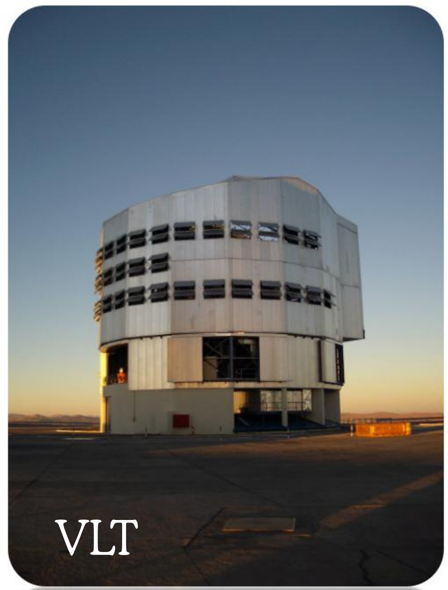
telescope

FIES

spectrograph

E2V 42-40

CCD



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

concepts

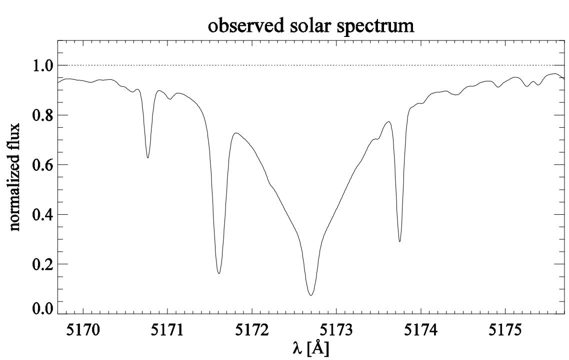
$$\frac{d}{dx}\mathcal{F} = 0$$

LTE

approximations

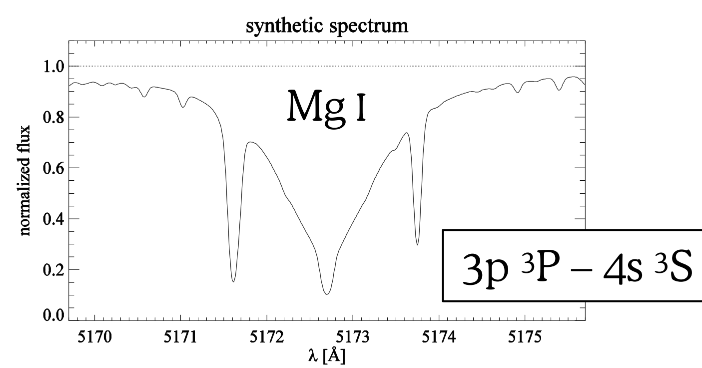
MLT

numerical model



comparison

