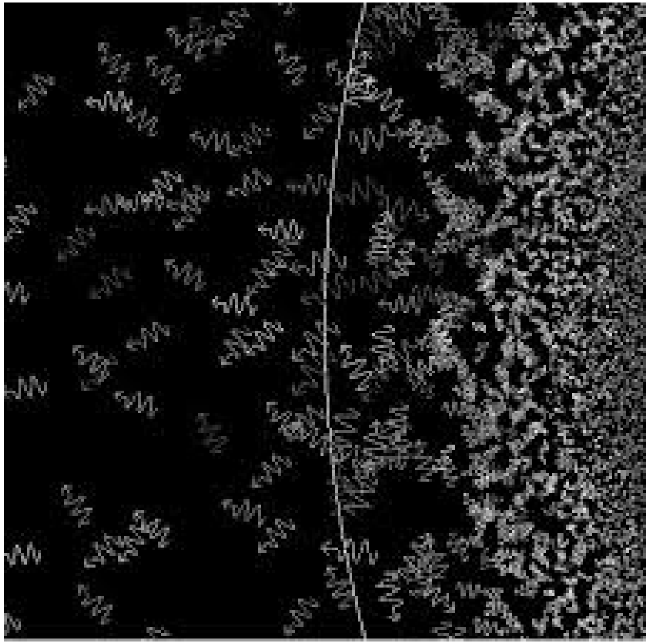
Challenges in NLTE diagnostics



Ivan Milić
(CU/LASP/NSO)
ivan.milic (at) colorado.edu; ivanzmilic (at) gmail.com; @WhisperinJay

NSO Brown Bag talk 03/10/2020

Takeaways

- NLTE (polarized) radiative transfer is by far the most numerically demanding component of today's forward models (either standalone RT or R(M)HD)
- We (think) we understand the physics, but we don't have enough (person?) computing power to tackle the most complicated problems
- There is work to be done at all the aspects :

  Iterative methods

  Response functions / diagnostics

  Multidimensional calculations

  Time dependent calculations

  PRD

- Radiative transfer and NLTE might be hard, but they are also fun!

What is NLTE and why do we care?

"… and the assumption of LTE no longer holds, a condition often referred to as non-LTE (NLTE), a description of what it is not rather than what it is."

(Michiel van Noort)

"In contrast, by the term non-LTE or (NLTE) we describe any state that departs from LTE"

(Ivan Hubeny & Dmitri Mihalas, Stellar Atmospheres 3rd edition)

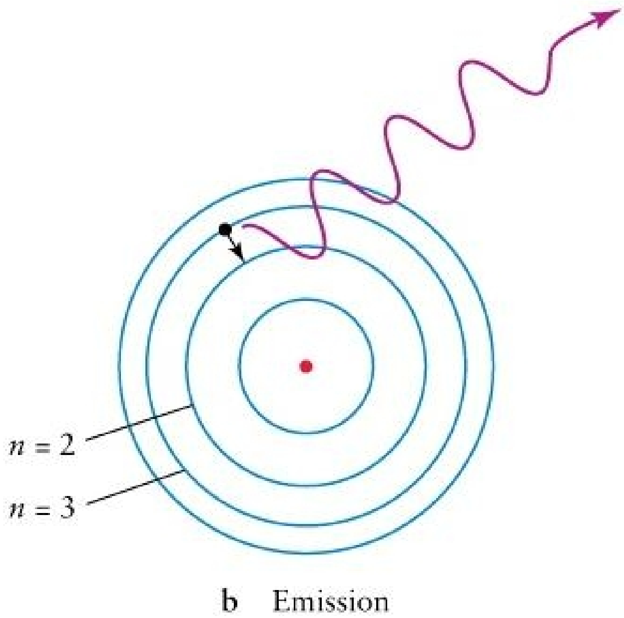
LTE:

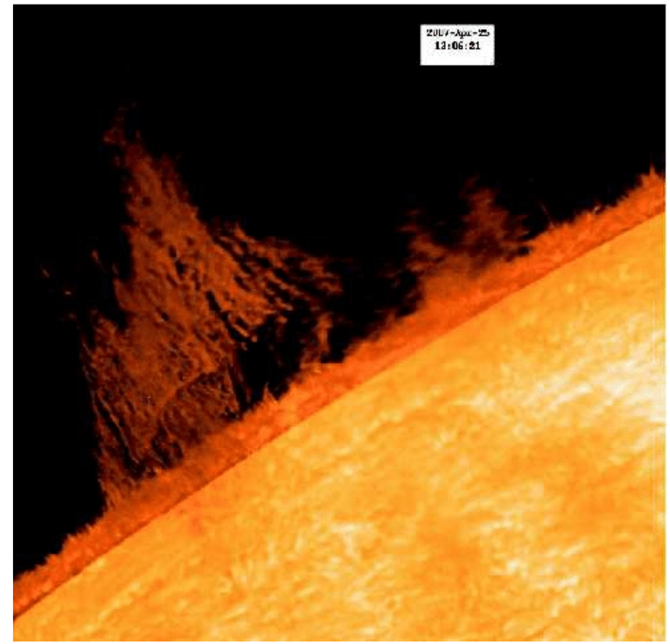
Ionization follows Saha distribution, exictation Boltzmann distribution, velocities Maxwellian distribution.

We will mostly focus on the departures from the first two.

The core of the NLTE problem

To paraphrase John Wheeler:

