BEYOND THE CLASSICAL MODELS OF STELLAR ATMOSPHERES AND SPECTRAL LINE FORMATION

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This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101008324 (ChETEC-INFRA)

INTRODUCTION

QUESTIONS TO ASK BEFORE SOLVING ANY ASTROPHYSICAL PROBLEM

- What kind of information is needed?
- How to obtain it?
- What methods and tools to use?
- How to interpret it?

INTRODUCTION

GOALS OF THIS LECTURE

- Bird’s-eye view of the advanced methods and tools for stellar spectroscopic analysis:
  - 3D hydrodynamical model atmospheres
  - Non-local thermodynamic equilibrium (NLTE) spectral line formation and abundance analysis
- Strategies for using them to study stars and stellar populations

INTRODUCTION

MAIN QUESTIONS TO BE ADDRESSED

- What are the pros and cons of using advanced methods and tools of stellar spectroscopic analysis?
- Where and how to apply them?
- What new information can be obtained?

INTRODUCTION

TOPICS **NOT** TO BE ADDRESSED

- Fundamentals of stellar spectroscopy and abundance analysis
- Detailed overview of various methods and tools for stellar abundance analysis
- Guidelines on how to use them

INTRODUCTION

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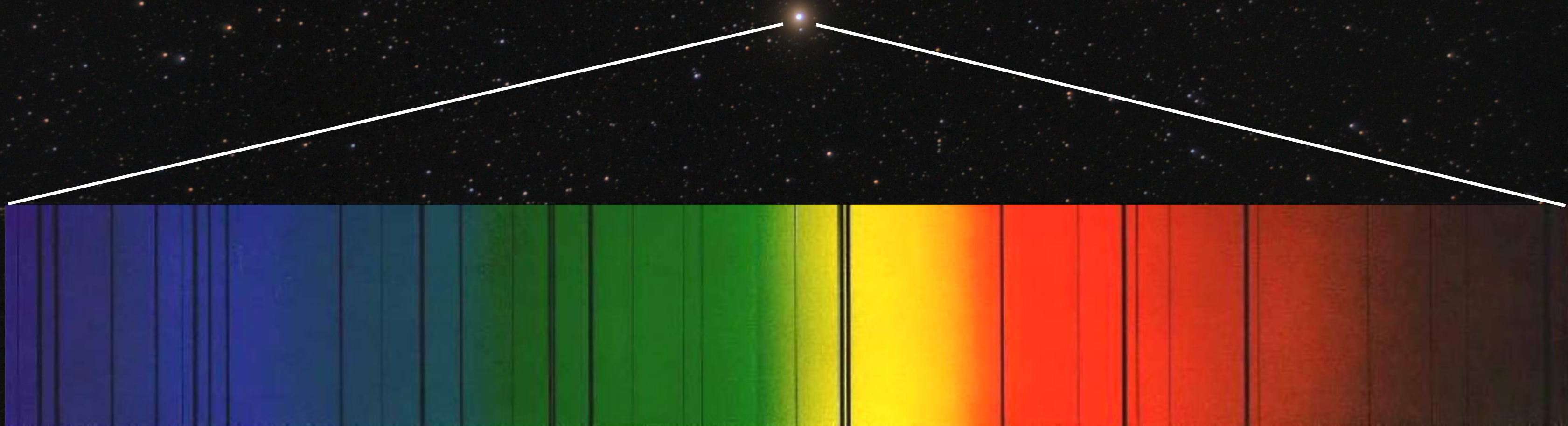
- Fundamentals of stellar spectroscopy and abundance analysis
- Detailed overview of various methods and tools for stellar abundance analysis
- Guidelines on how to use them

