Tools for analysing stellar spectra

3D non-LTE: the current state-of-the-art

Andrew Gallagher 27/07/2023

Who am I?

1. ***PhD from the University of Hertfordshire (UH), UK***
   2008 — 2012
   Thesis: *Modelling Barium isotopes in metal-poor stars*
   Andreas Korn was my external combatant…

2. ***Short-term (~1 year) postdoc at UH, UK***
   2012 — 2013
   Finished off PhD projects

3. ***Moved to the Observatory of Paris, France***
   2014 — 2017
   - working with Elisabetta Caffau and Piercarlo Bonifacio
   Other notable mentions:
   - Monique & François Spite
   - Roger Cayrel
   - Patrick François
   Worked on 3D molecular lines - first time anyone did this over such large wavelength ranges

4. ***Moved to the Max-Planck Institute for Astronomy in Heidelberg, Germany***
   2017 — 2021
   - working in Maria Bergemann's group along with Camilla Hansen
   Worked on improving 3D NLTE code Multi3D for more complicated model atoms

5. ***Moved to the Leibniz-Institute for Astrophysics in Potsdam (AIP), Germany***
   2021 — 2023
   - working with Matthias Steffen
   Working on the ChETEC-INFRA project to produce grids of 3D NLTE abundance corrections with newly developed tools

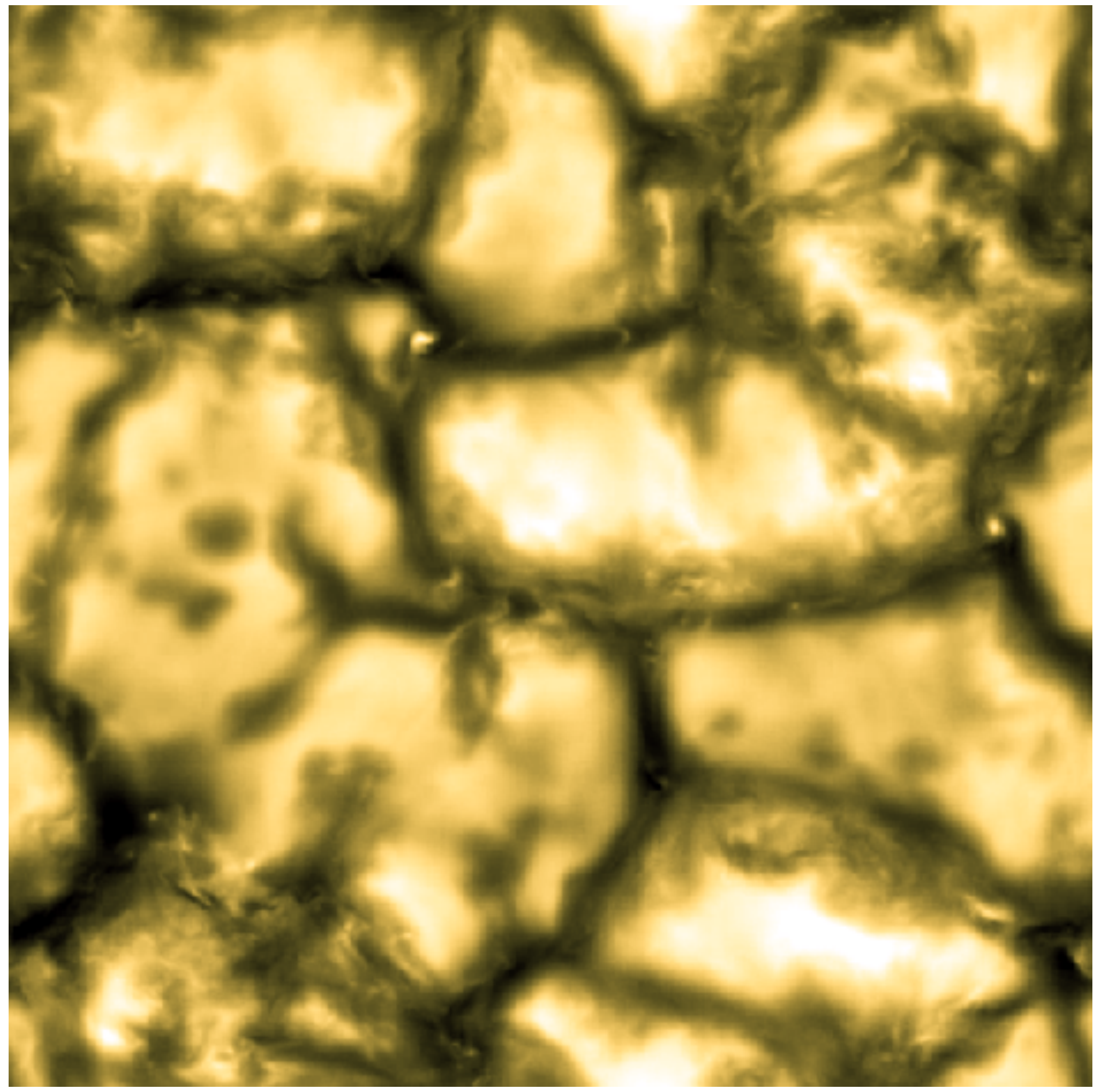
6. Responsible for the latest versions of Linfor3D
   The statistical equilibrium wrapper NLTE15D
   Known to some as "the barium guy"

Todays' topics covered

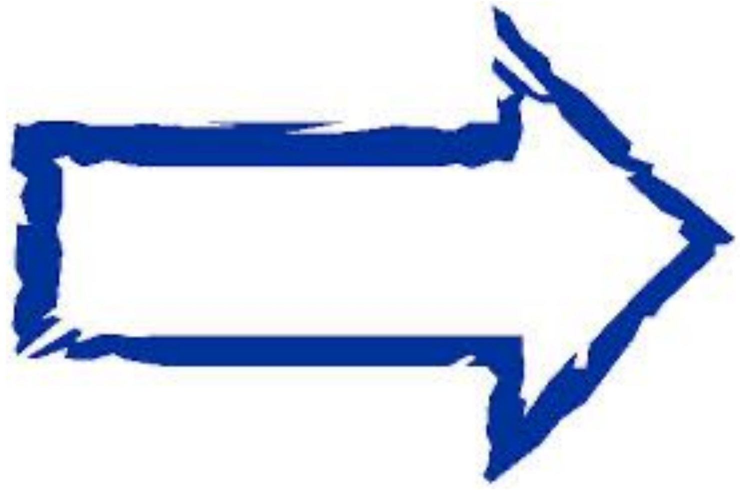
1. 3D model atmospheres
2. 3D spectrum synthesis
3. Non-LTE radiative transfer
4. Statistical equilibrium
   1. The model atom
   2. Departure coefficients
5. 3D non-LTE spectrum synthesis
6. Abundance corrections

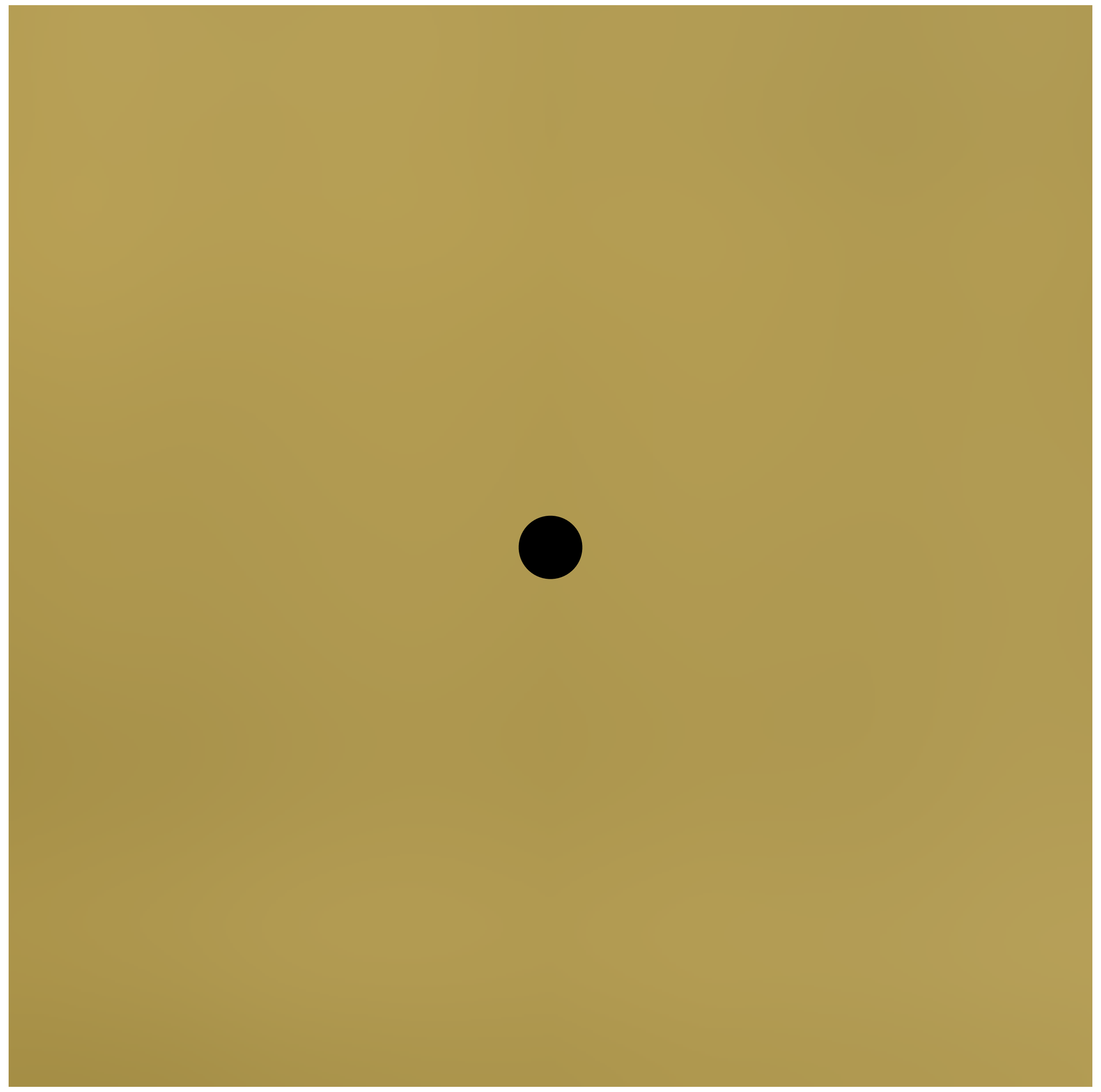
3D model atmospheres

Why model in 3D



High-resolution image of solar surface





1D model representation

- Sun as a typical star with outer convective envelope: horizontal T-inhomogeneities of $\Delta T \approx 1000\,\mathrm{K}$ evolving over minutes
- How accurate are predictions of stellar properties based on static 1D models?
    - *Abundances*
    - *Velocities*

Why model in 3D

1D modelling

- ✗ Static models
- ✗ Velocity field “fudge factors” required
- ✓ State-of-the-art micro-physics
  - ✓ Opacity sampling

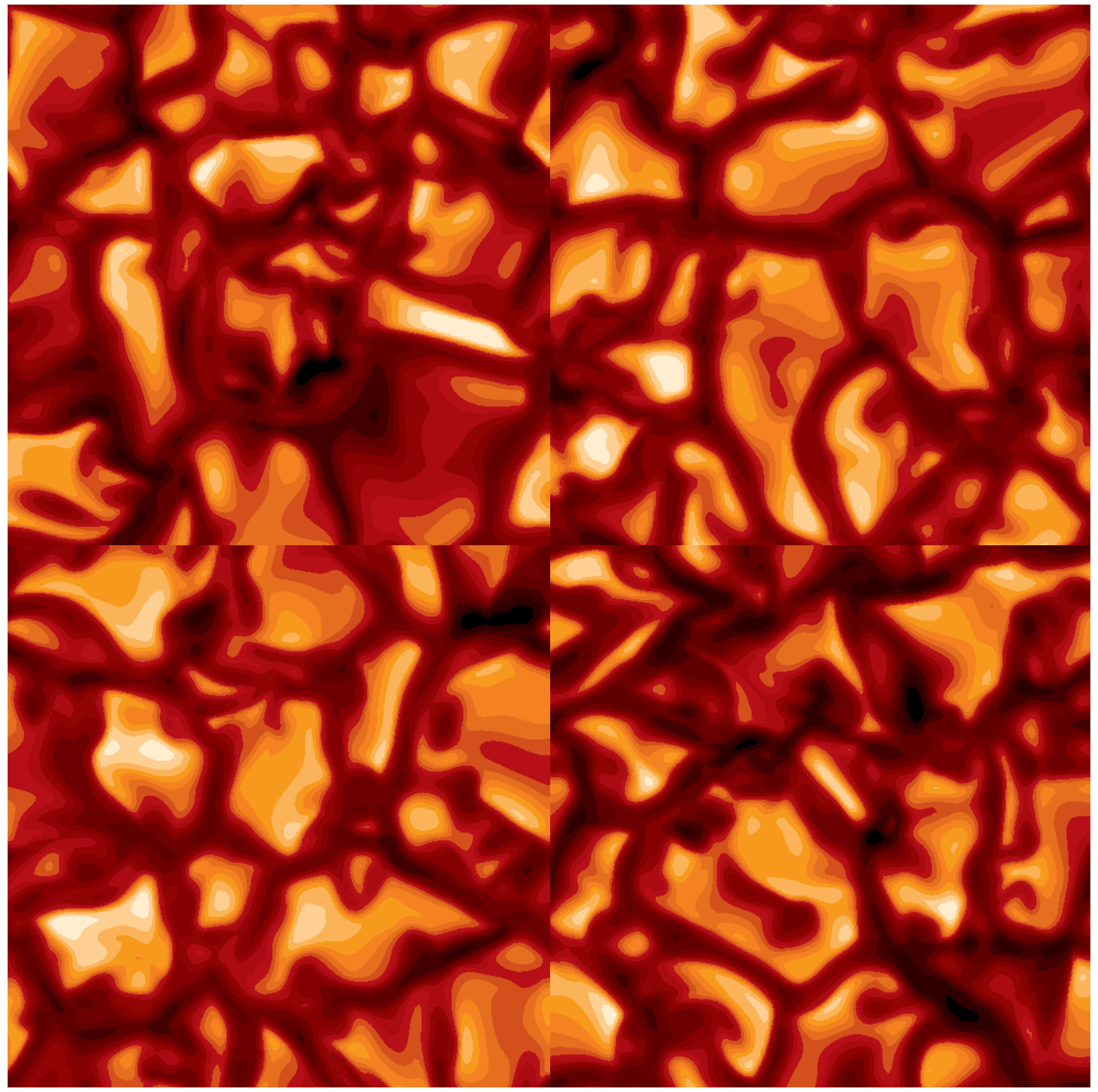
3D modelling

- ✓ Time-dependent dynamic models
- ✓ Intrinsic velocity field (*no more fudge factors*)
- ✗ Limited micro-physics
  - ✗ Opacities are binned

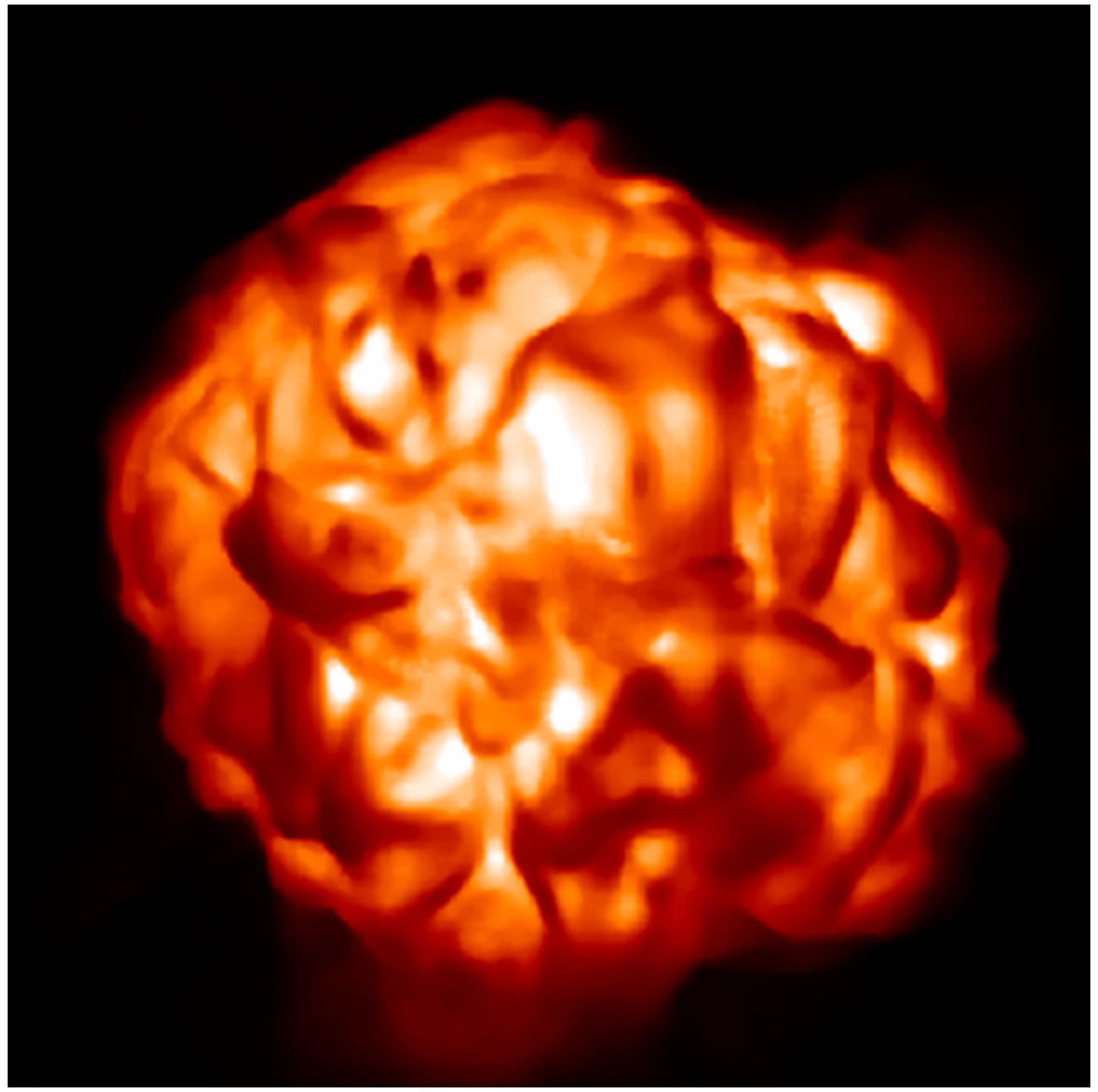
CO5BOLD

COnservative COde for the COmputation of COmpressible COnvection in a BOx of L Dimensions with L=2,3

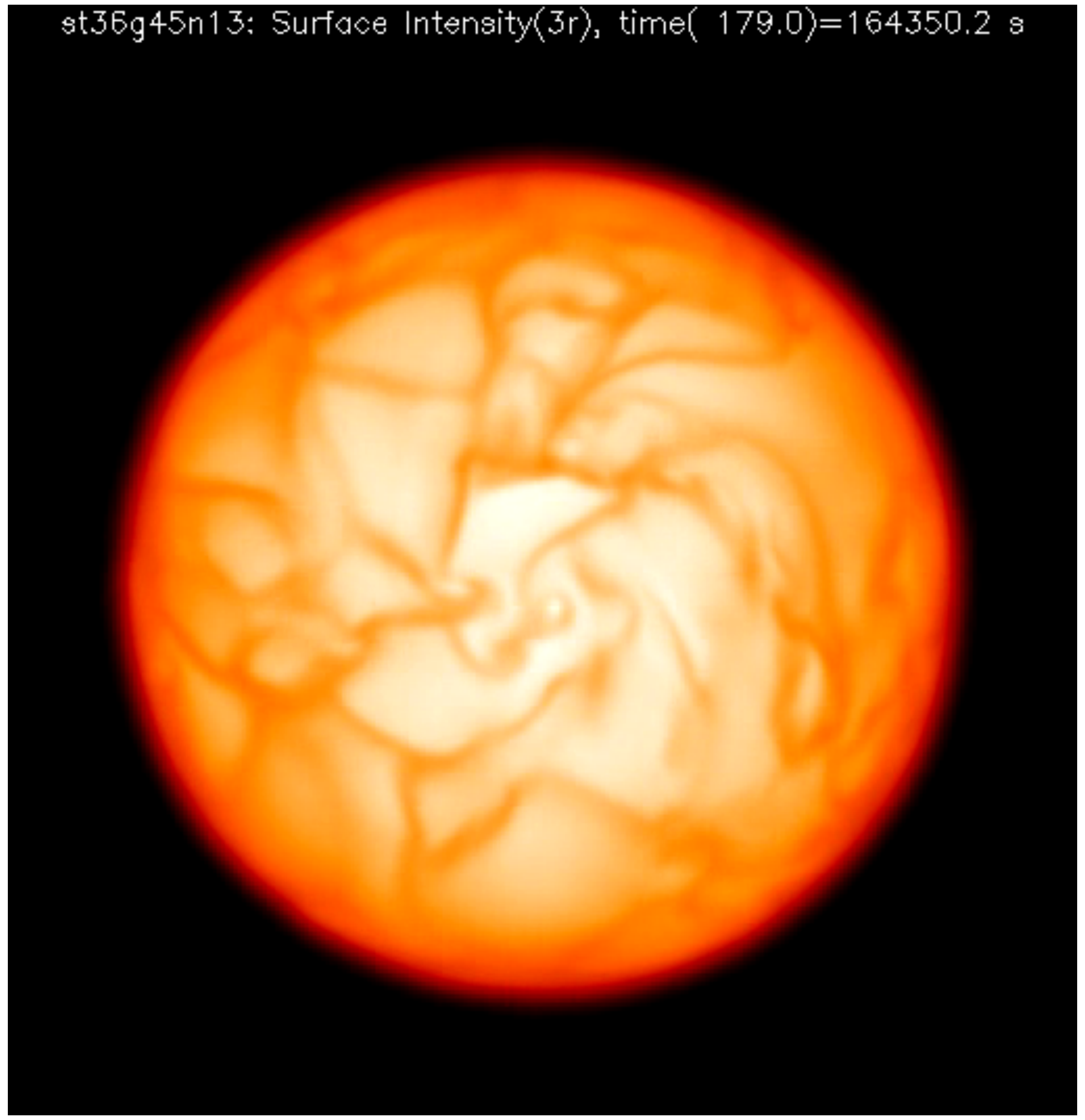
Bernd Freytag, Matthias Steffen, Hans-Günter Ludwig, Sven Wedemeyer, W. Schaffenberger, & Fabio Riva



Local models
(box in a star)



Global models
(star in a box)

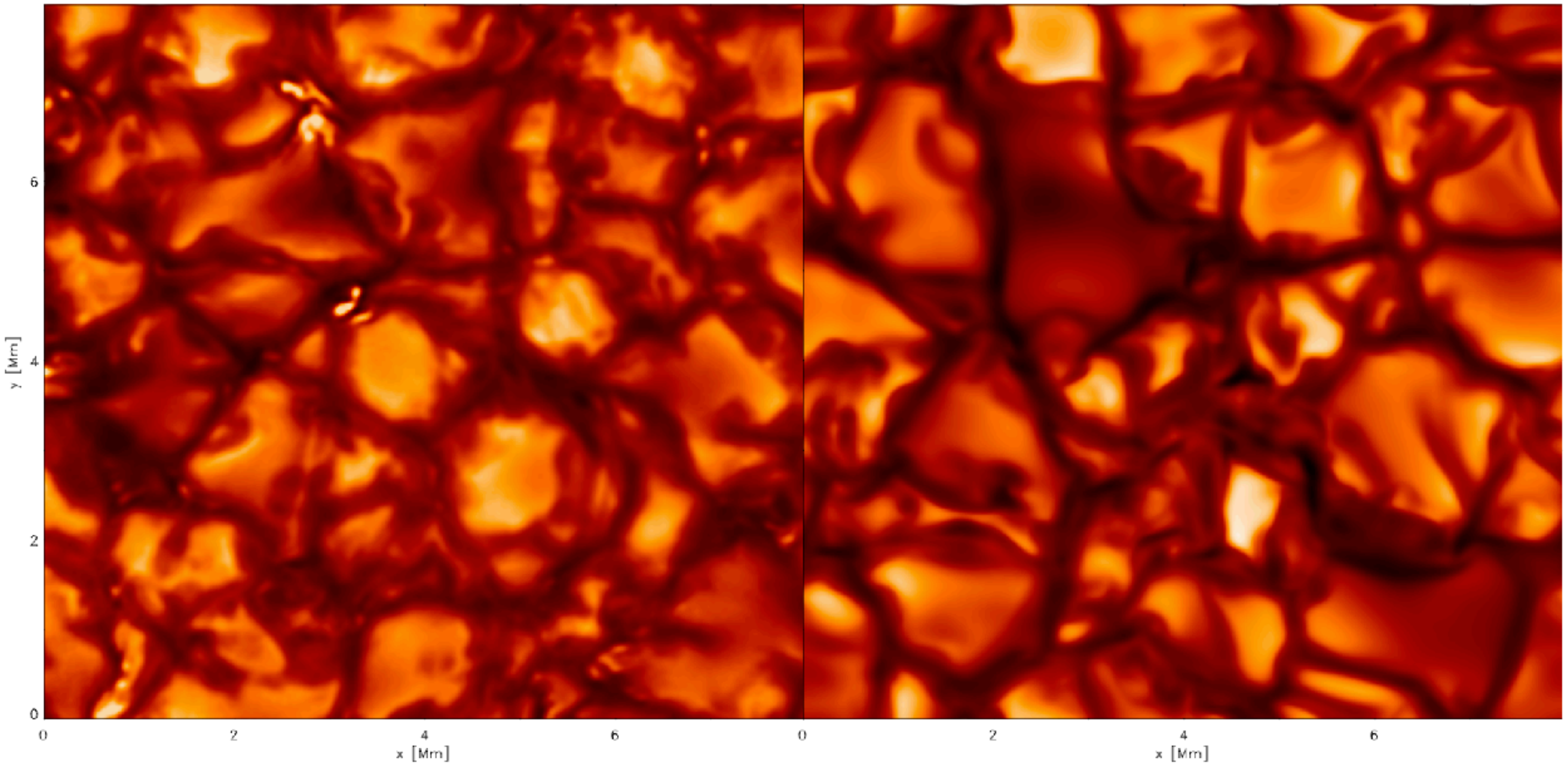


Rotation models
(star in a box)