to constrain thermodynamic variables and abundances



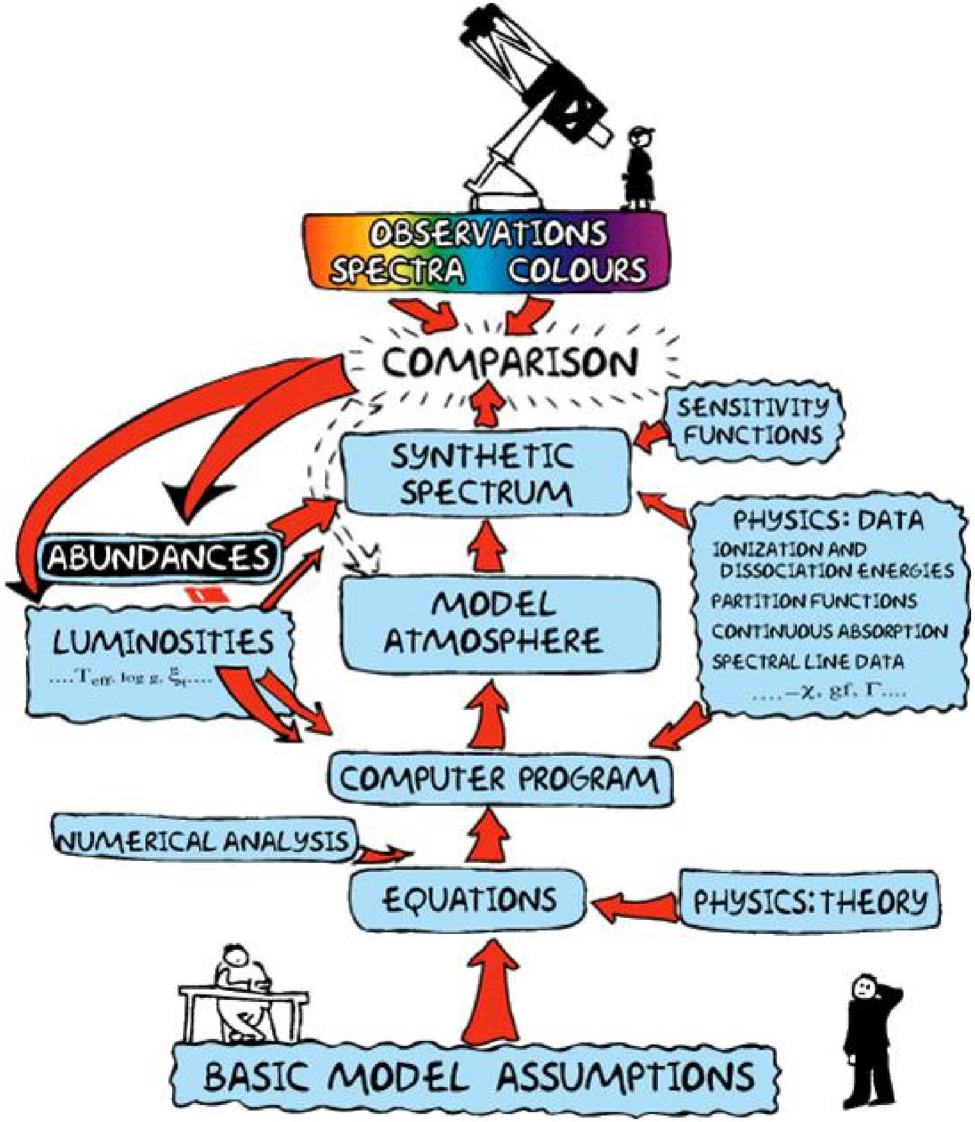
Modelling stellar spectra

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

* the computation of an appropriate model atmosphere

and

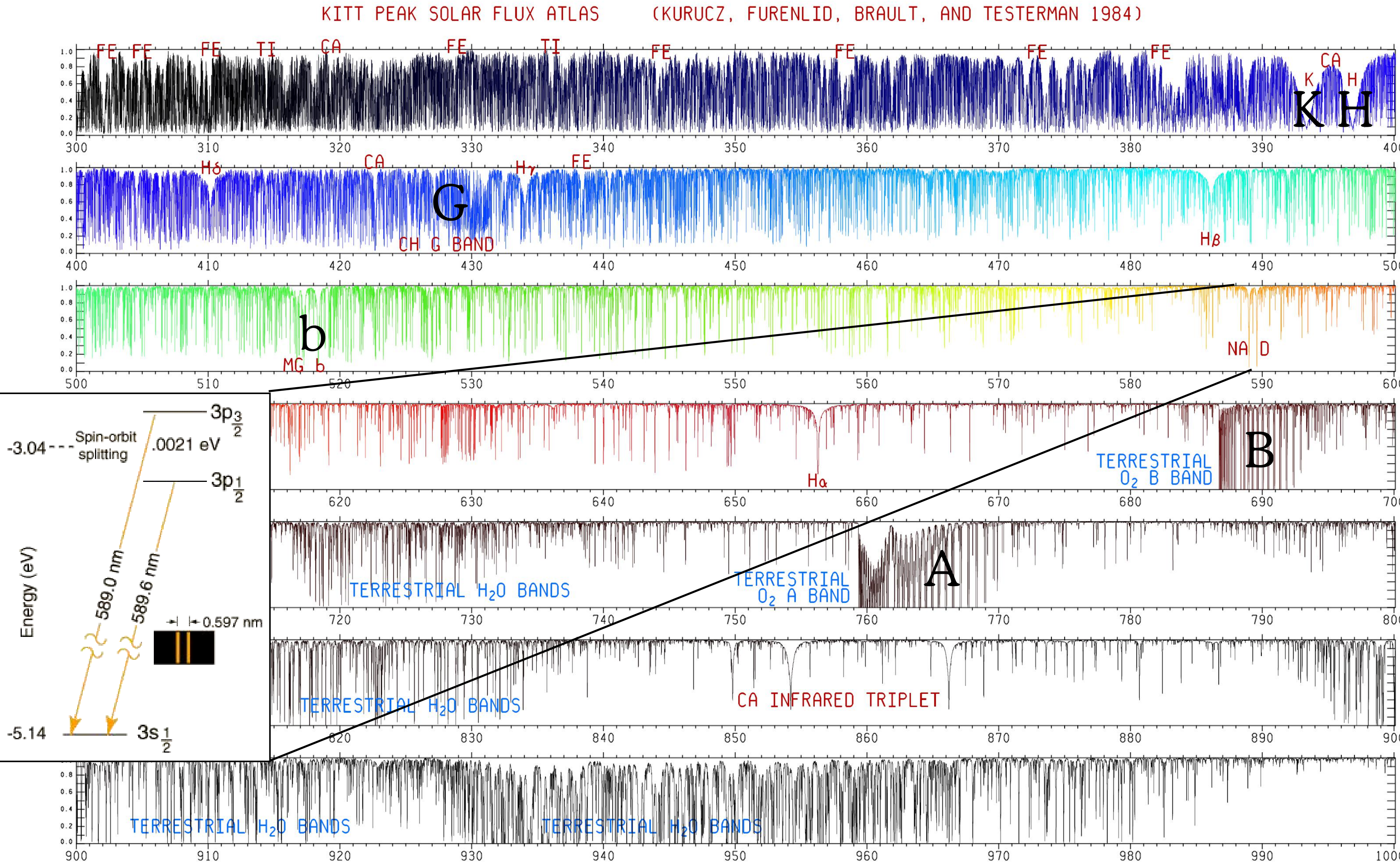
* the computation of a synthetic stellar spectrum.