FURTHER RESOURCES

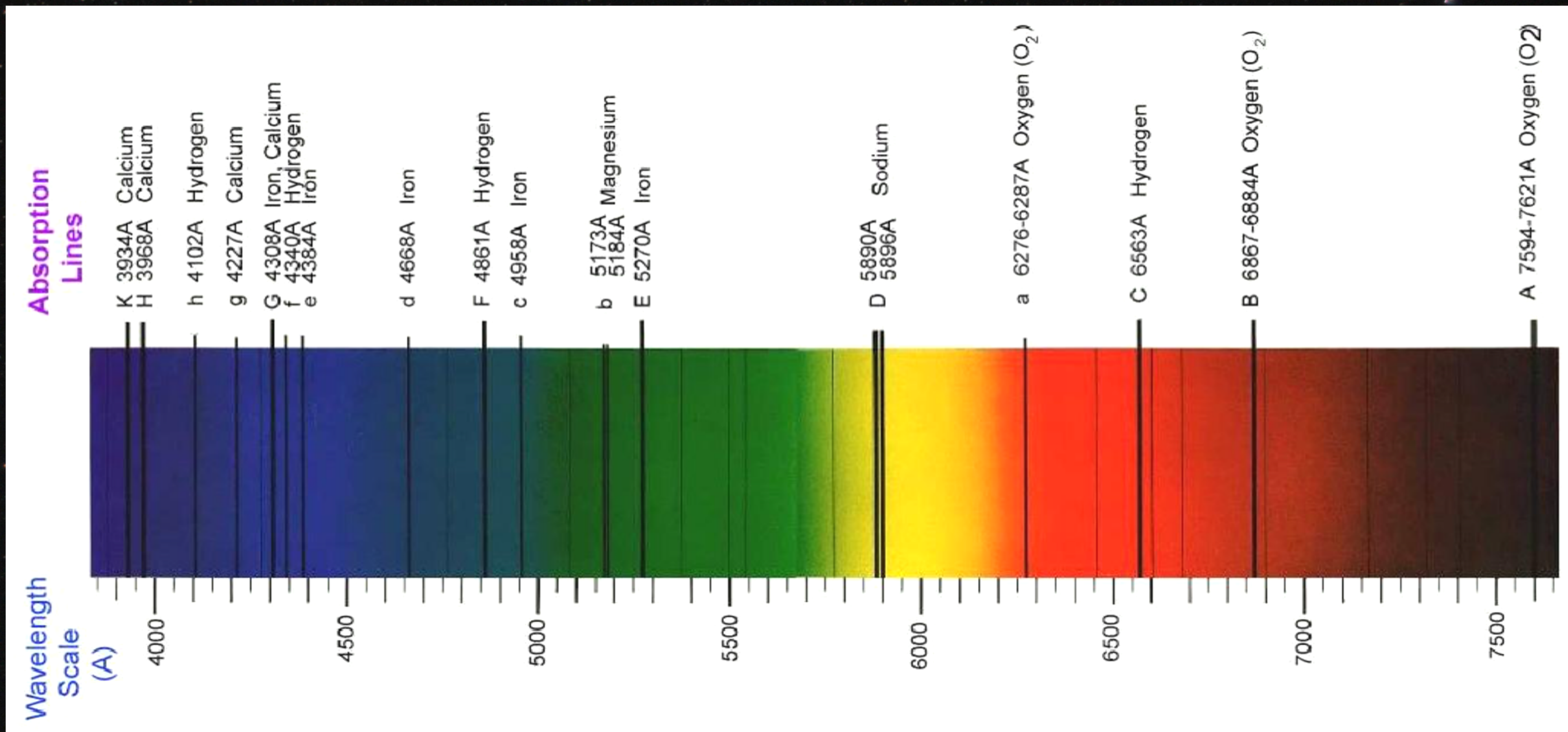
- This lecture: a bird's-eye overview!
- Talks by Brankica, Tiina, Camilla, Gabriele earlier this week
- Various internet resources: introductory lectures/courses on classical and advanced stellar spectroscopy, stellar atmosphere modelling, and radiative transfer in stellar atmospheres

