Tools and techniques for modelling stellar spectra beyond 1D/LTE

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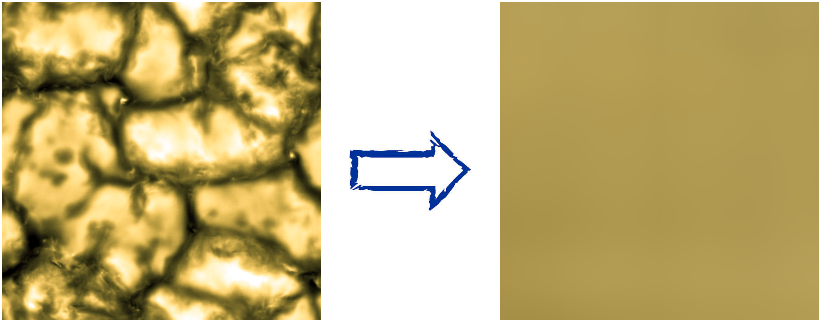
AIP

3D model atmospheres

Are stellar atmospheres horizontally homogeneous and static?



Hi-res image of solar surface 1D model representation

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

Future of observational data

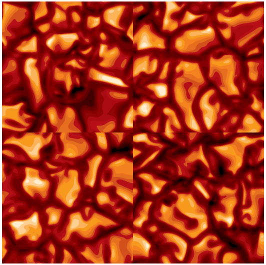
- 8m-class telescopes are capable of attaining very high quality data
- Complex stellar phenomena start to be resolvable
  - Asymmetric line profiles
  - Result from asymmetric velocity fields from stellar granulation
- 1D modelling cannot replicate this
- Observational quality will improve with new generation *GIANT* telescopes
  $\longrightarrow$ E-ELT
  $\longrightarrow$ TMT

3D atmosphere codes

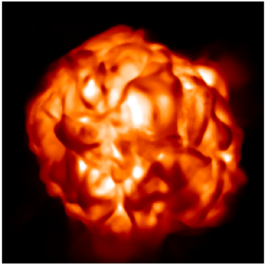
CO^5BOLD

COnservative **CO**de for the **CO**mputation of **CO**mpressible **CO**nvection in a **BO**x of **L D**imensions, with L=2,3

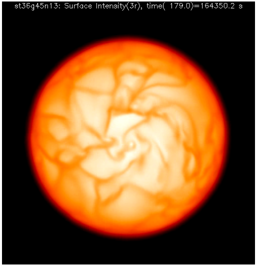
Bernd Freytag, Matthias Steffen, Hans-Günter Ludwig, Sven Wedemeyer, & W. Schaffenberger



local models



global models

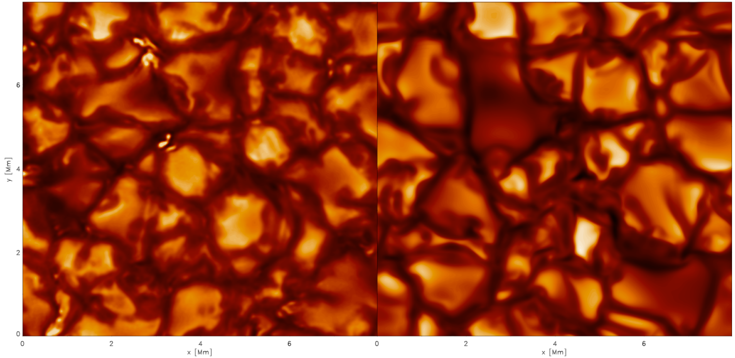


rotation models

3D atmosphere codes

STAGGER

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



Swedish Solar Telescope image ($R \approx 25\,\mathrm{km}$)