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

Bengt Gustafsson

The solar spectrum



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:

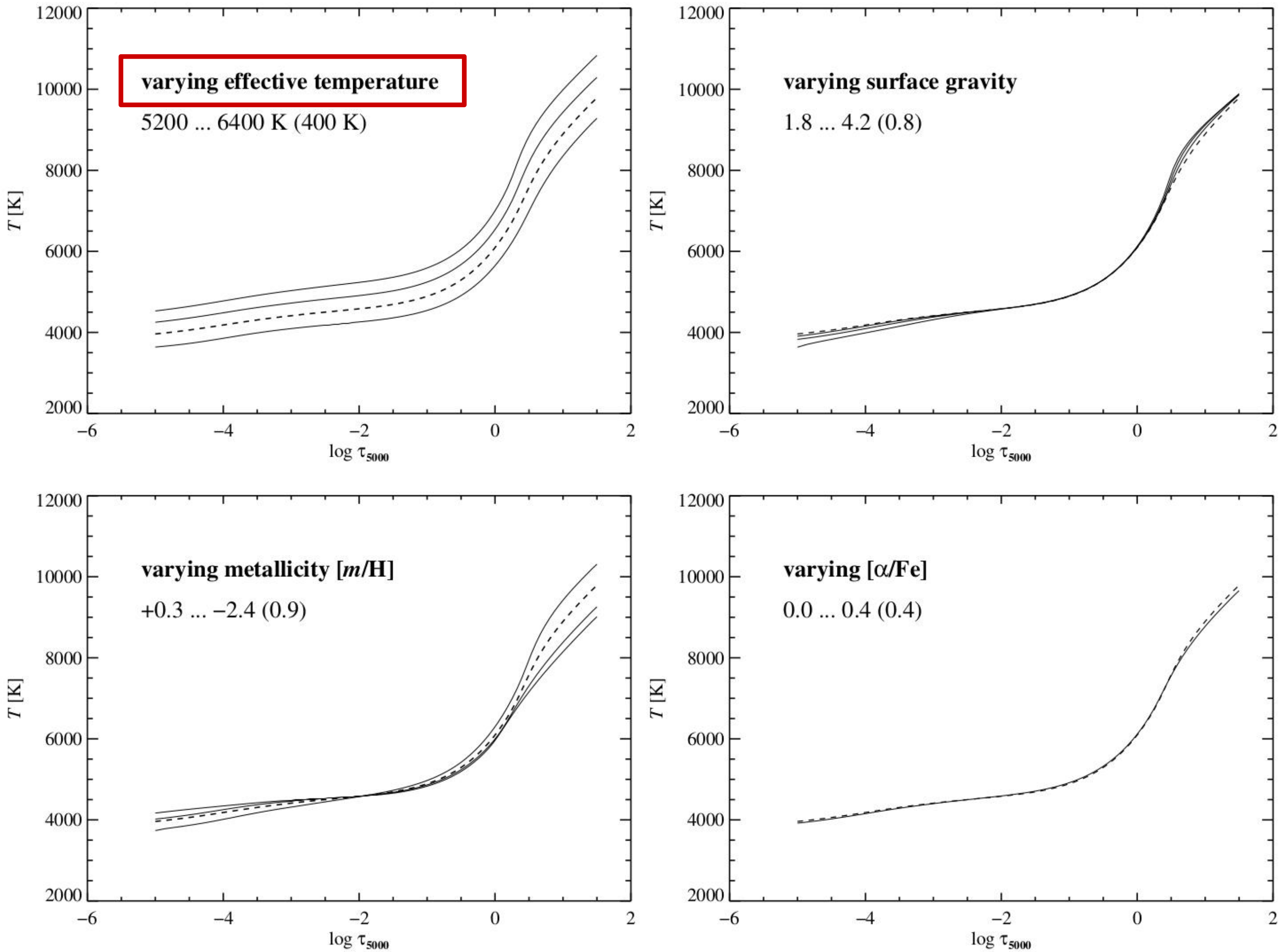
$$\frac{dI_\nu}{d\tau_\nu} = -I_\nu + S_\nu$$