STAGGER

R. Collet, A. M. Amarsi, M. Asplund, Z. Magick, Åke Nordlund, K. Galsgaard

Swedish Solar Telescope image ($R \approx 25$ km)



STAGGER numerical simulation

Bifrost

B. V. Gudiksen, M. Carlsson, V. H. Hansteen, W. Hayek, J. Leenaarts, & J. Martinez-Sykora

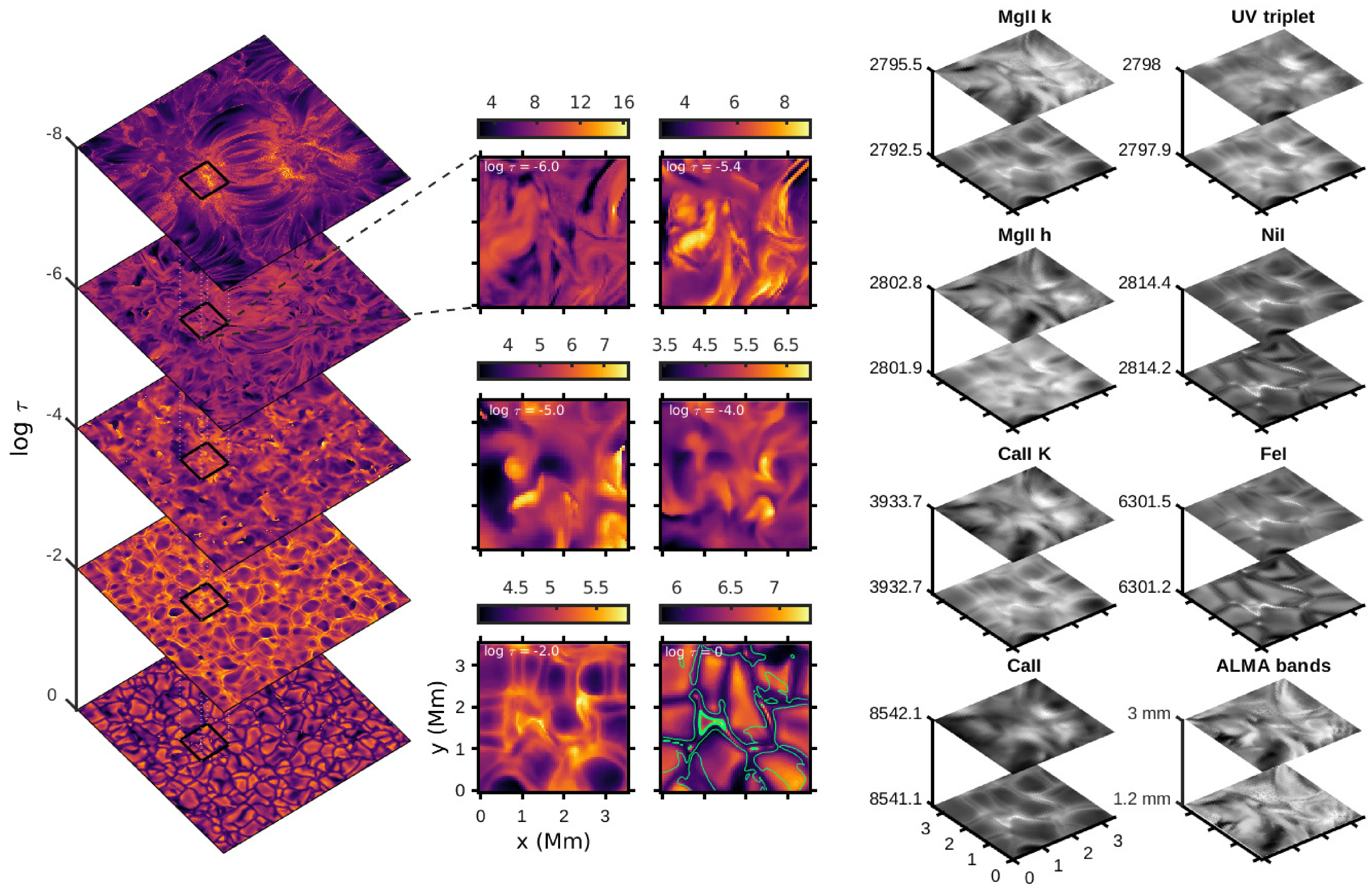


Image from da Silva Santos et al. (2018, A&A, 620, A124)

MURaM

MPS/University of Chicago Radiative MHD

A. Vögler, J. H. M. J. Bruls, M. Schüssler, S. Shelyag, F. Cattaneo, T. Emonet, & T. Linde

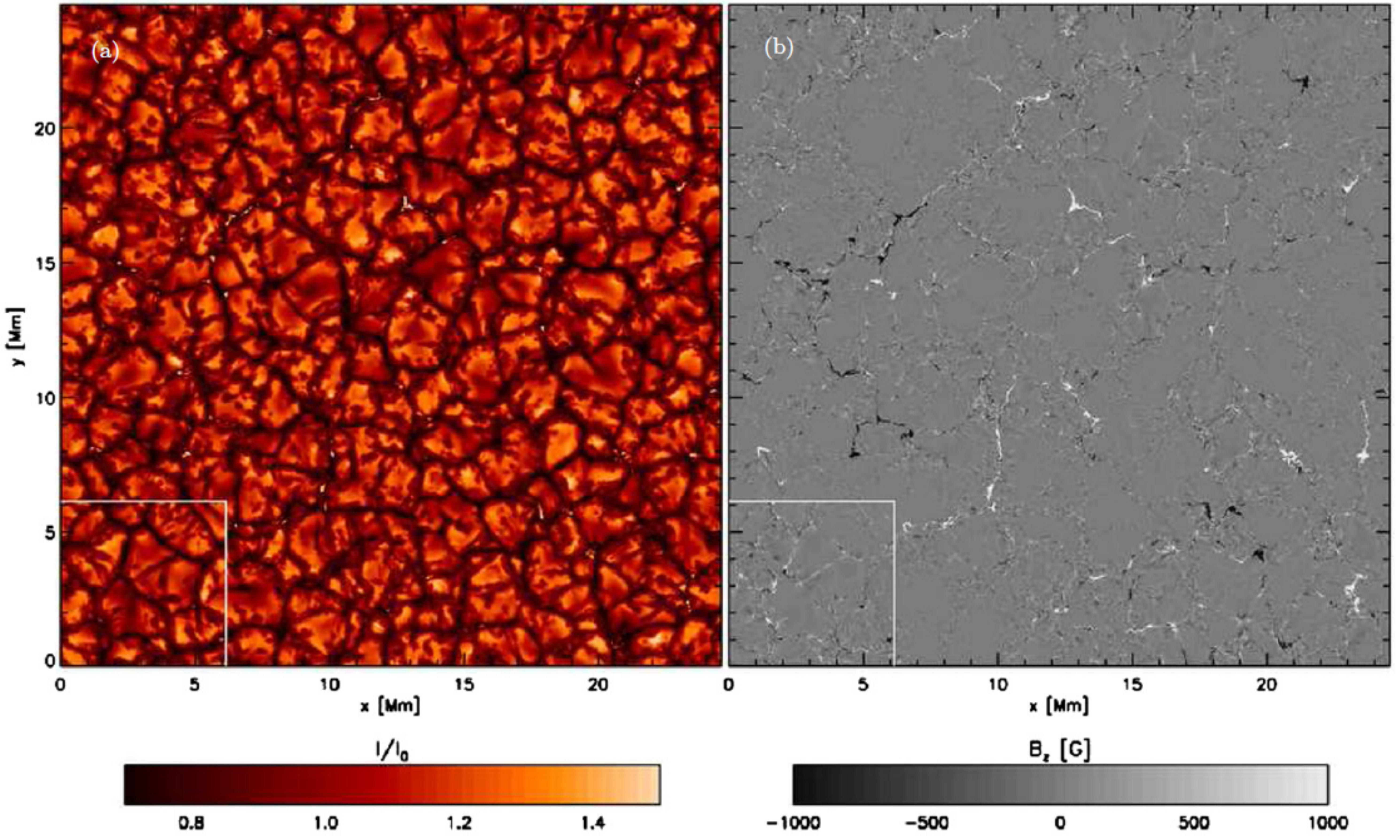


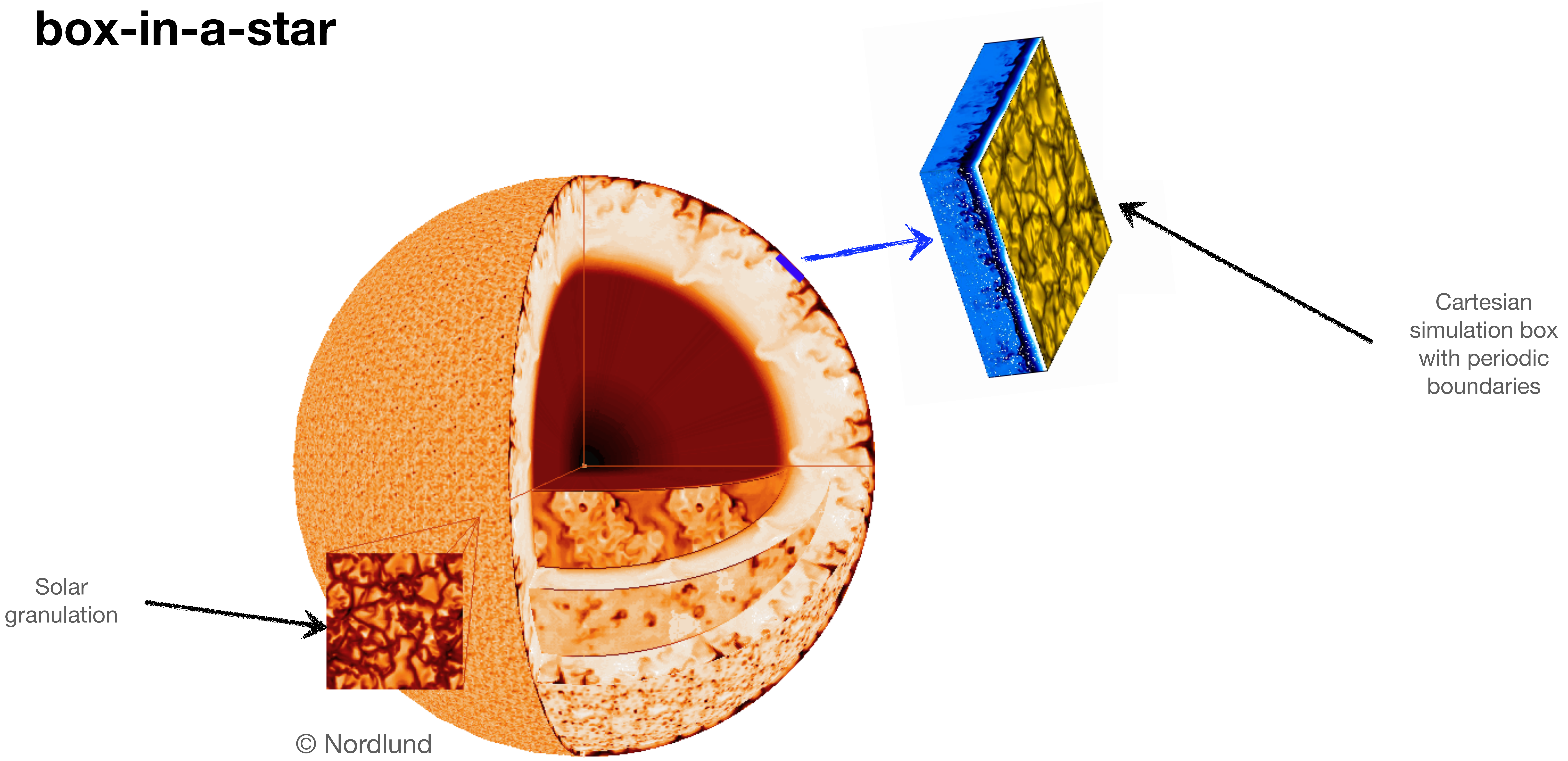
Image from Rempel (2014, ApJ, 789, 132)

What is modelled?

- Solution of the RHD or MHD equations coupled with the radiative transfer equation
- Kinetics & transport for molecules and dust grains; non-equilibrium chemistry
- Result: realistic gas flow and energy transport from sub-photosphere to just below chromosphere
- All codes run box-in-a-star mode. CO5BOLD can also run star-in-a-box
- Bifrost and MURaM also models the chromosphere in extremely high resolution models

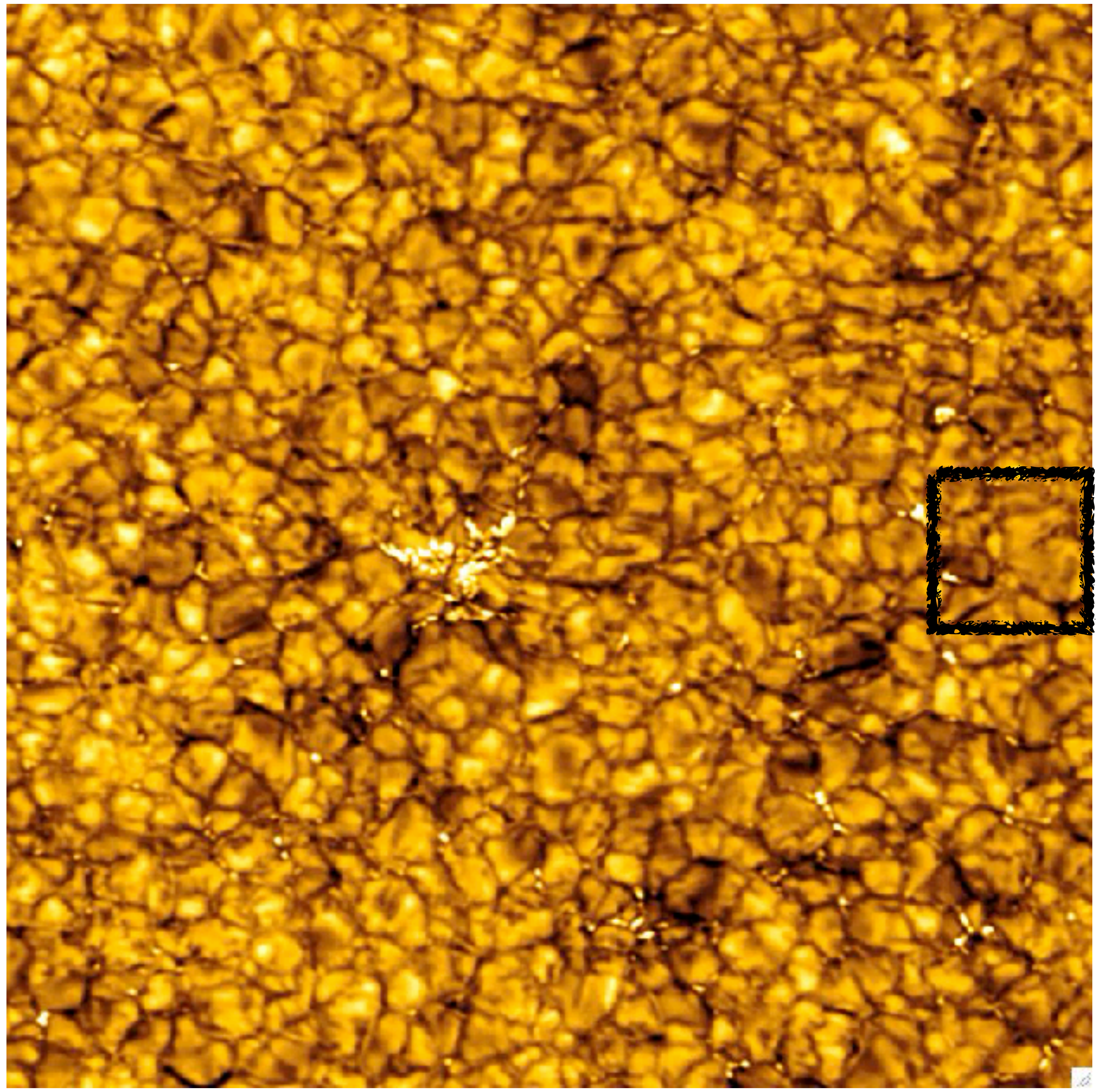
What is modelled?

box-in-a-star

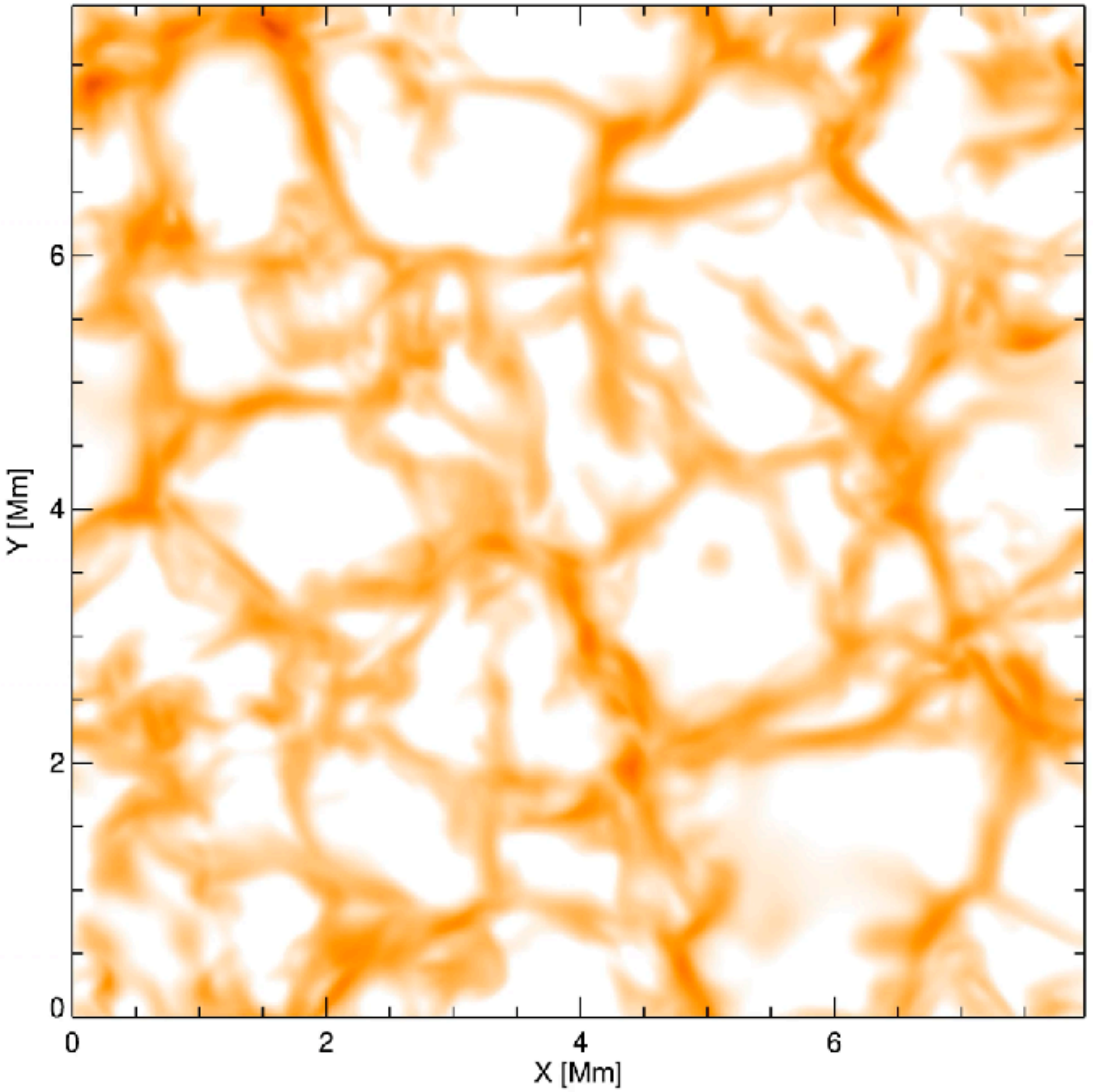


Granulation

2D solar intensity



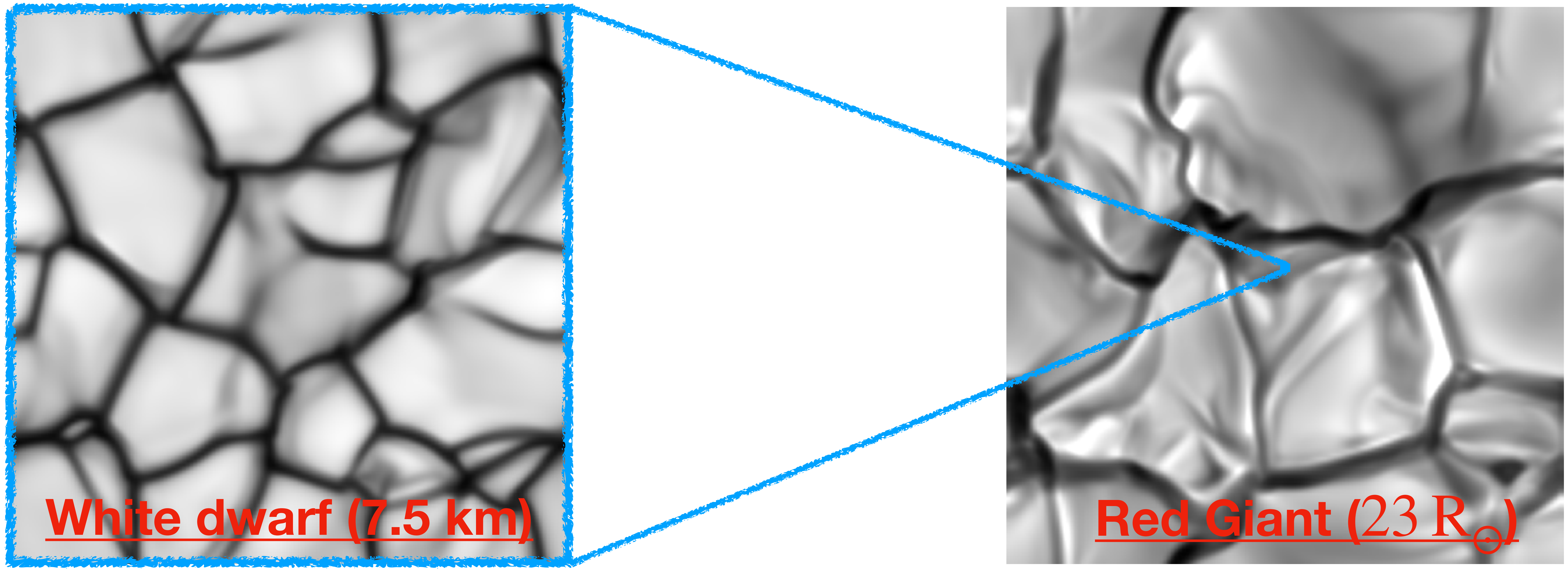
SST quiet Sun



CO5BOLD solar simulation msc600

Granulation

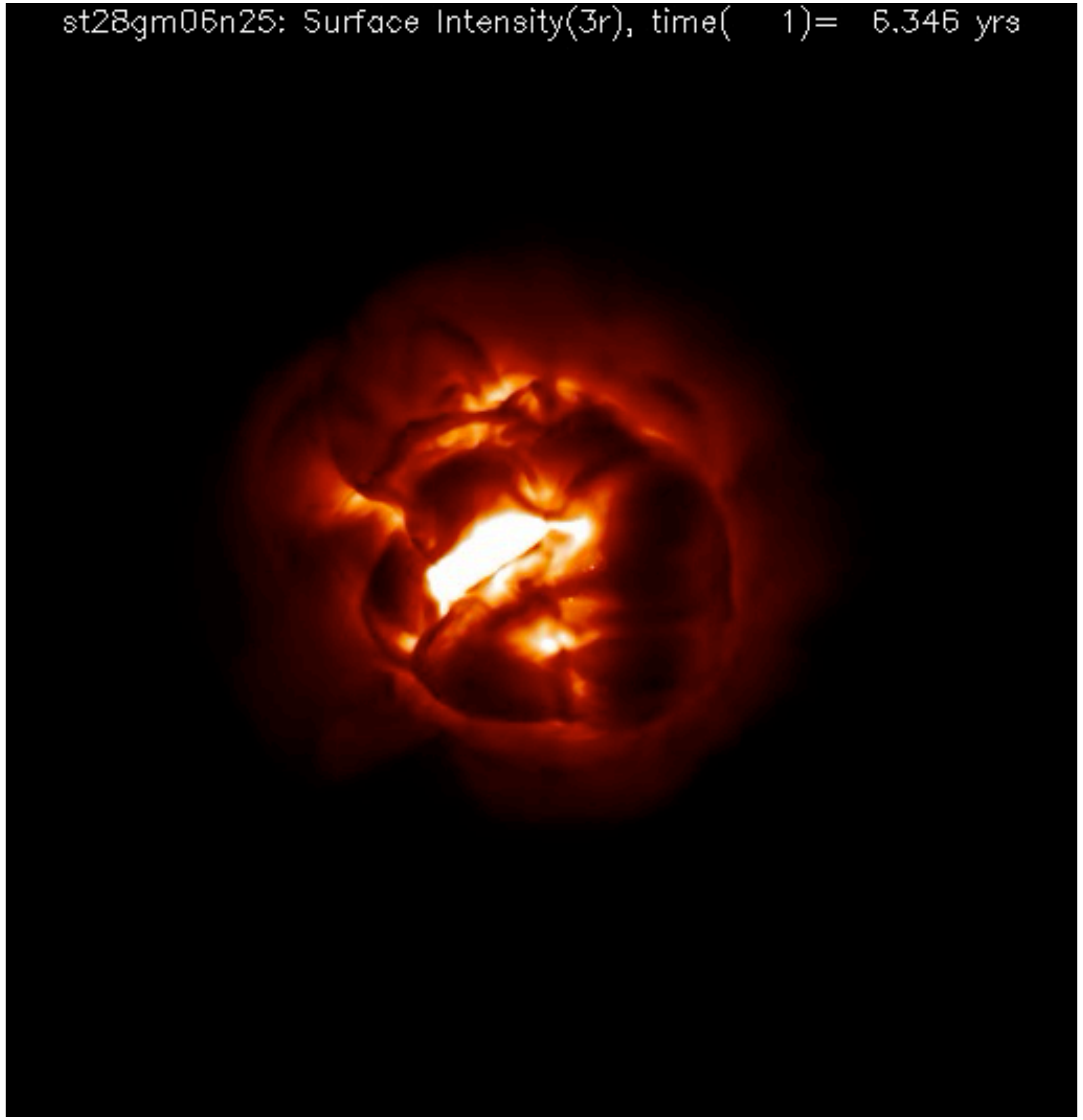
Across the Hertzsprung-Russell diagram



- From the Sun to stars with largely different parameters
  - Robustness!
- Spatial scale ratio in figures: 2×10^6

