

Spectroscopy Workshop

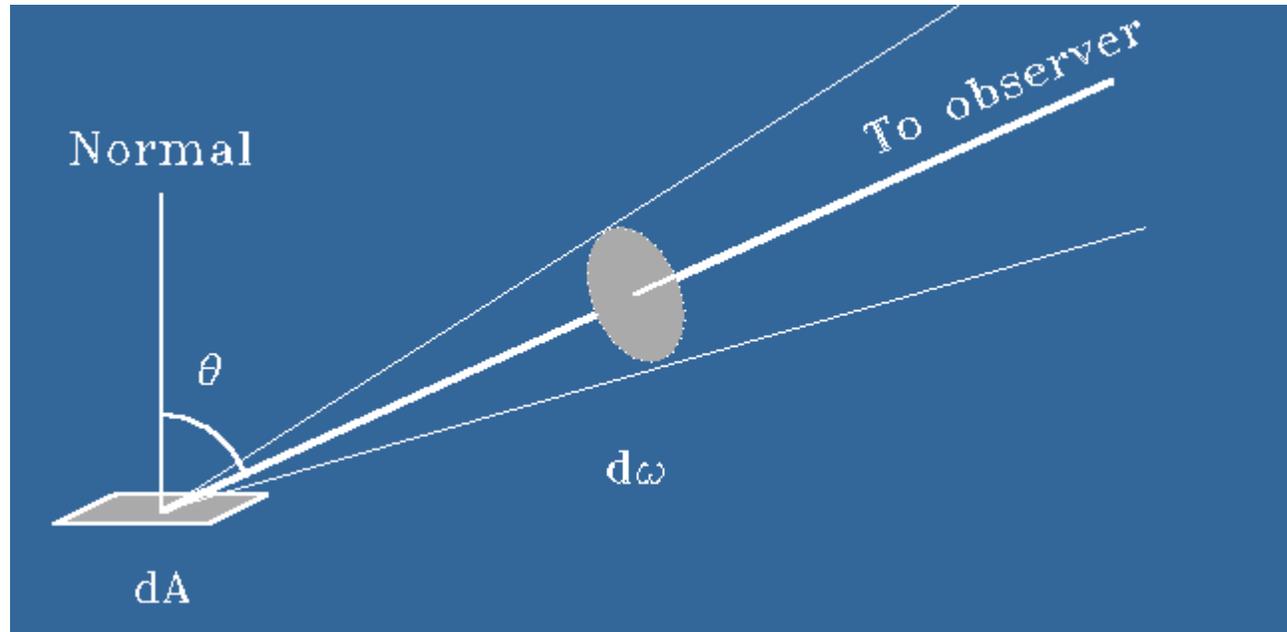
EXOHOST project

Nikolai Piskunov
Uppsala University

Introduction: Main Concepts and Definitions

$$\left. \begin{aligned} dE_\nu &= dA d\omega dt d\nu \\ dE_\lambda &= dA d\omega dt d\lambda \end{aligned} \right\} \text{definitions of intensity}$$

$$I_\lambda d\lambda = I_\nu d\nu, \text{ units } I_\nu [\text{erg}/(\text{s}\cdot\text{cm}^2\cdot\text{rad}^2\cdot\text{Hz})]$$



Useful quantities

Intensity	$\Delta E = I_\nu \left[\text{erg/s} \cdot \text{cm}^2 \cdot \text{Hz} \cdot \text{ster} \right] \cdot \Delta t \cdot \Delta \sigma \cdot \Delta \nu \cdot \Delta \Omega =$ $= I_\lambda \left[\text{erg/s} \cdot \text{cm}^2 \cdot \text{\AA} \cdot \text{ster} \right] \cdot \Delta t \cdot \Delta \sigma \cdot \Delta \lambda \cdot \Delta \Omega$ $I_\nu = I_\lambda \lambda^2 / c$
Flux	[erg/s cm ² Hz]
Mean intensity	J_ν [erg/s · cm ² · Hz], J_λ [erg/s · cm ² · Å]
Absorption coefficient	$\Delta I_\nu = -\alpha_\nu I_\nu \Delta x = -\kappa_\nu \rho I_\nu \Delta x$ $\alpha_\nu \left[\text{cm}^{-1} \right], \kappa_\nu \left[\text{cm}^2 \cdot \text{g}^{-1} \right]$
Emission coefficient	$\Delta E = j_\nu^{\text{Vol}} \left[\text{erg/s} \cdot \text{cm}^3 \cdot \text{Hz} \cdot \text{ster} \right] \cdot \Delta t \cdot \Delta V \cdot \Delta \nu \cdot \Delta \Omega =$ $= j_\nu^{\text{mass}} \left[\text{erg/s} \cdot \text{g} \cdot \text{Hz} \cdot \text{ster} \right] \cdot \rho \cdot \Delta t \cdot \Delta V \cdot \Delta \nu \cdot \Delta \Omega$
Optical path	$d\tau_\nu = \alpha_\nu(x) \cdot dx = k_\nu(x) \cdot \rho \cdot dx$ [unitless!]
Source function	$S_\nu = j_\nu / k_\nu$ [units of intensity!]

- Absorption and emission contain the “true” part (*energy is transferred between kinetic/internal energies of the gas and the radiation field*) and the scattering part (*energy of re-emitted photons*).
- Radiation-dominated gas: pure scattering.
- Collision-dominated gas: pure absorption.

- In general case:

$$\kappa_\lambda = k_\lambda + \sigma_\lambda, \quad S_\lambda = S_\lambda^A + S_\lambda^S$$

- For isotropic scattering and thermal equilibrium:

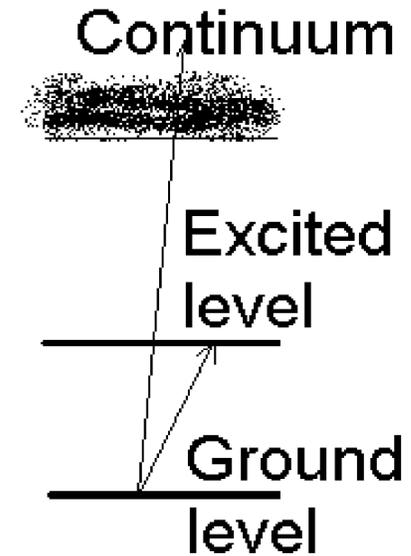
$$S_\nu = \frac{\sigma_\nu}{k_\nu + \sigma_\nu} J_\nu + \frac{k_\nu}{k_\nu + \sigma_\nu} B_\nu$$

We distinguish 3 types of absorption processes:

- ***b-b*** - radiative transitions
- collisional transitions
- ***b-f*** - ionization and recombination
- ***f-f*** - absorption/emission

Radiative ***b-b*** transitions: absorption, spontaneous and stimulated emission.

Collisional ***b-b*** transitions: excitation and de-excitation



- Equation of radiative transfer connects the change in intensity along a ray as function of absorption and emission:

$$dI_\nu = -\kappa_\nu \rho I_\nu dx + j_\nu \rho dx$$

or

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

- The formal solution (home work: derive this):

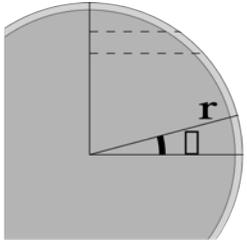
$$I_\nu(\tau_\nu'') = I_\nu(\tau_\nu') \cdot e^{-(\tau_\nu'' - \tau_\nu')} + \int_{\tau_\nu'}^{\tau_\nu''} S_\nu(t) e^{-(\tau_\nu'' - t)} dt$$

Stellar atmosphere models

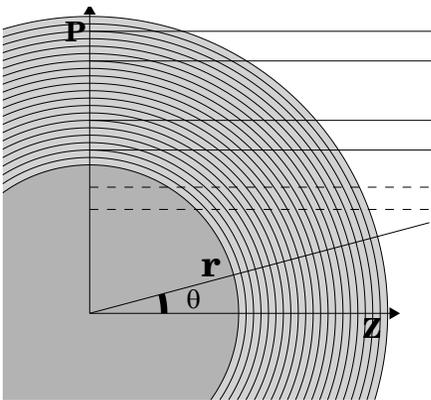
1D LTE model atmospheres base on flux conservation:

1. Setup the initial vertical structure.
2. Compute pressure based on hydrostatic equilibrium.
3. Compute temperature using ideal gas approximation, pressure and density.
4. Compute opacities and source functions for every layer.
5. Solve RT for every wavelength bin (10000-40000).
6. Add radiative pressure to gas pressure gradient.
7. Adjust Pressure-Temperature structure and iterate from 3 to achieve flux conservation.