SPECROSCOPIC ANALYSIS OF STARS



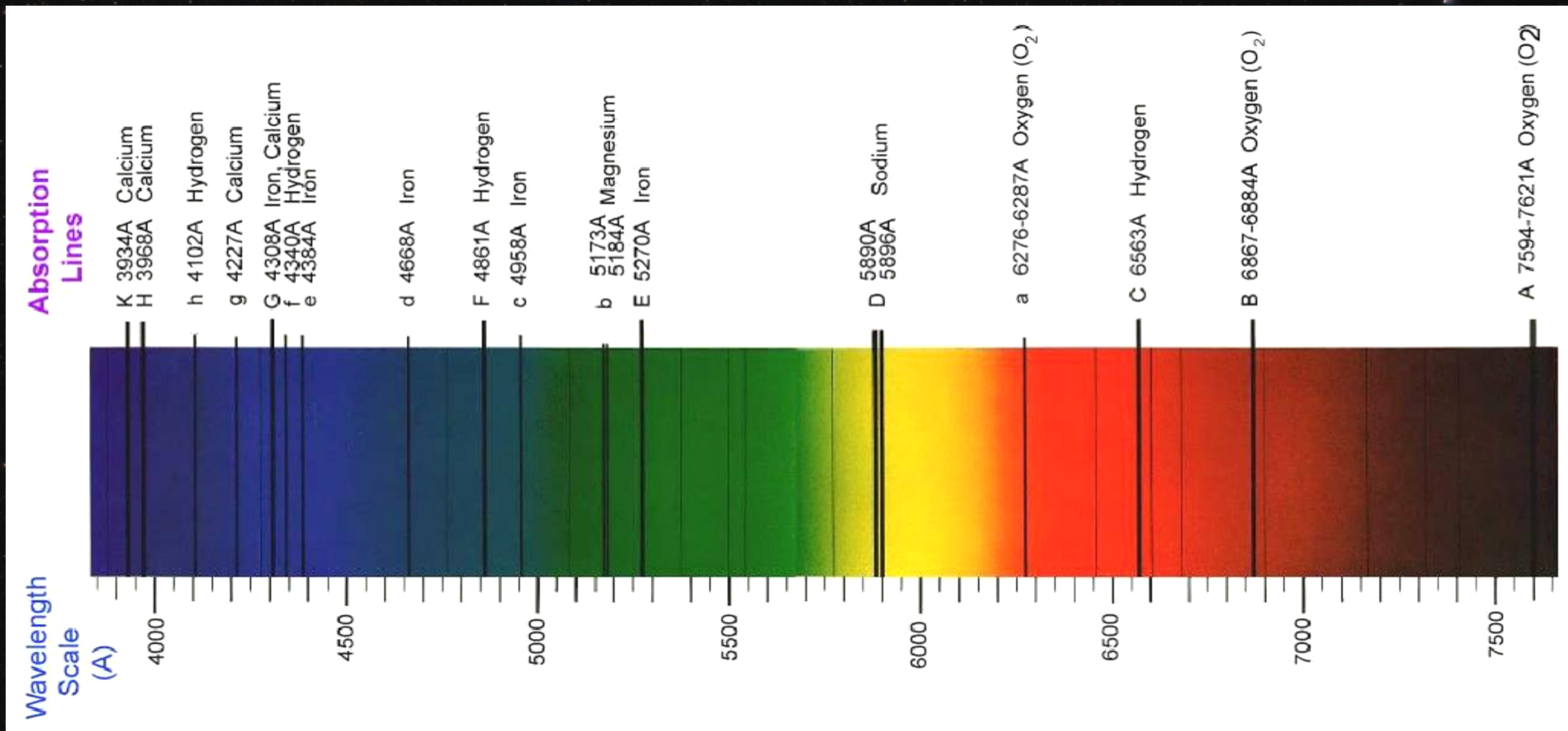
SPECROSCOPIC ANALYSIS OF STARS

PHOTONS = INFORMATION!



SPECROSCOPIC ANALYSIS OF STARS

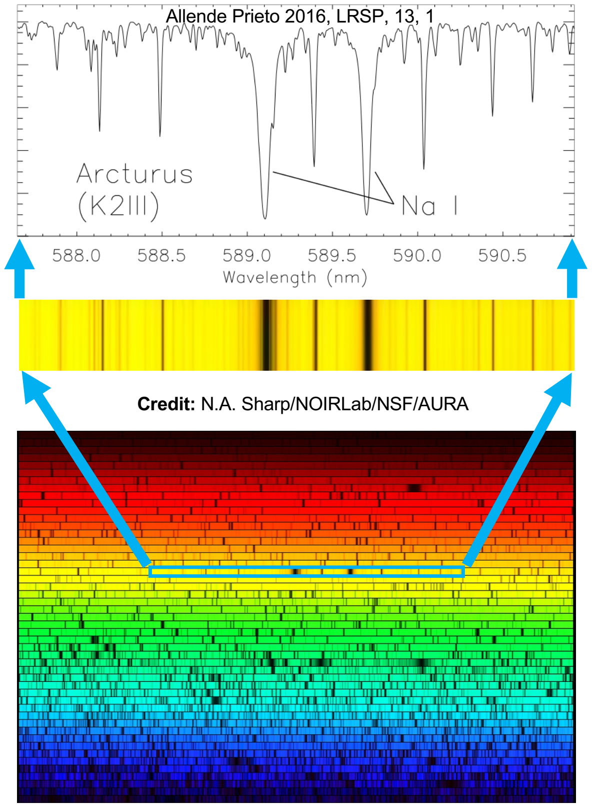
HOW TO ANALYSE STELLAR SPECTRA?