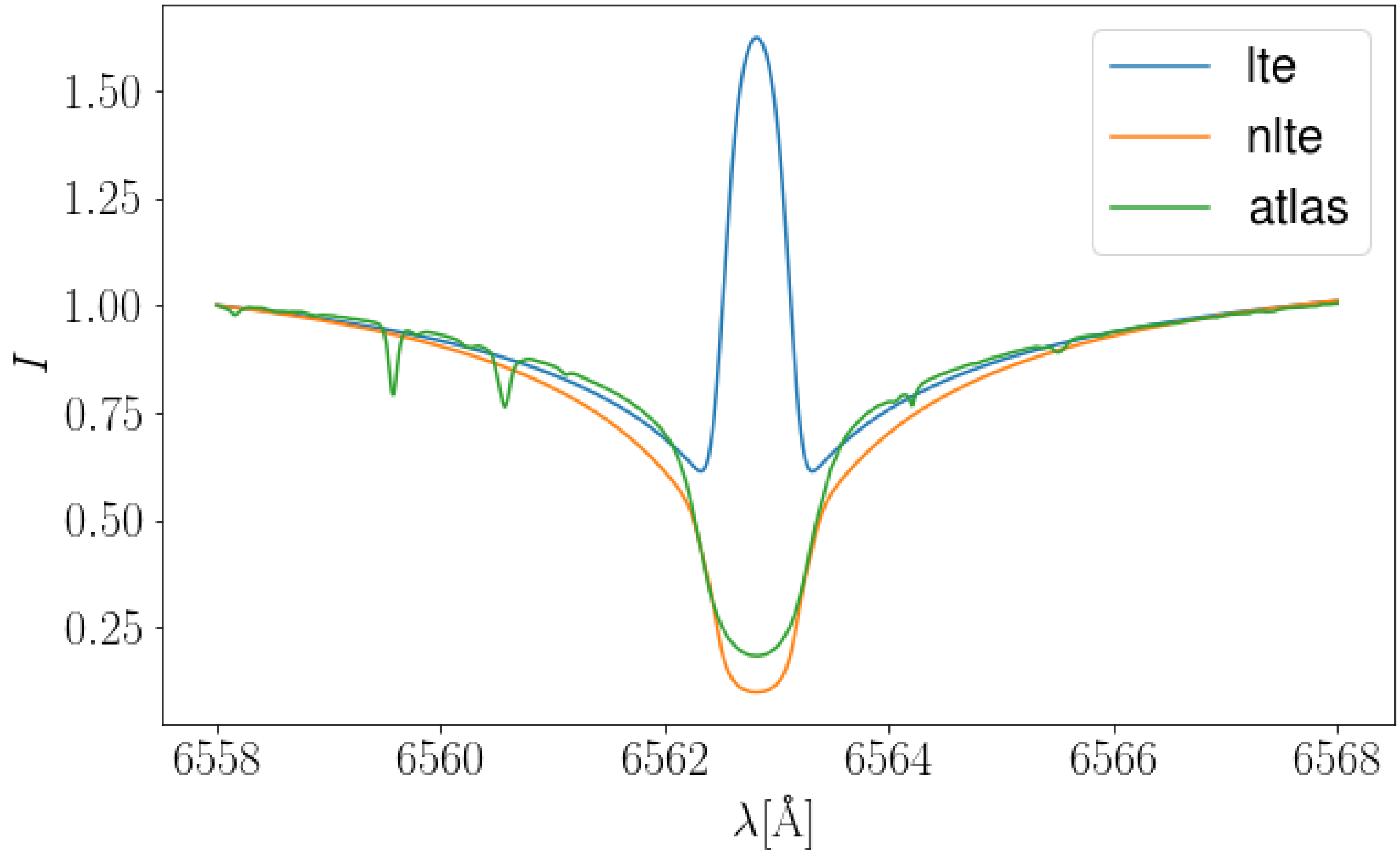




Credits: HINODE/SOT

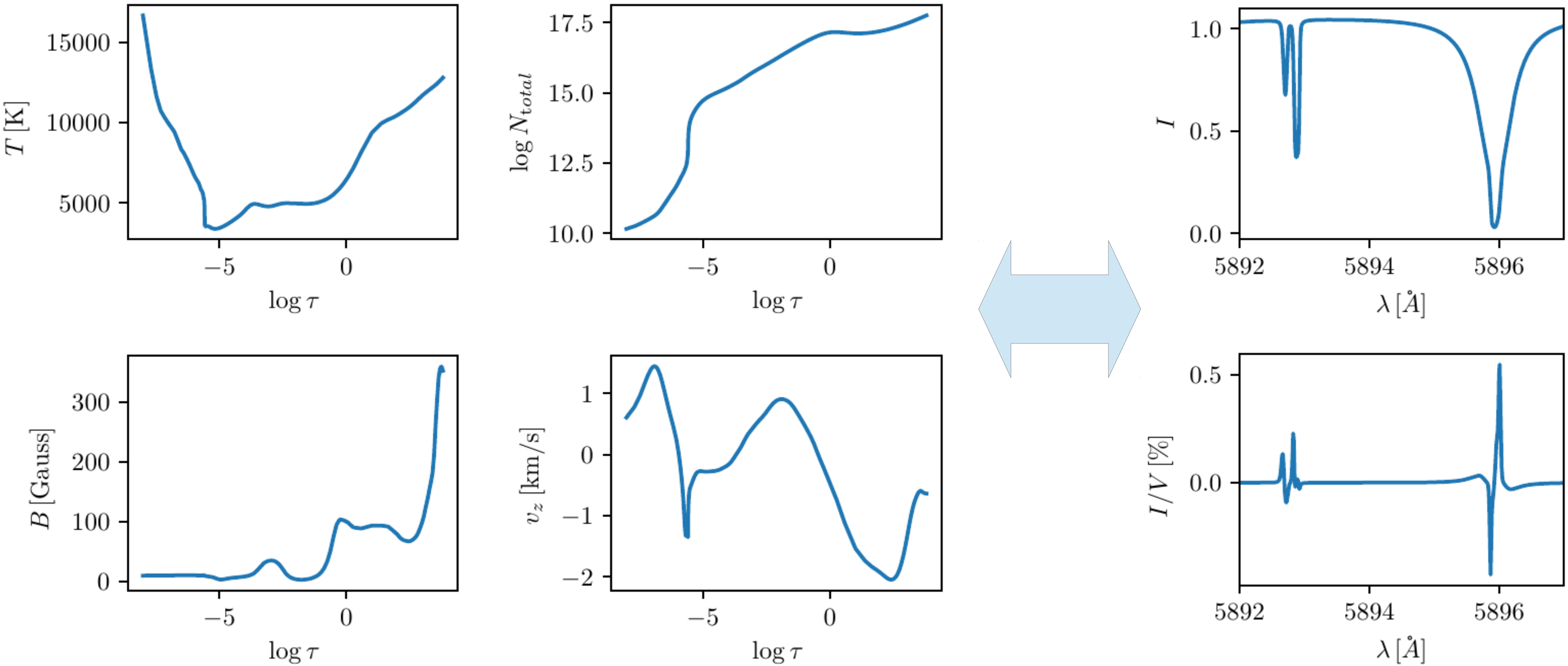
"Excitation tells the levels how many photons to emit,
photons tell the levels how to excit(e)."

Is NLTE important?

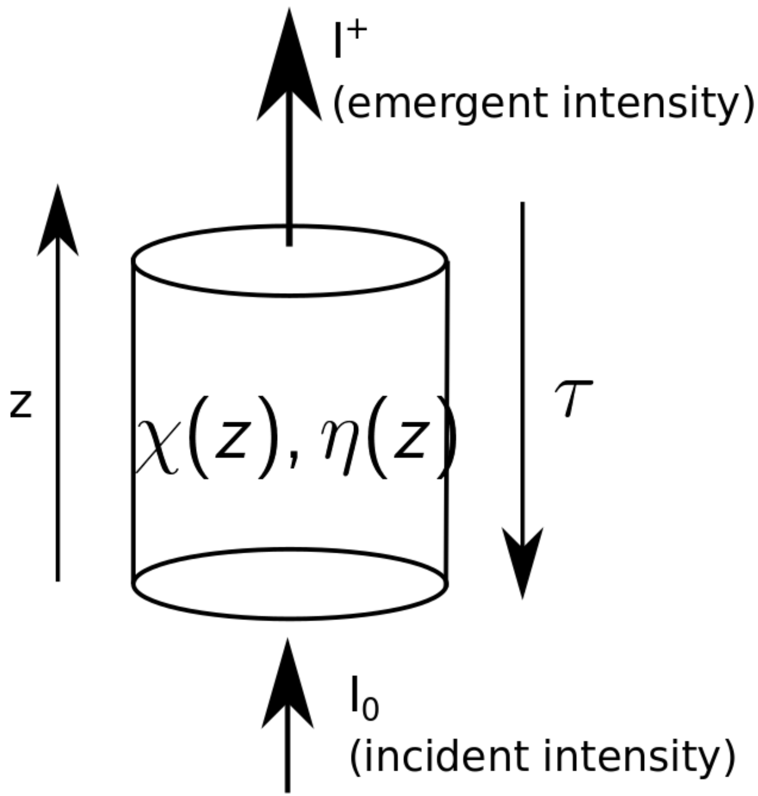


Why does this specific line (H-alpha) turn from emission to absorption?
What is the mystery behind this?

Step by step – how do we calculate the spectrum?



Step by step – how do we calculate the spectrum?



$$\frac{dI_\lambda(z)}{dz} = -\chi_\lambda(z) I_\lambda(z) + j_\lambda(z)$$

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

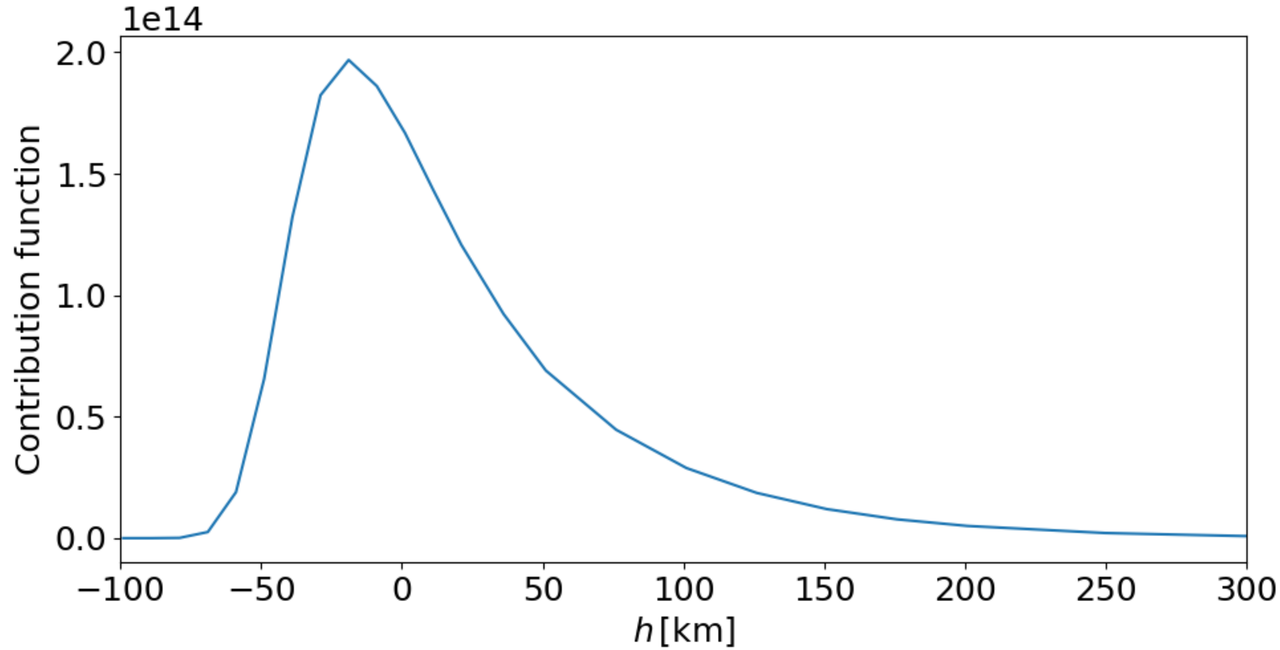
$$I_\lambda(\tau_\lambda) = \int_{\tau_\lambda}^{\infty} S_\lambda(t) e^{t-\tau_\lambda} dt$$

Given: boundary conditions, physical parameters
→ opacity / emissivity → **SPECTRUM.**

Inverse problem: Much harder

Ok, well that does not sound so bad...

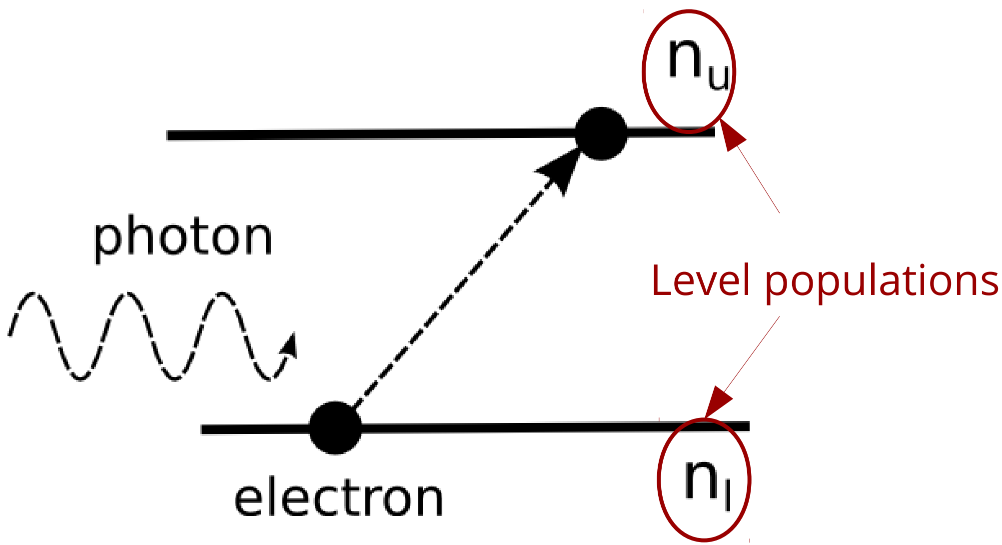
Well, it is, because this makes our problem non-local.



$$I_\lambda(\tau_\lambda) = \int_{\tau_\lambda}^{\infty} S_\lambda(t) e^{t-\tau_\lambda} dt$$

Strictly speaking, everything "upwind" from the point in question contributes.