Plane parallel models versus spherical models



Atmospheric thickness is very small in comparison to the stellar radius. One can assume that all layers are parallel to each other. Geometrical thickness of layers along a ray scales by $1/\cos \theta$.



Atmospheric thickness is not so small in comparison to the stellar radius. One treats sphericity properly but assumes central symmetry.

Completed model atmosphere

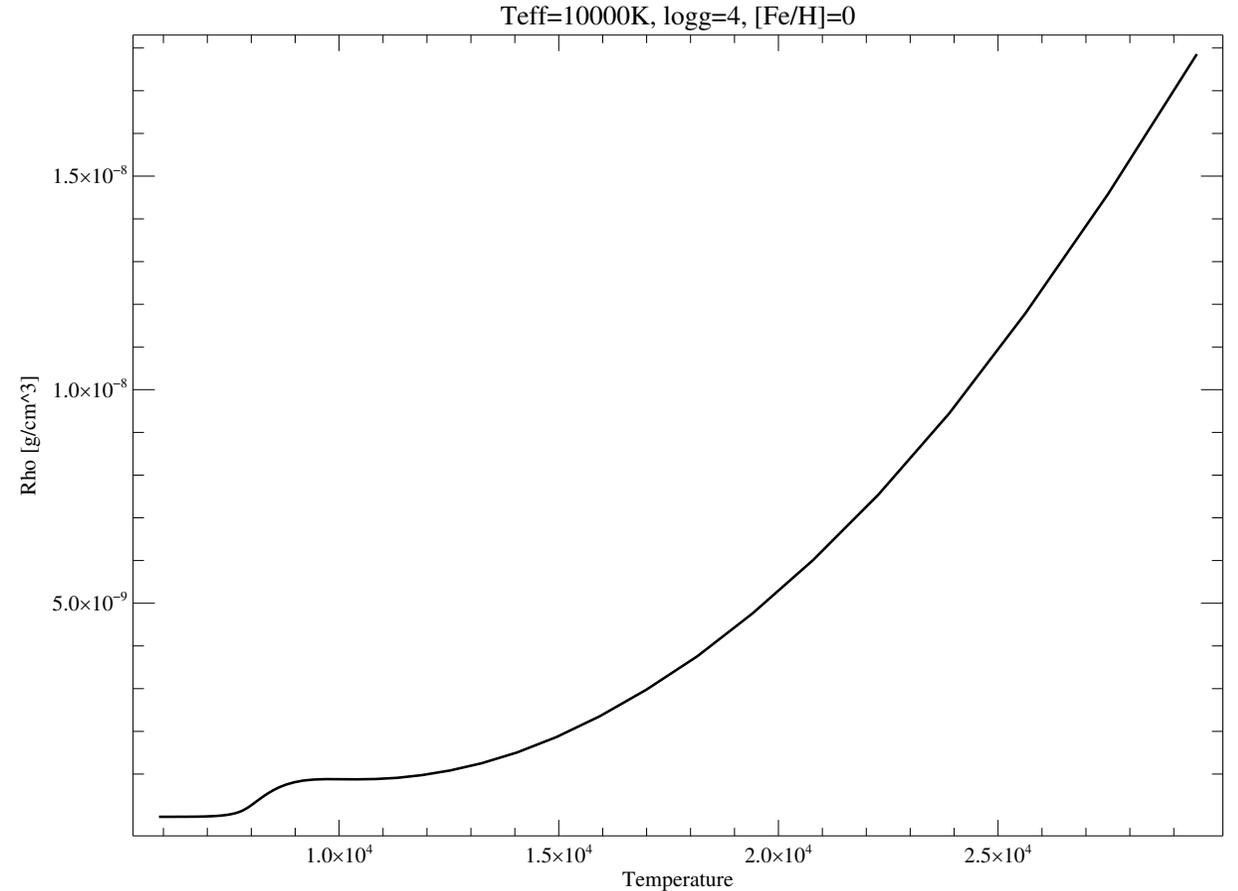
- The input parameters for the model are T_{eff} that gives bolometric flux, surface gravity $\log g$ assumed to be constant that sets pressure gradient, chemical composition and microturbulence.
- There could be a couple of extra parameters, such as mixing length and extra pressure components due to magnetic fields.
- Once the variations in temperature for every layer are smaller than the threshold (typically 5-10K) model is converged.
- The output contains model parameters and model structure (next slide), flux spectrum and possibly other data, such as opacity tables.

Model structure

```

TITLE [0.0] VTURB=2 L/H=1.25 NOVER NEW ODF
T EFF=10000. GRAV= 4.0 MODEL TYPE= 0 WLSTD= 5000.
1 1 1 1 1 1 1 1 1 1 1 1 1 1 0 1 0 0 0 0 0 - Opacity switches
 0.920 -1.11 -10.94 -10.64 -9.49 -3.52 -4.12 -3.21 -7.48 -3.96
-5.71 -4.46 -5.57 -4.49 -6.59 -4.71 -6.54 -5.64 -6.92 -5.68
-8.87 -7.02 -8.04 -6.37 -6.65 -4.54 -7.12 -5.79 -7.83 -7.44
-9.16 -8.63 -9.67 -8.63 -9.41 -8.73 -9.44 -9.07 -9.80 -9.44
-10.62 -10.12 -20.00 -10.20 -10.92 -10.35 -11.10 -10.27 -10.38 -10.04
-11.04 -9.80 -10.53 -9.87 -10.91 -9.91 -10.87 -10.46 -11.33 -10.54
-20.00 -11.03 -11.53 -10.92 -11.69 -10.90 -11.78 -11.11 -12.04 -10.96
-11.98 -11.16 -12.17 -10.93 -11.76 -10.59 -10.69 -10.24 -11.03 -10.91
-11.14 -10.09 -11.33 -20.00 -20.00 -20.00 -20.00 -20.00 -20.00 -11.95
-20.00 -12.54 -20.00 -20.00 -20.00 -20.00 -20.00 -20.00 -20.00 72
9.288976660E-07, 5899.7, 3.30300E+09, 8.06257E+09, 1.69011E-14,
1.248617530E-06, 5922.8, 4.19700E+09, 1.10170E+10, 2.30941E-14,
1.708896780E-06, 5937.4, 5.31800E+09, 1.54584E+10, 3.24036E-14,
2.375643730E-06, 5963.1, 6.88800E+09, 2.18646E+10, 4.58317E-14,
3.334604780E-06, 5992.9, 9.00200E+09, 3.11627E+10, 6.53211E-14,
4.696885350E-06, 6029.8, 1.18800E+10, 4.43524E+10, 9.29677E-14,
6.603563120E-06, 6072.9, 1.57900E+10, 6.27059E+10, 1.31438E-13,
9.228735530E-06, 6122.2, 2.10500E+10, 8.77771E+10, 1.83989E-13,
1.278494030E-05, 6176.1, 2.80600E+10, 1.21359E+11, 2.54379E-13,
1.753312510E-05, 6233.8, 3.73200E+10, 1.65794E+11, 3.47516E-13,
...
RHOX          T          Ne          Na          RHO

```



Libraries and Formats

- Kurucz (Harvard) <http://kurucz.harvard.edu/grids.html>
- MARCS (Uppsala) <https://marcs.astro.uu.se/>
- LL models (Göttingen) <https://doi.org/10.1051/0004-6361:20034169>
- Phoenix (Hamburg) <https://doi.org/10.1051/0004-6361/201219058>

All models are offered in proprietary formats and there is a KRZ format that the top three grids are available in. There are also conversion tools between proprietary formats and KRZ.

Specialisation

- *Kurucz* – best for main sequence stars hotter than 4500K even though it covers the range of T_{eff} : 3500 to 50000K and $\log g$ 2.5 to 5.5. All models are plane parallel.
- *MARCS* – best below 6500K down to 2500K and $\log g$ 0.0 to 5.5. There are several alpha-abundance options depending on the metallicity. Models for $\log g$ larger than 3.5 are plane-parallel. Below 2.5 are spherical. In between – both.
- *LL* covers T_{eff} 4500K to 22000K with variable step and $\log g$ from 2.5 to 5.0. All models are plane parallel.
- *Phoenix* covers T_{eff} from 2300K to 12000K, $\log g$ from 0.0 to 6.0. Also, some alpha-abundance variations.