STAGGER numerical simulation

Image from https://staggergrid.wordpress.com/convection/

3D atmosphere codes

Bifrost

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

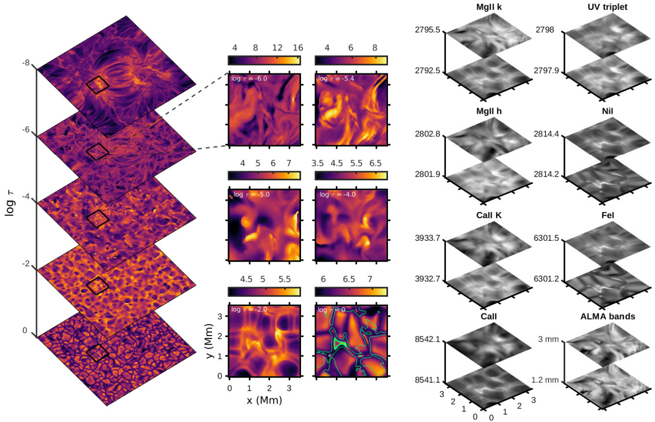


Image from da Silva Santos + (2018, A&A, 620, 124)

3D atmosphere codes

MPS/University of Chicago Radiative MHD
MuRAM

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

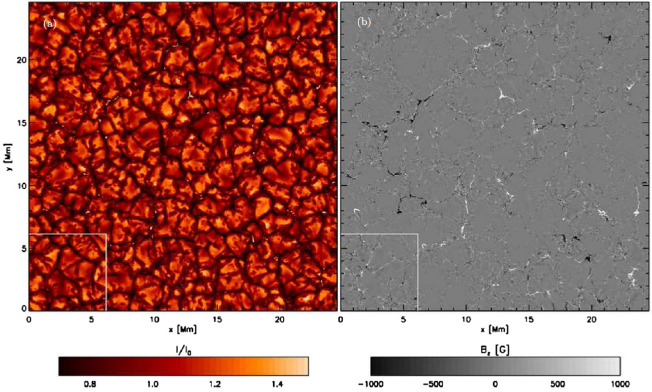
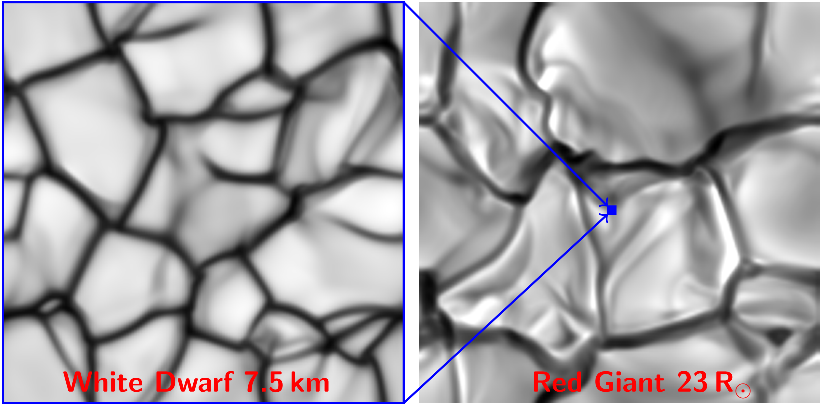


Image from Rempel (2014, ApJ, 789, 132)

What is modelled?

- Solution of the RHD or MHD equations coupled with radiative transfer
- Kinetics & transport for molecules and dust grains, non-equilibrium chemistry
- CO^{5}BOLD not limited to local models: "box-in-a-star" $\longleftrightarrow$ "star-in-a-box"
- Result: realistic gas flow and energy transport from sub-photosphere to chromosphere
- Bifrost & MURaM: Models of the Chromosphere, extremely high resolution

Granulation across the Hertzsprung-Russell diagram



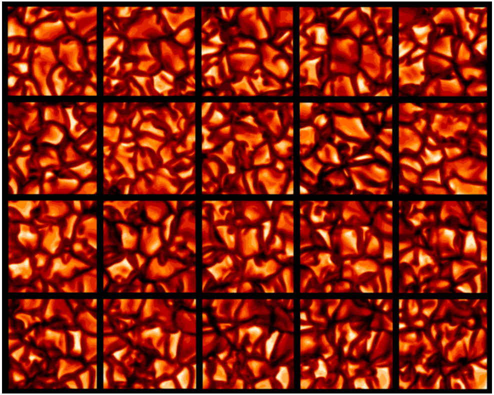
- From the Sun to stars with largely different parameters $\rightarrow$ robustness
- Spatial scale ratio in figures: 2×10^6 $\rightarrow$ box not to scale!