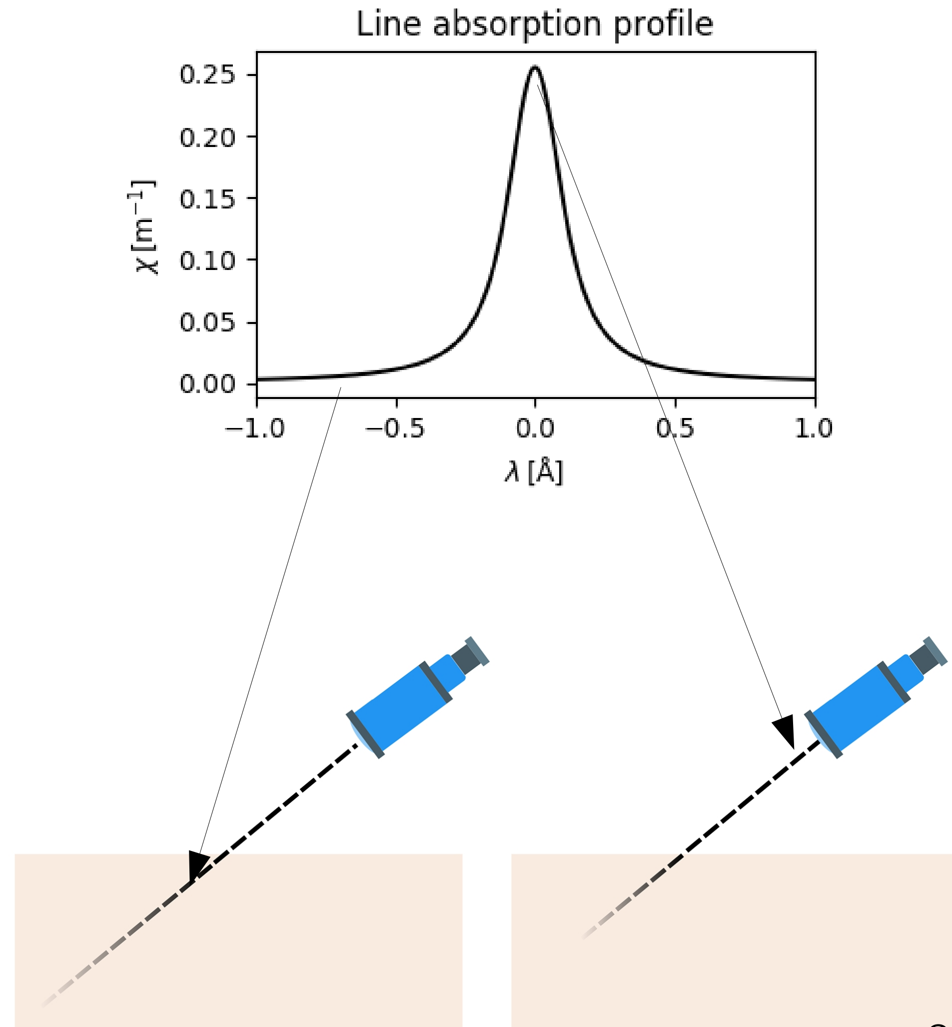
Let’s focus on spectral lines for the moment



Einstein coefficients

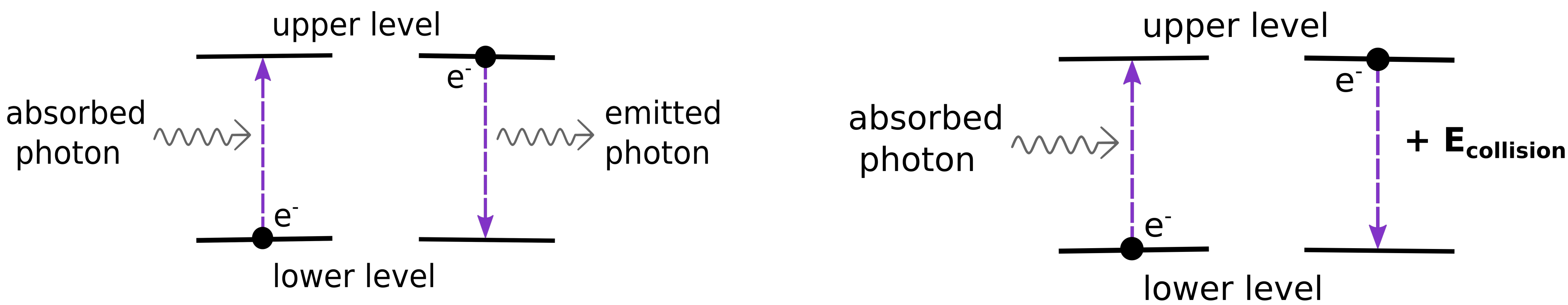
$$j(\lambda) = \frac{hc}{4\pi\lambda} n_u A_{ul} \phi(\lambda)$$

$$\chi(\lambda) = \frac{hc}{4\pi\lambda}(n_l B_{lu} - n_u B_{ul})\phi(\lambda)$$



NLTE complicates the calculation of the level populations

Radiation can alter the level populations (e.g. photoinization, optical pumping)



We replace Saha-Boltzmann with statistical equilibrium equation:

$$\frac{dn_i}{dt} = \sum_j n_j T_{ji} - n_i T_{ij} = 0$$

$$\boxed{I_\lambda(\tau_\lambda) = \int_{\tau_\lambda}^{\infty} S(t) e^{-t} dt}$$

$$T_{ij} = R_{ij} + C_{ij}$$

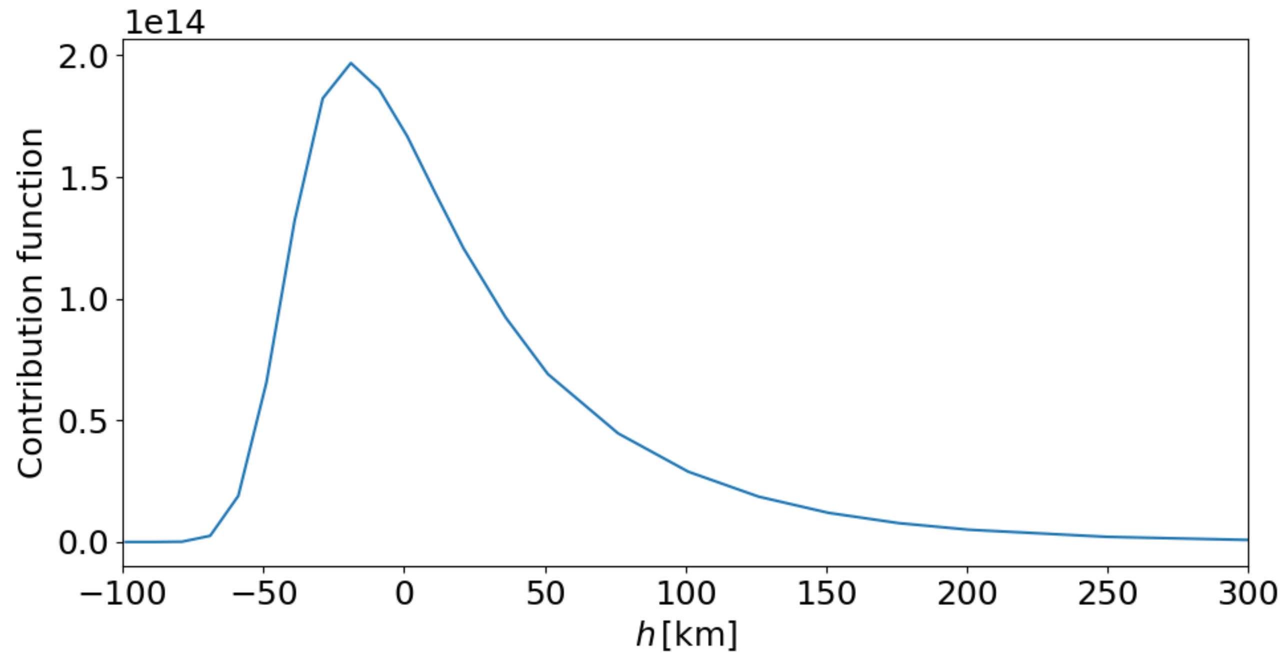
$$\boxed{j(\lambda) = \frac{hc}{4\pi\lambda} n_u A_{ul} \phi(\lambda)}$$

$$R_{ij} = A_{ij} + B_{ij} \oint \int I(\lambda, \Omega) \frac{d\Omega}{4\pi} \phi(\lambda) d\lambda$$

Ok, well that **still** does not sound so bad...

Well, it is, because this makes our problem non-local. **And non-linear.**

This is where the level populations are hiding.



$$I_\lambda(\tau_\lambda) = \int_{\tau_\lambda}^{\infty} S_\lambda(t) e^{t-\tau_\lambda} dt$$

Strictly speaking, everything "upwind" from the point in question contributes.

Now we have a non-local and non-linear problem

- Intensity in a given point depends on the level populations everywhere.
- Level populations in the given point depend on the local intensity.
- **Level populations in the given point depend on the level populations everywhere: Coupling.**
- To solve it, we need to calculate all the relevant intensities for:

$$R_{ij} = A_{ij} + B_{ij} \oint \int I(\lambda, \Omega) \frac{d\Omega}{4\pi} \phi(\lambda) d\lambda$$

- For a 1D atmosphere with 100 points, 10 directions, 20 wavelenghts per line, 5 lines atom (i.e. Ca II 8542): **100 000 unknowns.**
- Or, said in another way: 5 x 20 x 10 x 20 (iterations) = **20 000 formal solutions .**

The simplest example – 2 level atom.