MARCS online database

<https://marcs.astro.uu.se>

Using model atmospheres

- Spectral synthesis is using model atmospheres.
- When fitting the observations we allow small inconsistencies by changing the abundances of trace elements we are trying to fit.
- Change of abundance enters through opacities, density and equation of state.
- Even significant abundance changes for trace elements like Eu will not change the atmospheric structure.
- On the other hand Iron-peak elements may affect the atmospheric structure directly is significant opacity contributors and electron donors.
- This is why we use 3D model grids: T_{eff} , $\log g$, $[M/H]$ and also subgrids for specific cases.

Line lists

- For the spectral synthesis we need line data.
- For each line this includes the species (atom, molecule, ionization stage), energy levels involved, the wavelength, transition probability (oscillator strength), line broadening parameters and some others.
- There are three types of data produced by atomic and molecular physics:
 1. Purely experimental lab spectroscopy. Produces the most accurate data but usually covers a very short wavelength range, incomplete and frequently suffers from misidentification (assigned quantum numbers may be wrong).
 2. Purely theoretical, ab initio calculations. By definition complete and correct within the selected framework, predicts broadening parameters but energy levels are hard to get to the observational precision and therefore the wavelengths are not accurate. The calculations are getting much better even in this aspect.
 3. Hybrid calculations, where the potential surfaces of atomic models are adjusted to match the observed transitions. The best of two worlds: complete and accurate.

Line repositories

- Molecular and atomic data producers are not very good at publishing the data. Different formats, strange sorting, separate locations etc.
- Data precision and accuracy is estimated using different methodologies and systematics is often not included.
- Data for the same transitions is often available from multiple sources and this data could differ by a lot.
- Thus there are groups in the world that collect the data from producers, homogenize the format, assess accuracy and precision, sort the data and even merge line list from different sources.

NIST Atomic Spectra Database

<https://physics.nist.gov/PhysRefData/ASD>

- NIST maintains separate databases for molecular species and atoms.
- The focus is on the most reliable and accurate data, so this is not the most complete source (<150000 transitions).
- What is there is the most reliable data that was studied, intercompared and weighted by experts.
- Flexible interface focussed on species.
- Still, this is a never ending story and so there are issues present in NIST and other data repositories that take some time to fix.

VALD atomic and molecular spectroscopy database.

<http://vald.astro.uu.se/>

- The largest line data collection for astronomy (>5,000,000 lab and hybrid transitions, >600,000,000 predicted transitions) covering the range from 10 Å to 0.2mm.
- Largest contributions are coming from R.L. Kurucz, Wisconsin, UCL, NIST, Liege, Montpellier, Lund etc.
- VALD is line-oriented.
- All original data (380) are converted to the internal records and stored separately.
- Merger between different sources is happening on the fly following the ranking list.
- More than 3000 users from 156 countries. Average of 200 requests per day.

VALD ranking: configuration file

0.05,5000.,9,150.

; wavelength window in Angstroem, reference wavelength in Angstroem,

; maximum ionization stage and maximum excitation potential of the lower level in eV

```
;
'/CVALD3/ATOMS/H_lines_NIST+Kurucz',          2,    1,    1,  0,3,3,3,3,3,3,3,3,3,3, 'NIST H-lines complemented by Kurucz NLTE'
'/CVALD3/ATOMS/He_nlt_V3',                    10,   2,    3,  0,3,3,3,3,3,3,3,3,3,3, 'NLTE lines: He'
'/CVALD3/ATOMS/B_nlt_V3',                     20,  11,   11,  0,3,3,3,3,3,3,3,3,3,3, 'NLTE lines: B'
'/CVALD3/ATOMS/C2_nlt_V3',                    30,  17,   17,  0,2,2,2,2,2,2,2,2,2,2, 'NLTE lines: C'
'/CVALD3/ATOMS/gfemq0601_obs_2014',           111,  17,   17,  0,4,3,3,3,3,3,3,3,3,3, 'Kurucz obs. energy level: C 2'
'/CVALD3/ATOMS/gfemq0803_obs',                120,  32,   32,  0,5,5,5,5,5,5,5,5,5,5, 'Kurucz obs. energy level: O 4'
'/CVALD3/ATOMS/gfemq1400_obs',                130,  92,   92,  0,3,3,3,3,3,3,3,3,3,3, 'Kurucz obs. energy level: Si 1'
...
'/CVALD3/ATOMS/Hf2U_bell_V3_a',              1160, 2557, 4188, 0,2,2,2,2,2,2,2,2,2,2, 'Hf 1 - U 2 Bell'
'/CVALD3/ATOMS/cr2_ru_V3',                   1170,      278, 278, 0,2,5,2,2,2,2,2,2,2,2, 'Cr 2: Raassen & Uylings'
'/CVALD3/ATOMS/fe2_ru_V3_a',                 1180,  327,  327, 0,2,5,2,2,2,2,2,2,2,2, 'Fe 2: Raassen & Uylings'
...
'/CVALD3/ATOMS/CNO-Na1-Mg1_NIST',            1220,  16,   67,  0,4,5,4,4,0,0,0,0,4, 'C 1-6, N 1-7, O 1-8, Na 1, Mg 1: NIST 2010'
...
'/CVALD3/ATOMS/Si1_exp_V3',                  1820,  92,   92,  0,3,4,3,3,3,3,3,3,3,3, 'Si exp.'
'/CVALD3/ATOMS/vdw_Mg1_OBL',                 1851,  67,   67,  2,0,1,1,1,1,1,1,9,1, 'Mg1 OBL Van der Waals data',0.05
'/CVALD3/ATOMS/vdw_barklem_IS',              1852,   4,  5048, 2,0,1,1,1,1,1,1,9,1, 'Iron peak OBP Van der Waals data',0.05
'/CVALD3/ATOMS/Cr1_Wallace_wl',              1860,  277,  277, 2,9,1,9,9,1,1,1,1,1, 'Cr 1 Wallace wavelength data',0.08
'/CVALD3/MOLECULES/Ti460_Plez_Nordlander',   2160, 10036, 10036, 1,2,2,2,2,2,2,2,2,2,2, 'Plez 2012 Ti46O, polynomial fits to Phillips obs. wavelengths, Nordlander molecular constants'
...
```

You can use either the default configuration file or your own personal one.

VALD request

VALD queries are wavelength-oriented:

- ShowLine: shows all available data in a small region centred on a given wavelength as well as how this data will be merged.
- Extract All: extracts all transitions in a given wavelength range.
- Extract Element: extracts transitions of specified atoms, molecules or ions in a given wavelength range.
- Extract Stellar: extracts transitions in a given wavelength range that will be deeper than a certain fraction of continuum in a given stellar atmosphere model.

There is a 5th option for opacity table calculations that is only available on local installation.

VALD query modifiers

- Long or short format.
- Å, nm or cm^{-1} for the wavelengths. Å and nm can be in air or in vacuum.
- Energies can be in eV or cm^{-1} .
- Oscillator strength can be scaled by the Solar system isotopic ratios.
- The extended version of the van der Waals with variable temperature dependence (the AOB approximation) is available for all strong lines of the Iron-peak elements and some other transitions.
- One can ask for computing the HFS and including it in the output.
- The results can be returned via email or an FTP link.

Query processing

- VALD server checks and process accumulated requests.
- The results are either included in the email reply (up to 10,000 transitions) or as a link to extraction data in VALD FTP site (up to 100,000 transitions).
- Every field in every transition also has a BibTeX key and the associated BibTeX file is attached to the response.
- One can check documentation for a short description of all data sources using the same key.
- The term description was standardized (if it was available in the original list) and is also described in the documentation.
- After the last request was processed VALD server takes 10 min coffee break and then checks for the new requests.

Special cases

- The showline request is instantaneous and can be performed online.
- Select Stellar requires additional parameters such as T_{eff} , $\log v_{\text{micro}}$ and $[M/H]$ or explicit abundance list. One also should specify the threshold. Zero threshold means all lines will be included but considering the size of VALD your request will likely be truncated once the output reaches maximum allowed extraction size.
- Extract Stellar returns an estimated central line depth for each transition that can be used for planning observations, line identification or even more advanced tasks, like LSD averaging.
- Complicated requests can take a long time and substantial computational effort.