Granulation

AGB star



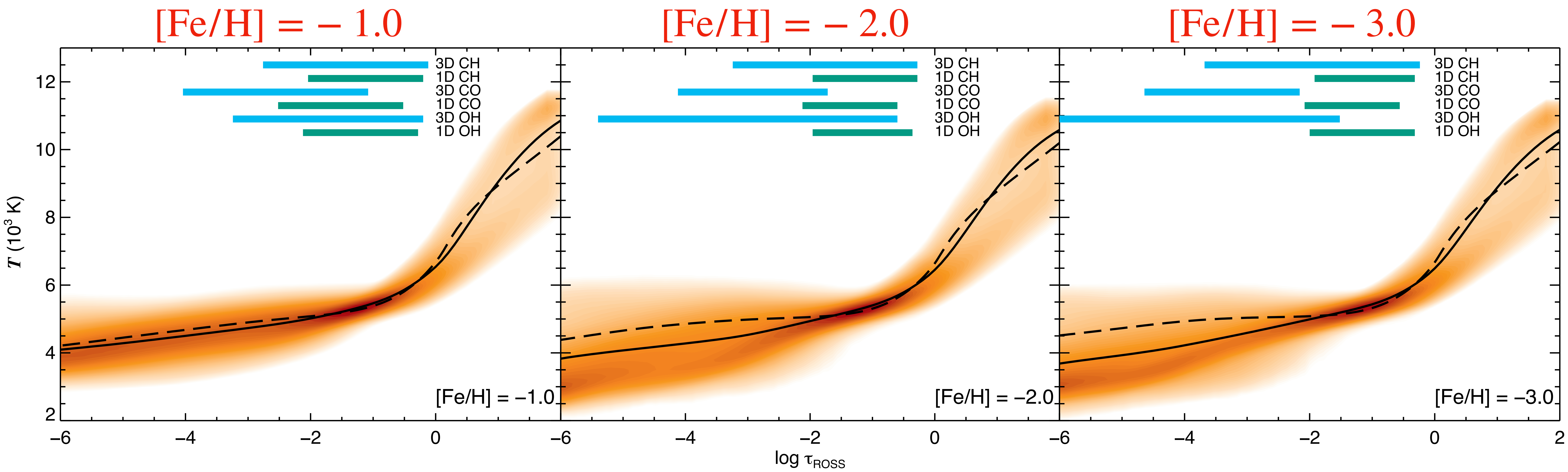
- 3D star-in-a-box simulations of asymptotic giant branch (AGB) star

$$
\begin{aligned}
M &= 1\,\mathrm{M}_\odot \\
L &= 6890\,\mathrm{L}_\odot \\
T_{\mathrm{eff}} &= 2727\,\mathrm{K} \\
\log g &= -0.6 \\
[\mathrm{M/H}] &= 0.0
\end{aligned}
$$

- Models the interior and inner atmosphere
- Variability of AGB stars through self-excited pulsations

Bernd Freytag: https://www.astro.uu.se/~bf/movie/AGBmovie.html

The 3D temperature structure

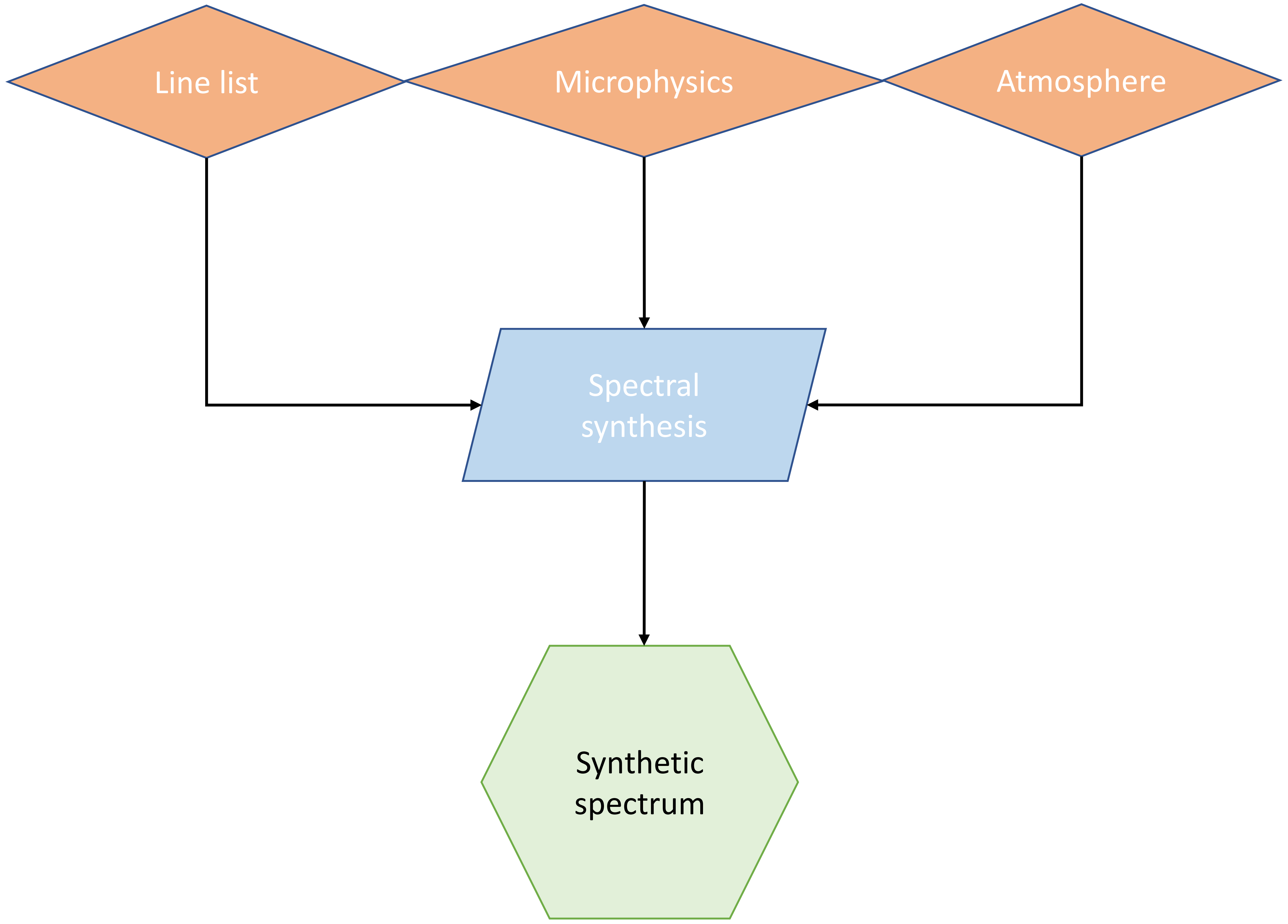


Gallagher et al. (2016)

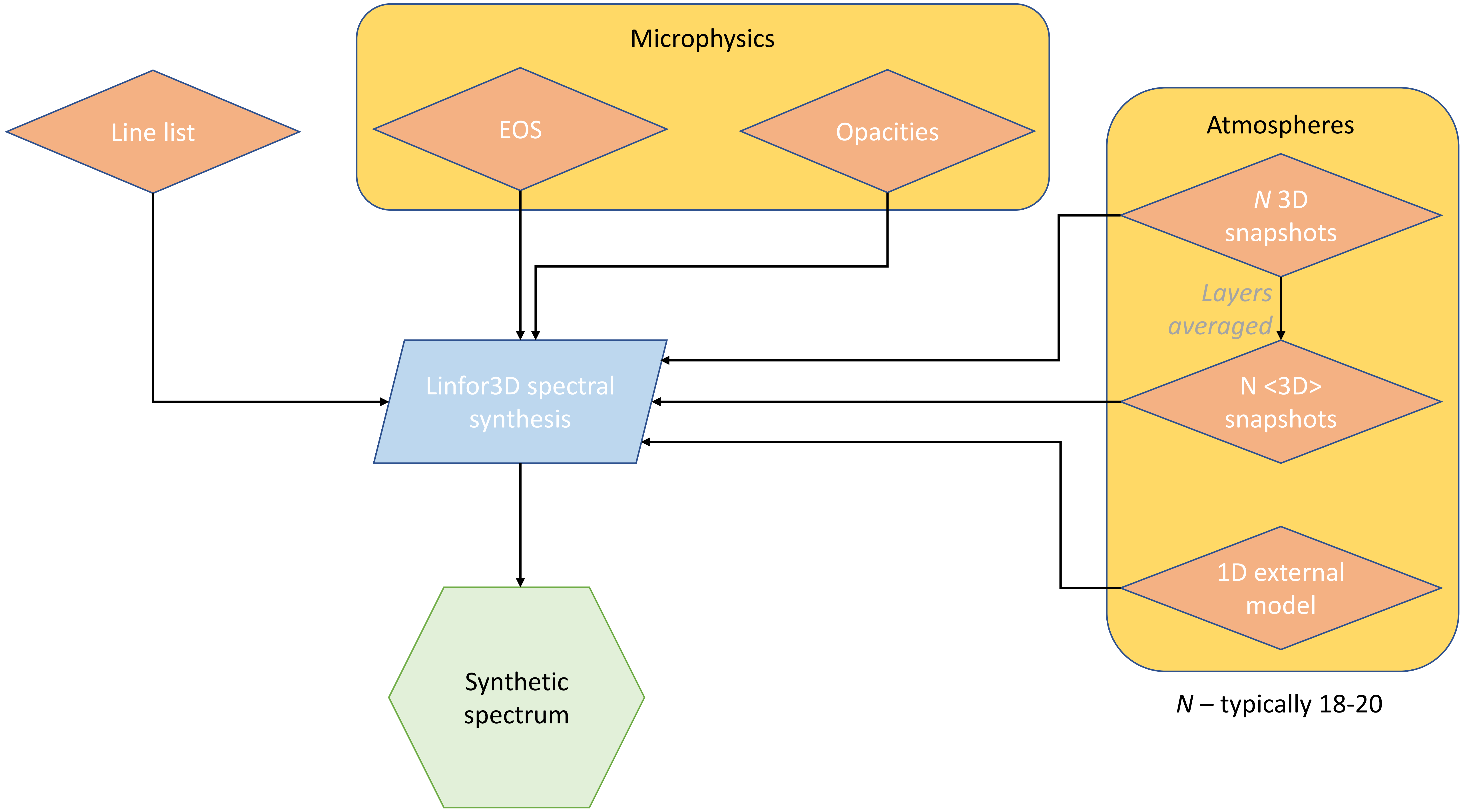
- Dashed lines: 1D LHD model
    - A 1D model computed using the same micro-physics as the 3D model
- Solid lines: <3D> model
    - A 1D model computed by spatially averaging 3D thermal structures over surfaces of equal optical depth
- 2D histogram: 3D model

3D spectrum synthesis

1D LTE spectral synthesis



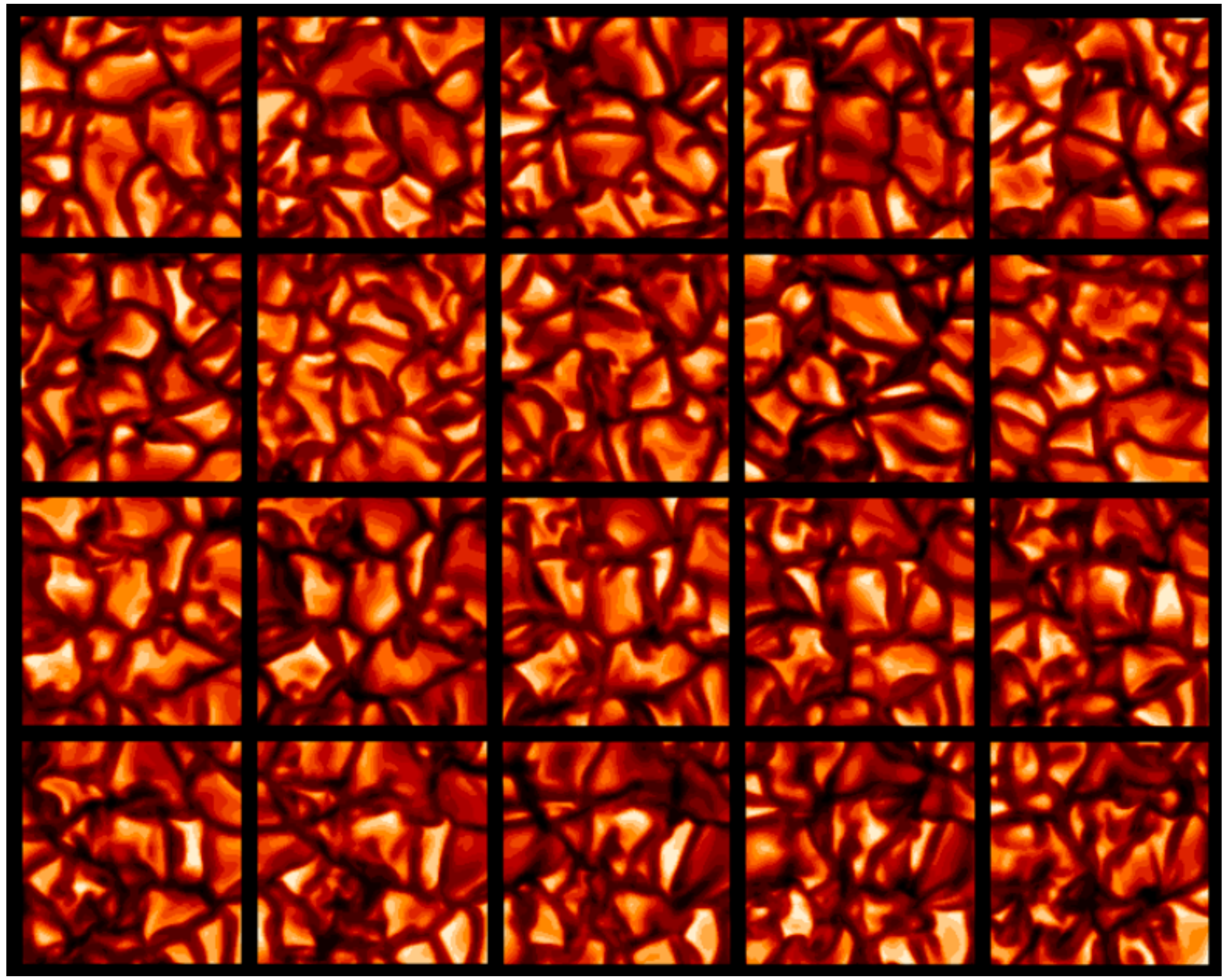
3D LTE spectral synthesis



Granulation

Ergodic approximation

- Assume that averaging over time equivalent to averaging over area
- CO5BOLD outputs computational boxes at regular instances in time (snapshots)
- Stellar disk resolved by computing *N* snapshots

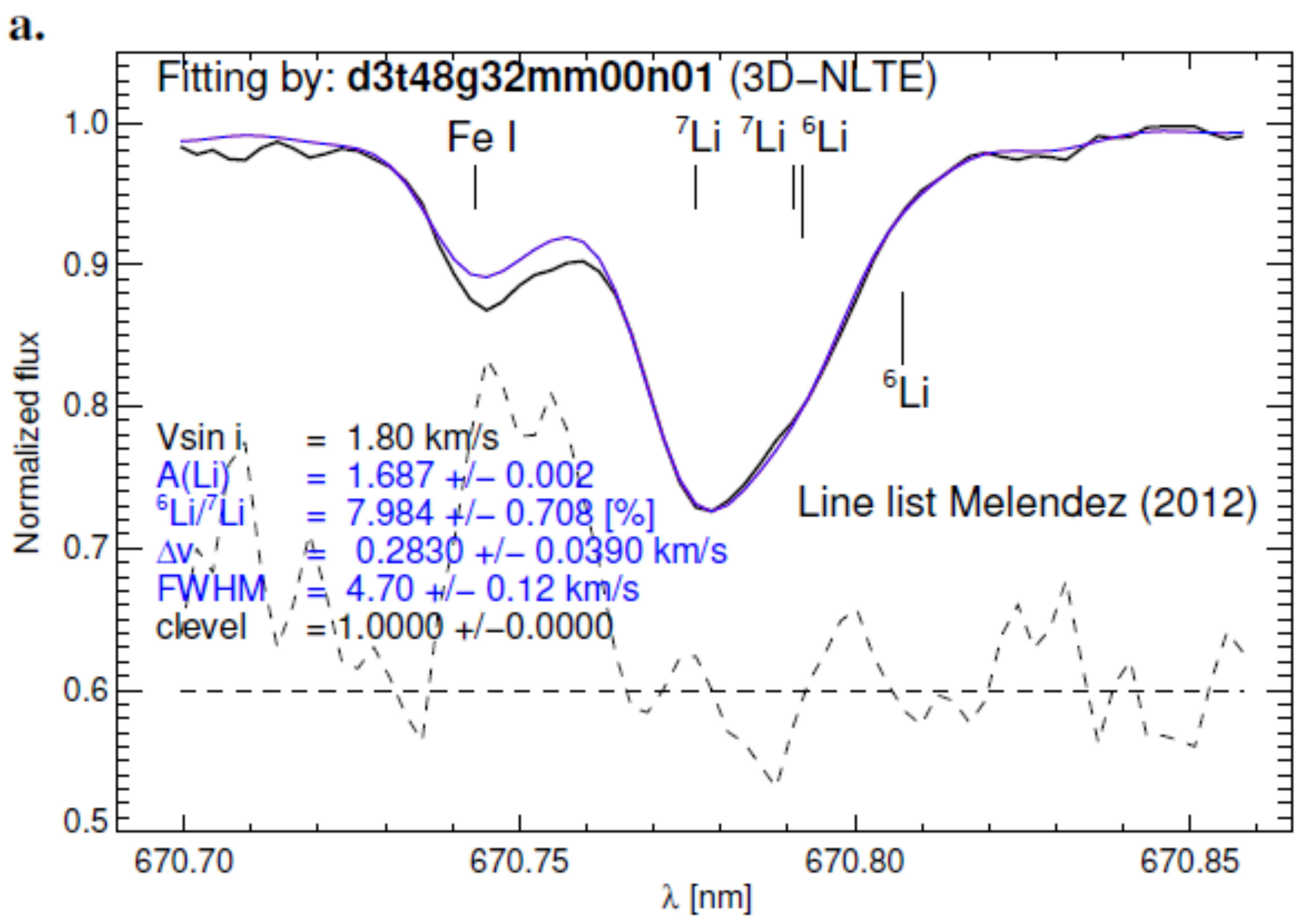


3D spectral synthesis codes

- Linfor3D *(private)*
  Steffen et al. (2023, Manual)
  3D CO5BOLD & STAGGER model atmospheres
  LTE/NLTE (with departures)
  MPI parallelised (fast)

- Optim3D *(private)*
  Chiavassa et al (2009)
  3D local and global CO5BOLD models
  LTE

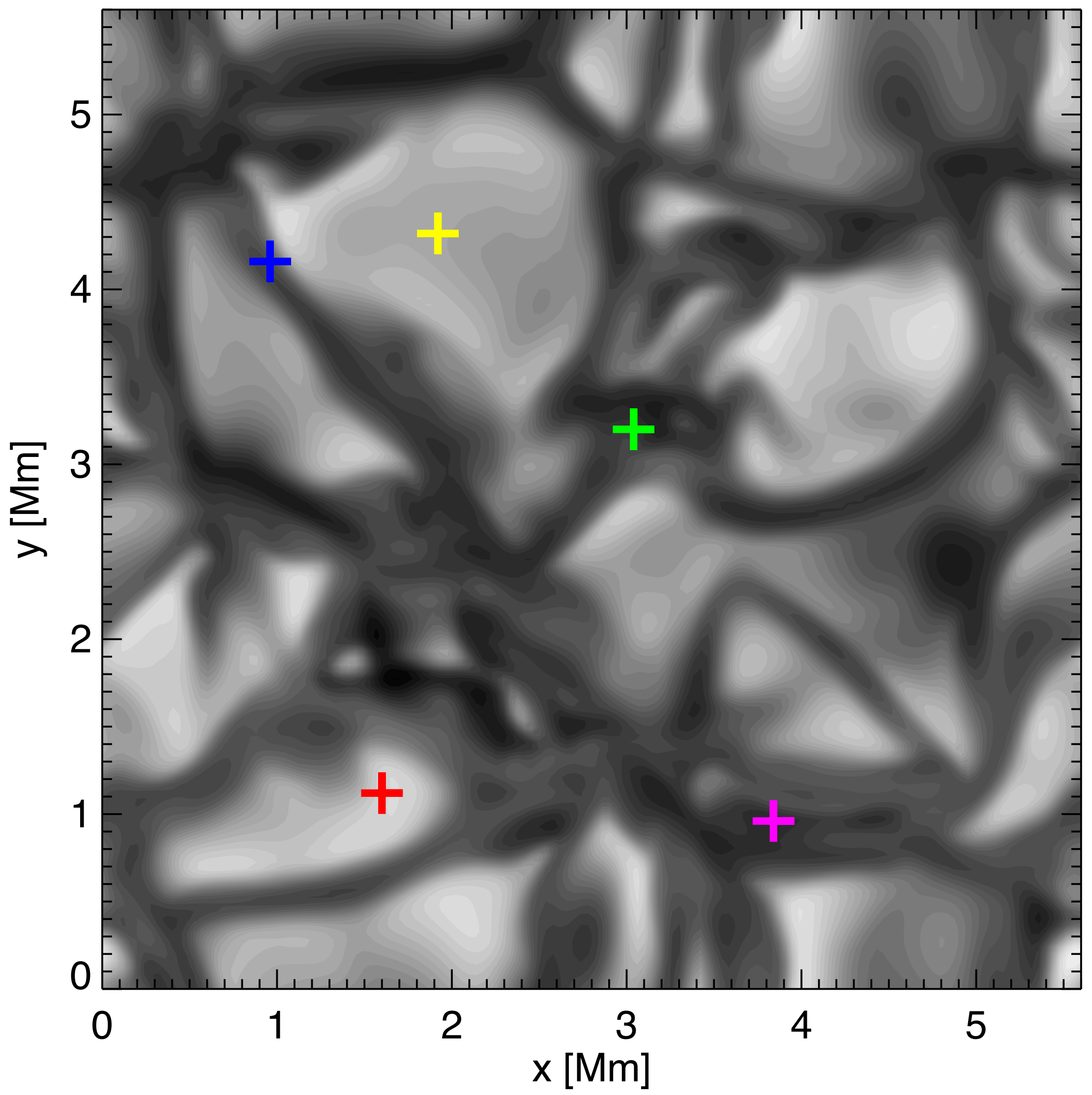
- SCATE *(private)*
  Hayek et al. (2011)
  3D STAGGER models
  LTE