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

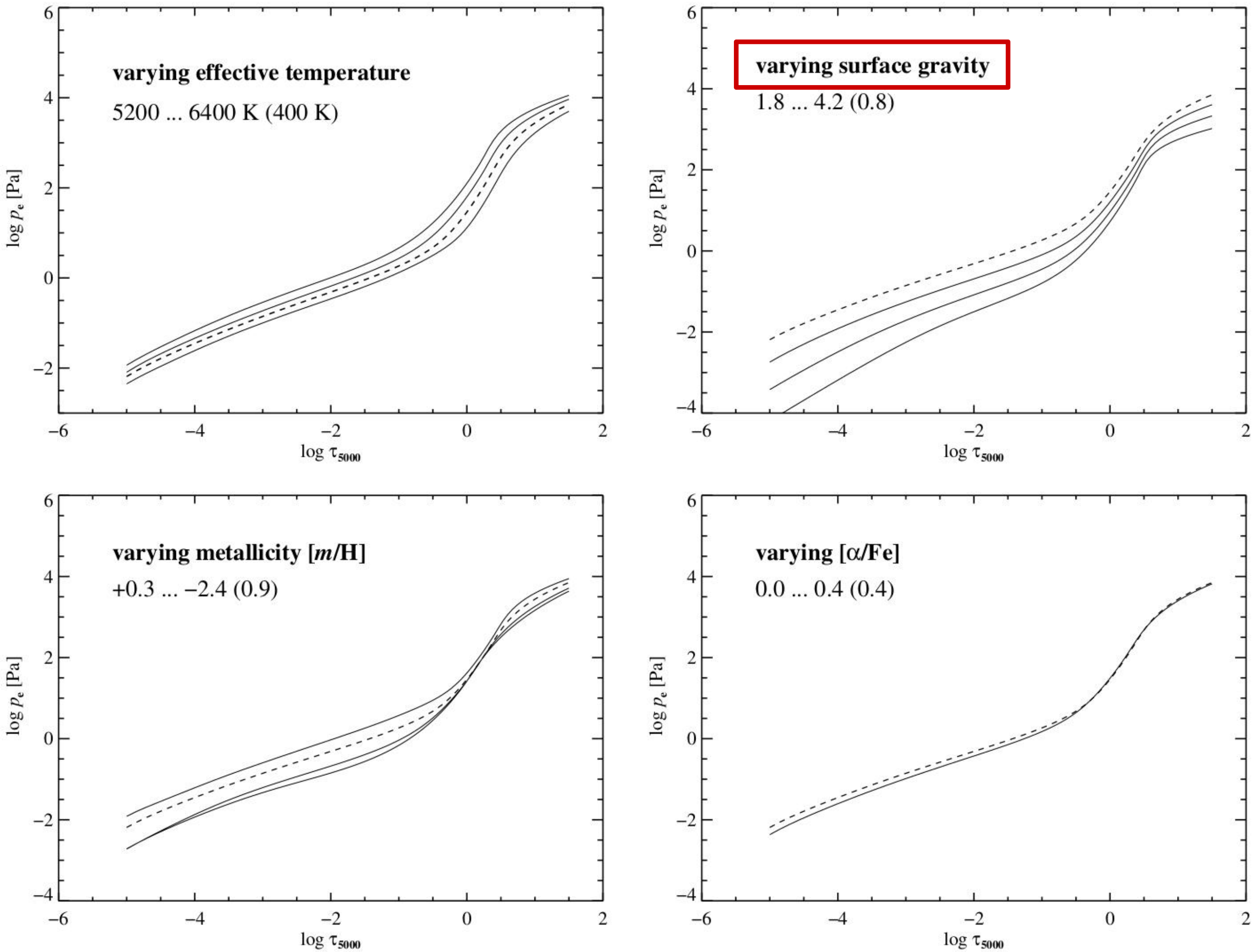
A model atmosphere tabulates two or more thermodynamic variables as a function of (optical) depth. It is one of the main inputs to calculations of synthetic stellar spectra.