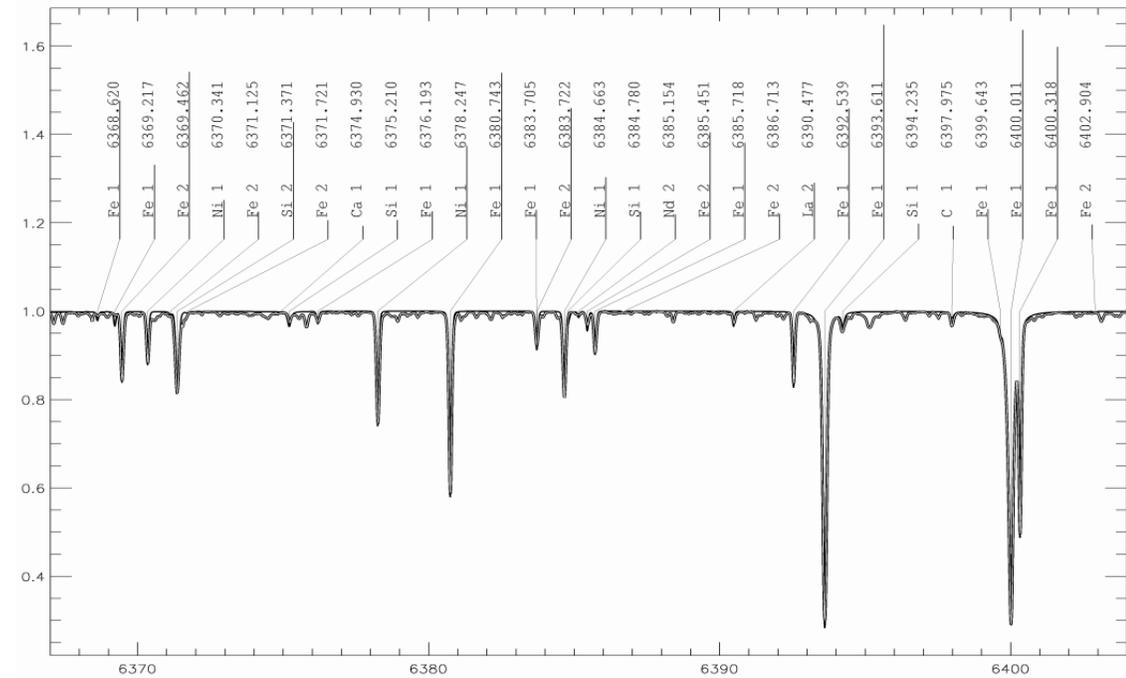
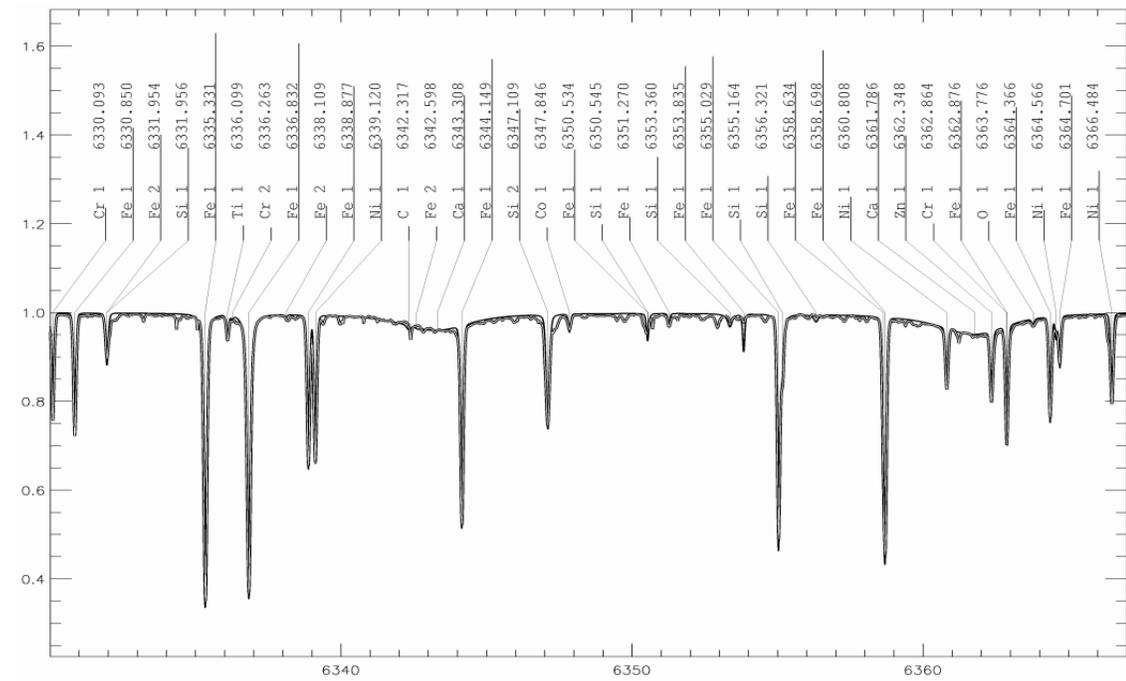
For tomorrow:

- Register in VALD: send an email to VALD admin specifying your name, affiliation, and email address that you will use for login (can be more than one).
- Submit two requests to VALD using extract stellar query.
- One for the Solar parameters (5770K, 4.4, $v_{\text{micro}}=1$) and one for hotter star, e.g. $T_{\text{eff}}=10000\text{K}$, $\log=4.0$, $v_{\text{micro}}=2$. Use solar metallicity (default) in both cases. Select one wavelength range out of the list below:

4855 – 4875 Å
5240 – 5260 Å
5160 – 5180 Å
6430 – 6450 Å
8480 – 8560 Å

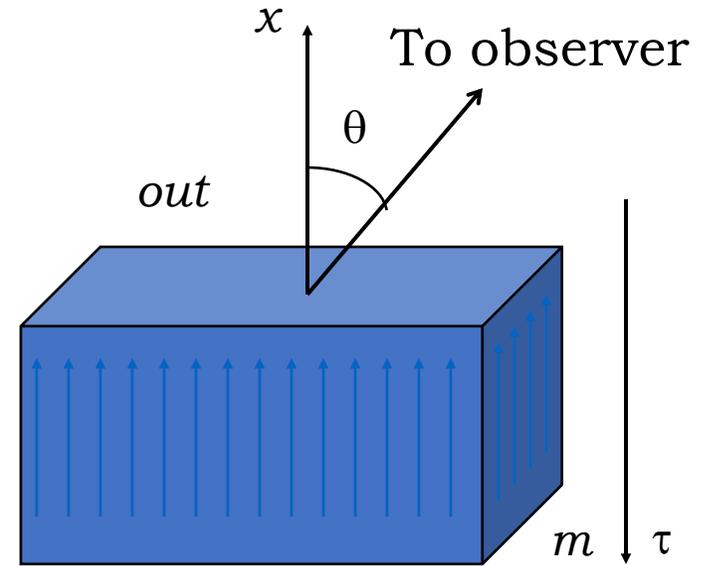
- Find identical lines selected at different temperatures. Check that you understand the change of the central depth.

Spectral synthesis



Coordinate system

o Orientation:



o We can introduce two depth variables:

$$d\tau_v = -k_v \rho dx \quad \text{optical depth and}$$

$$dm = -\rho dx \quad \text{column mass}$$

o The equation of hydrostatic equilibrium:

$$\frac{dP_{gas}}{dm} + \frac{dP_{rad}}{dm} = g \quad \text{or} \quad \frac{dP_{gas}}{d\tau_v} + \frac{dP_{rad}}{d\tau_v} = \frac{g}{k_v}$$

o The equation of radiative transfer:

$$\mu \frac{dI_v}{dm} = k_v I_v - k_v S_v \quad \text{or} \quad \mu \frac{dI_v}{d\tau_v} = I_v - S_v$$

o The relation between the two depth scales:

$$\frac{d\tau_v}{dm} = k_v \quad \text{with initial condition} \quad \tau_v \Big|_{m=0} = 0$$

Energy flux conservation

In a static plane-parallel atmosphere the total energy flux must be independent of depth:

$$\int_0^{\infty} \mathcal{F}_\nu d\nu + \mathcal{F}_{conv} = const = \sigma T_{eff}^4$$

where Stefan-Boltzmann constant:

$$\sigma \approx 5.67 \cdot 10^{-5} \text{ erg} \cdot \text{cm}^{-2} \cdot \text{s}^{-1} \cdot \text{K}^{-4}$$

If convection can be ignored then:

$$\begin{aligned} 0 &= \int_0^{\infty} \frac{d\mathcal{F}_v}{dm} dv = \int_0^{\infty} \oint \mu \frac{dI_v}{dm} d\omega dv = \\ &= \int_0^{\infty} \oint [k_v I_v - k_v S_v] d\omega dv \end{aligned}$$

or:
$$\int_0^{\infty} \oint k_v I_v d\omega dv = \int_0^{\infty} \oint k_v S_v d\omega dv$$

and assuming that the source function and extinction are isotropic:

$$\int_0^{\infty} k_v J_v dv = \int_0^{\infty} k_v S_v dv$$

Now we have the following set of equations:

- Equation of radiative equilibrium for intensity with T_{eff} as parameter;
- Equation of hydrostatic equilibrium for pressure and intensity with gravity as parameter.