Multiple snapshots as single model atmosphere

Why use multiple snapshots?

Single snapshot represents small region of stellar disk

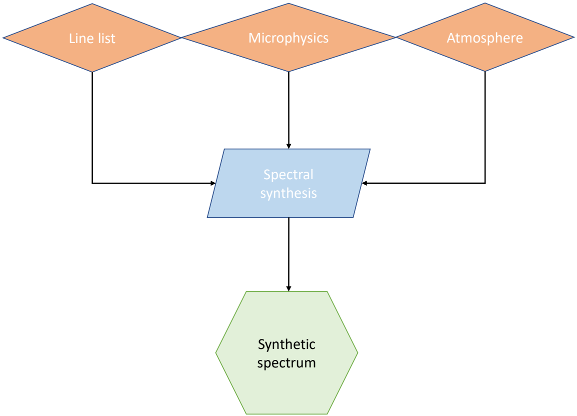
20 snaps
typical selection



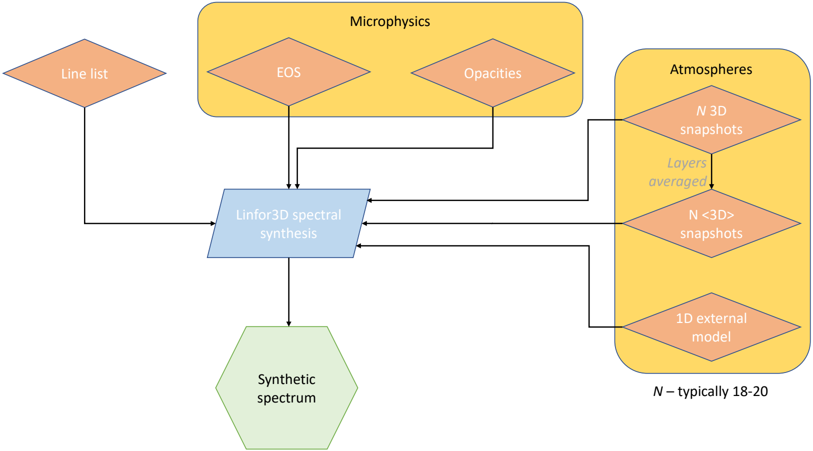
Ergodic approximation: **time** average $\equiv$ **spatial** average

3D Spectrum synthesis

LTE spectral synthesis in a nutshell



3D LTE spectral synthesis in a nutshell



3D spectral synthesis codes

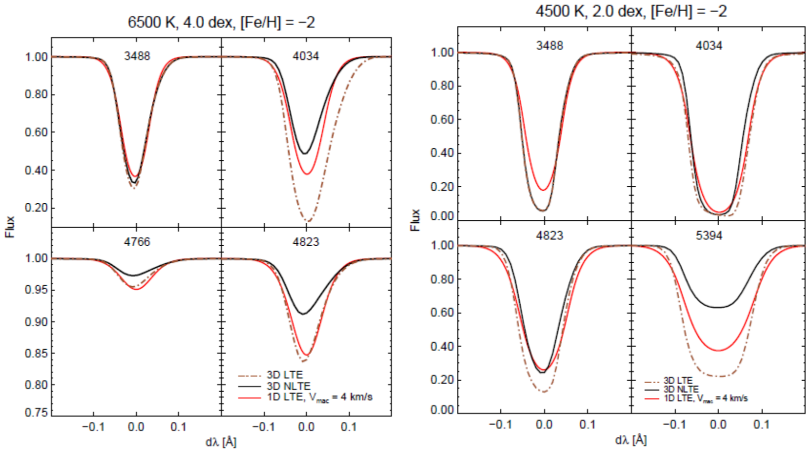
- **Linfor3D** *private*
  Steffen + (2020, Manual)
  - 1D/3D model atmospheres
  - LTE
  - Departures can be read
- **Optim3D** *private*
  Chiavassa + (2009)
  - 3D (local and global models)
  - Fast – precomputed extinction coefficients
  - SED production
- **SCATE** *private*
  Hayek + (2011)
  - 3D models
  - LTE