SPECTROSCOPIC ANALYSIS STARS

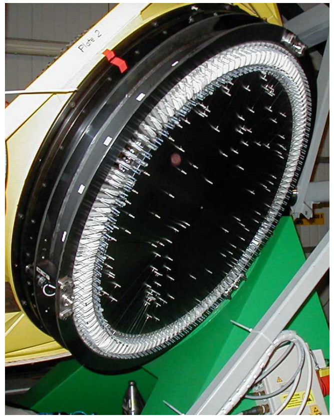
(1) OBSERVATIONS

Observed spectrum: Arcturus

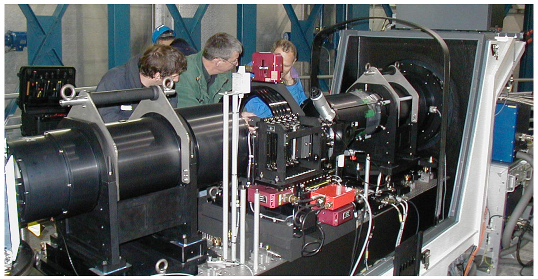


Credit: N.A. Sharp/NOIRLab/NSF/AURA

Telescopes, spectrographs



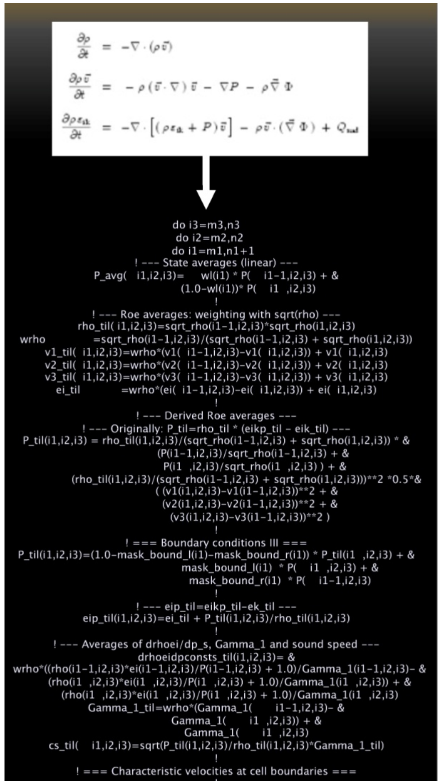
Credit: ESO



SPECTROSCOPIC ANALYSIS STARS

(2) THEORETICAL MODELS

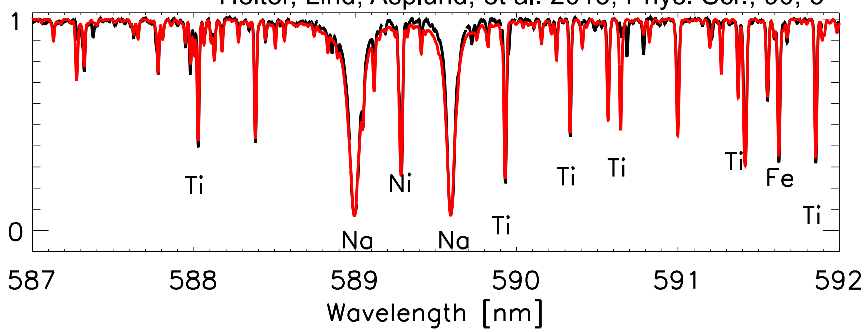
Assumptions about the physics; codes, computers