In addition we have RT equation, connecting the intensity with extinction and local thermodynamic quantities, and equation of state relating the chemical composition to the density which we will get to later.

It is time to formulate the relation between local macro- and micro-physics.

Equation of radiative transfer

The reason why RTE needs special attention is its non-linearity. Non-linearity arises from the dual nature of the source function. The emission coefficient has two parts:

$$j_{\nu} = k_{\nu}^s \rho J_{\nu} + k_{\nu}^a \rho B_{\nu}$$

The source function is therefore:

$$S_{\nu} = \frac{k_{\nu}^s}{k_{\nu}^s + k_{\nu}^a} J_{\nu} + \frac{k_{\nu}^a}{k_{\nu}^s + k_{\nu}^a} B_{\nu}$$

The absorption part of the extinction coefficient is often referred to as:

$$\varepsilon = \frac{k_v^a}{k_v^s + k_v^a}$$

Therefore: $S_v = (1 - \varepsilon)J_v + \varepsilon B_v$

No scattering: $S_v = B_v$

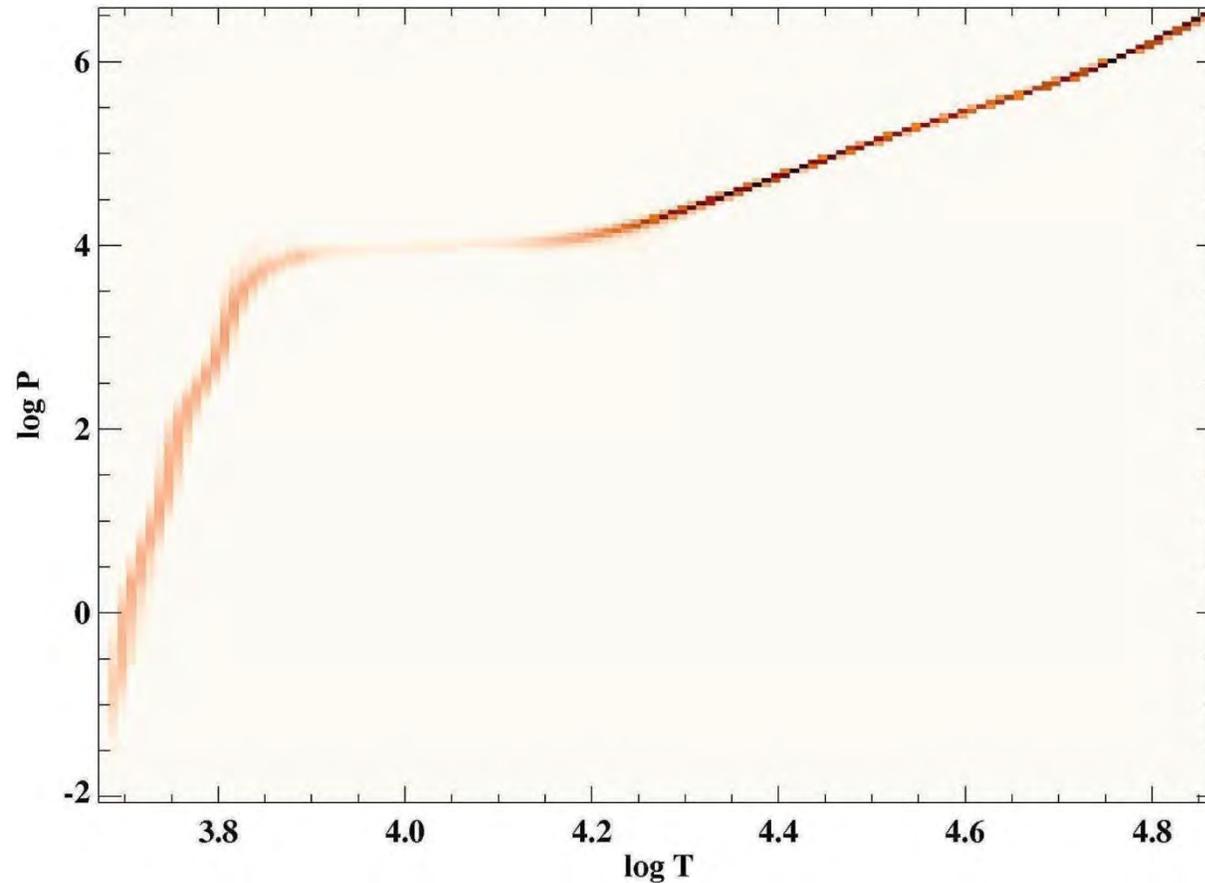
Pure scattering: $S_v = J_v$

Strict LTE

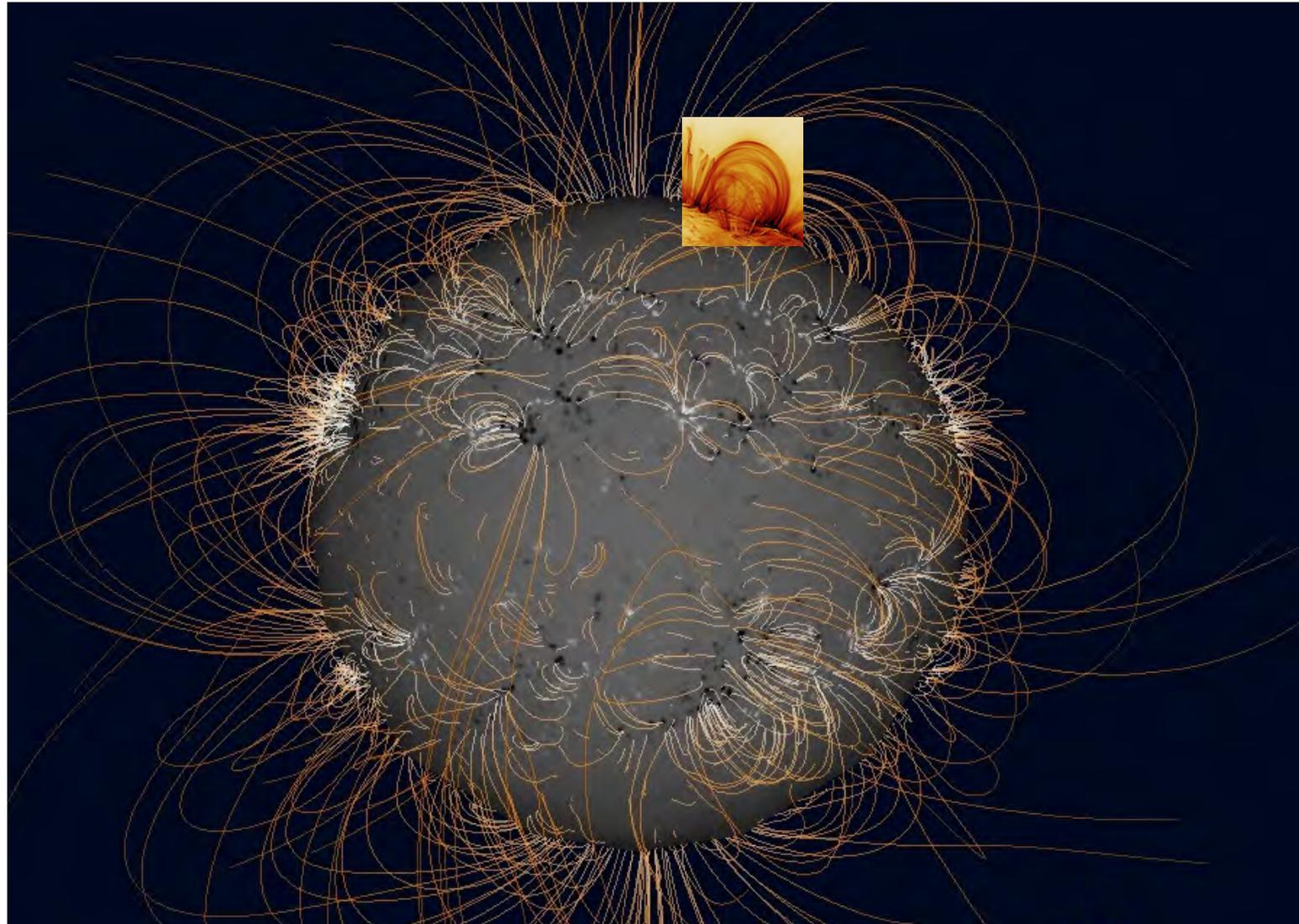
- o In strict LTE all the processes are in detailed balance.
- o There are no spectral lines in the spectrum of radiation inside the atmosphere.
- o The local mean radiation field J_ν is equal to the Planck function B_ν with the same temperature as the kinetic temperature of the gas. Therefore, the source function becomes Planck function independent of radiation field.
- o *Will strict LTE model predict spectral lines in emerging flux??? Why??????*