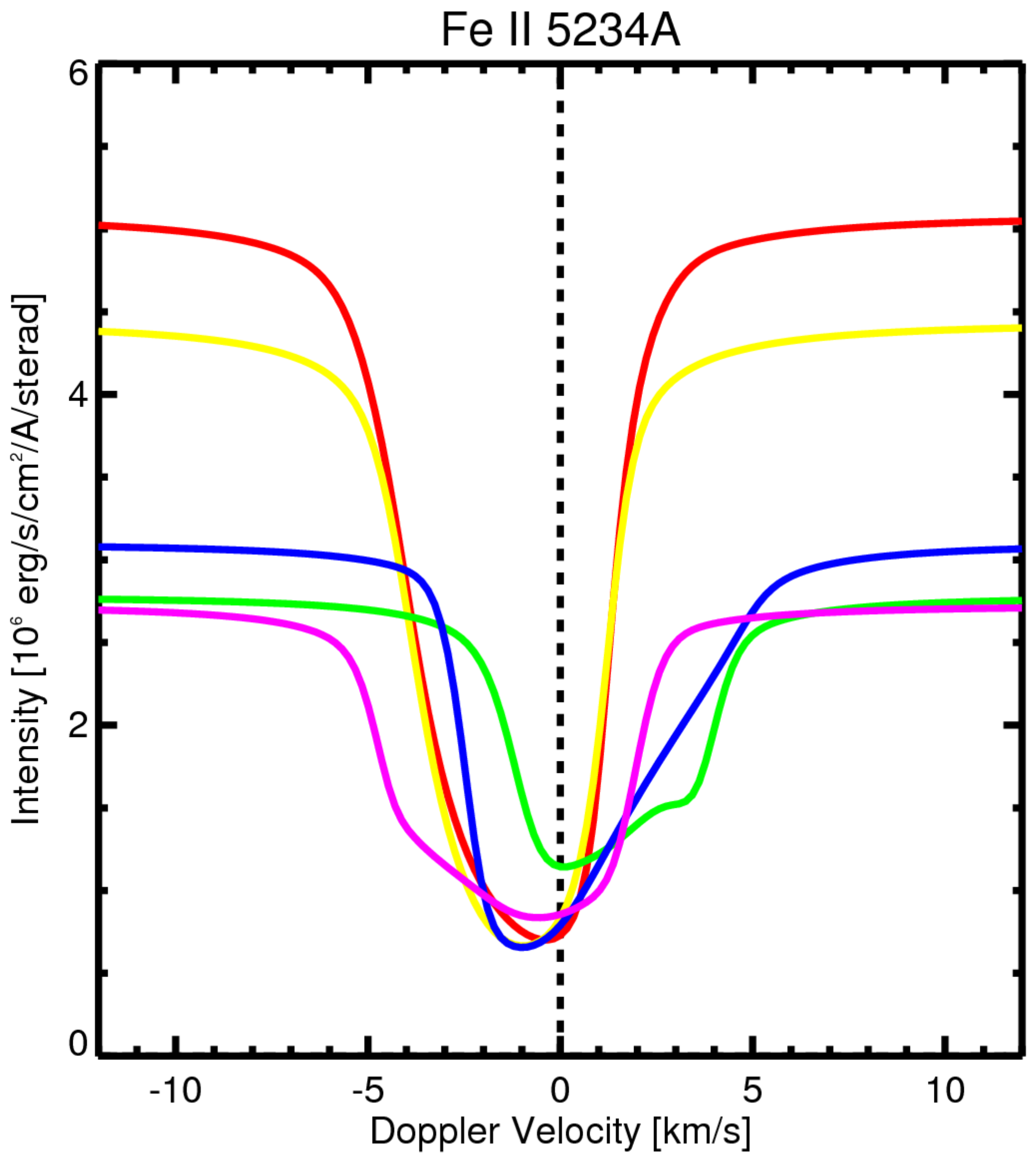


Mott et al. (2017)

3D spectrum synthesis
Asymmetries and wavelength shift

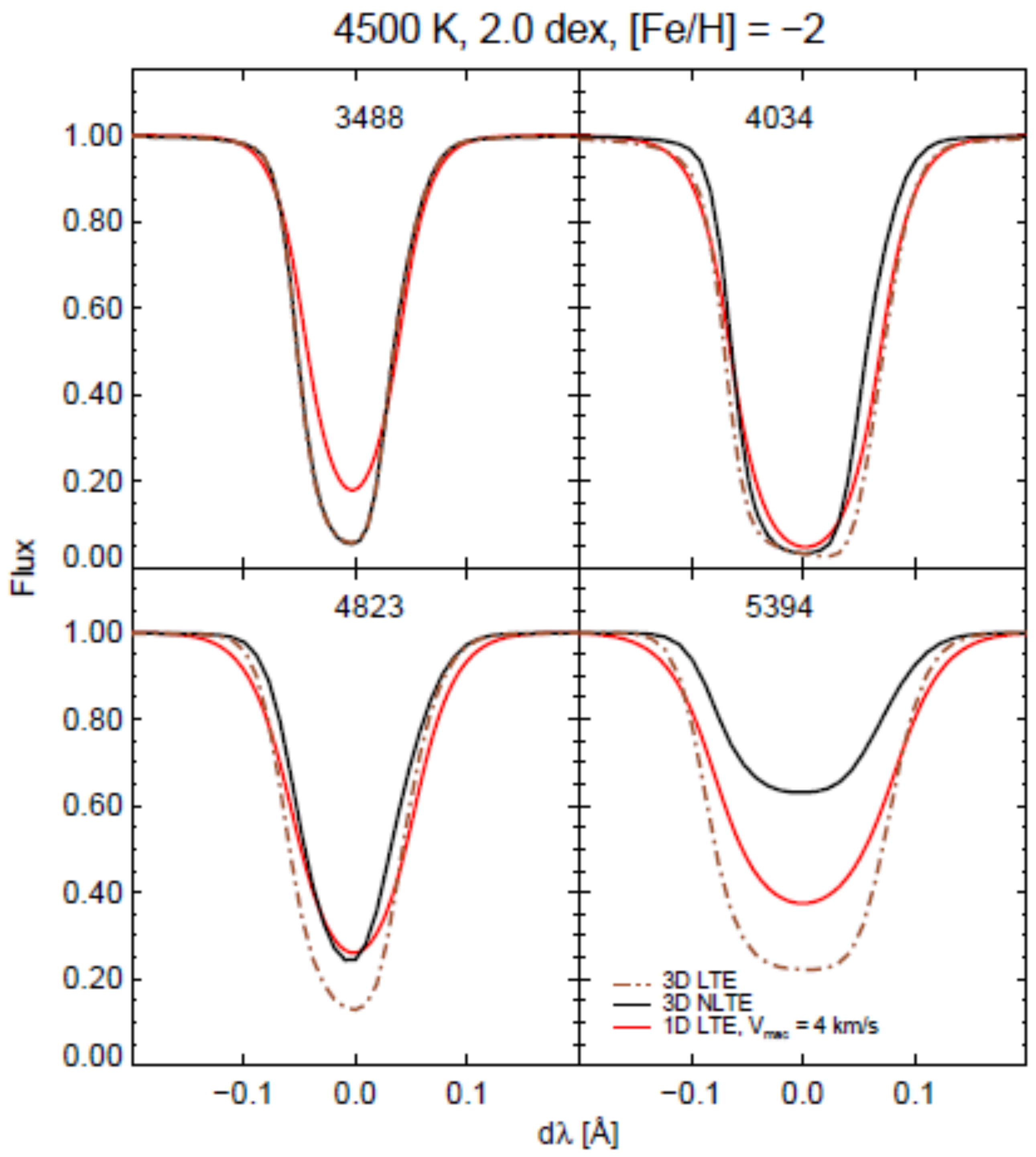
- Variations in line strength, width, shift, asymmetry across granulation pattern
- Non-linearities cause net effects in disk-integrated light
- Knowledge of detailed line shapes means no ad-hock “fudge factors” (ξ_{mic} and ξ_{mac})



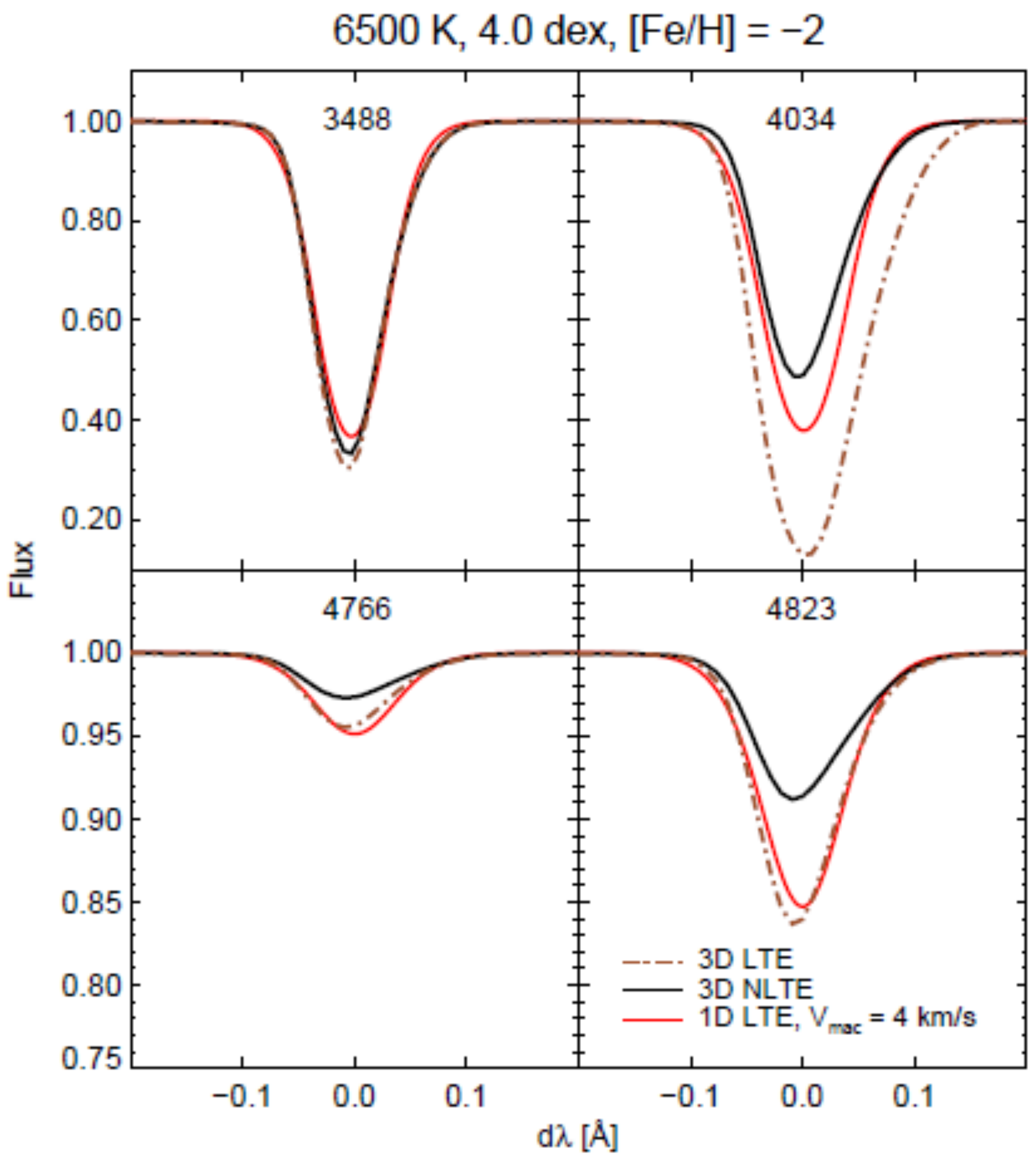


3D convective line shifts and asymmetries

Due to 3D velocity fields

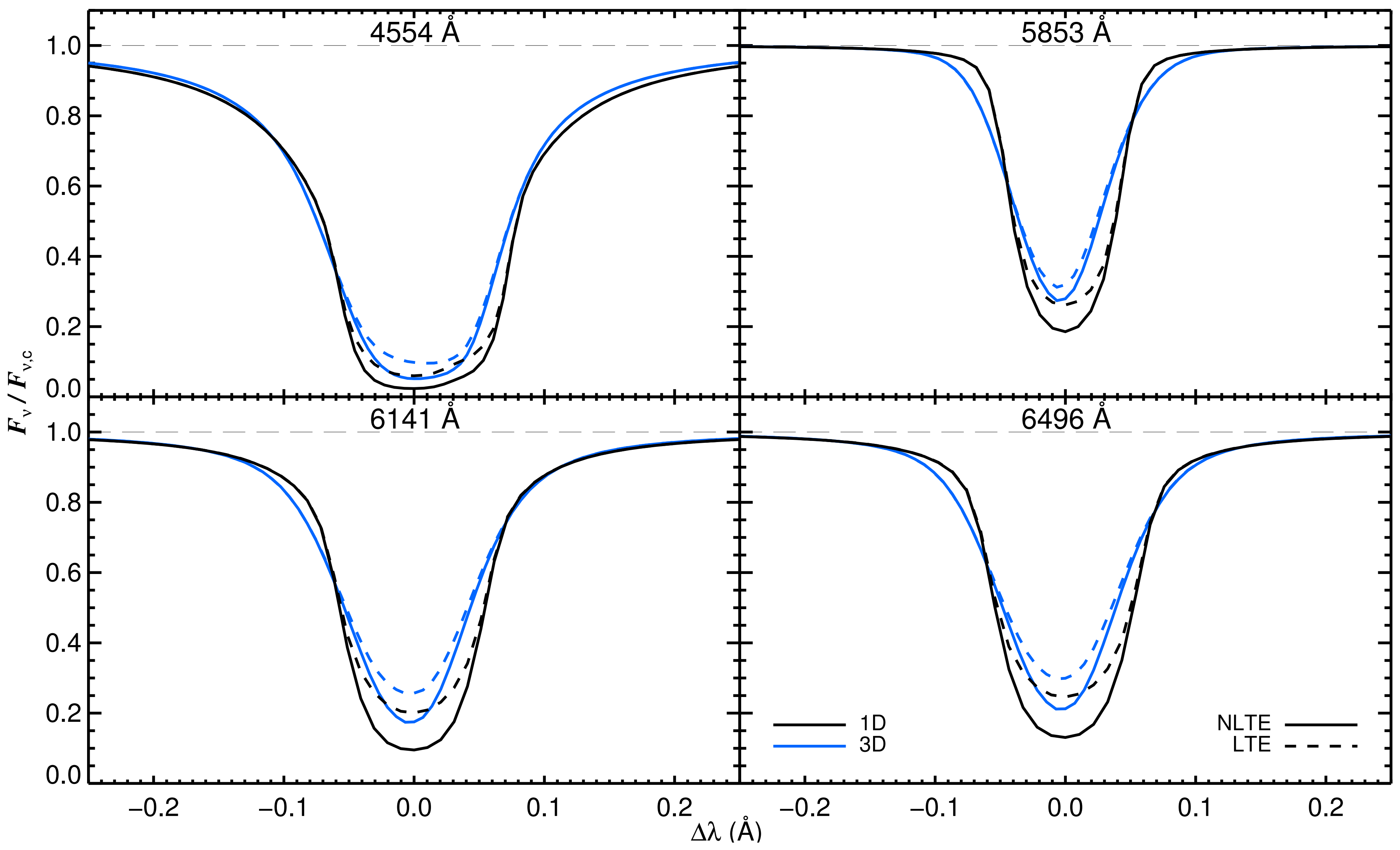


Metal-poor giant



Metal-poor dwarf

Manganese lines: Bergemann et al. (2019)



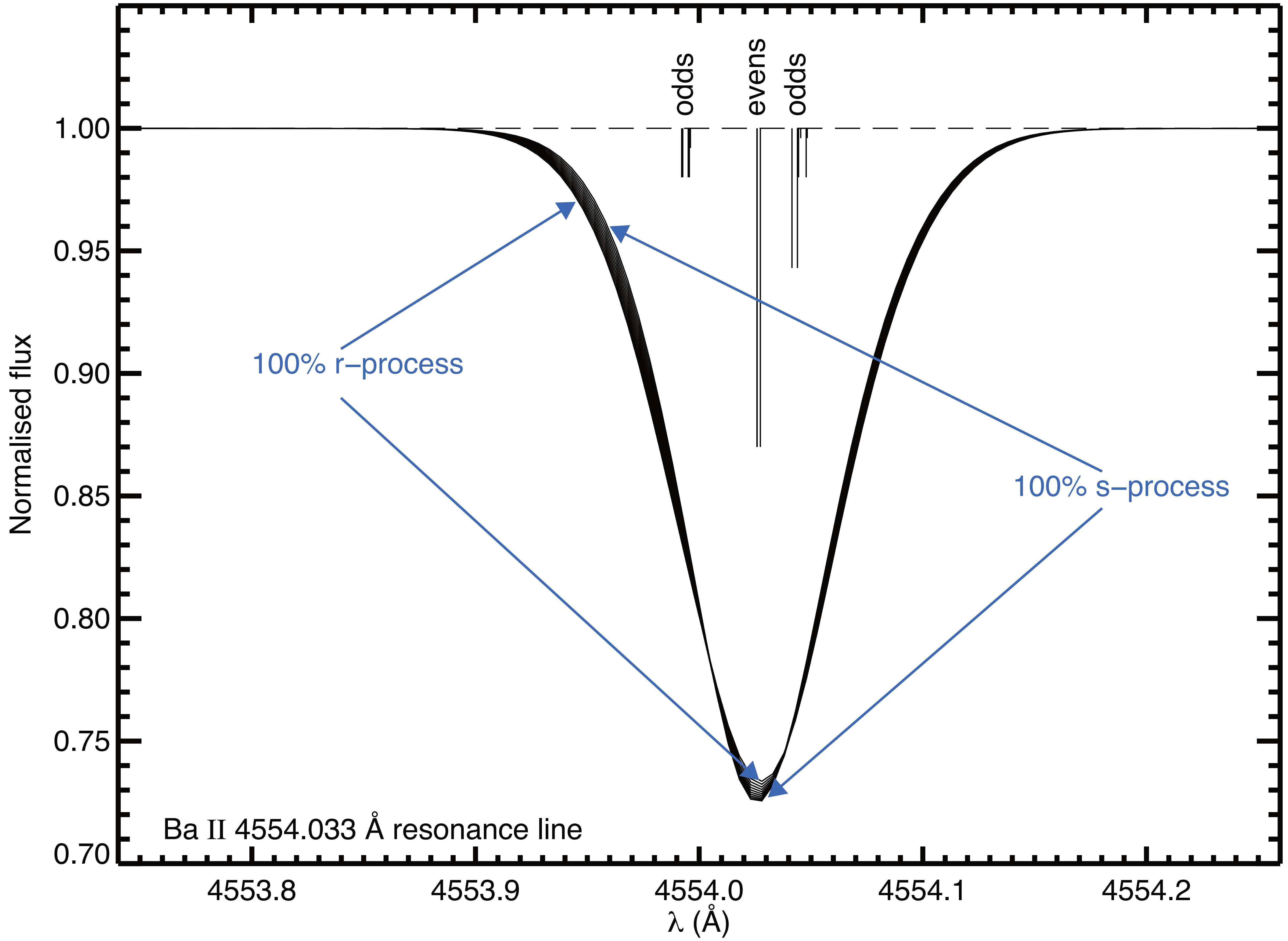
Barium lines in the Sun

Gallagher et al. (2020)

Isotopes

Barium resonance line

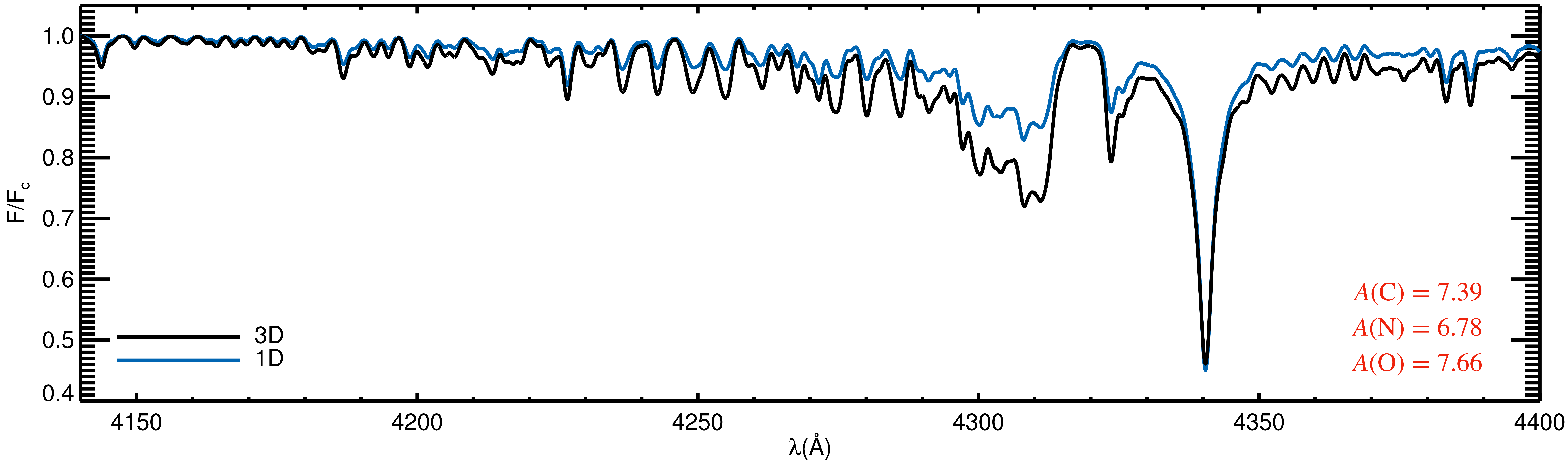
- Measuring line profiles leads to isotopic fraction measurement
- Shallower, broader lines are more r-process
- Deeper, narrower lines are more s-process



Molecular bands

3D LTE spectral synthesis

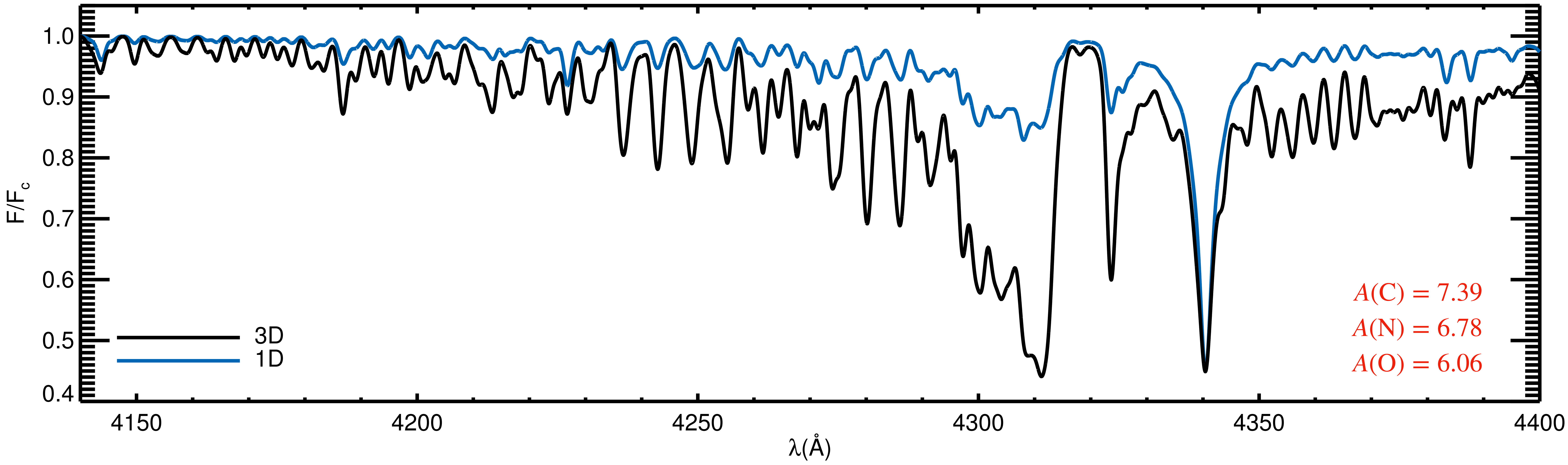
$$T_{\mathrm{eff}} = 6250\,\mathrm{K},\ \log g = 4.0,\ [\mathrm{Fe/H}] = -3.0,\ \mathrm{C/O} = 0.54$$



Molecular bands

3D LTE spectral synthesis

$$T_{\rm eff} = 6250\,{\rm K},\;\; \log g = 4.0,\; [{\rm Fe/H}] = -3.0,\; {\rm C/O} = 21.04$$



Non-LTE radiative transfer

LTE radiative transfer

LTE can be characterised by the following:

- The Boltzmann excitation distribution

$$\frac{n_i}{N_I} = \frac{g_i}{U_I} e^{-E_i/kT}$$

- The Saha ionisation distribution

$$\frac{N_I}{N_{I+1}} = n_e \frac{U_I}{U_{I+1}} \left(\frac{h^2}{2\pi m_e kT} \right) e^{\chi_I/kt}$$

- The Maxwellian velocity distribution of particles

$$f(v)dv = \left(\frac{m}{2\pi kT} \right)^{3/2} e^{mv^2/2kT} 4\pi v^2 dv$$

- all determined to solve …

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

The radiative transfer equation

LTE radiative transfer

LTE can be characterised by the following:

- Atomic processes $i \to j$ are in *detailed balance* with processes $j \to i$
- Collisions between particles are high, maintaining LTE
  collisional processes, C_{ij} & C_{ji}, dominate over radiative processes, R_{ij} & R_{ji}
- In ***very simple*** terms, the source function, S_ν, is equal to the Planck function (with no scattering)

$$S_\nu = B_\nu(T) \equiv \frac{2h\nu^3}{c^2}\frac{1}{e^{h\nu/kT} - 1}$$

$$\boxed{\mu\frac{\mathrm{d}I_\nu}{\mathrm{d}\tau_\nu} = B_\nu - I_\nu}$$

Non-LTE radiative transfer

Radiation escapes from a star, so LTE must break down

- Radiative rates of some transition dominate over collisional rates
- Radiation no longer follows a Planckian distribution

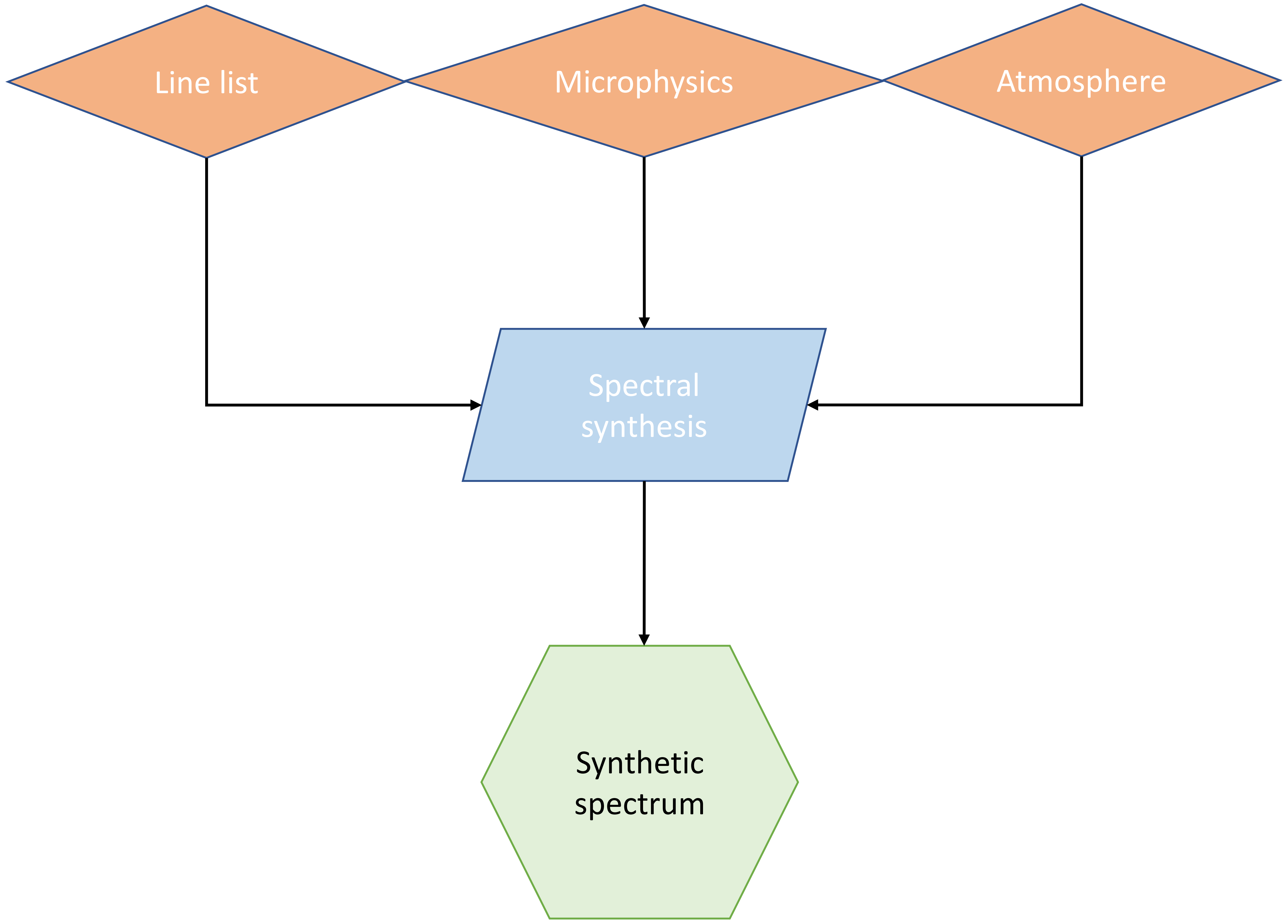
$$\therefore S_\nu \neq B_\nu(T);\;\; S_\nu = \frac{j_\nu}{k_\nu}$$

- Collisional rates are proportional to particle density; low densities → non-LTE
- Saha-Boltzmann distributions no longer determine level/excitation populations

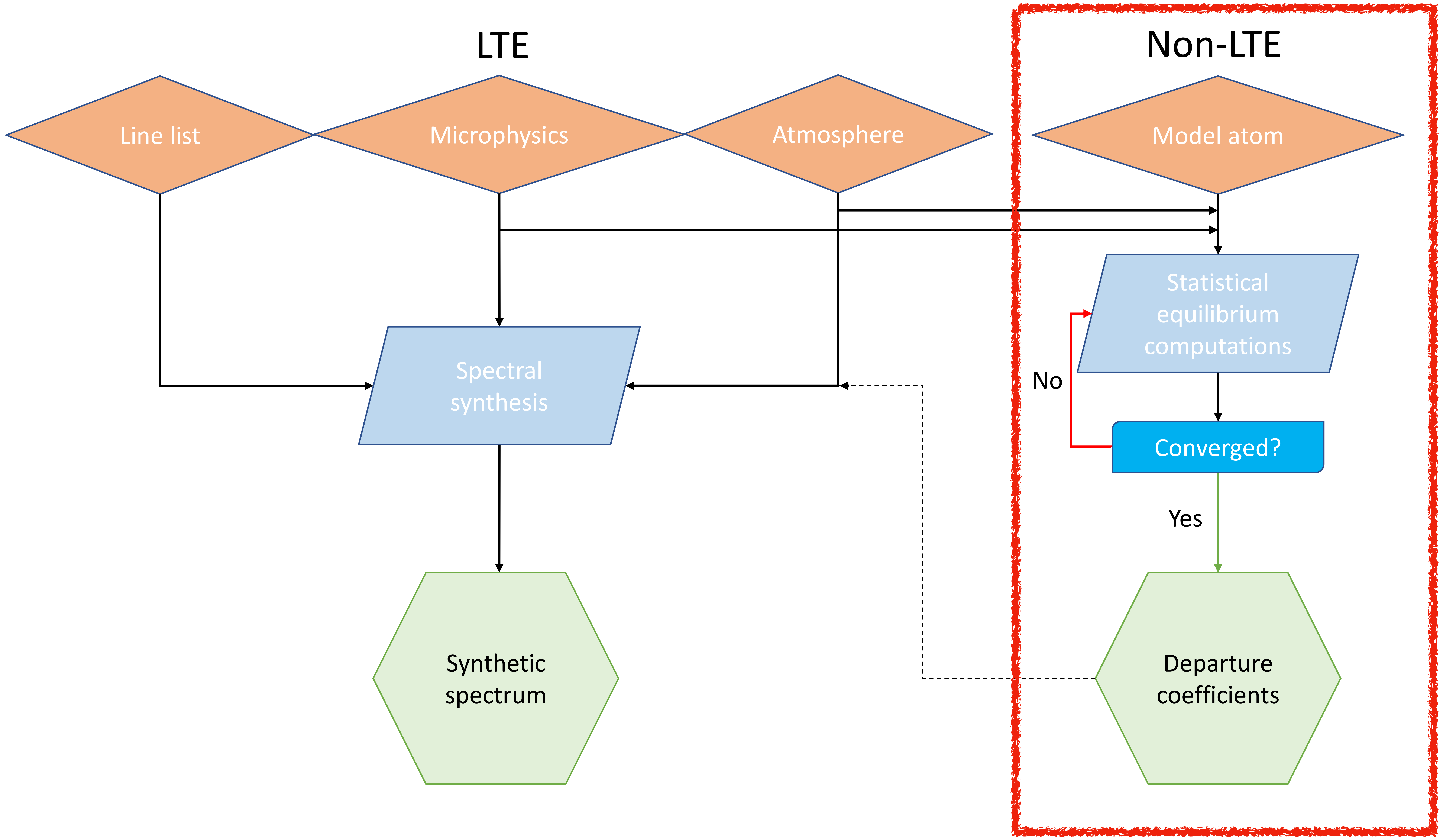
Kinetic equilibrium / Rate equation

$$n_i \sum_{j \neq i}^{NL} \left(R_{ij} + C_{ij}\right) = \sum_{j \neq i}^{NL} n_j \left(R_{ji} + C_{ji}\right)$$

LTE spectral synthesis



Non-LTE spectral synthesis



Statistical equilibrium

Statistical equilibrium

Codes on the "market"

- **MULTI** (public)
  1D code with a 3D wrapper
  Carlsson (1986)
  1D NLTE spectrum synthesis

- **DETAIL** (private)
  1D code
  Butler & Giddings (1985)

- **Multi3D** (private)
  3D / 1.5D code
  Leernaarts & Carlsson (2009)
  3D / 1.5D spectrum synthesis

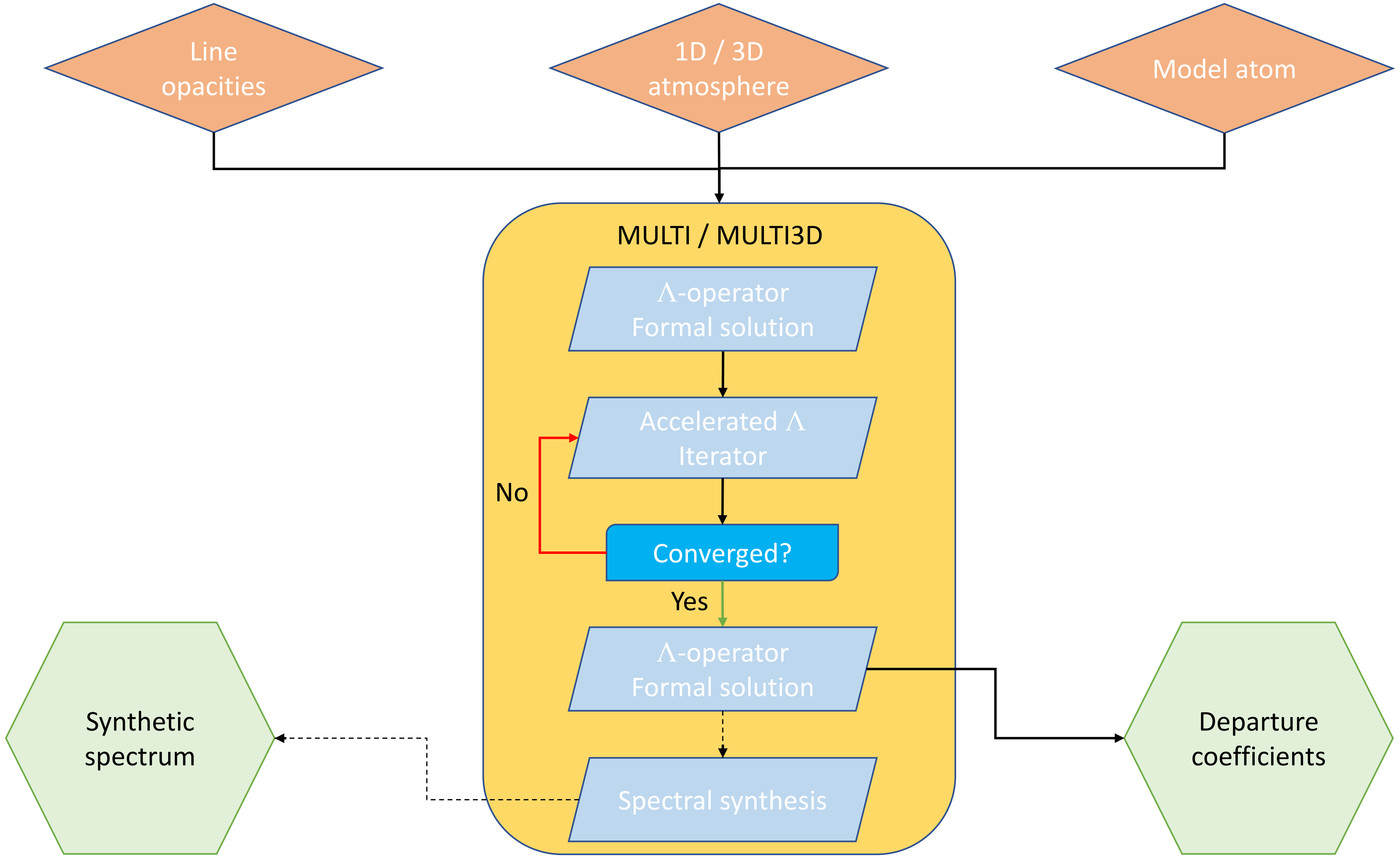
- **Balder** (private)
  3D / 1.5D code (based on Multi3D)
  Amarsi et al. (2016)
  Computes 3D / 1.5D spectral region

- **NLTE15D** (private, soon to be public)
  1.5D MPI wrapper for 1D codes
  Gallagher et al. (in prep)

- **NLTE3D** (private)
  3D code
  Steffen et al. (2012)

Statistical equilibrium

What is being computed?



Statistical equilibrium

What is being computed?

Formal solution using a Λ-operator:

1. Mean intensity, J_ν, initial guess
   Usually populations are set to LTE

2. Integrate the formal transfer solution with enough rays so that J_ν can be approximately calculated

3. Compute J_ν at all locations of the atmosphere, hence compute scattering emissivity, j_ν

4. Return to point (2) until J_ν appears to have converged
   In reality convergence is usually set by a user limit on the maximum relative change to the populations between iteration n and n-1

The model atom

The model atom

MULTI/Multi3D

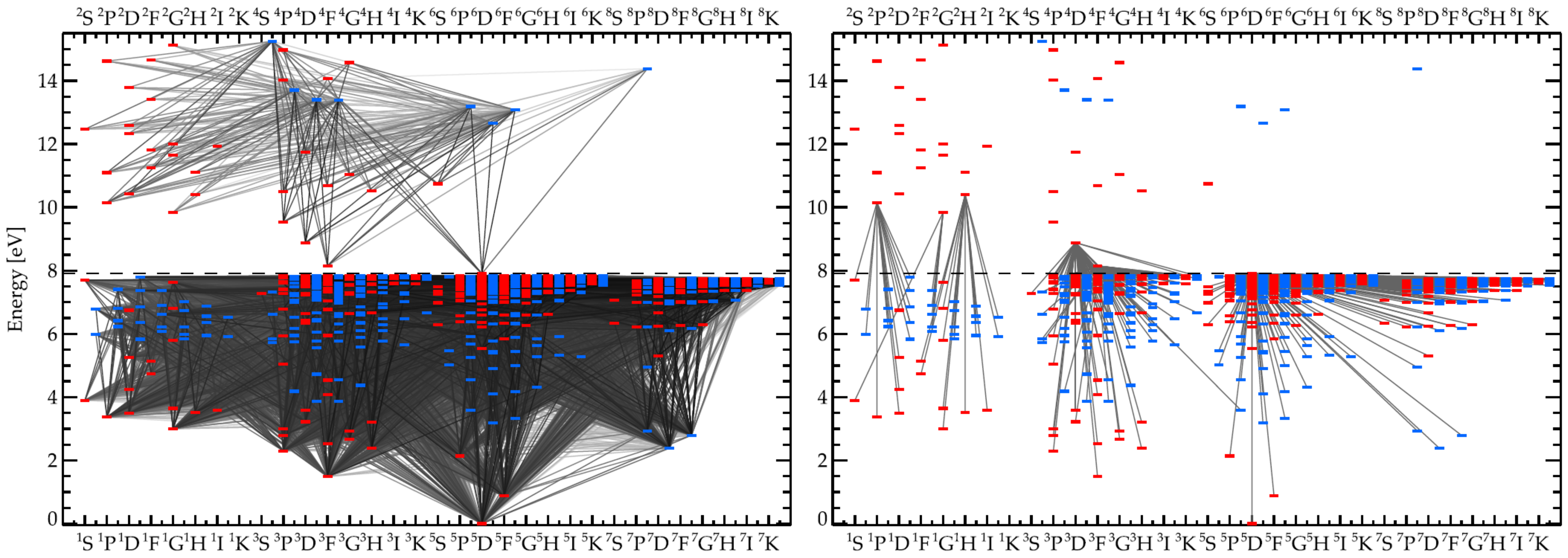
An ASCII table describing the behaviour of an atom

Only the atom modelled is considered to be in NLTE. Everything else considered is in LTE

1. A complete list of energy levels
2. A complete (*comprehensive*) list of all bound-bound transitions
3. A complete (*comprehensive*) list of all bound-free transitions
   Very complicated
4. An accompanying list of collisional data for any and all radiative data above
   Even more complicated

The model atom

Radiative data

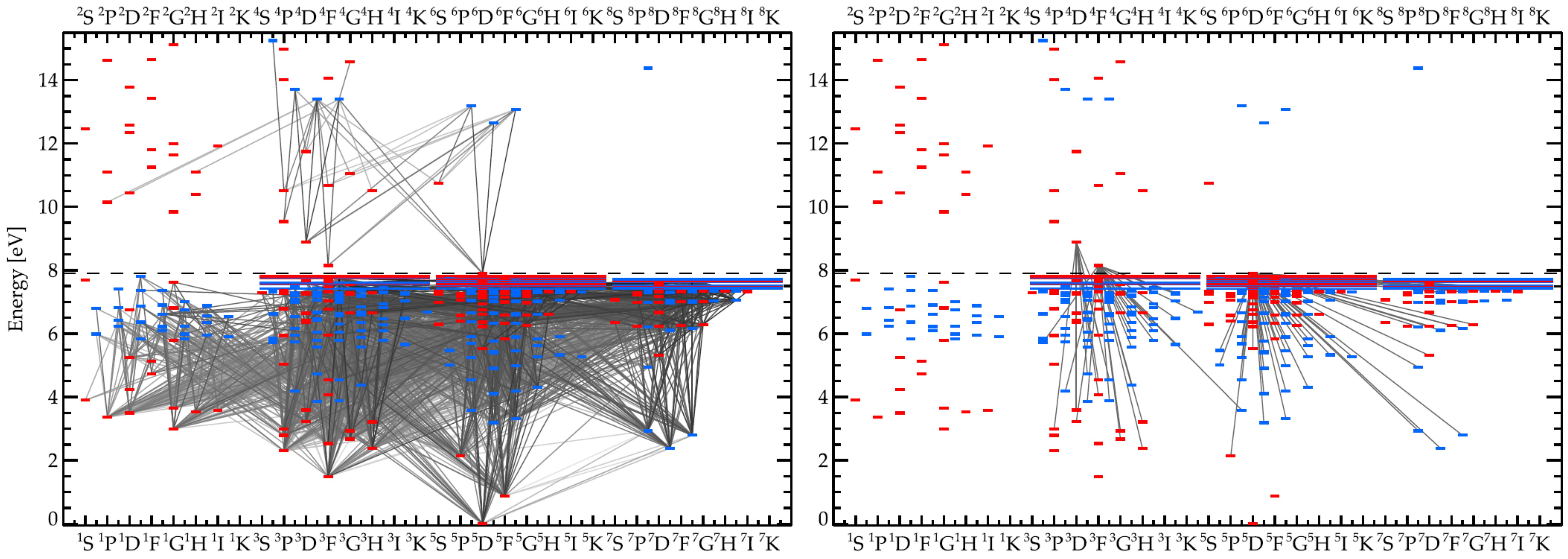


Iron atom Grotrian diagram: Lind et al. (2017)

- 2996 energy levels
- >500 000 B-B and B-F transitions for Fe I and Fe II

The model atom

Radiative data

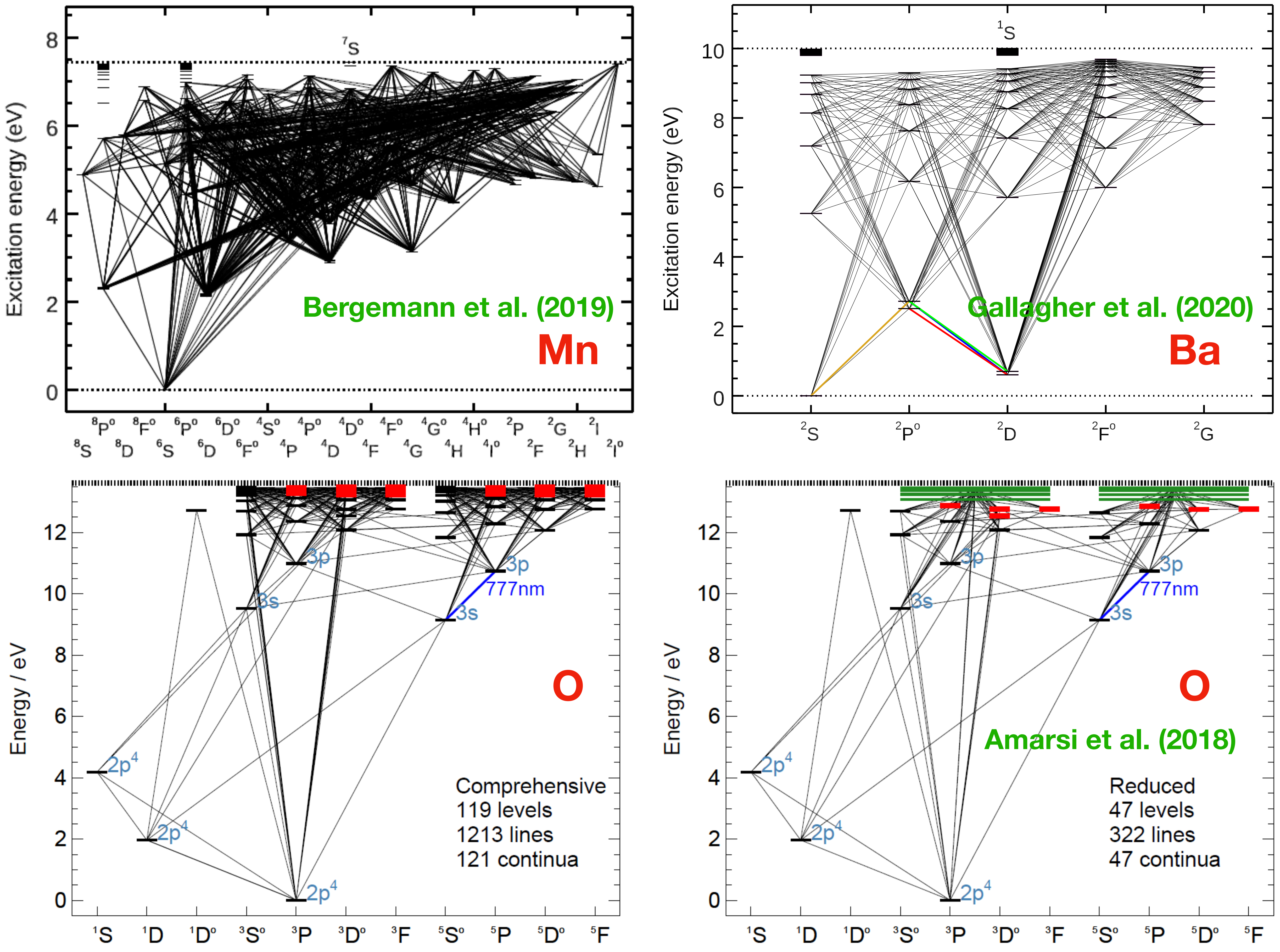


Reduced iron atom Grotrian diagram: Lind et al. (2017)

- 804 energy levels (2996)
- 3100 B-B and B-F transitions for Fe I and Fe II (>500,000)

The model atom

Radiative data



Not all atoms are as large …

Even so, it can sometimes be useful to do so anyway

The model atom

Collisional data

- Collsional rates computed for a series of temperatures for all radiative B-B and B-F transitions (where possible)

- Collisions with various particles are considered, for example:

$$\mathrm{A} + \mathrm{H} \qquad \mathrm{A}^{Z} + \mathrm{H} \rightarrow \mathrm{A}^{Z-1} + \mathrm{H}^{-} \qquad \mathrm{A} + e$$

<u>**Hard to compute!**</u>

- Drawins (1969) formula for hydrogenic collisional rates
  (order of magnitude estimate - requires empirically determined parameter, S_H)

- New ab initio quantum mechanical hydrogenic collisions for some atoms now available
  (see Belyaev & Yakovleva, 2018 for H, Barklem 2007 for *e*)