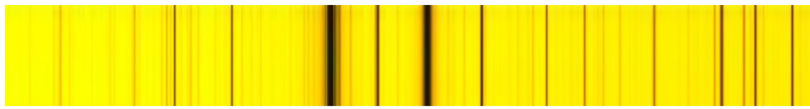


Credit: RIKEN; C. Jones, Oak Ridge National Laboratory

Fits of theoretical to the observed spectra

Heiter, Lind, Asplund, et al. 2015, Phys. Scr., 90, 5



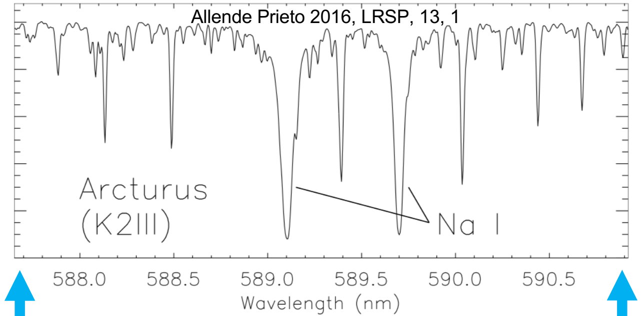


Credit: N.A. Sharp/NOIRLab/NSF/AURA

SPECTROSCOPIC ANALYSIS STARS

OBSERVATIONS VS THEORY

Observed spectrum



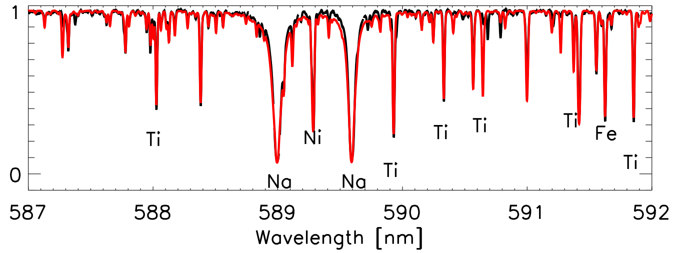
Credit: N.A. Sharp/NOIRLab/NSF/AURA

Credit: ESO

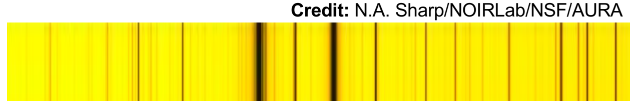
Comparison to constrain stellar parameters, thermodynamics, abundances, ...

Theory vs observations

Heiter, Lind, Asplund, et al. 2015, Phys. Scr., 90, 5



Credit: N.A. Sharp/NOIRLab/NSF/AURA

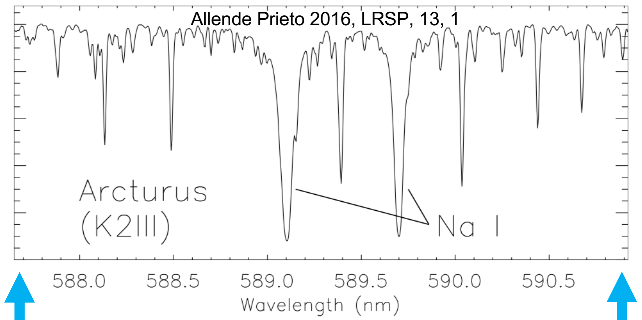


Credit: C. Jones, Oak Ridge National Laboratory

SPECTROSCOPIC ANALYSIS STARS

OBSERVATIONS VS THEORY

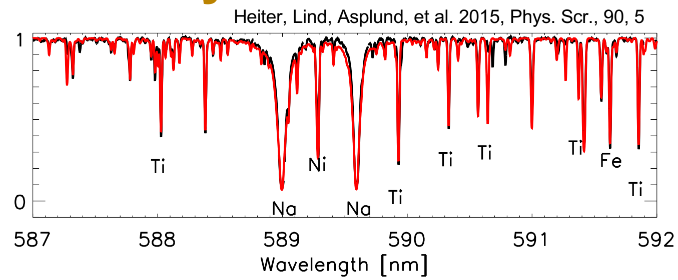
Observed spectrum



Credit: N.A. Sharp/NOIRLab/NSF/AURA

How to obtain spectra?
How to interpret them?
What can we learn?