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 tau



Pressure stratification: here P_e



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.

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.

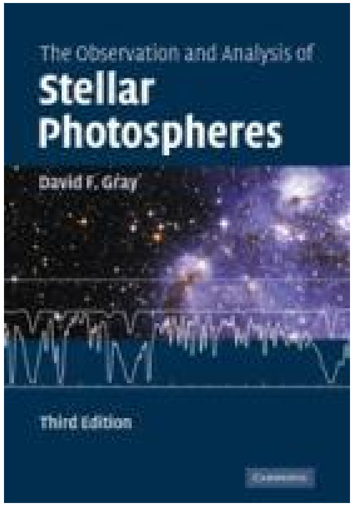
The strength of a spectral line is proportional to the ratio of the line vs the continuous absorption coefficient. It also depends on the gradient of the source function throughout the depths of line formation.

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

Line strength dependencies

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

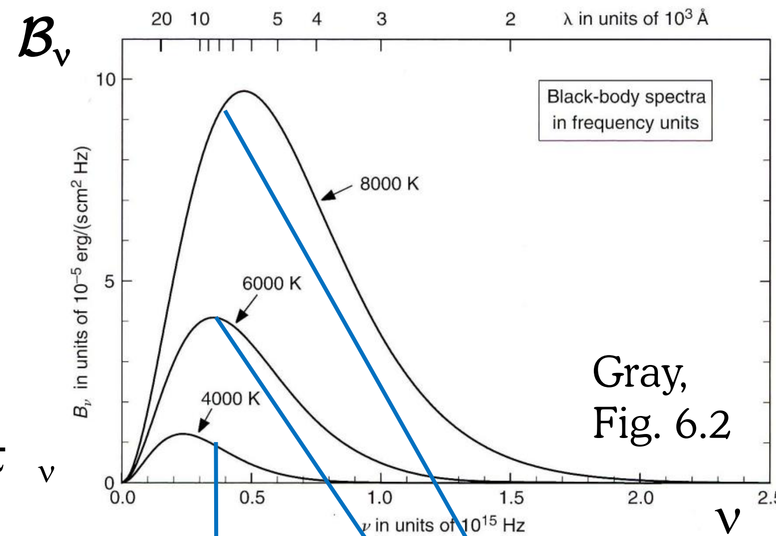
The left-hand side of the above equation is a measure of the line flux (subscript nu) eaten out of the continuum (subscript c). Integrate this and you get the line strength. The right-hand side shows important dependencies:
* gradient of the source function with optical depth and
* the ratio of line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