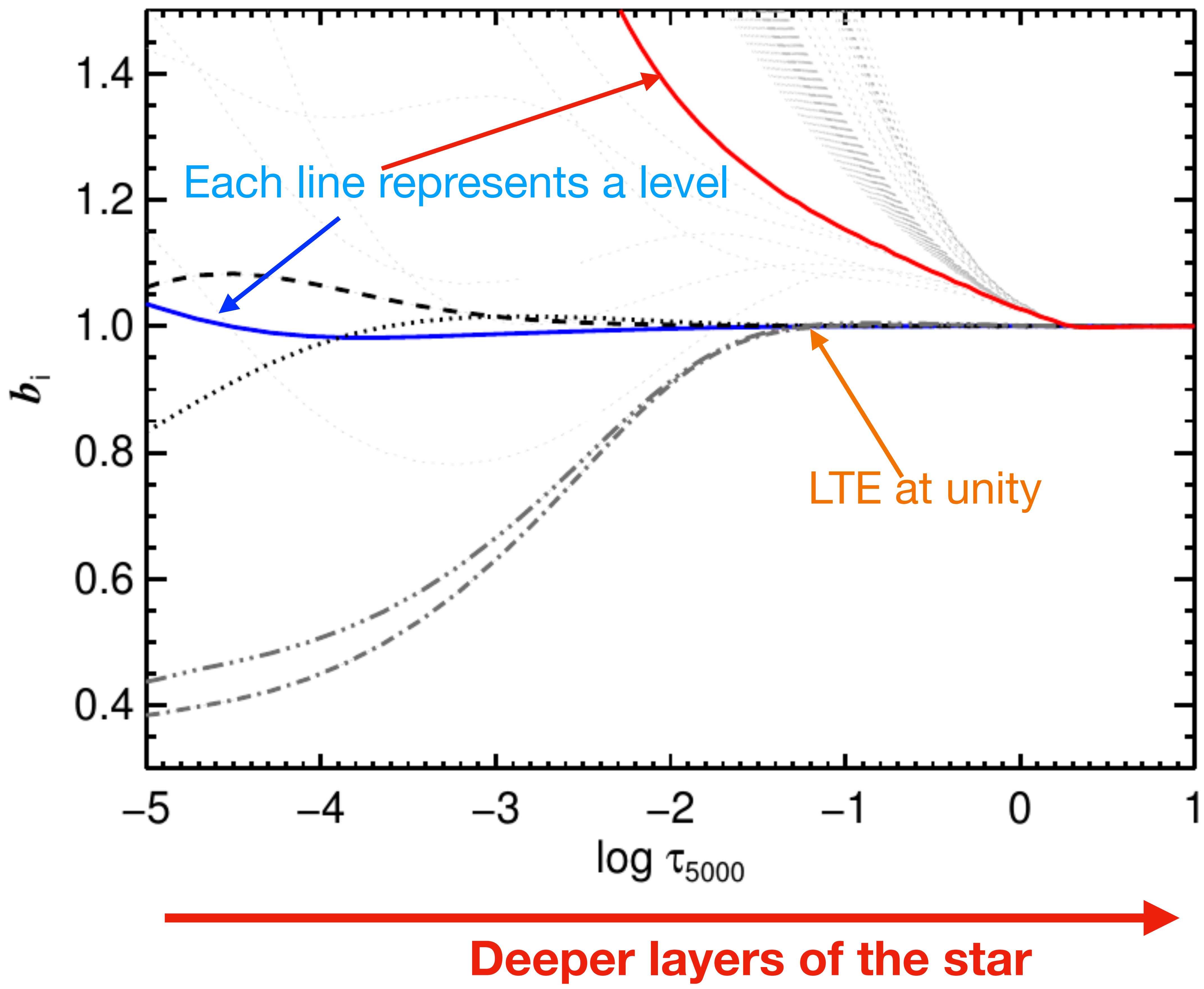
Departure coefficients

Departure coefficients

Energy levels affected by NLTE effects differently

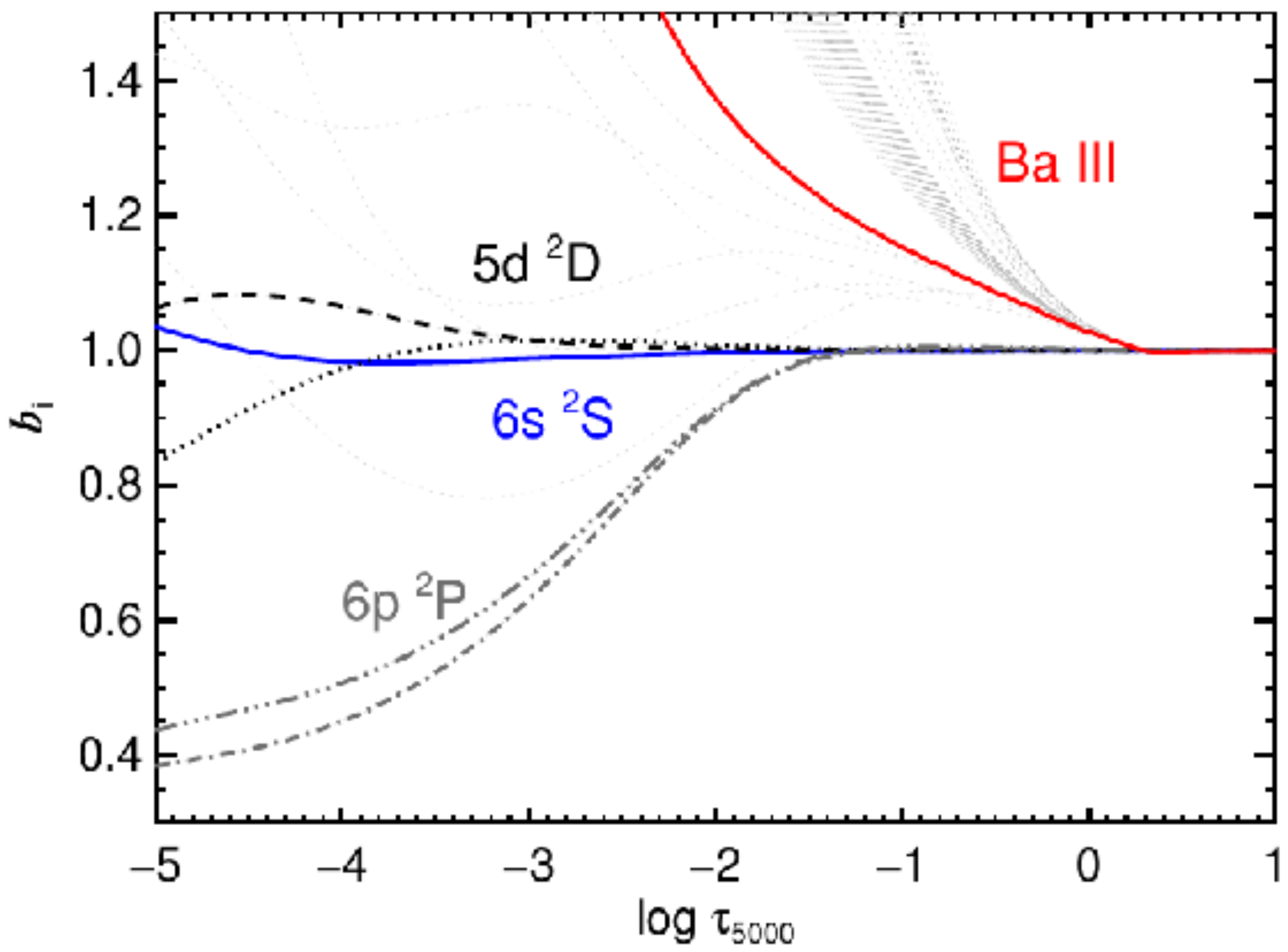
$$b_i = \frac{n_{i,\mathrm{NLTE}}}{n_{i,\mathrm{LTE}}}$$

n_i is the population of level i

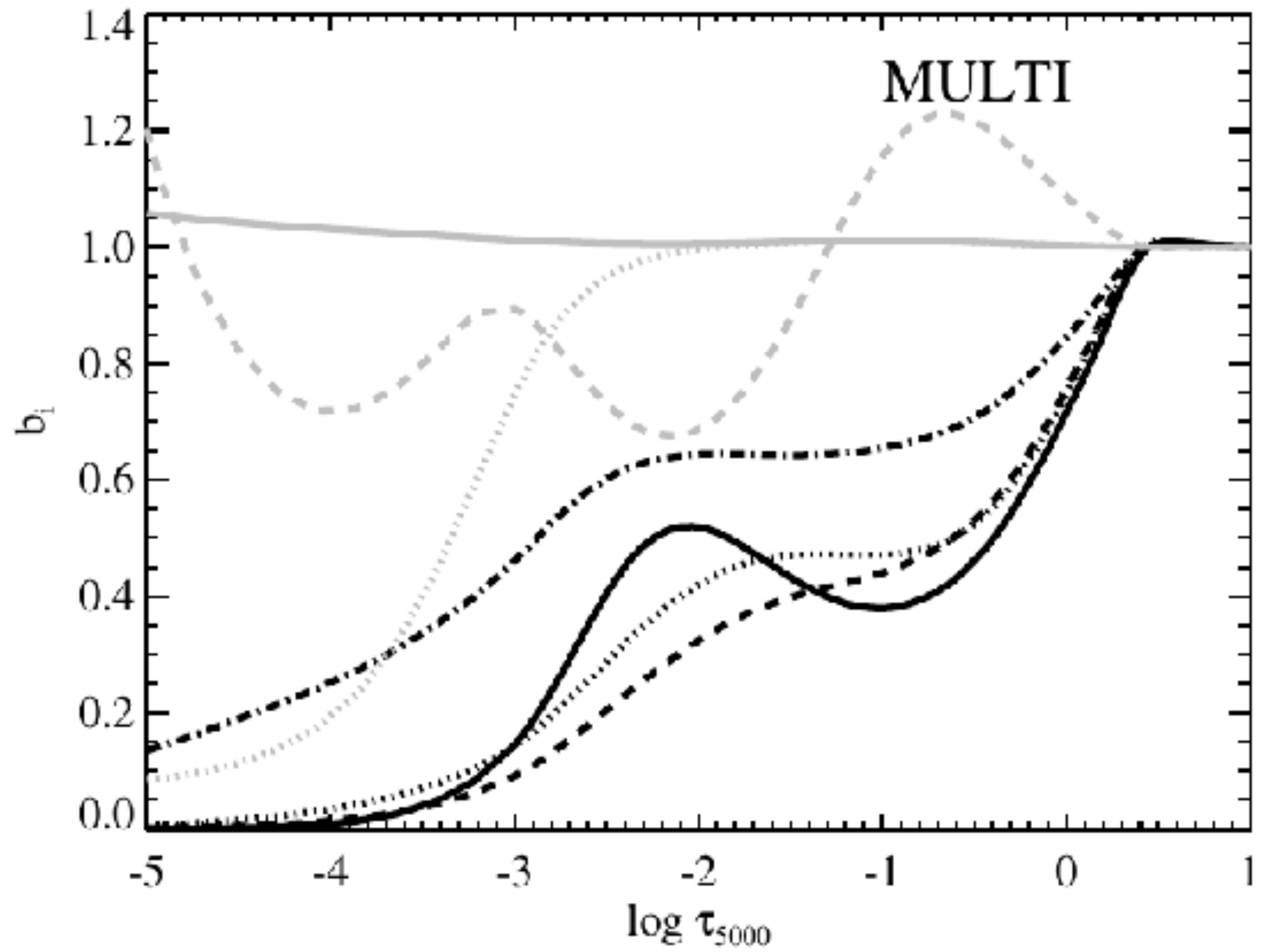


Departure coefficients

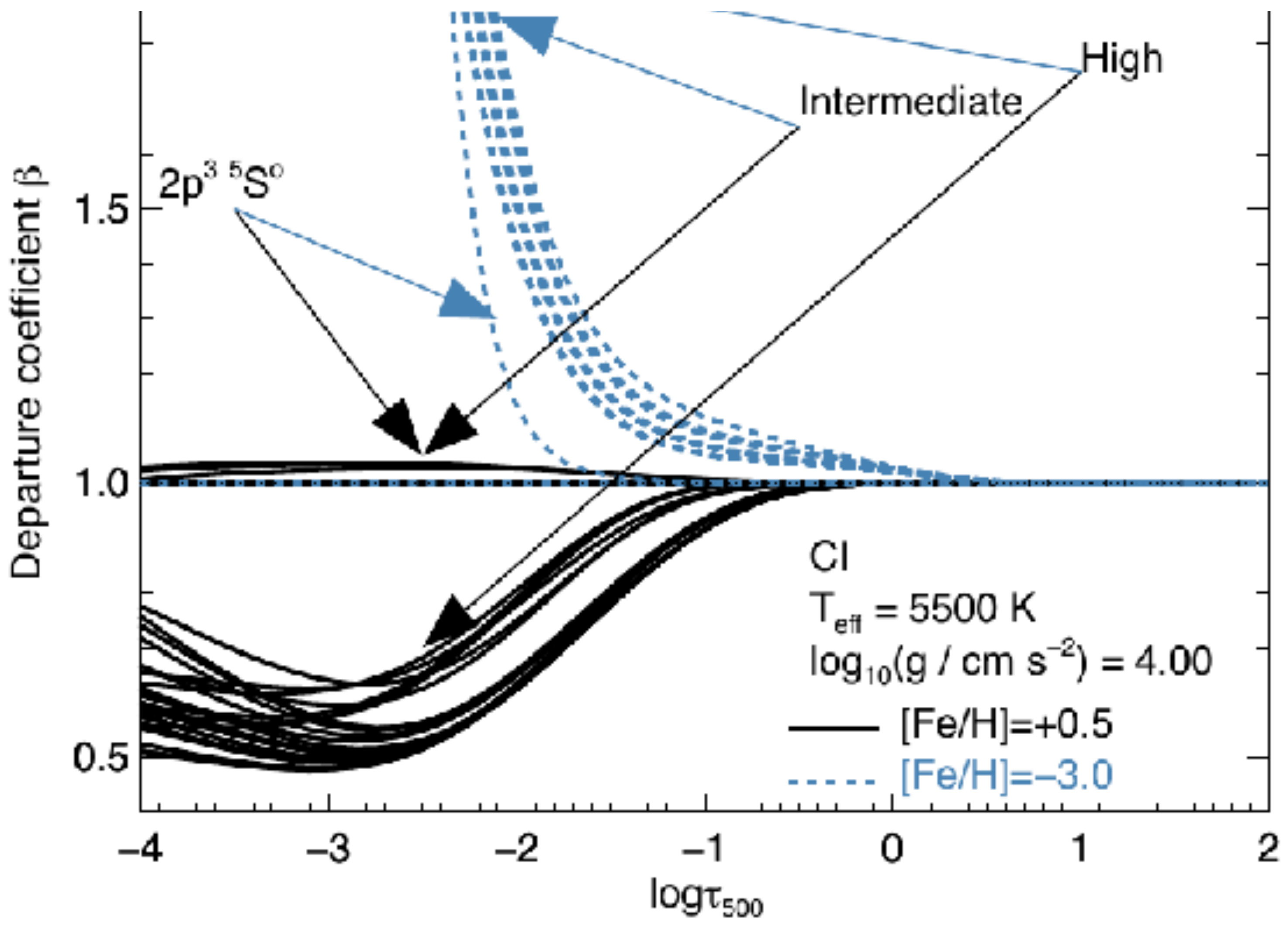
Ba
Gallagher et al. (2020)



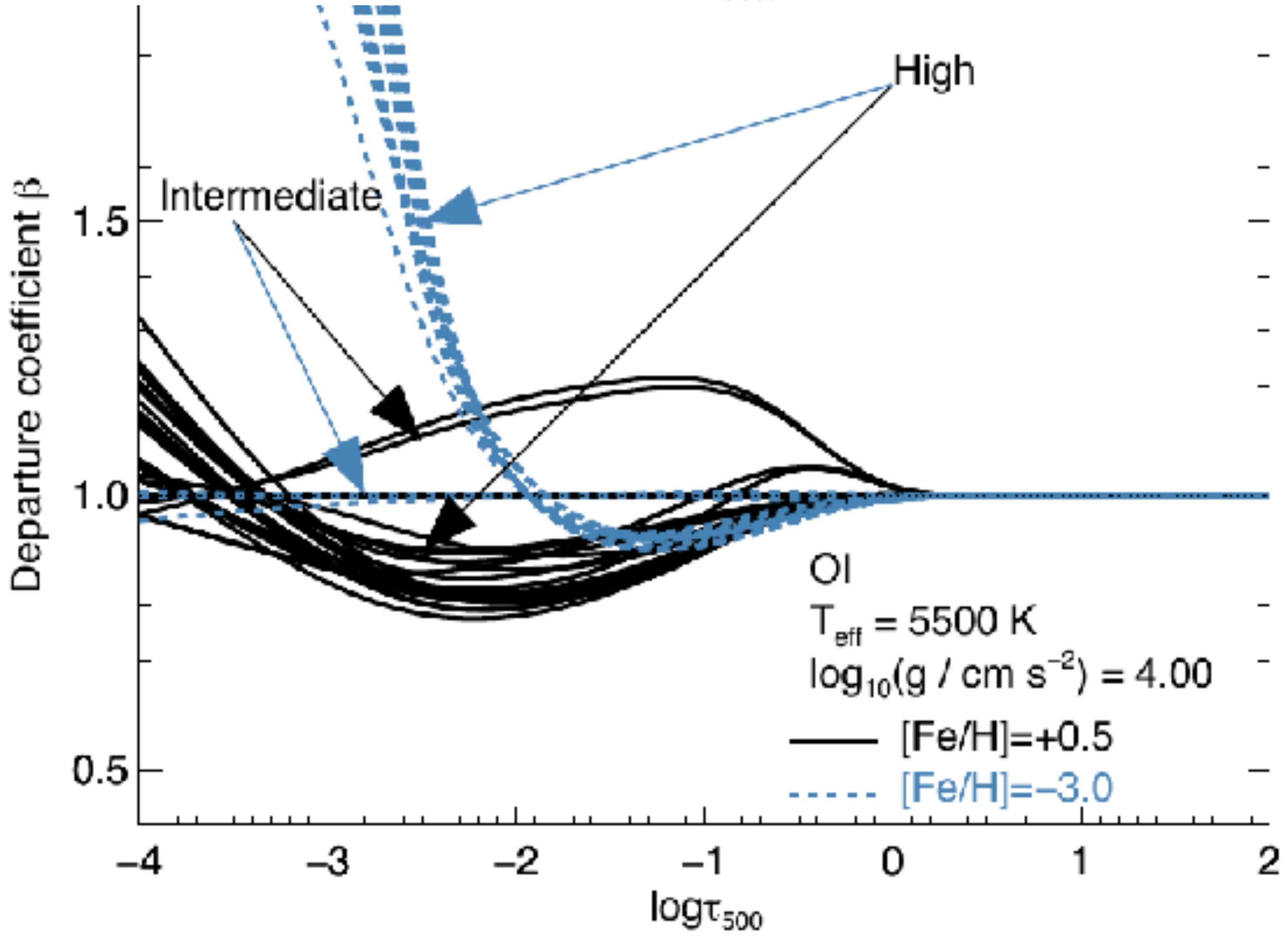
Mn
Bergemann et al. (2019)



C
Amarsi et al. (2019)



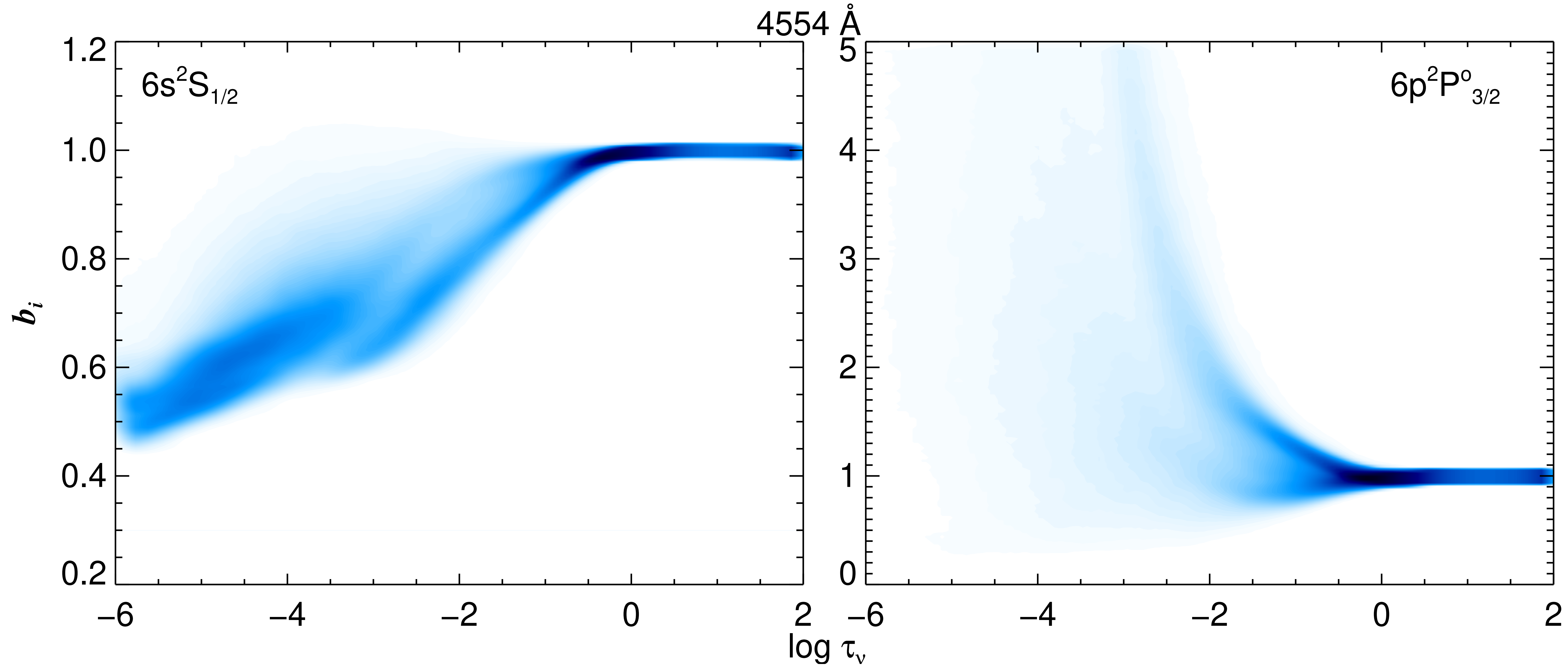
O
Amarsi et al. (2019)



Departure coefficients

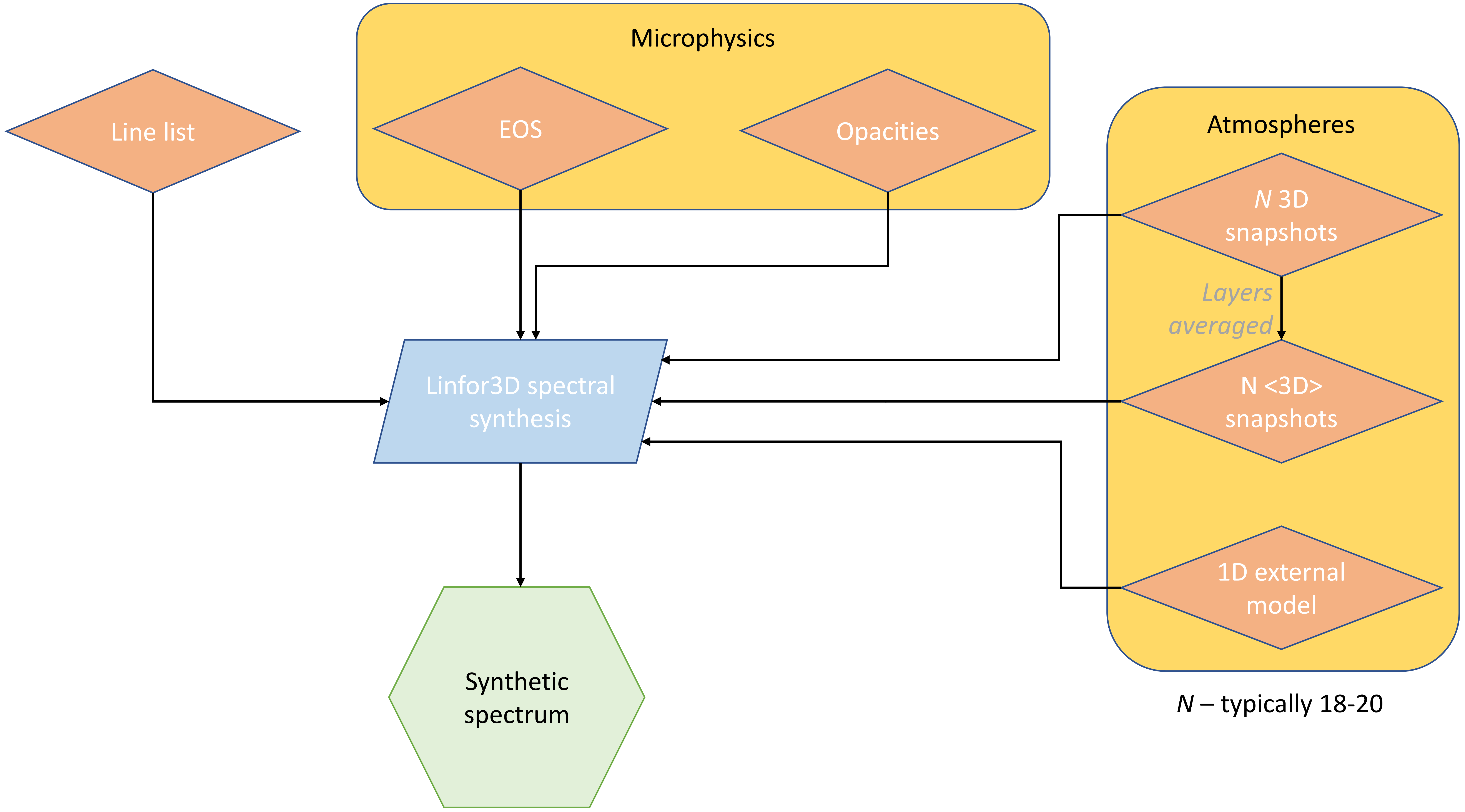
In a 3D atmosphere

- The scatter in the departures a sign of *T* and *P* inhomogeneities
- At every depth point there is a 2D surface