Theory vs observations



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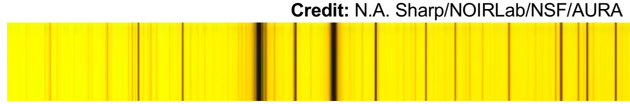


Credit: ESO

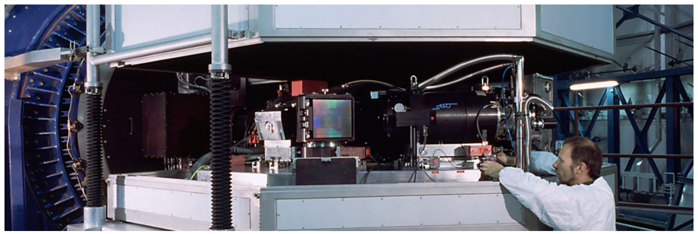
Credit: C. Jones, Oak Ridge National Laboratory

STELLAR SPECTROSCOPY: THE CLASSICS

OBSERVATIONS: "CLASSICAL" SINGLE-OBJECT SPECTROSCOPY

- Studies of individual objects: stars in Galactic streams, metal-poor stars, etc.
- Spectrographs available on small to large(st) telescopes (e.g. NOT+FIES -> VLT+UVES)
- Optimal number of objects to be studied: several to 10^2

VLT UT2 (8m)



UVES

Objects: up to 8 per exposure
Range (single setup): 300–500 nm (blue arm)
Resolution: R~80000 max (blue arm)

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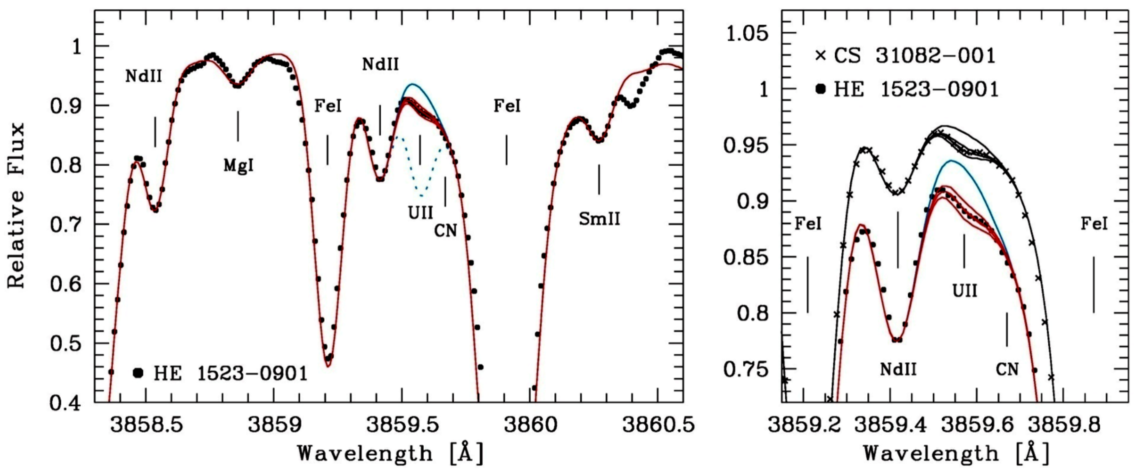

EXAMPLE: age determination of stars/stellar populations

Abundance of ^{238}U in the atmospheres of evolved stars CS31082-0018 (Cayrel et al. 2001; R=70000, S/N~150) and HE1523-0901 (Frebel et al. 2007; UVES, R=75000, S/N~350) obtained using the method of spectral synthesis.

A(U) / A(Th) → Age!

STELLAR SPECTROSCOPY: THE CLASSICS

OBSERVATIONS: "CLASSICAL" SINGLE-OBJECT SPECTROSCOPY

PROS

- Perfect to study a small number of individual targets scattered across the sky
- High resolution and high signal-to-noise ratio possible

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OBSERVATIONS: “CLASSICAL” SINGLE-OBJECT SPECTROSCOPY

PROS

- Perfect to study a small number of individual targets scattered across the sky
- High resolution and high signal-to-noise ratio possible