This is statistical equilibrium

This is radiative transfer

$$S = \epsilon B + (1-\epsilon) \int \oint I(\lambda, \hat{\Omega}) \frac{d\Omega}{4\pi} \phi_\lambda d\lambda \qquad I_d = \sum_{0}^{ND} w_{d,d'} S_{d'}$$

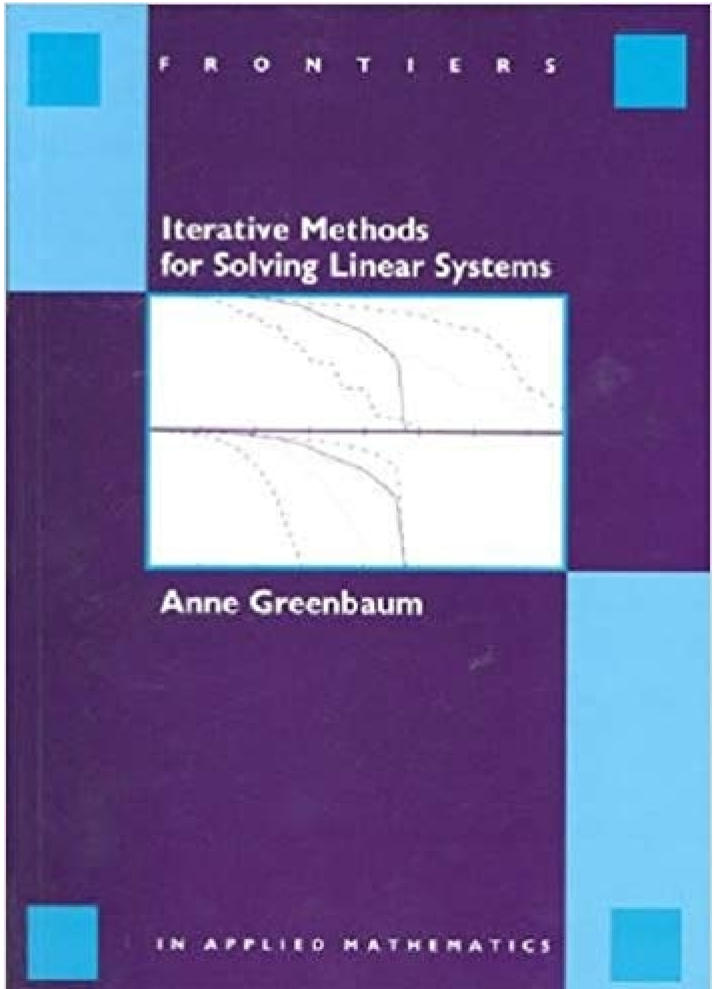
Let's merge them into one:

$$S_d = \epsilon_d B_d + (1 - \epsilon_d) \sum_{d'=0}^{ND} \Lambda_{d,d'} S_{d'}$$

Which is actually good old:

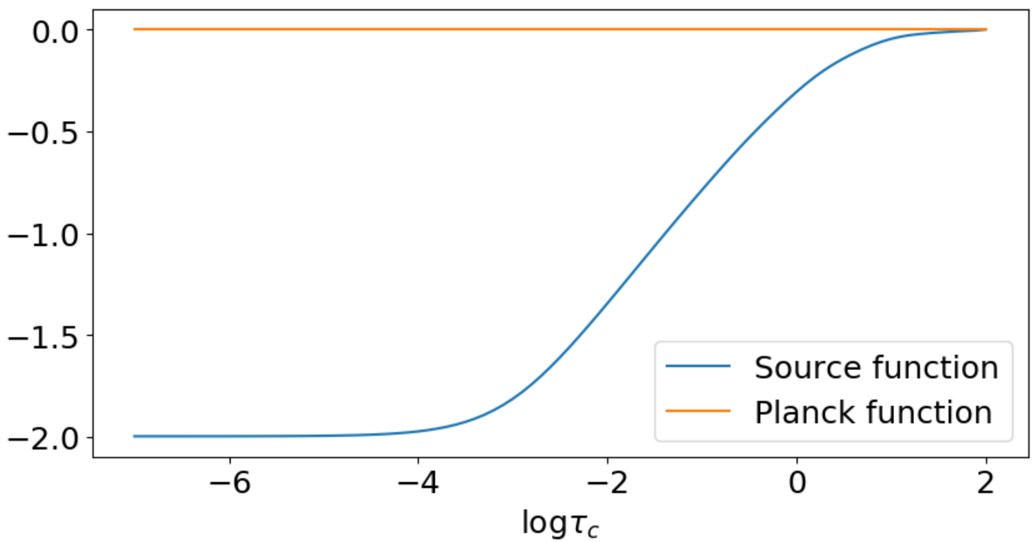
$$\boxed{\hat{A}\vec{x} = \vec{b}}$$

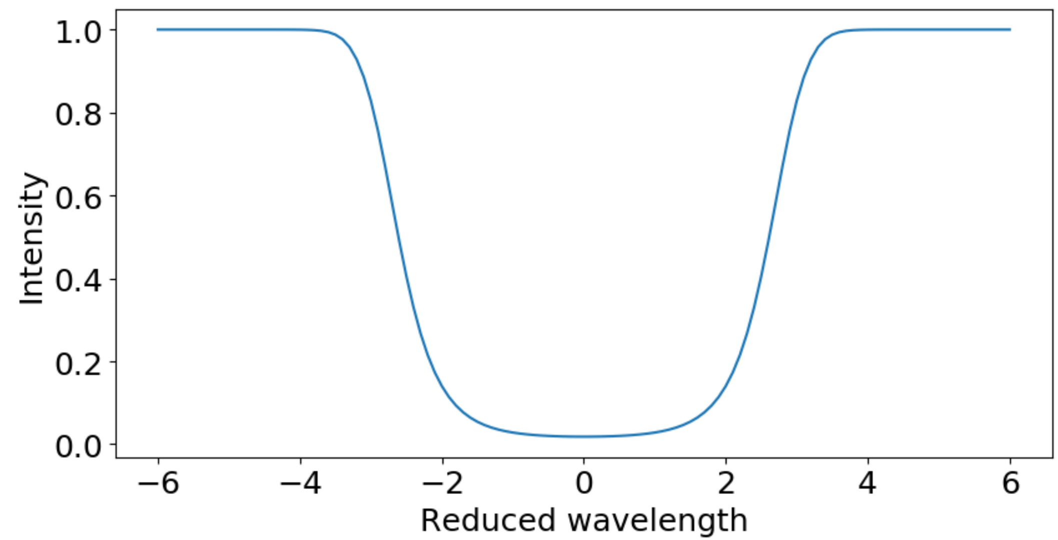
In 99.9% cases solved by iteration:

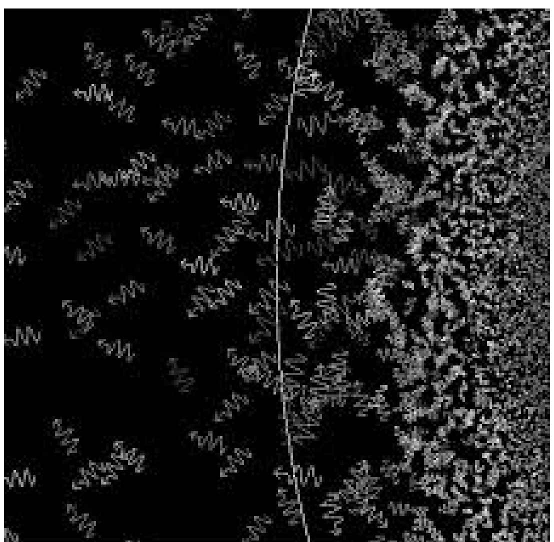


- ALI (Rybicki & Hammer) : easy, robust, well-tested. But, there are (much) faster ones:
- Gauss Seidel + SSOR (Trujillo Bueno & Fabiani Bendicho)
- Implicit lambda iteration (Atanackovic & Milic)
- Multigrid (Steiner, Stepan & Trujillo Bueno)
- Bi-conjugate Gradient (Anusha, Paletou)
- ***Something new?***
  (especially for 2-level atom like lines)

So what happens then?



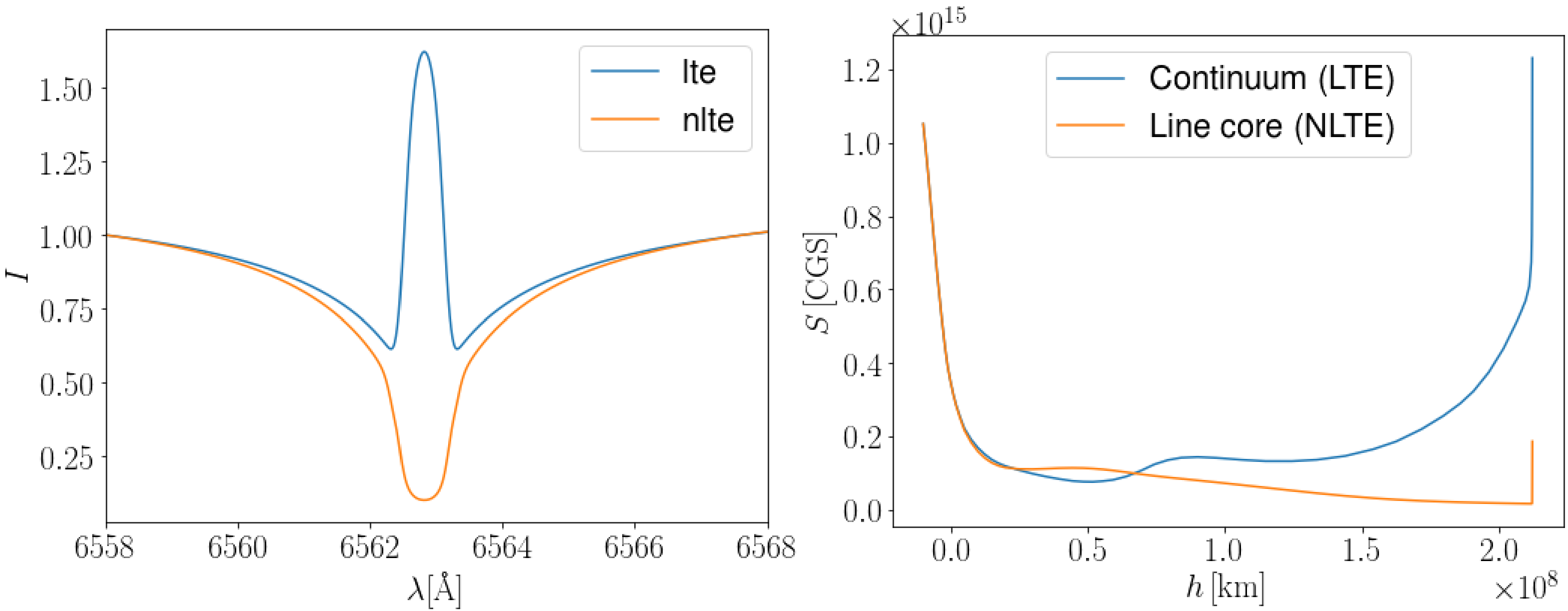




- Photons “leak” from the surface, there are few collisions, so upper level is under-populated.
- Source function decoupled from the local temperature (Planck function).
- Line appears even in an isothermal atmosphere.

Credits: Mats Carlsson

How does it look for our beloved H alpha?



Line shape tracks the depth run of the source function (wavelength maps to height!)

Now I will jump ahead and ask you something

How do we know where a spectral line forms?