How spectral lines originate

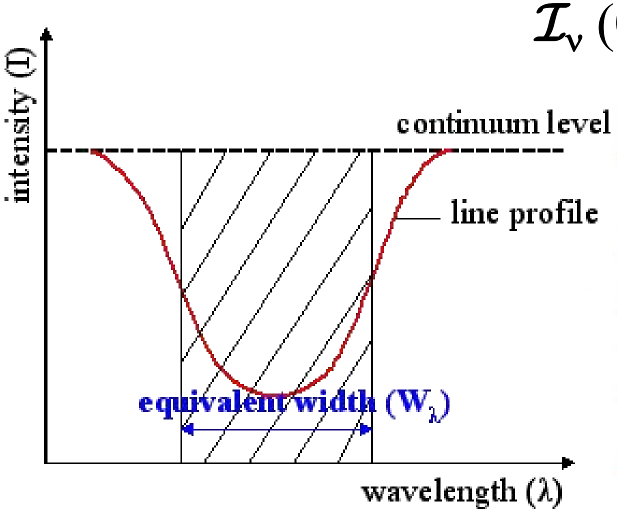
The formation of absorption lines can be qualitatively understood by studying how

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



Gray, Fig. 6.2

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



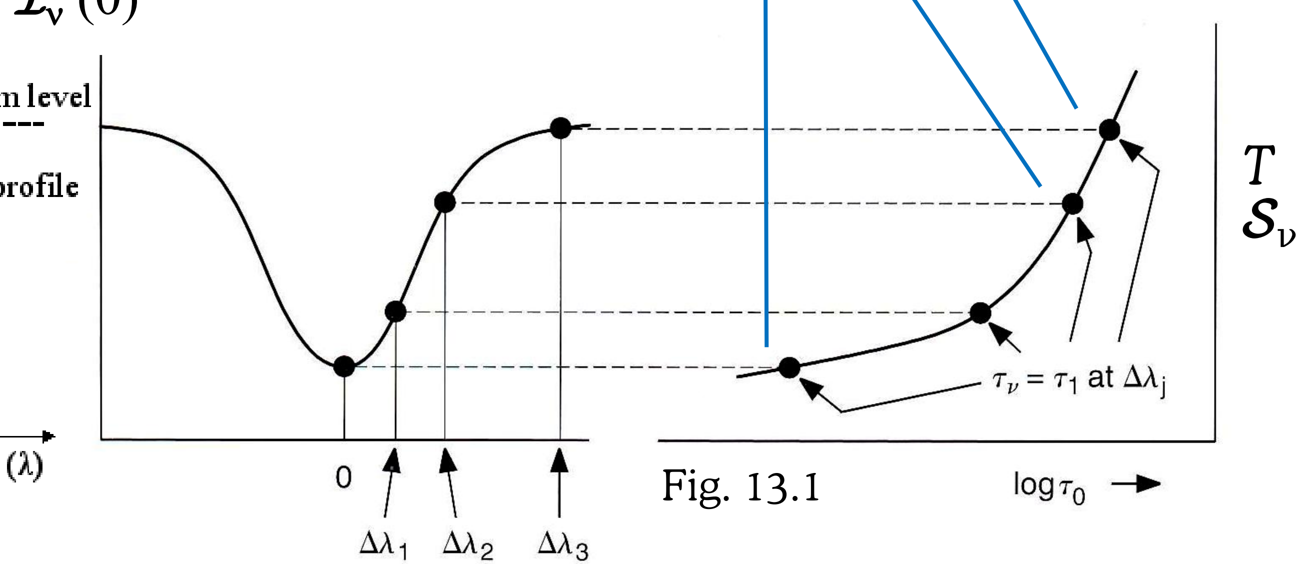


Fig. 13.1

l_ν / κ_ν: qualitative examples

Many species in cool-star atmospheres are predominantly singly ionized (e.g. Mg, Na, Ti, Fe, but not O). Why?

The continuous opacity in the optical and near-infrared of cool stars (< 8000 K) is dominated by H^-, the negative H ion (I = 0.75 eV). Its abundance is low, but can rival the abundance of neutral H in the n=3 level (producing the so-called Paschen continuum). One computes this abundance via the Saha equation which contains P_e, the electron pressure (which is proportional to log g).

Neutral lines of e.g. Fe thus turn out not to depend on log g.

Ionized lines do depend on log g. Please confirm this behaviour yourself with some spectral lines today!