Most are available upon request, subject to terms

3D Convective shifts

Intrinsic 3D velocities lead to convective shifts

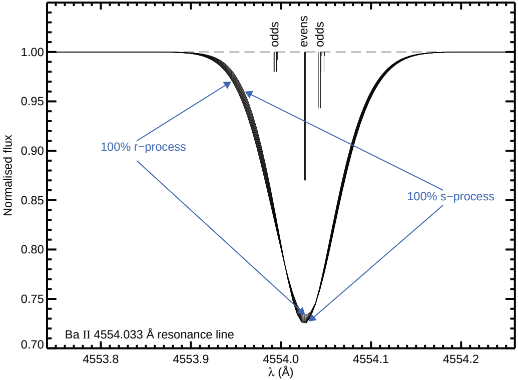
3D non-LTE 1D LTE 3D LTE



Bergemann + (2019)

Isotopes

The barium 4554 Å line as diagnostic of s- and r-process ratios.



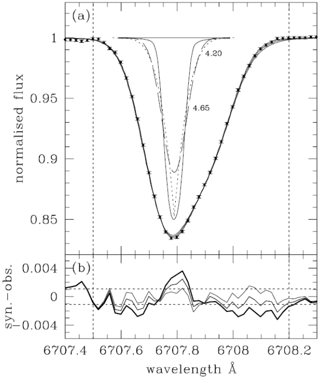
HD 140283 – **The metal-poor benchmark star** – Stellar parameters

- $T_{\mathrm{eff}} = 5750\,\mathrm{K}$
- $\log g = 3.7$
- $[\mathrm{Fe/H}] = -2.5$

Isotopes

Lithium

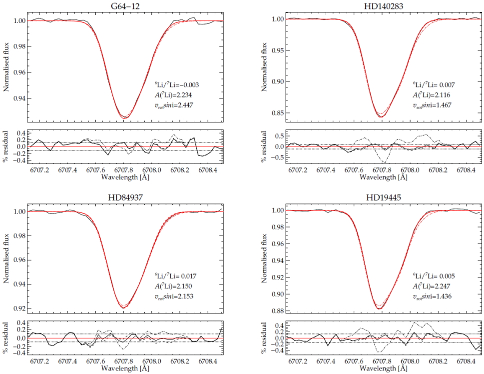
- ^{6}Li/^{7}Li isotope ratios in metal-poor stars offer constraints on Lithium production in BBN and the early Universe.
- Traditional 1D LTE isotopic studies find an over-abundance of ^{6}Li relative to model predictions.
- Issue one: symmetric adhoc broadening (1D $\rightarrow$ 3D)
- Issue two: a limited treatment of line formation (LTE $\rightarrow$ non-LTE)



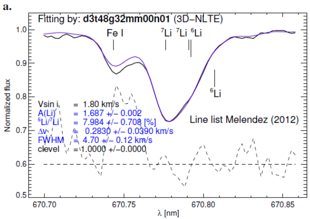
Aoki + (2004) found that the broadening mechanism was of major importance to the isotope ratio.

Isotopes

Lithium isotopes modelled in 3D non-LTE...



Need for ^{6}Li mitigated by inclusion of new physics in Lind + (2013)



New physics not enough to attribute all ^{6}Li in HD 123351 in Mott + (2017)

Non-LTE

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
  $\frac{N_I}{N_{I+1}} = n_e \frac{U_I}{U_{I+1}} \left(\frac{h^2}{2\pi m_e kT} \right)^{\frac{3}{2}} e^{\chi_I/kT}$
- The Maxwellian velocity distribution of particles
  $f(v)\,dv = \left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}} e^{-\frac{mv^2}{2kT}} 4\pi v^2\,dv$