- Well, strictly speaking it depends on a model atmosphere.
- We can model the spectrum, and extract some relevant quantities.
- **Tau = 1 point (surface)** : the simplest measure of the “height” of formation
- **Contribution function**
- **Response function**

Let's apply it to our academic 2-level atom problem

This is statistical equilibrium

This is radiative transfer

$$S_d = \epsilon B_d + (1-\epsilon)\sum_m \sum_l w_m w_l I_{d,l,m} \quad I_d = \sum_0^{ND} w_{d,d'} S_{d'}$$

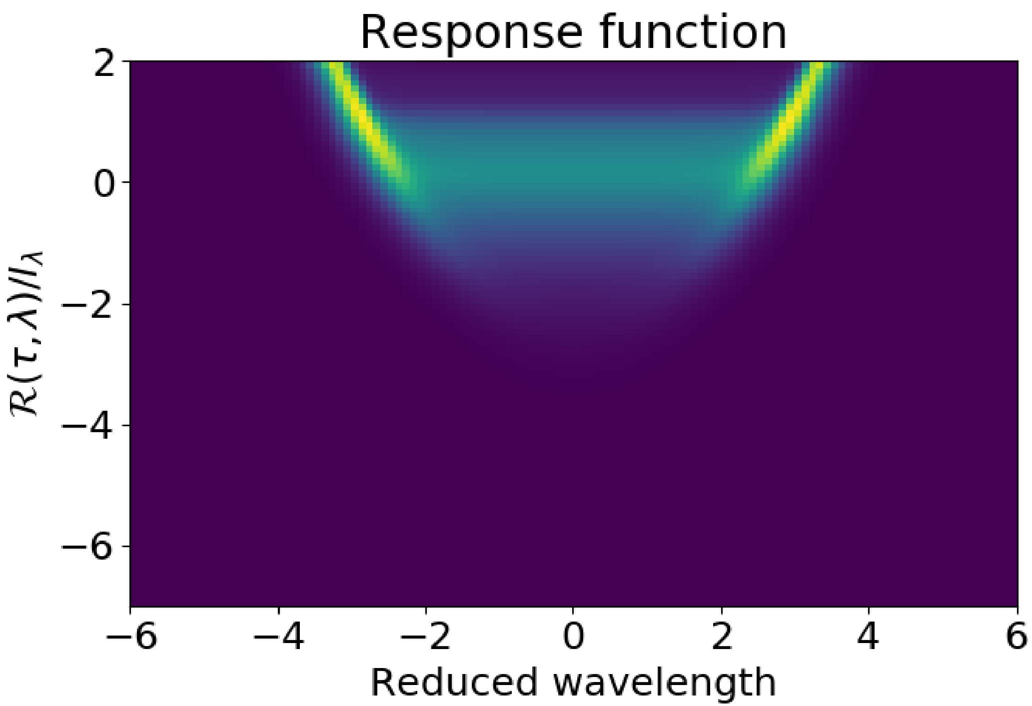
This is the contribution function

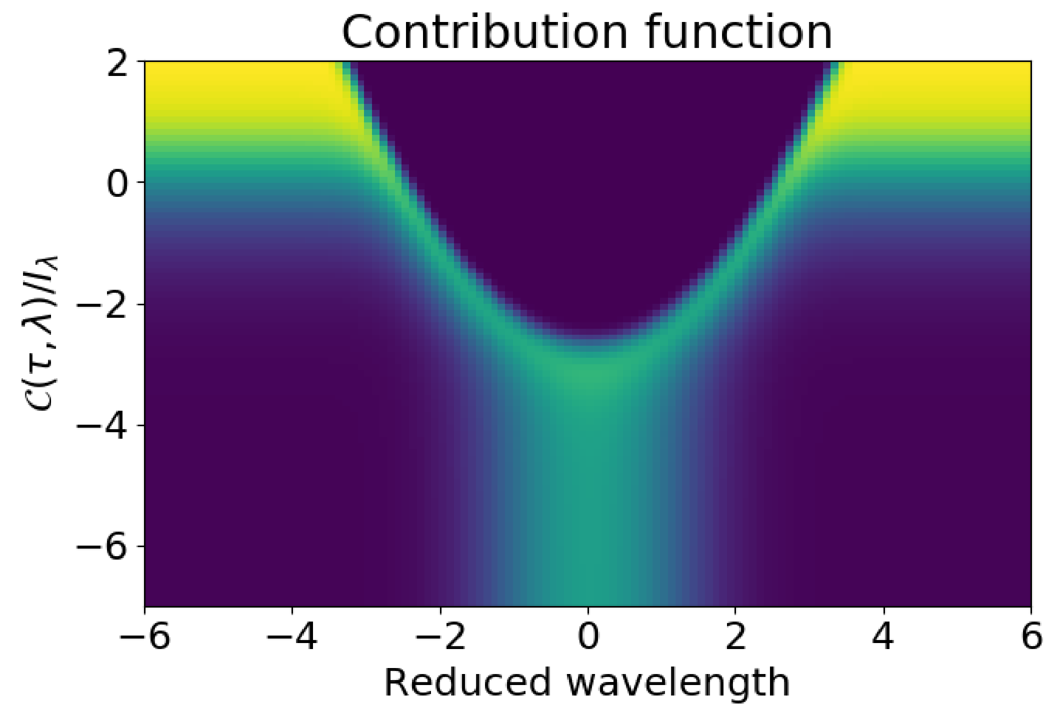
Let's merge them into one:

$$S_d = \epsilon_d B_d + (1-\epsilon_d)\sum_{d'=0}^{ND} \Lambda_{d,d'} S_{d'}$$

To get the response function, we need to calculate derivative of the last equation to each B and plug it back into the formal solution

Let's do it!

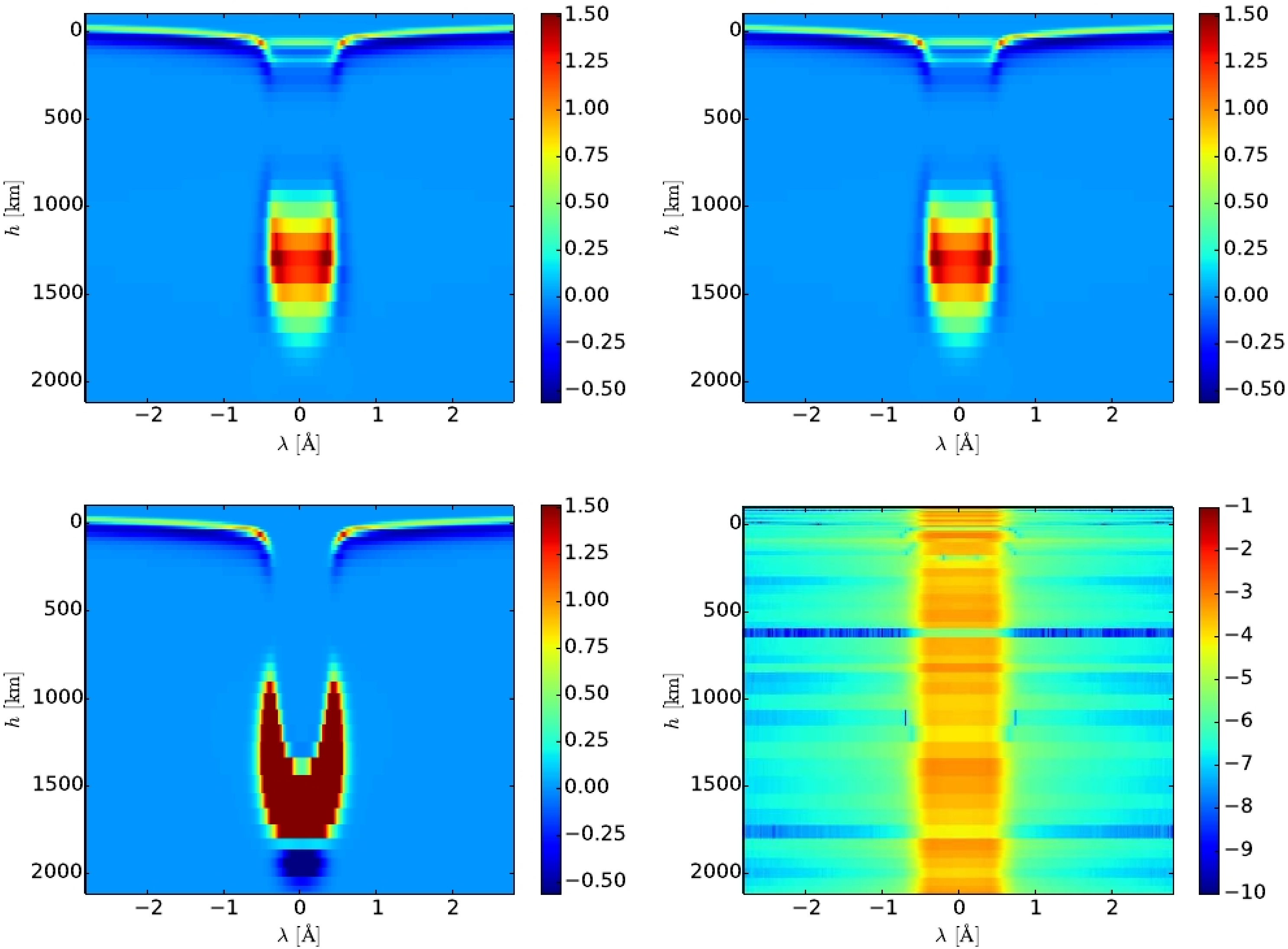




$$S = \epsilon B + (1-\epsilon)\hat{\Lambda} S$$
$$(I - (1-\epsilon)\hat{\Lambda})S = \epsilon B$$
$$\frac{dS_d}{dB_{d'}} = (I - (1-\epsilon)\hat{\Lambda})^{-1} \epsilon\, \delta_{d,d'}$$

- This algebra shows us how the Source function responds to temperature
- From there we can easily calculate intensity response function

Real life example (well, sort of): H alpha – like 2 level atom



- Generalization of the method presented above to multilevel problems
- We can capture exactly all the spatial and inter-level dependencies
- Note the double peak of the RF