Spectral lines as a function of abundance

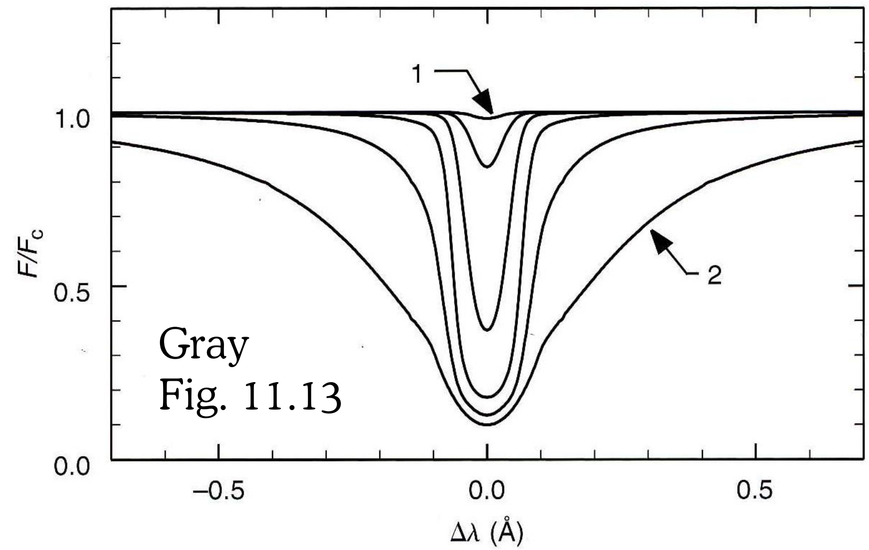
Starting from low log ε (low log *gf*), the line strength is directly proportional to *f* and n_X:

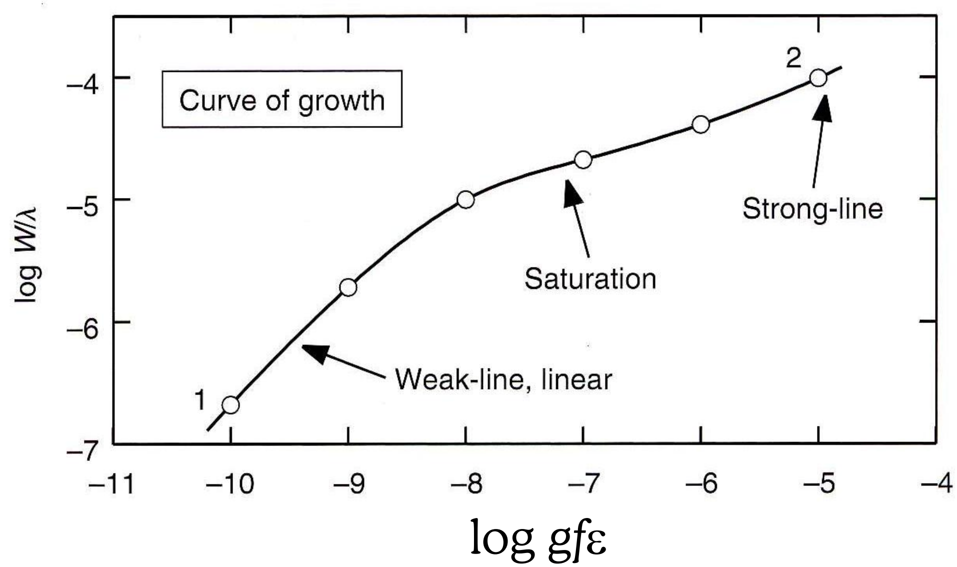
$$W_\lambda \propto gf\, n_X$$

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 (blending!)





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.

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 ε(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.

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)

4. Well-mixed atmospheres

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

6. *Can you think of other approximations?*

Stellar spectroscopy with iSpec

This week, we will derive semi-quantitative results with a suite of classical tools integrated into a software called **iSpec**.

iSpec allows you to plot, manipulate and fit stellar spectra of cool stars with a variety of approaches, model atmospheres and line-formation codes. See the documentation.

The author, Sergio Blanco Cuaresma, provides the iSpec code (written in Python 3) for download. He even provides a VM file to be run in VirtualBox (Python 2).