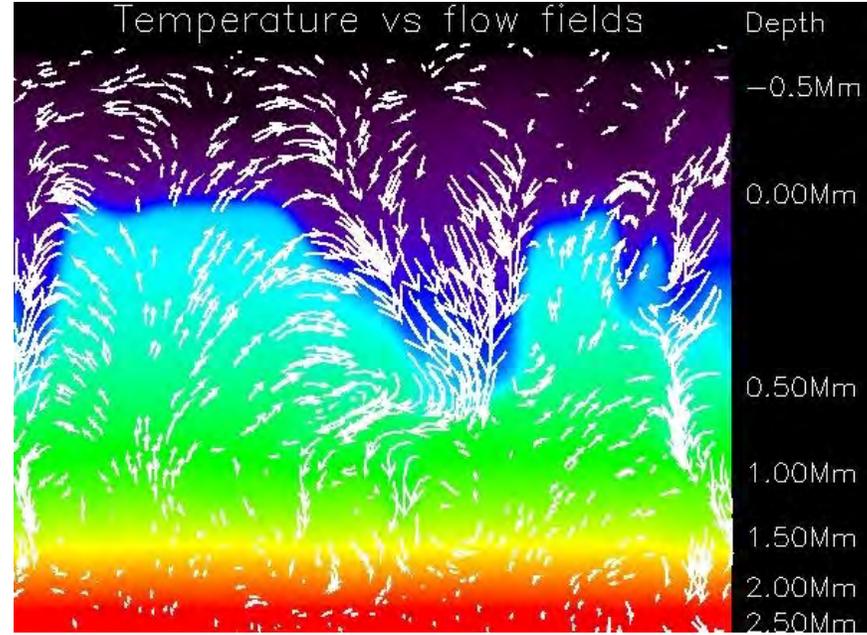
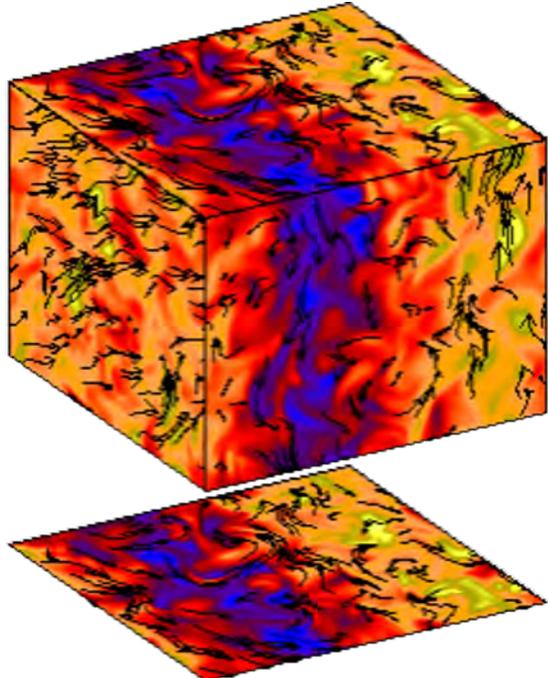
Model atmosphere

Why 1D hydrostatic atmosphere models work?

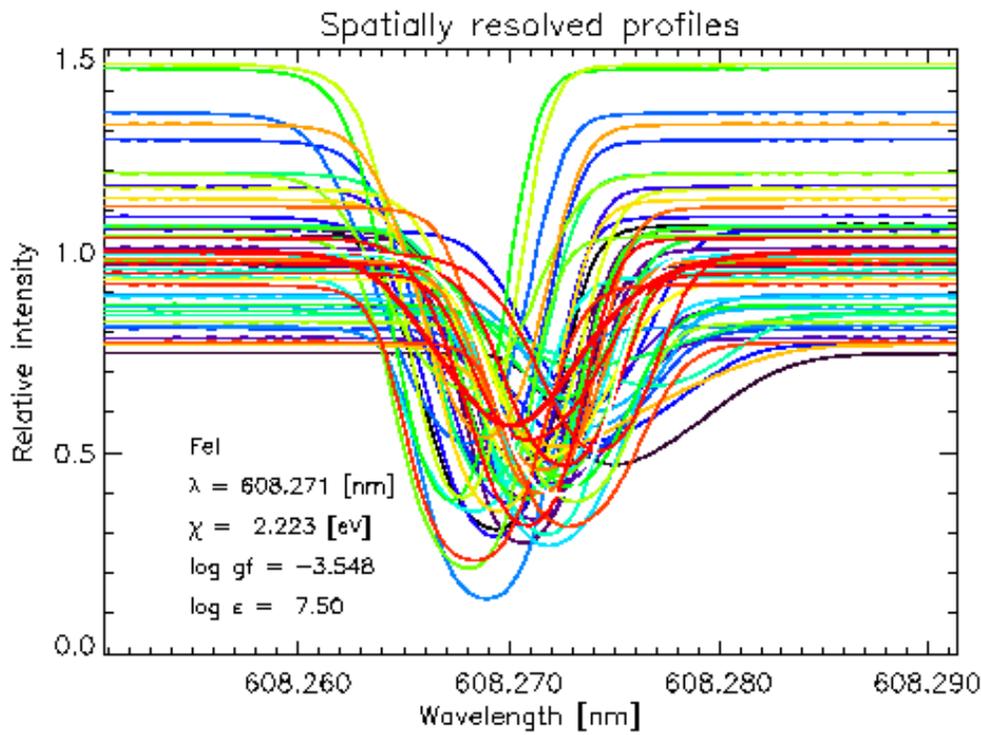
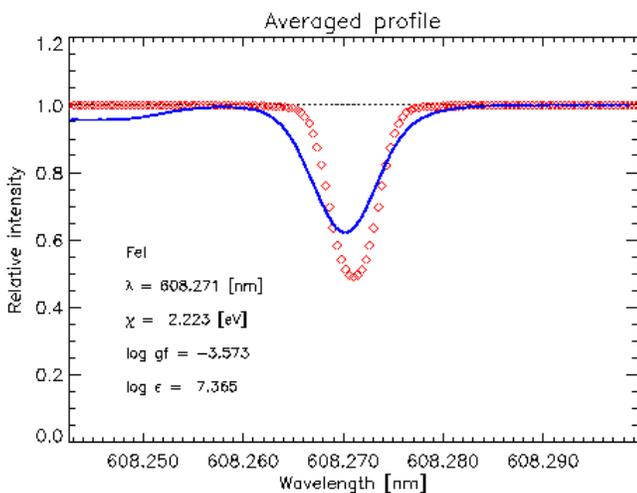


Convective stars are more complex





3D dynamic



Spectral synthesis

**Equation of state -> Level
population -> Opacities -> Intensity**

Intensity Opacity

- Intensity is affected by opacities through the RT equation.
- Opacities depend on the number of absorbers and absorption coefficient (per particle).
- Absorber means “a species in a given energy level”.
- “Species” can be an atom, an electron, an ion, a molecule or a dust particle. To get the density of these we need to solve the EOS.
- “Level population” means number of species per unit volume at a given energy level. This is described by statistical equilibrium equation.