Milic & van Noort 2017

More on the response functions

- An essential ingredient of inversion codes (Jaime's talk)
- They also tell us something about line formation
- That is, after solving this problem we know:

$$\frac{\partial I_d(\hat{\Omega}, \lambda)}{\partial T'_d}$$

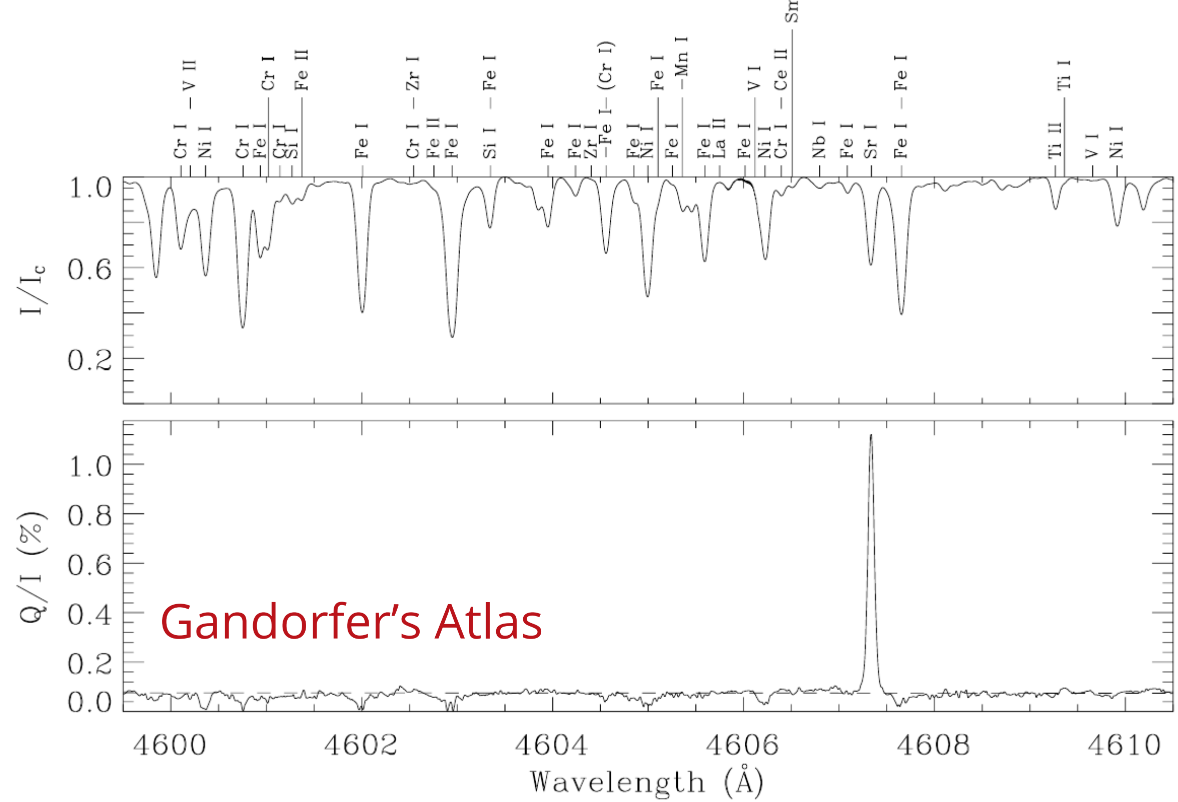
everywhere in the atmosphere.

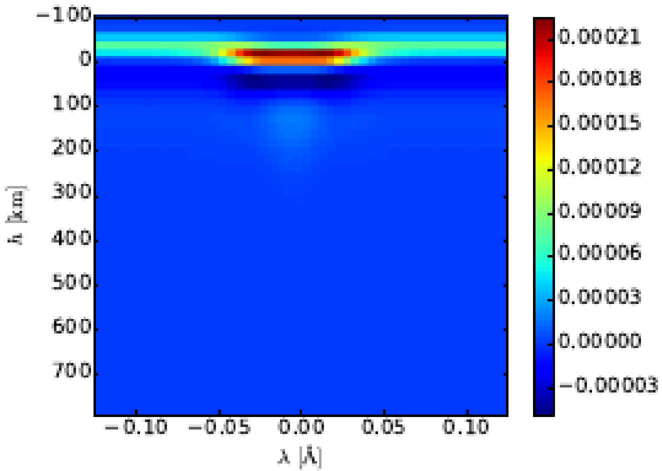
- Now can also calculate the response of any moment of the intensity to T
- Why not anisotropy? It determines the scattering polarization

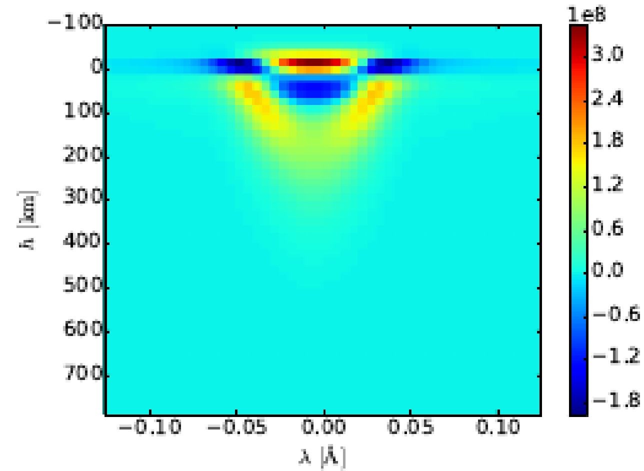
$$J_0^2 = \frac{1}{2\sqrt{2}} \int \oint I(\lambda, \hat{\Omega})(1 - 3\mu^2)\frac{d\Omega}{4\pi}\phi\lambda d\lambda$$

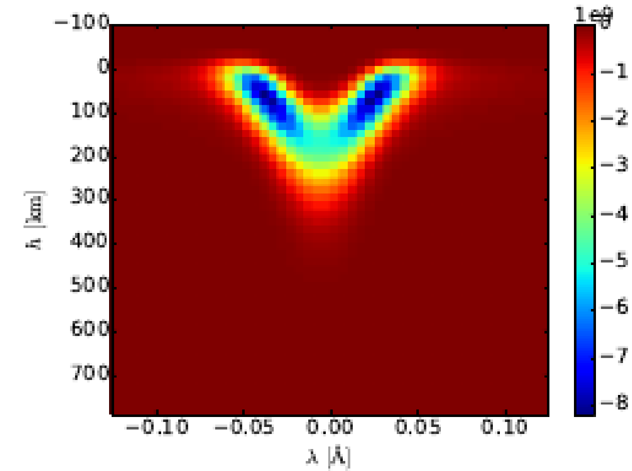
Response functions for scattering polarization

- Beloved Si 4607 line.
- Modeled as 2lvl + continuum
- A promising tool for quiet Sun magnetism (DKIST target)
- Complements Fe I 6300 lines







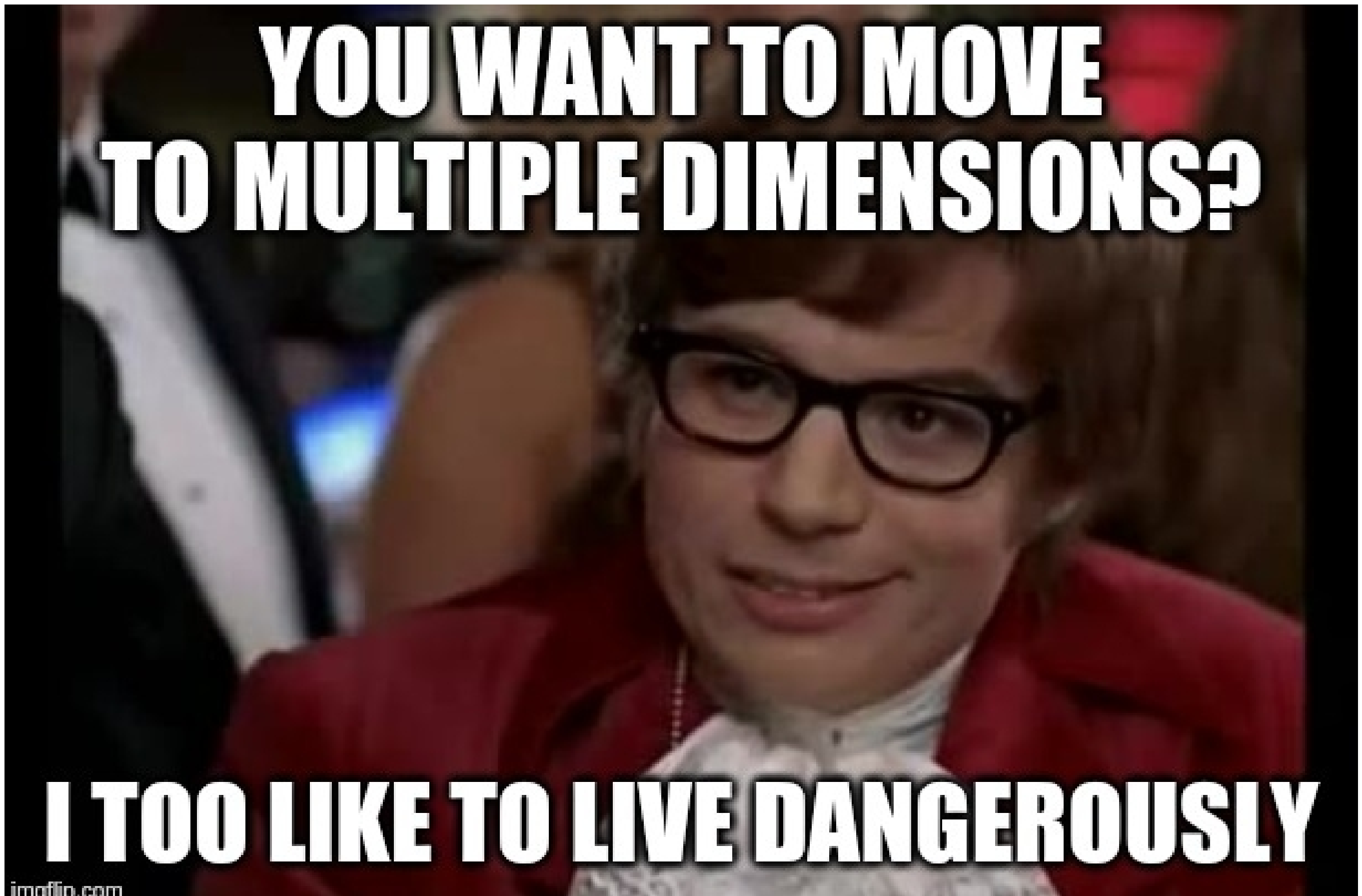


Recap:

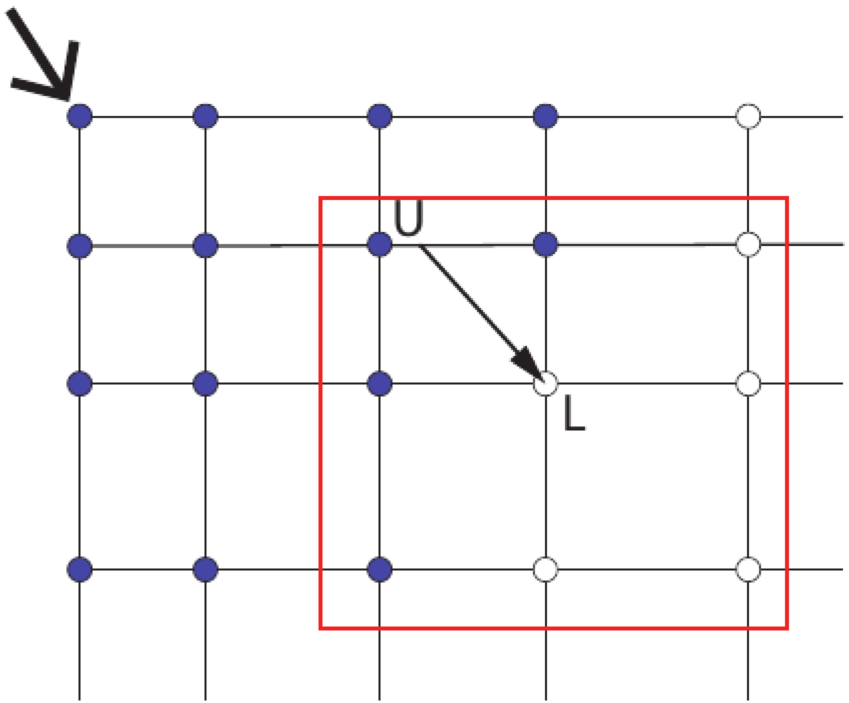
- NLTE is a non-local and non-linear coupling between level populations and radiation
- Or more precisely said, a non-local and non-linear coupling between all the level populations, in all the atoms, *everywhere*
- Without NLTE, there is no scattering polarization.
- The problem is solved numerically.
- The dimension of the problem is very large.
- Still, we have it under control :-)

Wait Ivan, you said RT is non-local, that means…

- That we also need to think about the light that travels laterally!



Multidimensional NLTE radiative transfer



Milic, PhD thesis

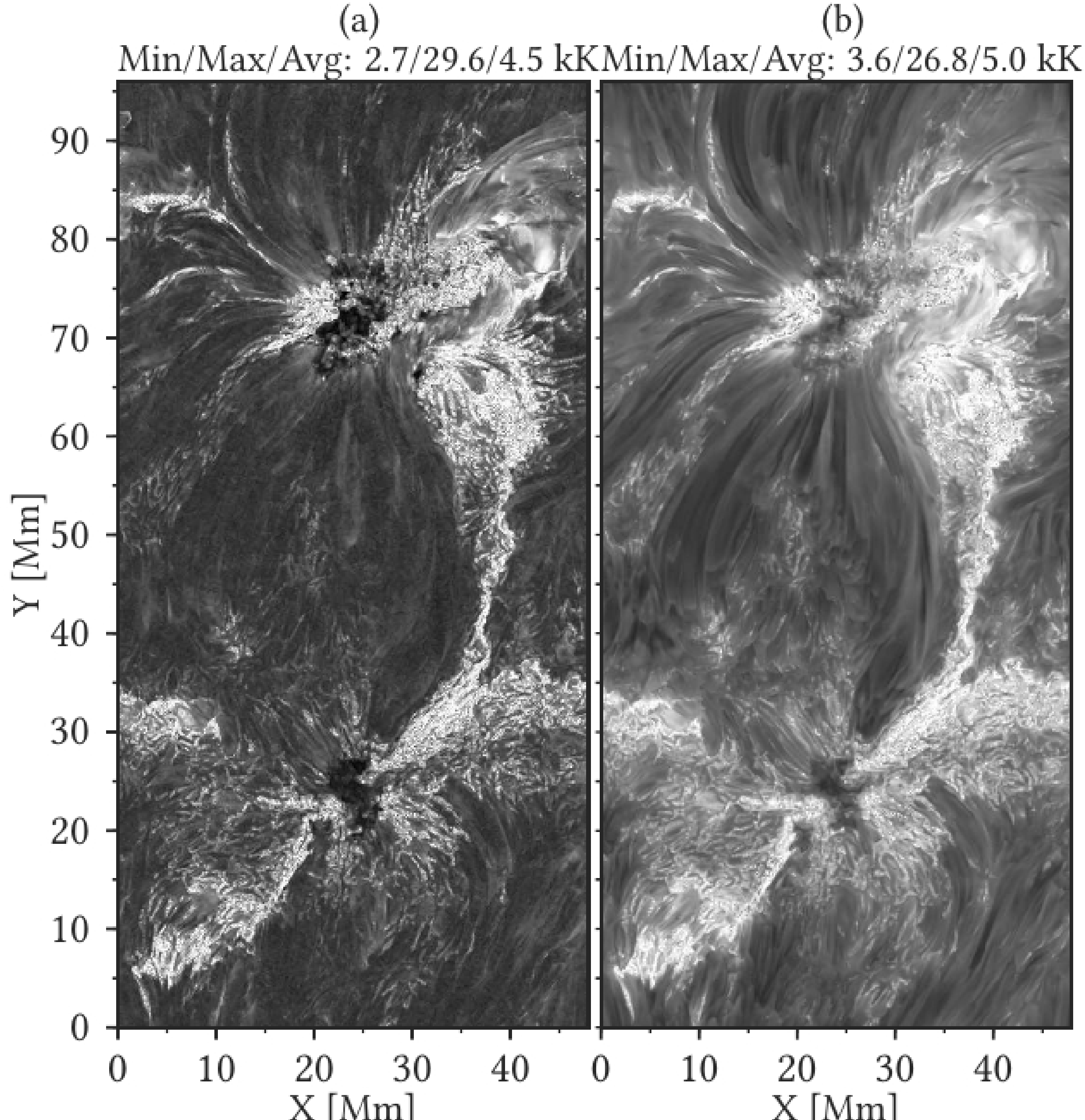
- Increased number of spatial points (100-10000 times more).
- Additional angle dependence
- “Upwind” point does not lie on the grid, we need to interpolate quantities there.

$$I_L = I_U e^{-\Delta} + \int_0^{\Delta} S(t) e^{-t} dt$$

$$I_L = I_U e^{-\Delta} + w_L S_L + w_U S_U + \ldots$$

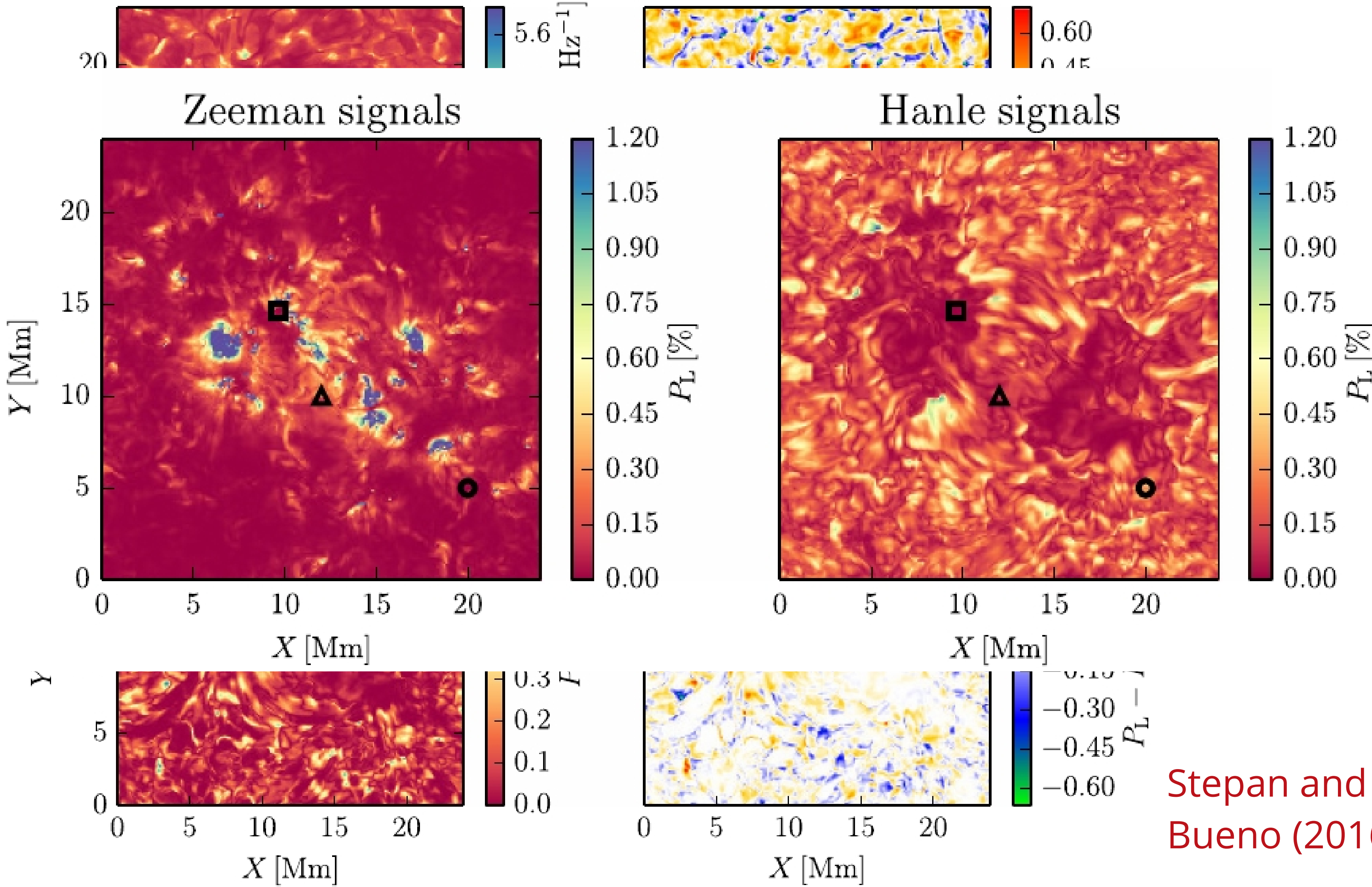
Couples the atmosphere – smooths the source function

- 3-level Hydrogen atom, with CRD, and nlte ionization
- MHD simulation similar to Cheung et al (2018)
- NLTE solution and synthesis using Multi3D
- Note lower contrast by higher average brightness in 3D!