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

Non-LTE radiative transfer

Radiation escapes from a star, so LTE must break down

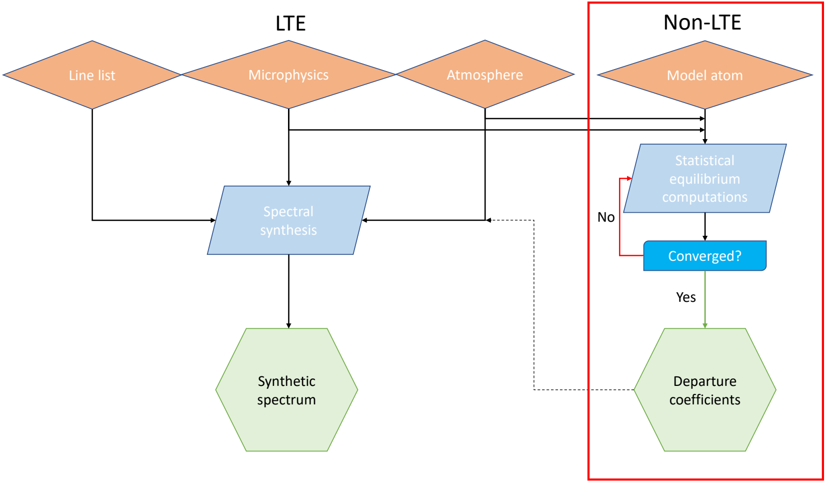
- Radiative rates of some transitions dominate over collisional rates
- Radiation no longer follows a Planckian distribution $\therefore S_\nu \neq B_\nu(T)$; $S_\nu = j_\nu / \kappa_\nu$
- Collisional rates are proportional to particle density; low densities $\rightarrow$ non-LTE
- Saha-Boltzmann distributions no longer determine level/excitation populations

Kinetic equilibrium / Rate equation

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

All transitions at every possible energy level included

Non-LTE spectral synthesis in a nutshell



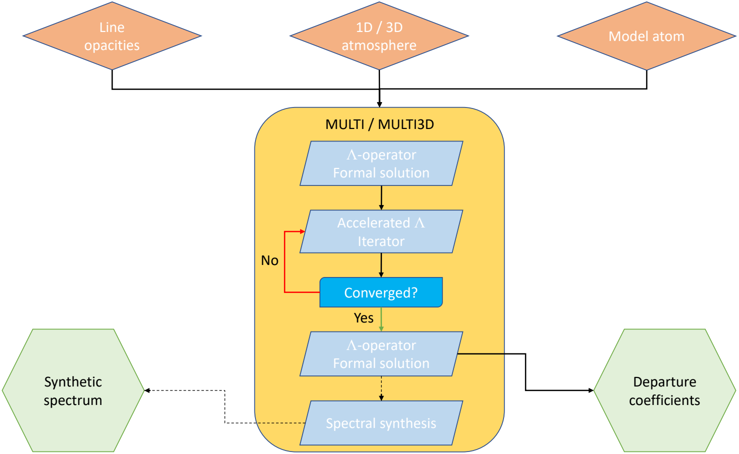
Statistical equilibrium

Several codes on the market to compute these important calculations:

- **MULTI** - 1D S.E. code *public*
  Carlsson (1986)
  Also computes basic 1D non-LTE spectrum synthesis
- **DETAIL** - 1D S.E. code *private*
  Butler & Giddings (1985), Maskonkina + (2011)
- **Multi3D** - 3D S.E. code *private*
  Leenaarts & Carlsson (2009)
  Also computes basic 3D non-LTE spectrum synthesis from atom
- **Balder** - 3D S.E. code *private*
  Amarsi + (2016), Amarsi + (2018), Amarsi + (2019)
  Also computes *full* 3D spectrum synthesis

Most are available upon request subject to terms

Statistical equilibrium



Statistical equilibrium

What's being computed?

Formal solution solved using a Λ-operator:

1. Mean intensity, J_ν, initial guess (usually populations are LTE or 0)
2. Integrate formal transfer solution with enough rays so that J_ν can be approx. calculated
3. Compute J_ν at all locations of atmosphere, hence compute scattering emissivity, j_ν
4. Return to point (2) until J_ν appears to have been converged

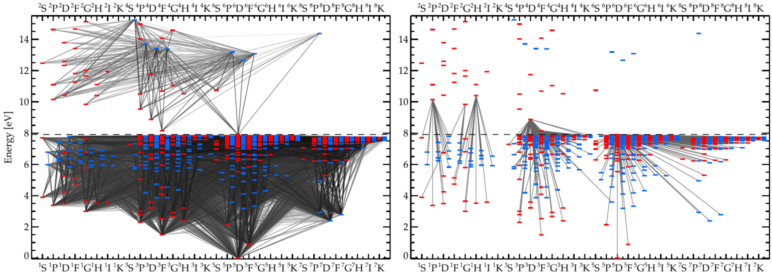
In reality, convergence is usually set by user and governed by changes in population

The model atom

Radiative data

An ASCII table describing the behaviour of an atom

Only the atom modelled is considered in non-LTE. Everything else is LTE!