Molecular-ionization equilibrium

- What do we know? P, T, abundances
- What else can assume in equilibrium? For chemical reactions the reactants and the product are in balance controlled by the temperature. The same is true for ionization.
- We can also assume charge neutrality

Expressing what we know as equations

- Abundances (if $Z_A = n_A / n_{tot}$)

$$\sum_{sp} P_{sp} \left(n_A^{sp} - Z_A n_{tot}^{sp} \right) = 0$$

- Particle conservation (q^{sp} is charge)

$$\sum_{sp} P_{sp} \left(1 + q^{sp} \right) = P_{gas}$$

- Charge neutrality

$$\sum_{sp} P_{sp} q^{sp} = P_{elec}$$

The expression for partial pressures

- Molecular and ionization equilibria:

$$\frac{P_A \cdot P_B}{P_{AB}} = Kp^{sp}(T); \quad \frac{P_{sp^+} \cdot P_{e^-}}{P_{sp}} = Ip^{sp}(T)$$

$$\frac{\prod_A P_A^{n_A^{sp}}}{P_{sp}} = Kp^{sp}(T); \quad \frac{P_{sp^+ \dots} \cdot P_{e^-}^{q_{sp}}}{P_{sp}} = Ip^{sp}(T)$$

- Partial pressure of a species is then:

$$P_{sp} = \frac{Ip(T)}{Kp(T)} P_{e^-}^{-q_{sp}} \prod_A P_A^{n_A^{sp}}$$

... and what are these Kp 's and Ip 's?

- Chemical equilibrium constant:

$$Kp(T) = kT \left(\frac{2\pi T}{h^2} \right)^{3/2} \left(\frac{m_A \cdot m_B \cdot \dots}{m_{sp}} \right)^{3/2} \frac{U_A \cdot U_B \cdot \dots}{U_{sp}} e^{-\frac{D_{sp}}{kT}}$$

- Ionization equilibrium constant:

$$Ip(T) = kT \left(\frac{2\pi T}{h^2} \right)^{3/2} m_{e^-}^{3/2} \cdot \frac{2 \cdot U_{sp^+}}{U_{sp}} e^{-\frac{I_{sp}}{kT}}$$

Let's count equations and unknowns

- First, what are the unknowns?

P_A and P_{e^-}

- How many unknowns?

$N_A + 1$

- How many equations?

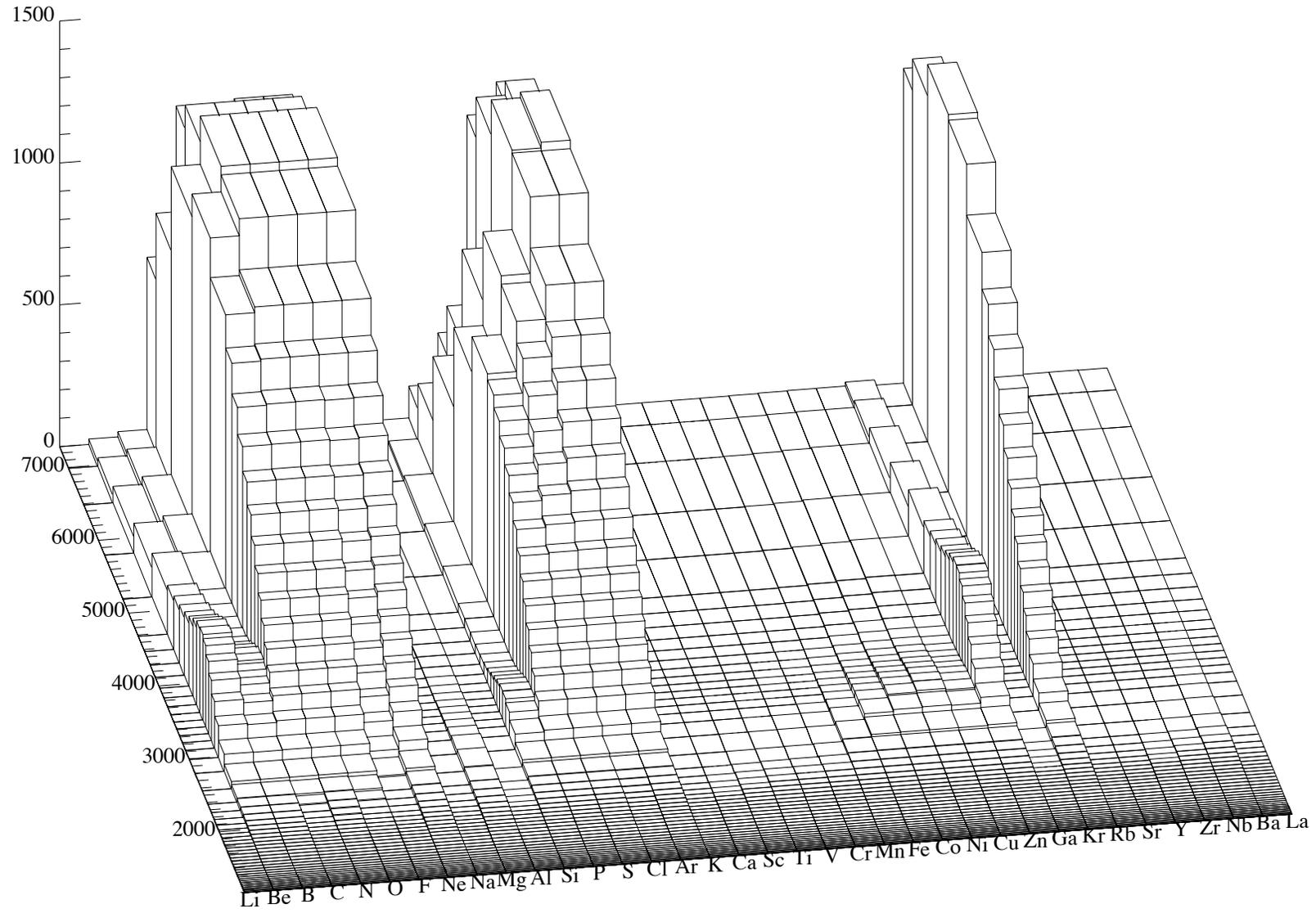
N_A for abundances + total pressure + charge conservations = $N_A + 2$!

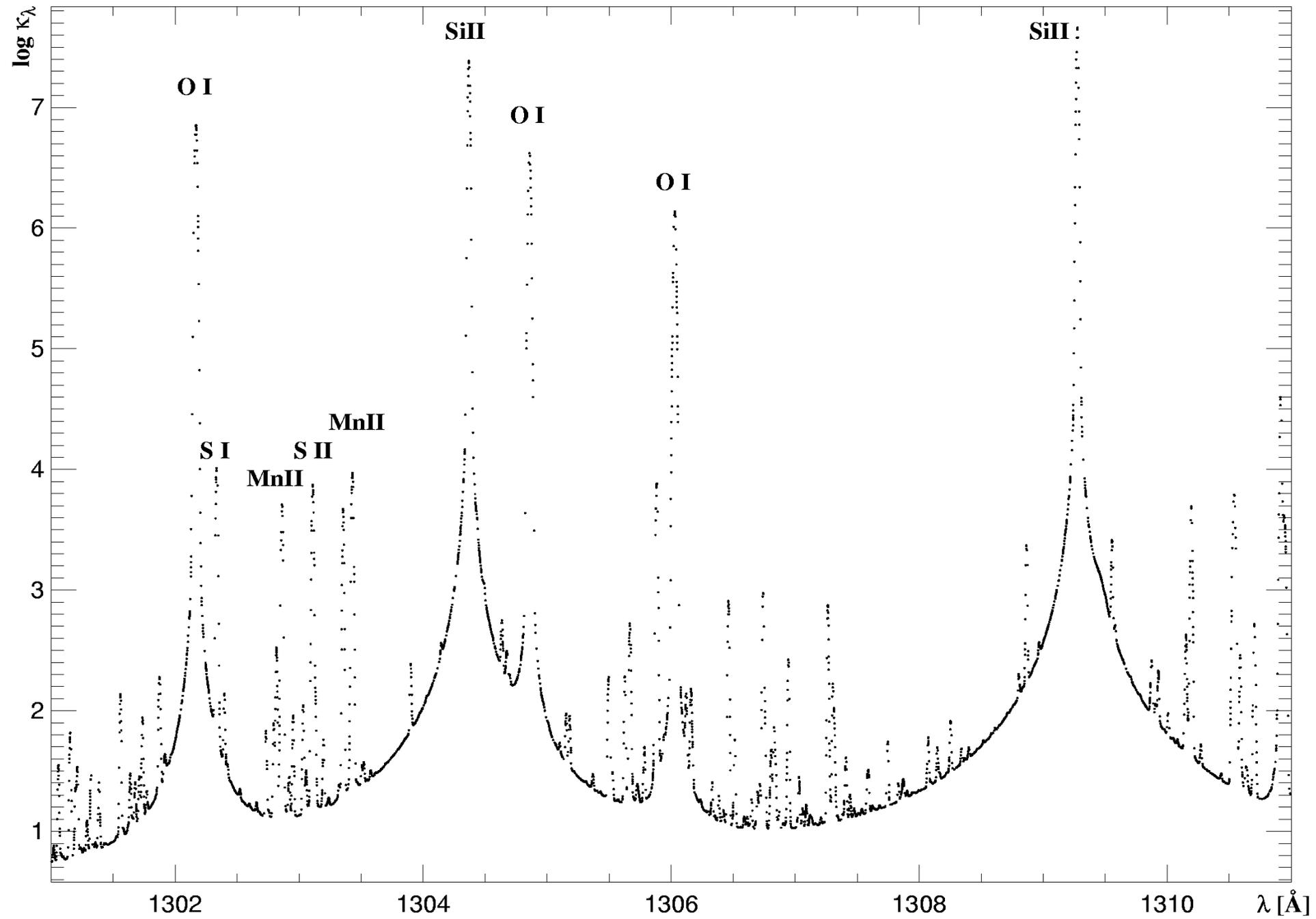
- Help!