I suggest each group installs at least one of these on one of their laptops. (If you use two different versions, you can check their consistency.)

iSpec: download or native install

https://www.blancocuaresma.com/s/iSpec

The VM file will work with VirtualBox. Certain functionality (USB support, drag&drop) may not work. This may make file transfer a bit cumbersome (go via a web service). Can be helped by installing Guest additions (ask me).

The Python3 version of the code should install if your Python installation fulfills the following dependencies:
astropy==4.3.1, Cython==0.29.32, dill==0.3.4, lockfile==0.12.2, matplotlib==3.5.2, numpy==1.21.5, pandas==1.3.5, pudb==2022.1.2, python_dateutil==2.8.2, scipy==1.8.0, statsmodels==0.13.2

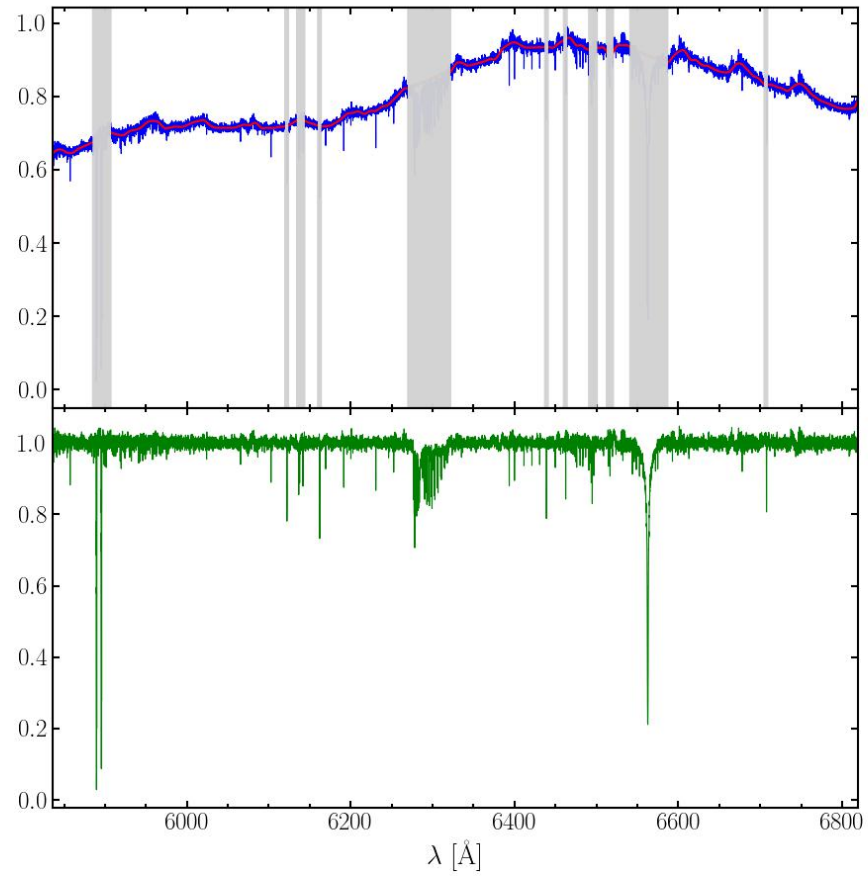
Rtfm!

A small helper: normalizer

Sometimes, iSpec struggles with providing a decent normalization.

To this end, we can load the NOT (or UVES) spectra into a normalization tool by ChETEC-INFRA postdoc Johannes Puschnig (UU):

https://github.com/astrojohannes/normalizer



Summary of your task

This is an exploratory open-ended exercise. You can design your own scientific project, if you want to. Talk to me and Camilla!

As a baseline, we would like you to select, observe and analyse stars for which Gaia provided n-capture abundances (Zr, Ce, Nd) as part of Data Release 3.

Assuming that the stellar parameters provided by Gaia (GSP-phot or GSP-spec) are correct, can you confirm the n-capture abundance with additional spectral lines in the wide wavelength coverage of FIES@NOT?

What extra assumptions do you need to make?

Can you derive an estimate of the uncertainties?

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

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!)

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 a factor of 200 000 below the Sun (Christlieb *et al.* 2002) ($[\mathrm{X/H}]_\odot \equiv 0$)

Feedback

Please get back to me, if you find mistakes, errors or have suggestions to improve this exercise. Thank you!

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