CONS

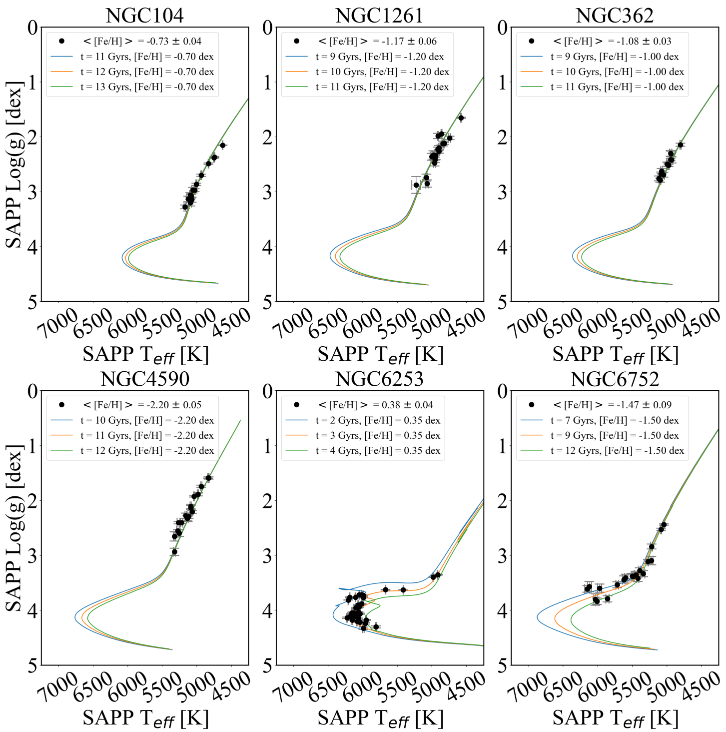
- Studies of large numbers of objects tedious and time-consuming
- Competition for observing time may be high, in particular, for instruments that can be used both in single and multi-object modes

STELLAR SPECTROSCOPY: THE CLASSICS

THEORY: "CLASSICAL" 1D LTE SPECTROSCOPIC ANALYSIS

- 1D hydrostatic model atmospheres
- Assumption of local thermodynamic equilibrium (LTE) in spectral line synthesis

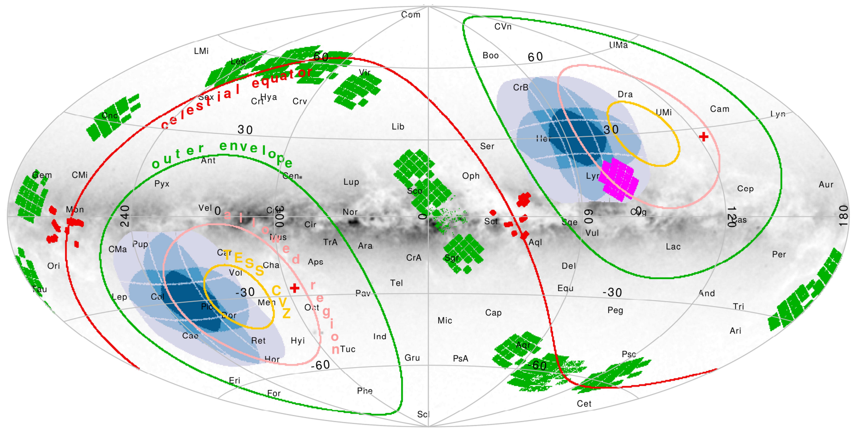
Gent et al. 2022, A&A, 658, A147



EXAMPLE: stellar parameter and abundance pipeline for PLATO

Below: PLATO fields (in blue). **Left:** Surface gravities determined using the PLATO SAPP pipeline for several Galactic globular clusters (the SAPP was "calibrated" using the 1D MARC model atmospheres).

Rauer et al. 2025, Exp. Astron., 59, i26



STELLAR SPECTROSCOPY: THE CLASSICS

THEORY: “CLASSICAL” 1D LTE SPECTROSCOPIC ANALYSIS

PROS

- Fast and easy computation of model atmospheres and line synthesis
- Suitable for many tasks, still the main horse in stellar abundance analysis
- Can be automated/scaled for the analysis of large numbers of stars
- Grids of 1D model atmospheres are readily available

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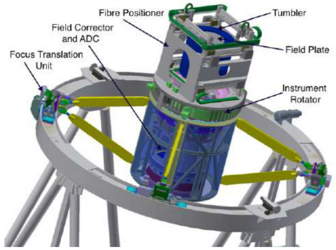
CONS

- 1D – symmetry and homogeneity in all directions
- Hydrostatic – nothing moves
- Convection is parametrized, not modelled