Iron Lind + (2017)

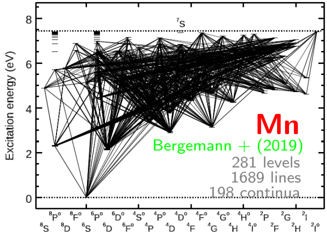
1. Energy levels
2. b-b and b-f transitions

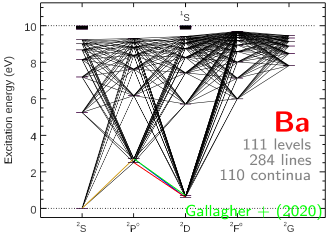
1. 2980 for Fe I, 116 for Fe II
2. $> 500\,000$ for iron

The model atom

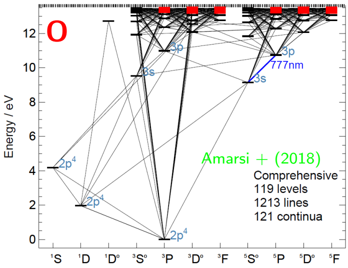
Radiative data

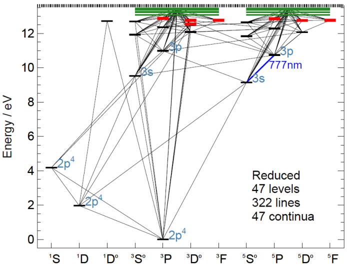
Not all atoms are as large...





Even so, sometimes it is sensible to reduce one's atom





The model atom

Collisional data

Collisional rates computed for a series of temperatures for all radiative b-b and b-f transitions (where possible)

Collisions with various particles:

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

Hard to compute!

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

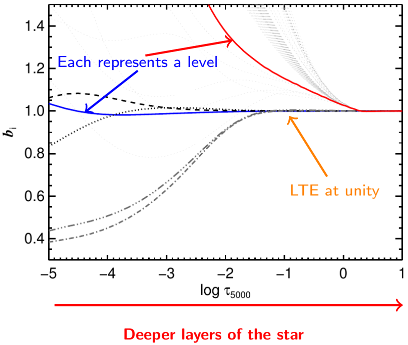
New ab initio quantum mechanical collisions for some atoms now becoming available for H (see Belyaev & Yakovleva 2018), e (see Barklem 2007)

Departure coefficients

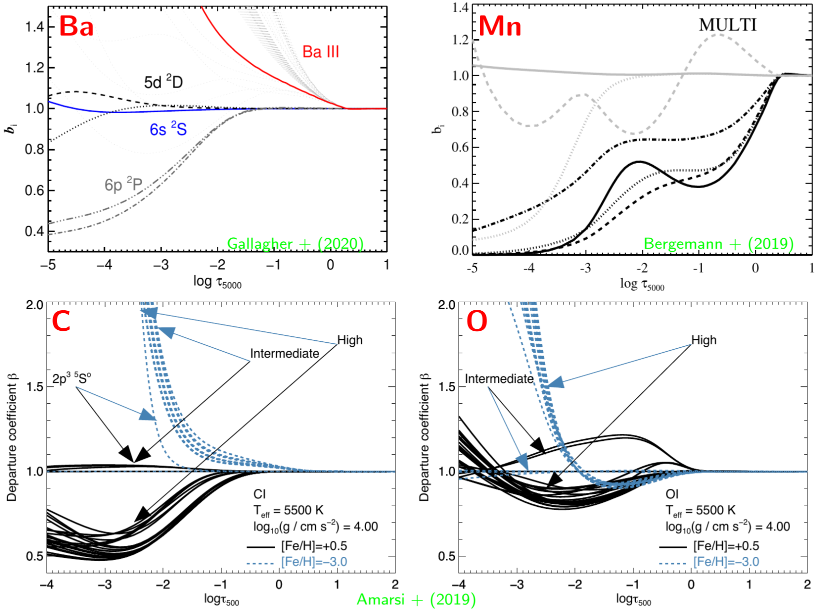
Energy levels affected by effects of non-LTE differently