Solving the EOS

- Equations are non-linear so we need to use Newton-Raphson.
- Remember that N-R requires the initial guess on the same “slope” where the solution is.
- Here is an elegant way of getting one:
 1. Construct P_A 's using abundances: $P_A = Z_A * P_{\text{gas}}$
 2. Compute total pressure
 3. If it's too small – scale up all P_A 's; too large – scale them down and repeat 2.
 4. Stop, when approximately ($\pm 10\%$) matching

Effects of molecular equilibrium





Attenuation operator solver

- Solution of RT over one grid cell can be written:

$$I_{\nu}(\tau_{i+1}) = e^{-(\tau_{i+1}-\tau_i)} \cdot I_{\nu}(\tau_i) + \int_{\tau_i}^{\tau_{i+1}} S_{\nu}(t) \cdot e^{-(\tau_{i+1}-t)} dt$$

where τ is the optical path along the ray

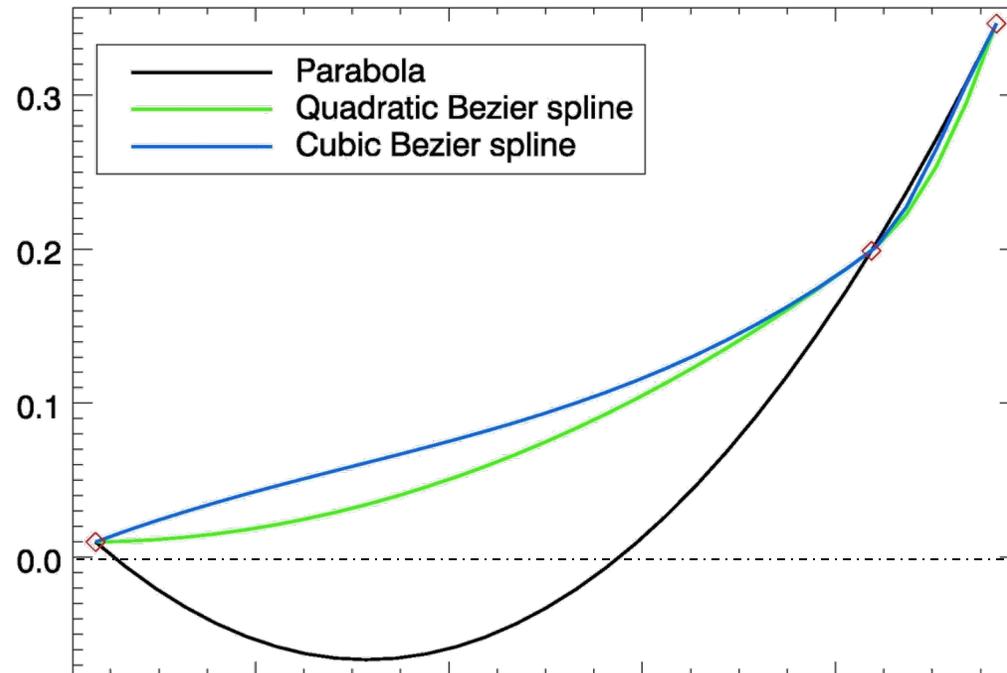
- Suppose S slowly changes with τ which can be approximated by a linear function. Then we can take the integral analytically!

$$S_{\nu}(\tau) = \left[\frac{(\tau_{i+1} - \tau)}{(\tau_{i+1} - \tau_i)} S_{\nu,i} + \frac{(\tau - \tau_i)}{(\tau_{i+1} - \tau_i)} S_{\nu,i+1} \right]$$

$$I_{\nu}(\tau_{i+1}) = I_{\nu}(\tau_i) \cdot e^{-(\tau_{i+1}-\tau_i)} + \eta_{\nu,i}$$

Source Function Approximation

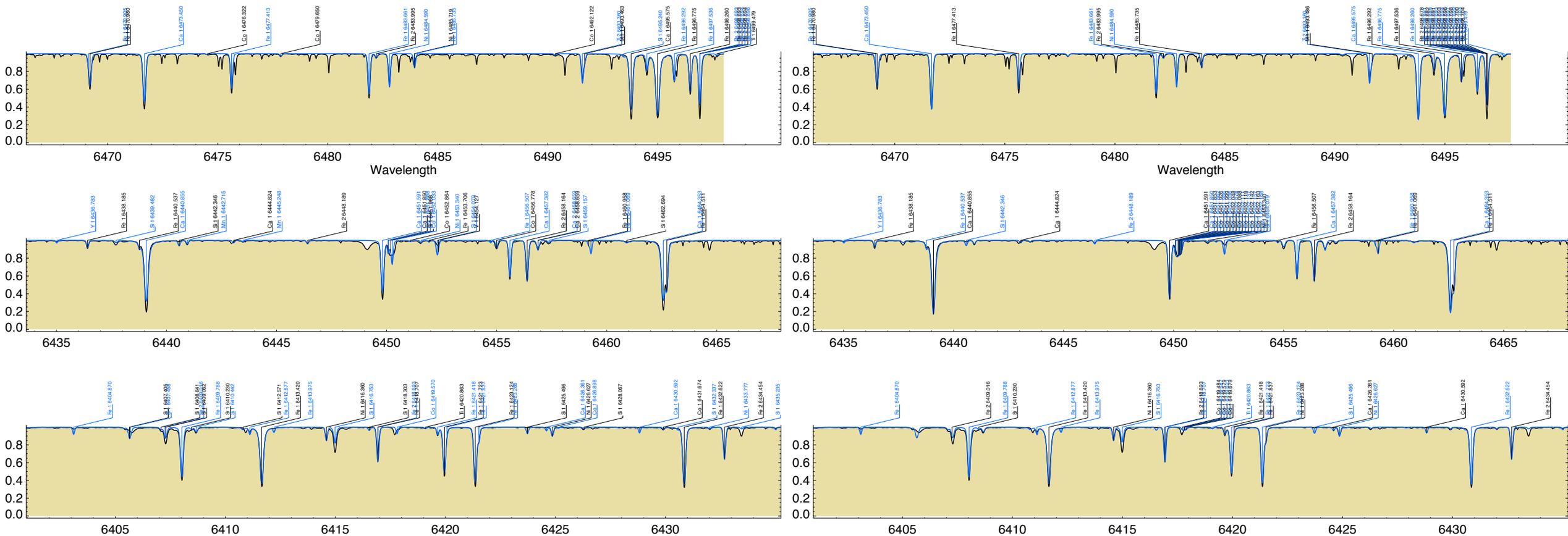
Quadratic approximation for the source function is better than linear, but ...



Bezier splines are a much more robust alternative

SME in action

- Spectroscopy Made Easy (Valenti & Piskunov, 1996 A&AS 118, 595; Piskunov & Valenti, 2017, A&A 597, 16)



SME is ...

- A spectral synthesis tool.
- A spectral fitting tool.

It also includes:

- Solar flux atlas.
- 3 grids of stellar atmospheres (Kurucz, MARCS, LL).
- NLTE departure coefficient tables for several elements.
- AOB van der Waals approximation.
- Quadratic Bezier spline RT solver.
- Explicit disk integration to account for v_{rot} and v_{macro} .

Original (IDL) SME consists of two parts

- GUI
- Solver

and they both work ...

pySME replaced the IDL parts with Python code and ... we will see tomorrow.