Halpha line core, calculated by Bjorgen et al. 2019

And modifies the radiation anisotropy



Stepan and Trujillo Bueno (2016)

How hard are these calculations?

"I am writing a new 3D NLTE code right now, I think it is going to be a good practice." - Every enthusiastic PhD student, ever

- It is a great practice! But, there are a number of things to think about:
- Typical MHD simulation is, say 512 x 512 x 100 points. We need typically 50 angles and some 100 wavelengths:

  10E11 quantities (intensities) per iteration.
- This must be done in parallel, using efficient techniques and robust codes.
- Radiative Transfer calculations are always going to be orders of magnitude slower than (M)HD ones, because we have **3 extra dimensions** (wavelength, direction)
- Calculation of a self-consistent 3D NLTE RT problem takes days if not weeks.

3D Diagnostics (future):

- Spectropolarimetric inference in 1D:

$$\mathcal{F}_{1D}[T(z), v(z), B(z)...] = \hat{I}_\lambda$$

- Inference in "2D" (actually 3D, e.g. van Noort, 2012)

$$PSF(x,y) \star \mathcal{F}_{1D}[T(x',y',z), v(x',y',z), B(x',y',z)...] = \hat{I}_\lambda(x,y)$$

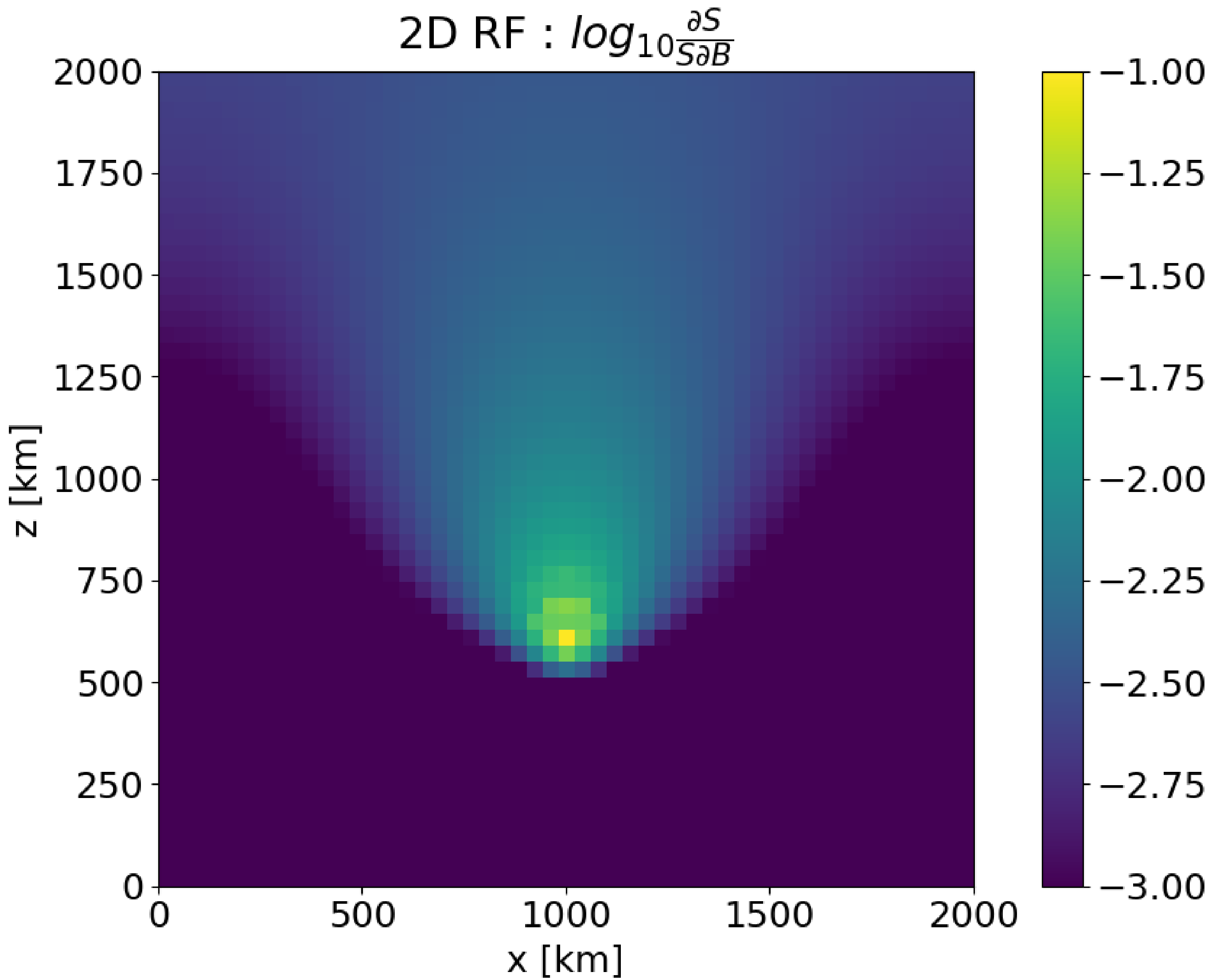
- Inference involving 3D radiative transfer (we do not have it **yet**):

$$\mathcal{F}_{3D}[T(x',y',z'), v(x',y',z'), B(x',y',z')...] = \hat{I}_\lambda(x,y)$$

- This would be a response function in 3D (~1E15 quantities)

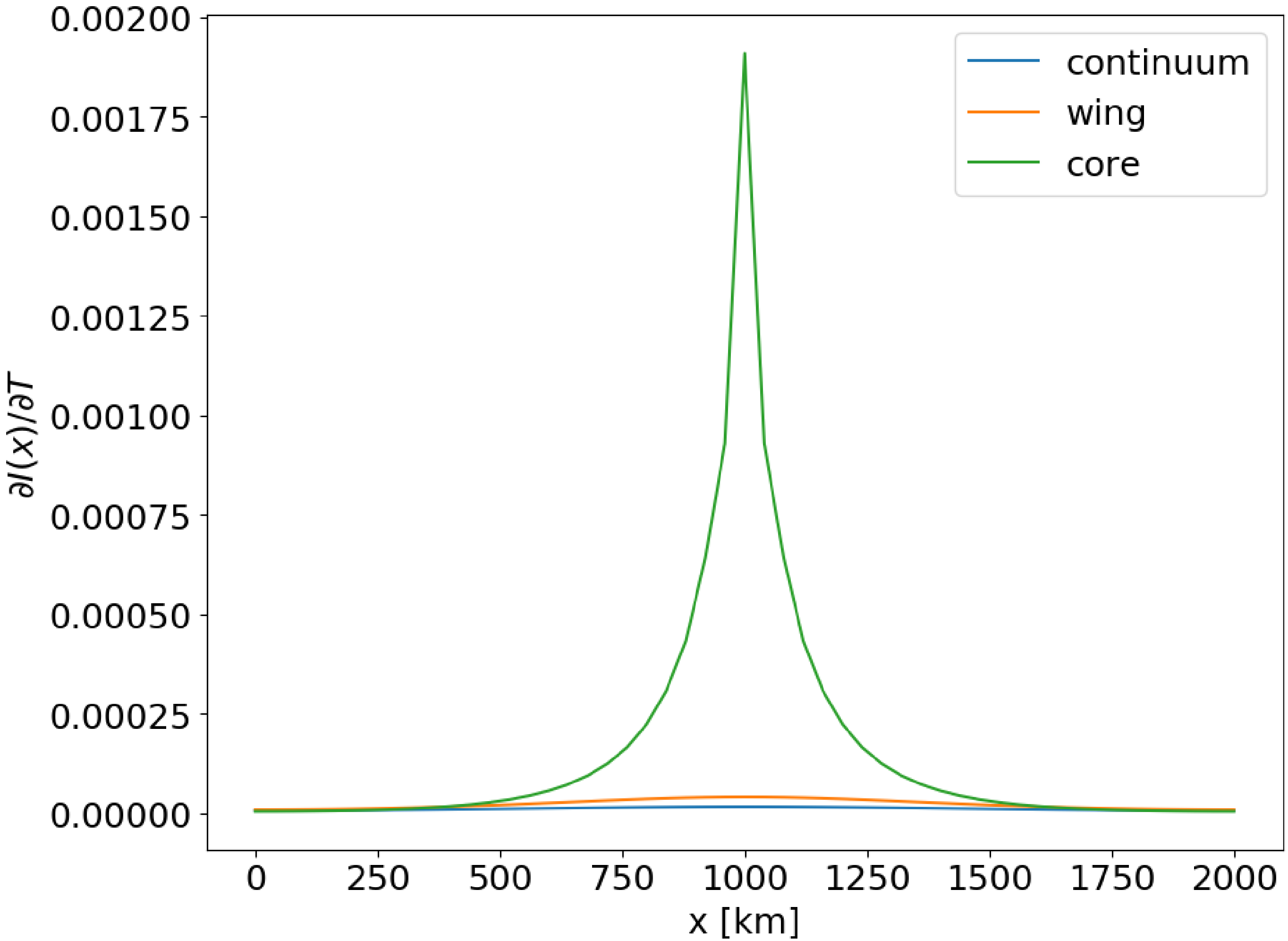
$$\frac{\partial I_\lambda(x,y)}{\partial T(x',y',z')}$$

Multidimensional response functions:



- 2-level prototype line with total line-center optical depth of 10^5
- Isothermal atmosphere, perturbed at various depths (recall NLTE Rfs)
- This plot illustrates how temperature perturbation "diffuse" because of the line scattering

Multidimensional response functions:



- 2-level prototype line with total line-center optical depth of 10^5
- This is how the emergent intensity responds to the perturbation.
- Width of the response ~ **few 100s of km!**
- Easily resolvable by DKIST!

What is there to be done:

- We need a way to understand how 3D scattering influences the observable in the real-life examples.
- This is especially true for scattering polarization.
- Even without 3D, having a way to “invert” or diagnose spatially resolved “atmospheric” (i.e. not 10830) scattering polarization is needed.
- Finding a way to, at least statistically, compensate for 3D scattering, would be a huge step forward.
- We still need to work on faster and more stable self-consistent NLTE solutions, if we want to use realistic atom and atmosphere models.
- **Questions? Comments? Critics? Suggestions?**