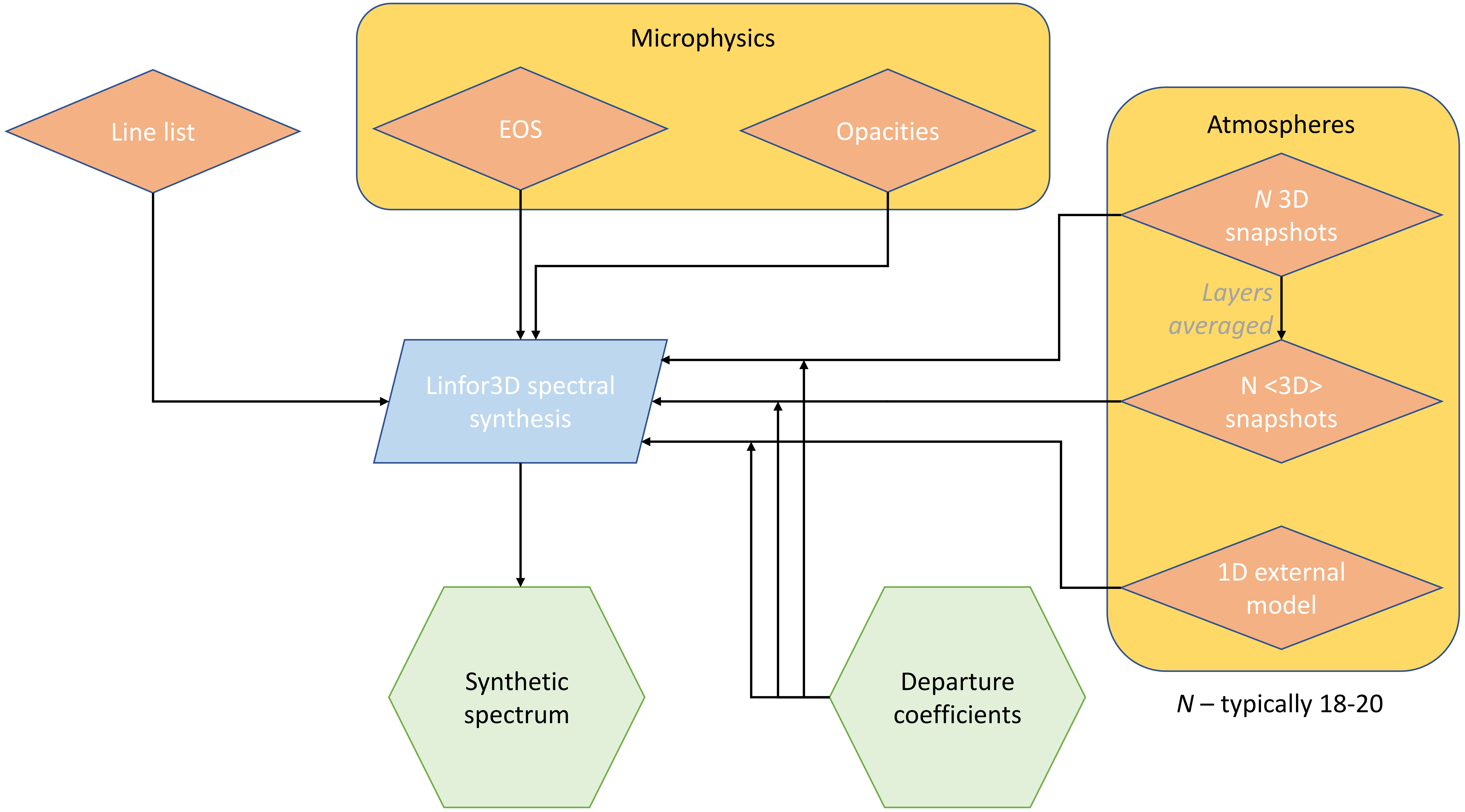


3D NLTE spectrum synthesis

3D LTE spectral synthesis

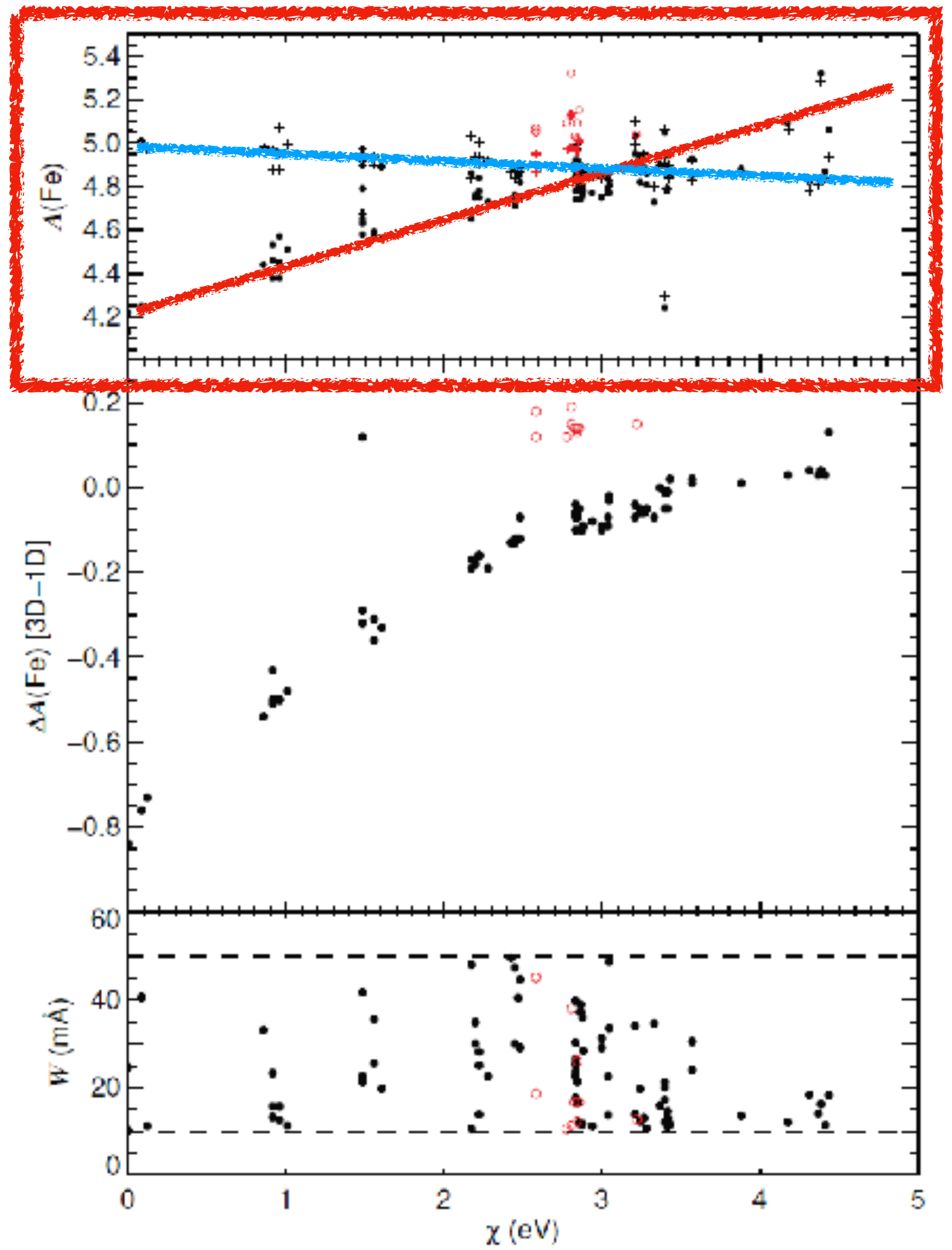


3D NLTE spectral synthesis



N – typically 18-20

3D NLTE iron



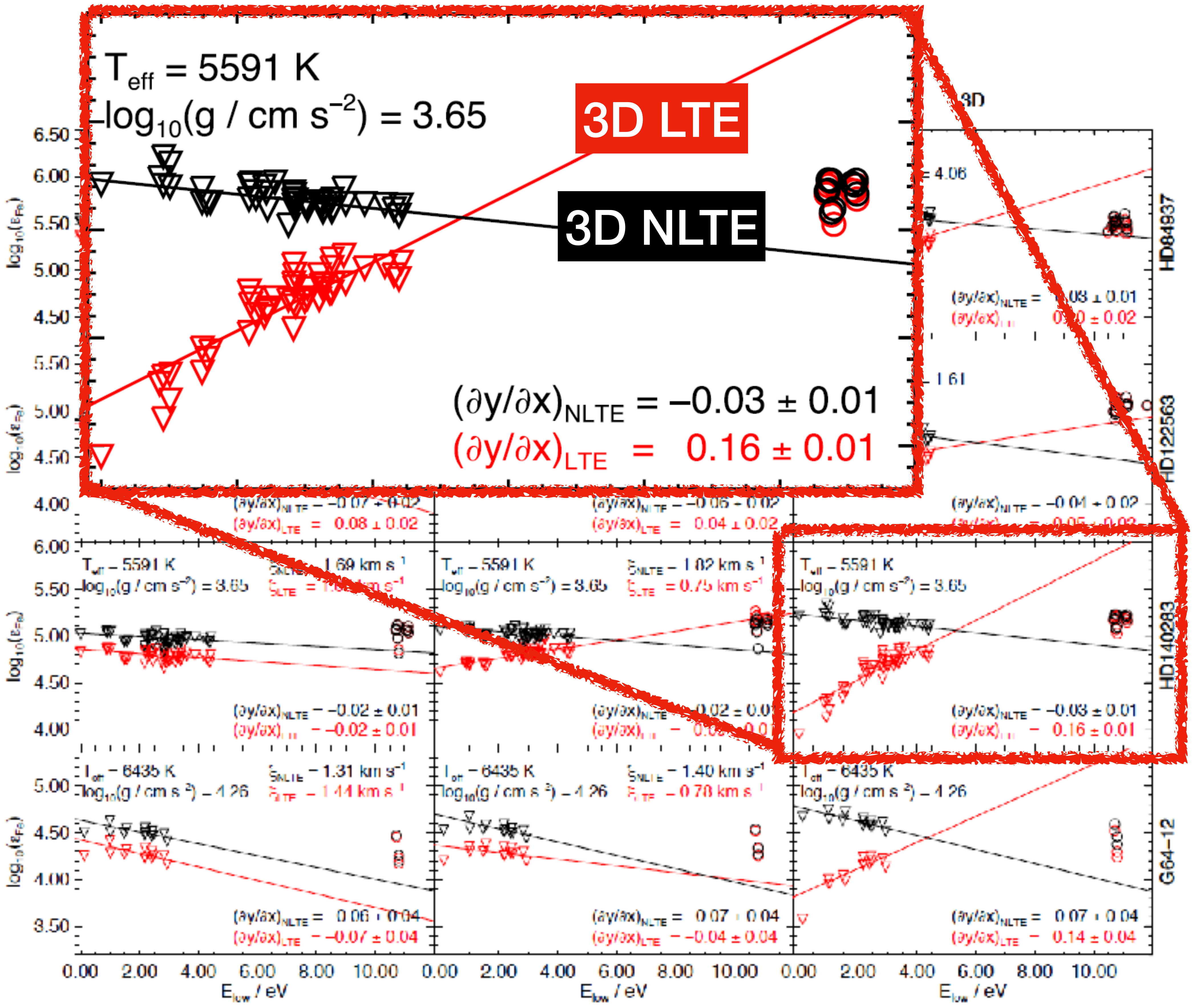
Gallagher et al. (2015)

Fe I lines show large dependence on their excitation potential, χ, in 3D LTE

1D Fe I & 3D Fe II do not

3D abundance - 1D abundance enhances and highlights issue

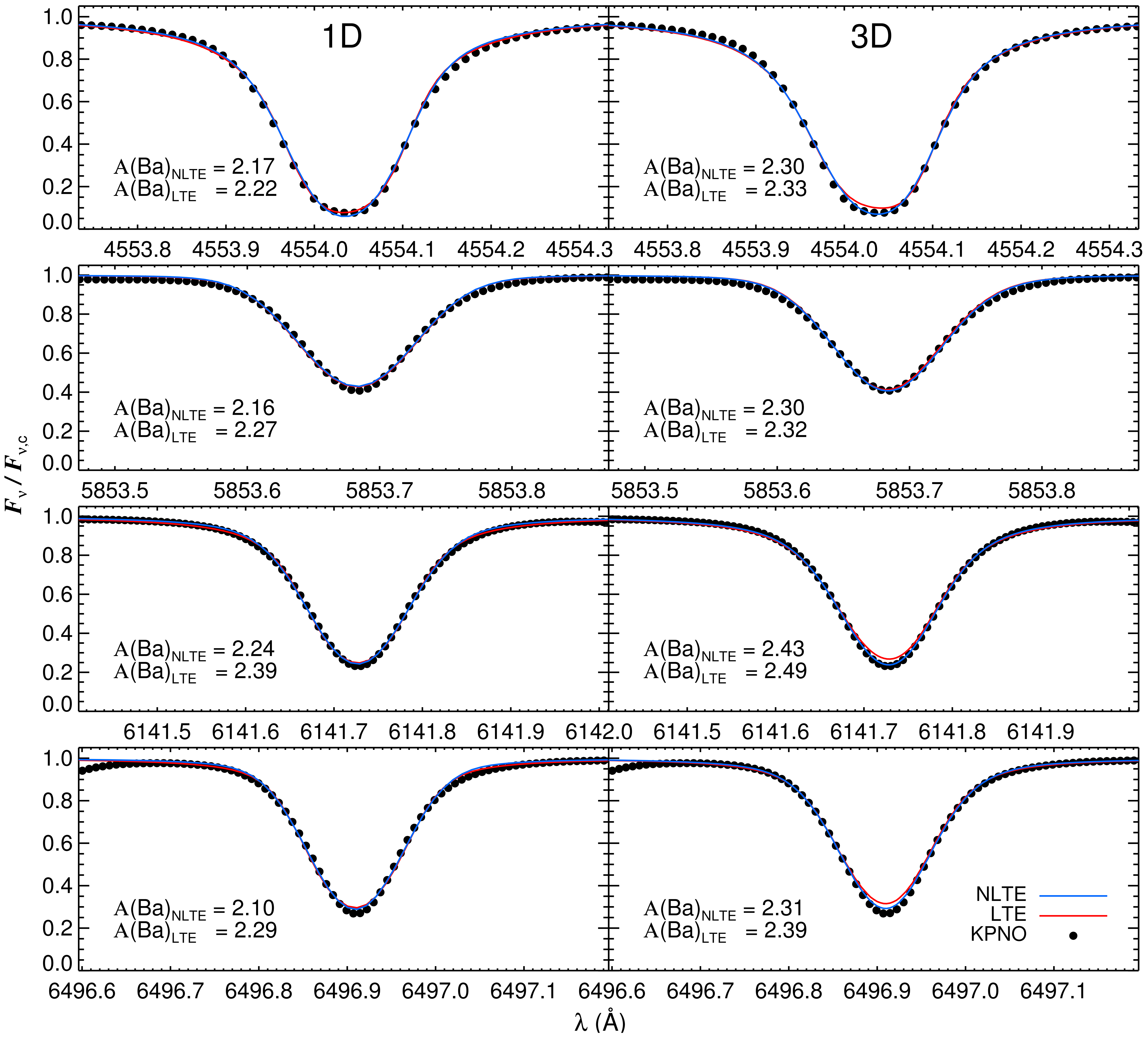
No dependence seen in the line strength



Amarsi et al. (2016)

3D NLTE spectrum synthesis

- ***Extremely*** time consuming
- Single lines can take *hours* of computing
  (S.E. to compute departures + 3D NLTE synthesis)
- Computing 3D NLTE grids to fit features not practical
- Better to use correction grids instead



Gallagher et al. (2020)

Abundance corrections

Abundance correction

- The difference in absolute abundance of some caveat, relative to 1D LTE
- $\Delta = A(\mathrm{X})_A - A(\mathrm{X})_{\mathrm{1D\ LTE}}$

  where 1D LTE refers, in general, to the observed study, and *A* represents some caveat other than 1D LTE

  - 1D NLTE modelling
  - 3D LTE modelling
  - 3D NLTE modelling

- Easy to apply to most observational studies …

3D NLTE correction grids

1. Fit a line / feature using the standard 1D LTE technique
   Determine line strength and absolute abundance of transition

2. Use a precomputed grid of 3D NLTE corrections
   Add an abundance correction to determined 1D LTE correction

But where are these grids?

Not many exist, but luckily ChETEC-INFRA has made a good start

Corrected corrections

"Real world" corrections

- 3D CO5BOLD models
- 1D LHD models
- $\Delta^{0}_{\mathrm{3D}} = A(\mathrm{X})^{0}_{\mathrm{3D\ NLTE}} - A(\mathrm{X})^{0}_{\mathrm{1D\ LTE}}$

"Ideal" corrections

- ~~3D MARCS models~~
- 1D MARCS models
- $\Delta^{1}_{\mathrm{3D}} = A(\mathrm{X})^{1}_{\mathrm{3D\ NLTE}} - A(\mathrm{X})^{1}_{\mathrm{1D\ LTE}}$

$$\Delta^{1}_{\mathrm{3D}} \neq \Delta^{0}_{\mathrm{3D}}$$

$$A(\mathrm{X})^{1}_{\mathrm{3D\ NLTE}} - A(\mathrm{X})^{1}_{\mathrm{1D\ NLTE}} \approx A(\mathrm{X})^{0}_{\mathrm{3D\ NLTE}} - A(\mathrm{X})^{0}_{\mathrm{1D\ NLTE}}$$

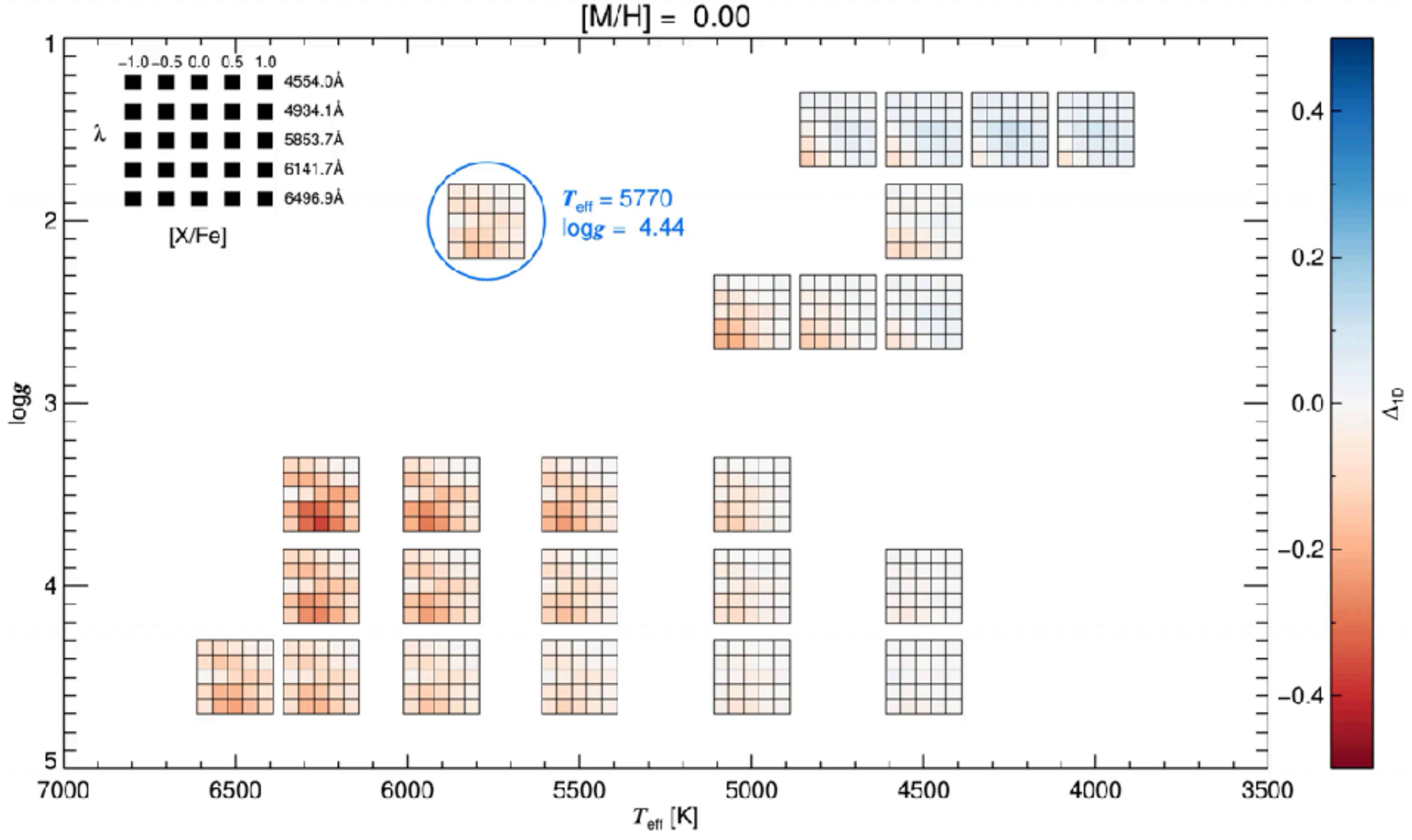
$$\Delta^{1}_{\mathrm{3D}} - \left(A(\mathrm{X})^{1}_{\mathrm{1D\ NLTE}} - A(\mathrm{X})^{1}_{\mathrm{1D\ LTE}}\right) = \Delta^{0}_{\mathrm{3D}} + \left(A(\mathrm{X})^{0}_{\mathrm{1D\ NLTE}} - A(\mathrm{X})^{0}_{\mathrm{1D\ LTE}}\right)$$

$$\Delta^{1}_{\mathrm{3D}} = \Delta^{0}_{\mathrm{3D}} + \left(\Delta^{1}_{\mathrm{1D}} - \Delta^{0}_{\mathrm{1D}}\right)$$

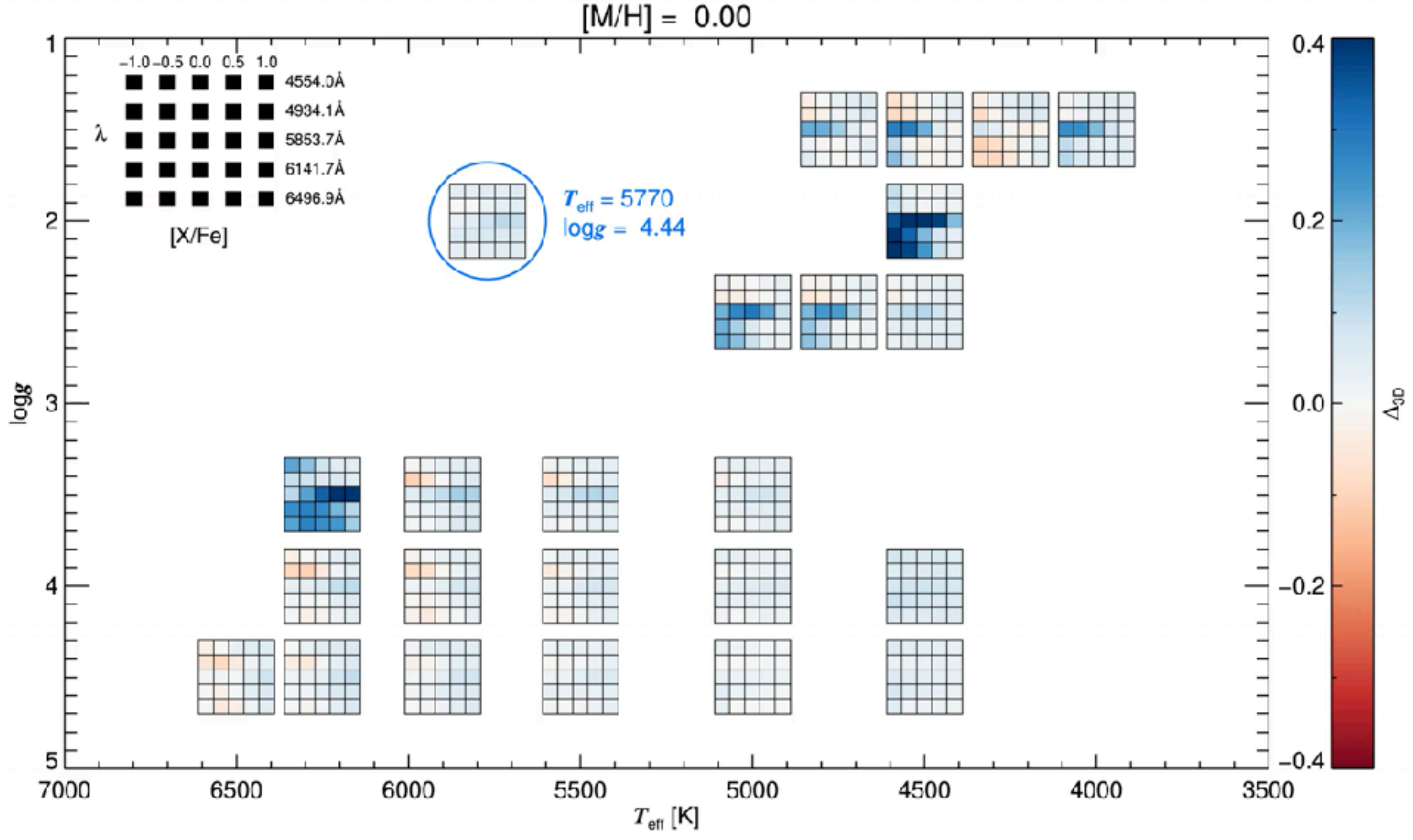
Barium abundance correction grid

ChETEC-INFRA WP 5.1

1D NLTE corrections



3D NLTE corrections



https://web.vu.lt/tfai/j.klevas/

The corrected correction grid

Barium

- **95** 3D CO5BOLD models spanning four metallicities

$$-1.0 \leq [\mathrm{M/H}] \leq \quad 0.0, \qquad -1.0 \leq [\mathrm{Ba/Fe}] \leq +1.0$$
$$-3.0 \leq [\mathrm{M/H}] \leq -2.0, \qquad -2.5 \leq [\mathrm{Ba/Fe}] \leq +2.0$$