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

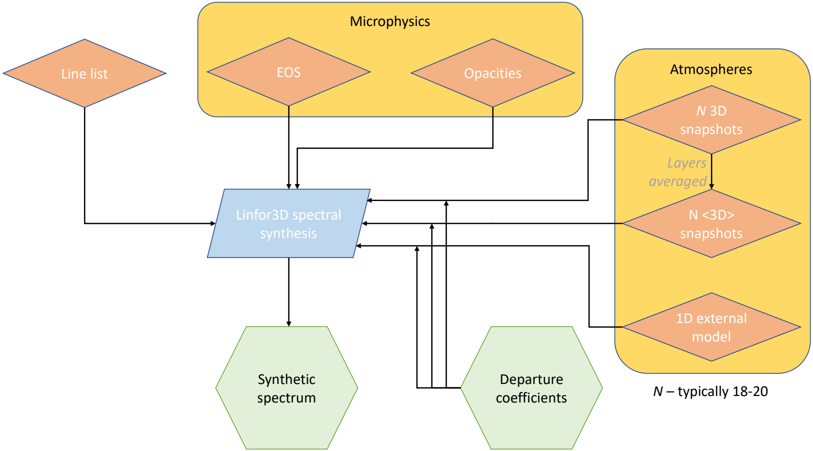
n_i – population of level i



Departure coefficients



3D non-LTE spectral synthesis in a nutshell



N – typically 18-20

Take away messages

3D non-LTE is going through a renaissance...

- Massive efforts leading to a high production of new results
  - 81 refereed papers so far (abundances, methodologies, isotopes, temperatures)
  - 13 since 2019
- Abundance corrections available for a number of key elements (e.g. Li, C, Fe, Mn, Ba, Sr, etc.)
- Currently limited to atoms (molecules are too big)
- Atom only thing treated in non-LTE; everything else assumed to be in LTE

Take away messages

Massive undertaking

- Building a model atom
  - data collation
  - computing collisional rates
- Running a 1D non-LTE simulation
  - Barium in the Sun took $\approx$ **15 seconds**
  - Strontium took $\approx$ **30 seconds**
  - $50 \leq N_{\mathrm{depth}} \leq 150$
- Running a 3D non-LTE simulation
  - Barium in the Sun took $\approx$ **15k hours!**
  - Strontium took $\approx$ **50k hours!**
  - $3,100,000 \leq \mathrm{voxels} \leq 25,000,000$

Take away messages

Ways to speed up 3D non-LTE computations

- Simplifying the atom
  - Atom only thing treated in non-LTE
  - Levels *carefully* collapsed into super levels to reduce size
- Reducing number of horizontal grid points
  - $240^3 \rightarrow 30 \times 30 \times 240$ STAGGER grid
  - $140 \times 140 \times 150 \rightarrow 30 \times 30 \times 150$ CO^{5}BOLD CIFIST grid
  - $280 \times 280 \times 300 \rightarrow 30 \times 30 \times 300$ CO^{5}BOLD hi-res
- 1.5D non-LTE departure coefficients
  - Departures computed for each vertical column in 1D
  - Columns combined to provide 1.5D departures
- Carefully chosen, 1D non-LTE can offer *some* compromise (see Bergemann + 2019)

Useful links/books

Books:

- **Theory of Stellar Atmospheres**
  Ivan Hubeny & Dimitri Mihalas
- **The Observation and Analysis of Stellar Photospheres**
  David F. Gray

Lecture series:

- Robert Rutten's *comprehensive* lecture series on radiative transfer
- C.P. Dullemond's lecture series of radiative transfer

Review papers:

- CO^{5}BOLD paper Freytag + (2012)
- Solar abundances, Asplund + (2021)

Manuals:

- CO^{5}BOLD user manual
- Linfor3D user manual