- **5** transitions - 4554, 4934, 5853, 6141, 6496 Å

- **41,685** 1.5D level population departure files
- **2,130** 1D LHD level population departure files
- **2,130** 1D MARCS level population departure files
- **31,950** 3D and 1D correction files

~9.6 million *CPU hours*

(or ~1100 years)

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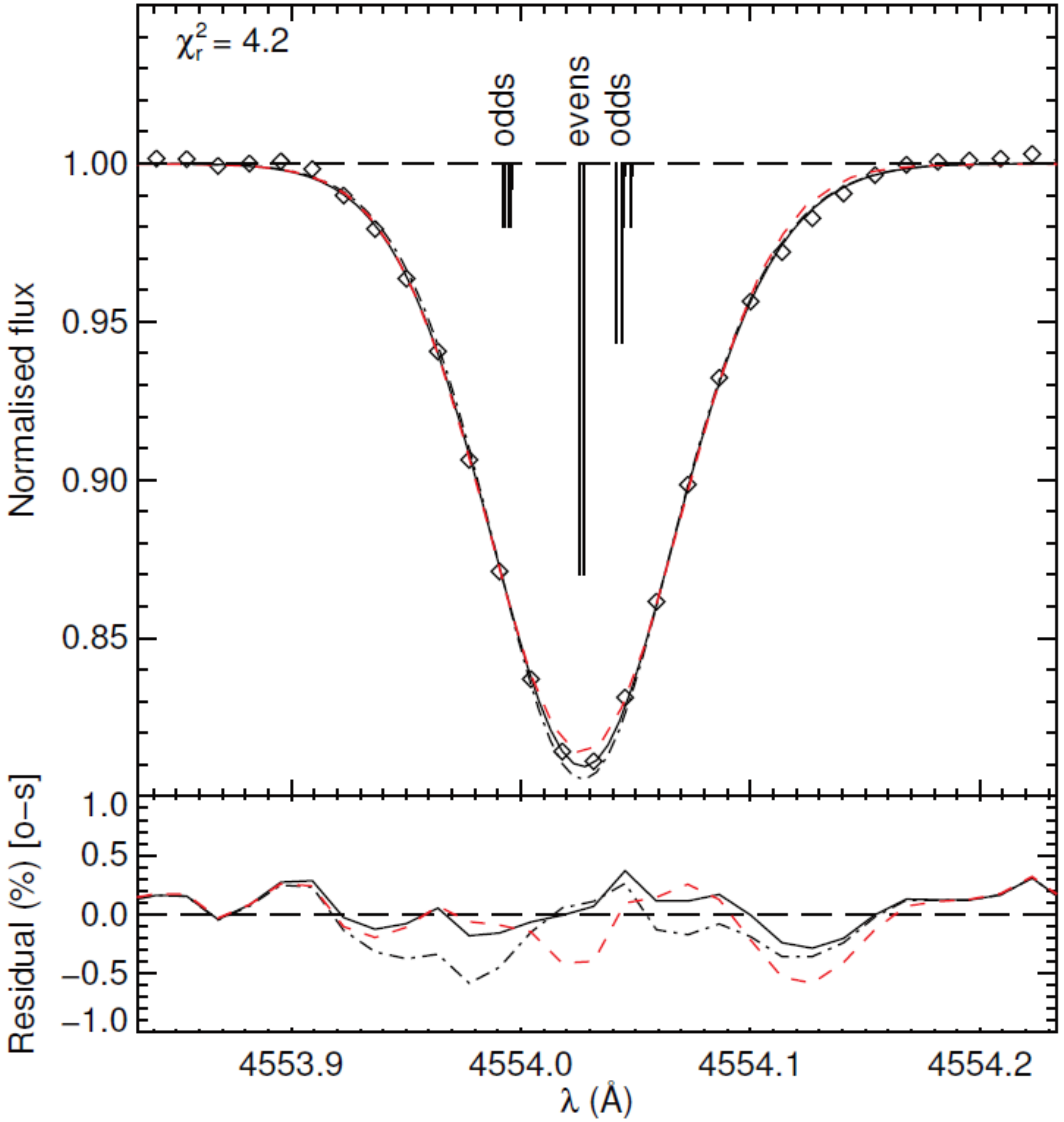
Using the corrections

1. Fit the spectral line in 1D LTE



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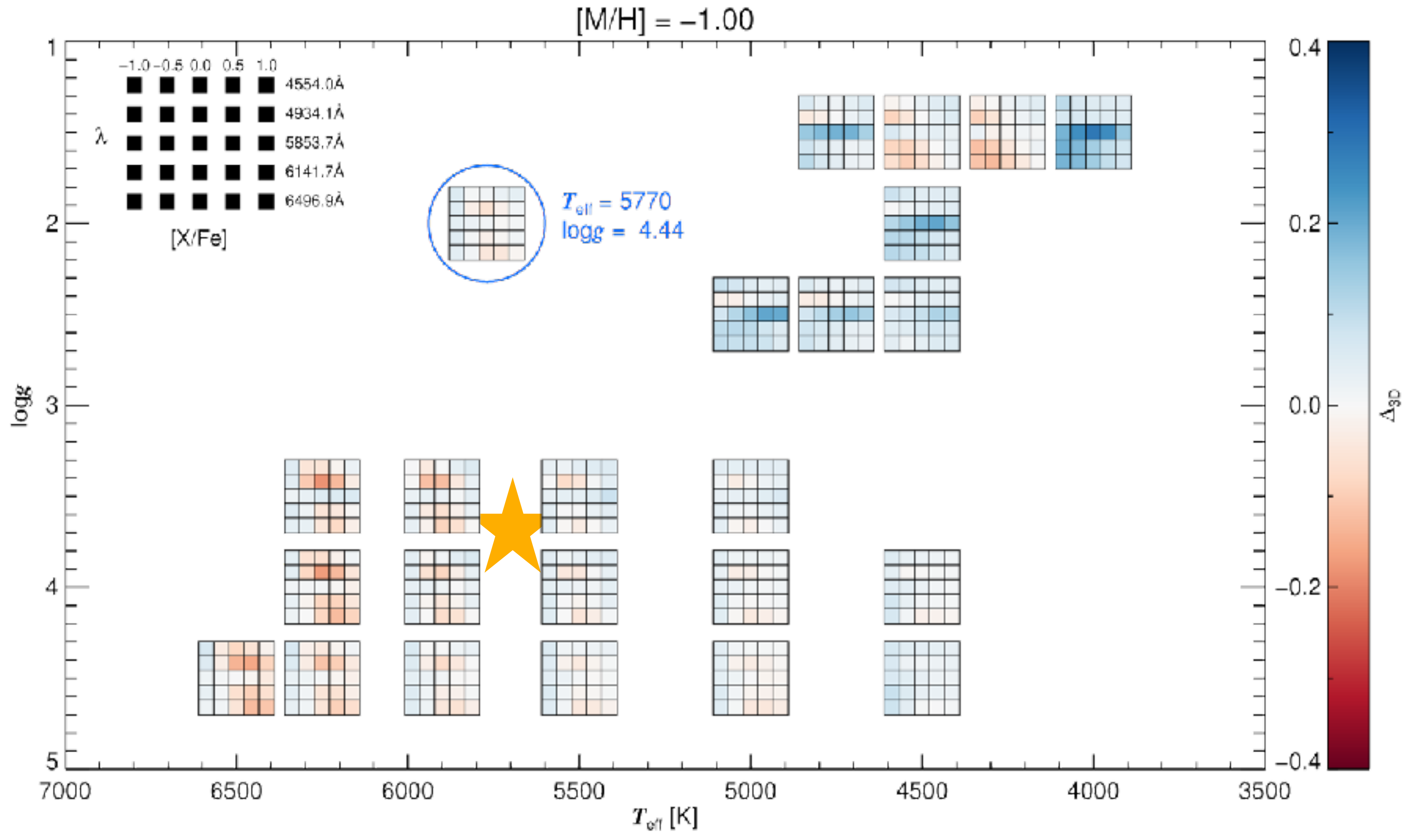
Using the corrections

1. Fit the spectral line in 1D LTE
2. Use the star's stellar parameters to select the necessary correction tables



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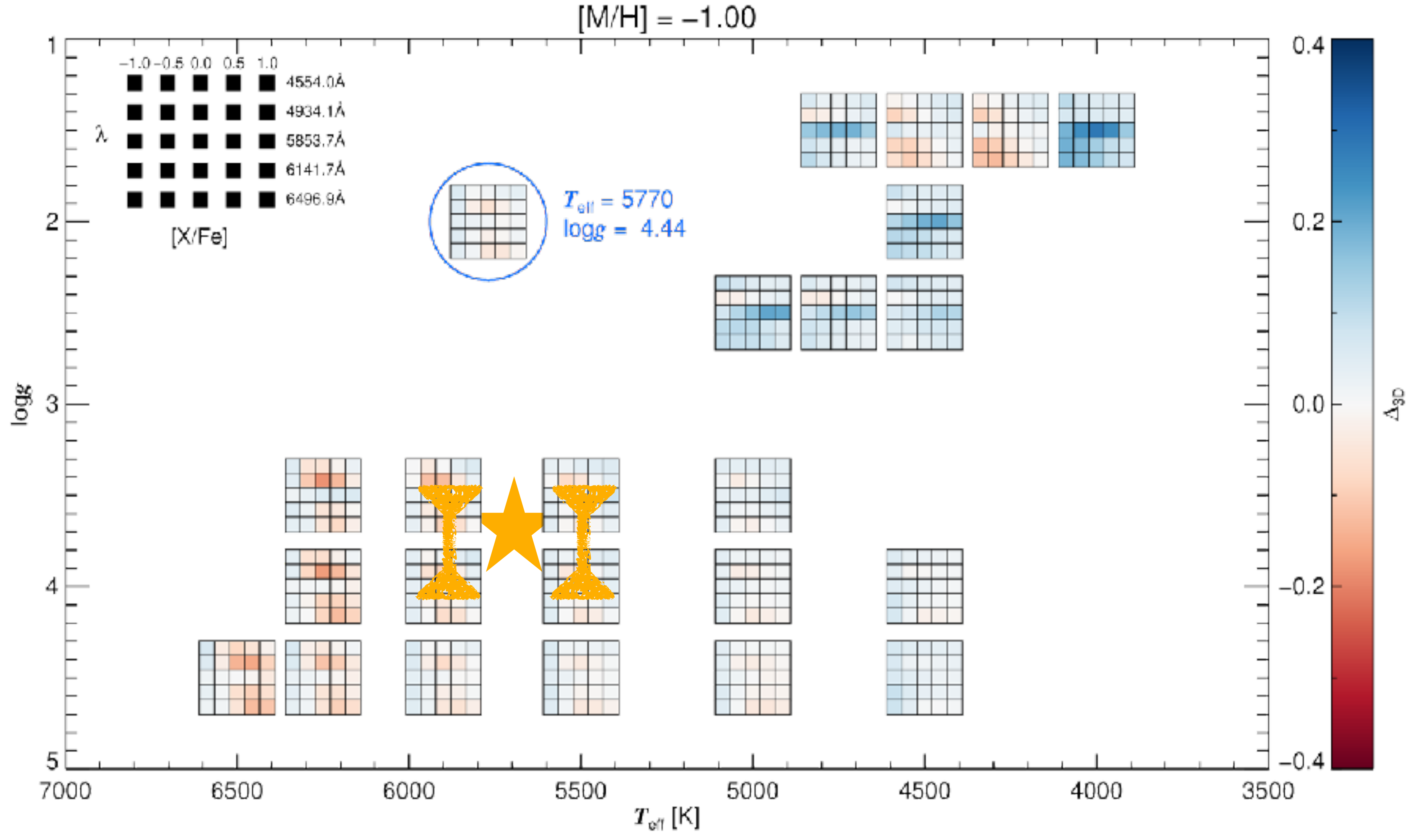
Using the corrections

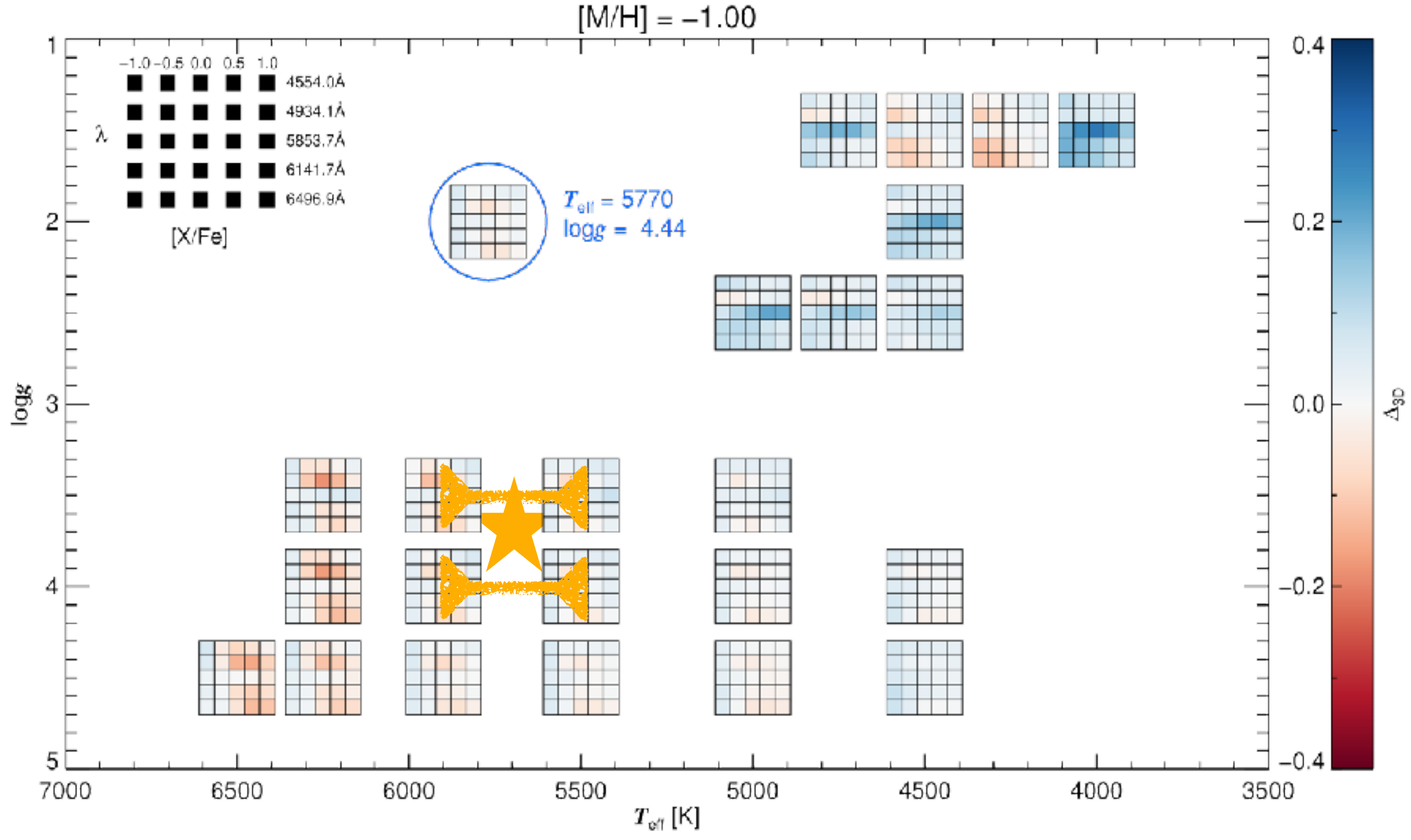
1. Fit the spectral line in 1D LTE
2. Use the star's stellar parameters to select the necessary correction tables
3. Interpolate the tables in the following order:
    1. By temperature



https://web.vu.lt/tfai/j.klevas/

Using the corrections

1. Fit the spectral line in 1D LTE
2. Use the star's stellar parameters to select the necessary correction tables
3. Interpolate the tables in the following order:
    1. By temperature
    2. By gravity



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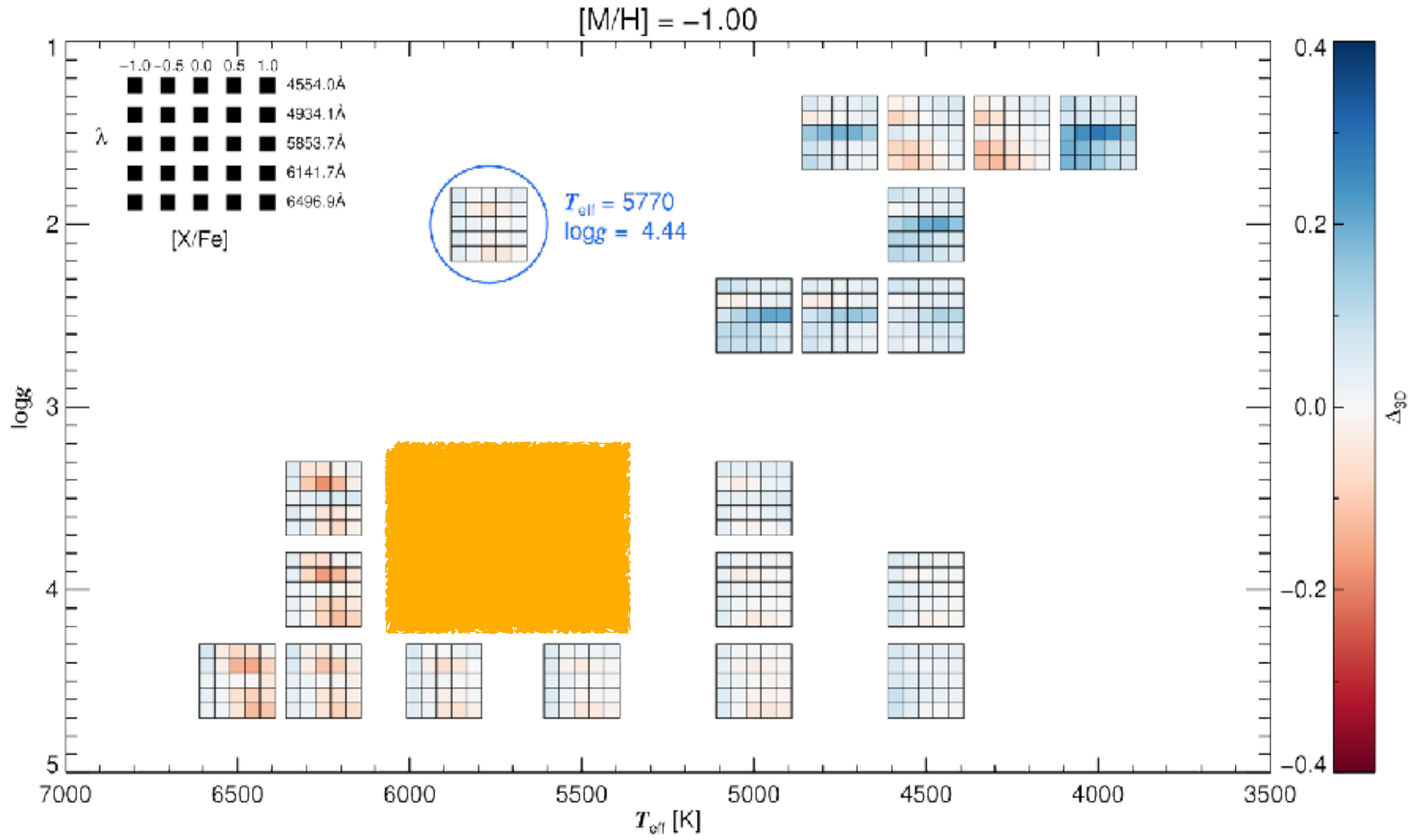
Using the corrections

1. Fit the spectral line in 1D LTE
2. Use the star's stellar parameters to select the necessary correction tables
3. Interpolate the tables in the following order:
    1. By temperature
    2. By gravity
    3. By metallicity



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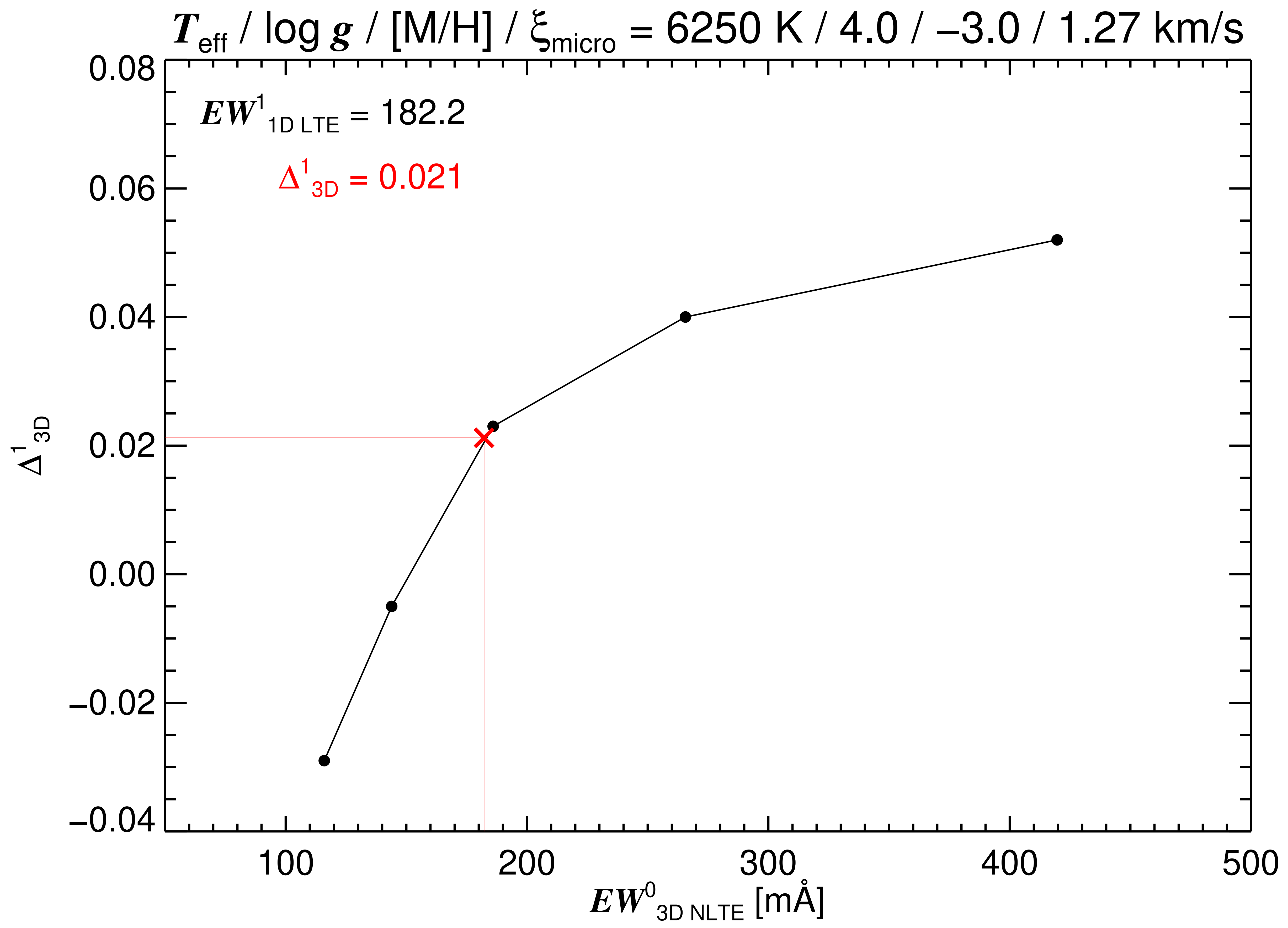
Using the corrections

1. Fit the spectral line in 1D LTE
2. Use the star's stellar parameters to select the necessary correction tables
3. Interpolate the tables in the following order:
    1. By temperature
    2. By gravity
    3. By metallicity
4. Interpolate the remaining abundance grid using the line strength



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Take aways

3D NLTE represents the state of the art, but …

- It is ***very*** complicated!
- It is ***very*** time consuming!
- For observers, it represents an **unrealistic approach** to analyse 10s, 100s, 1000s, … , of stars, or survey work
- New 3D NLTE abundance correction grids are slowly becoming available
- Our work represents the first large-scale correction grid for any element
- Corrections can be included in 1D LTE work to provide fast, full 3D NLTE abundances to a project

https://web.vu.lt/tfai/j.klevas/