STELLAR SPECTROSCOPY: BEYOND THE CLASSICS

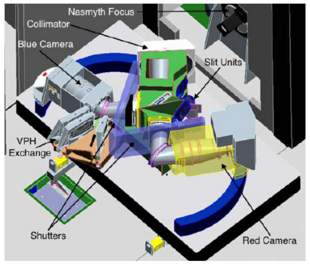
OBSERVATIONS: MULTI-OBJECT SPECTROSCOPY

- Dedicated spectroscopic surveys – spectra of large numbers of stars
  - Multi-object spectrographs



WHT (4.2m)

WEAVE
Fibers: 1004
Objects: ~850 per exposure
Range: 404–685 nm;
Resolution: 18000-30000



VLT UT2 (8m)

GIRAFFE
Objects: ~120 per exposure
(132 fibers with Medusa)
Range: 370–900 nm; ~20 nm per exp.
Resolution: 18000-30000

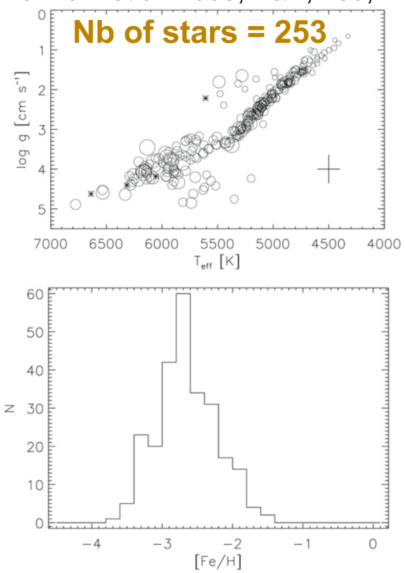
STELLAR SPECTROSCOPY: BEYOND THE CLASSICS

OBSERVATIONS: MULTI-OBJECT SPECTROSCOPY

- Dedicated spectroscopic surveys – spectra of large numbers of stars
  - Multi-object spectrographs
  - Number of objects: 10^5–10^6 stars

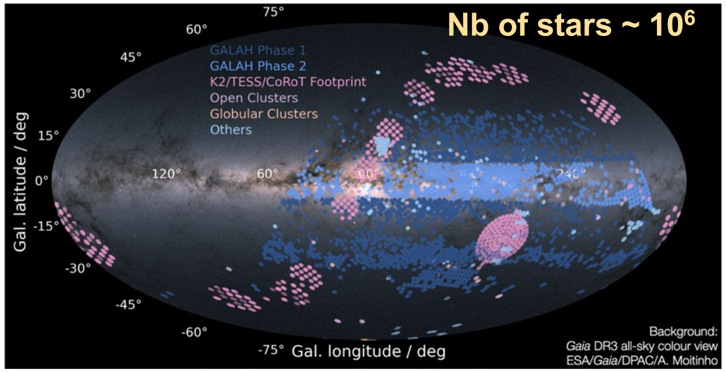
Initial HERES sample

Barklem et al. 2005, A&A, 439, 121



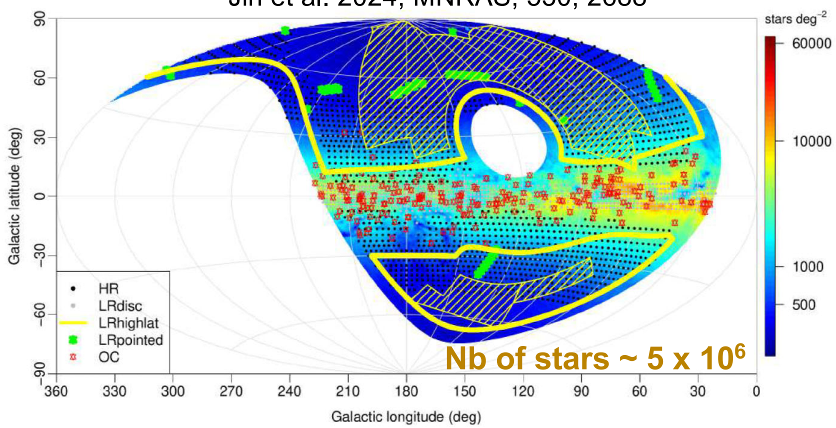
GALAH DR4

Buder et al. 2025, PASA, 42, e051



WEAVE GA surveys

Jin et al. 2024, MNRAS, 530, 2688



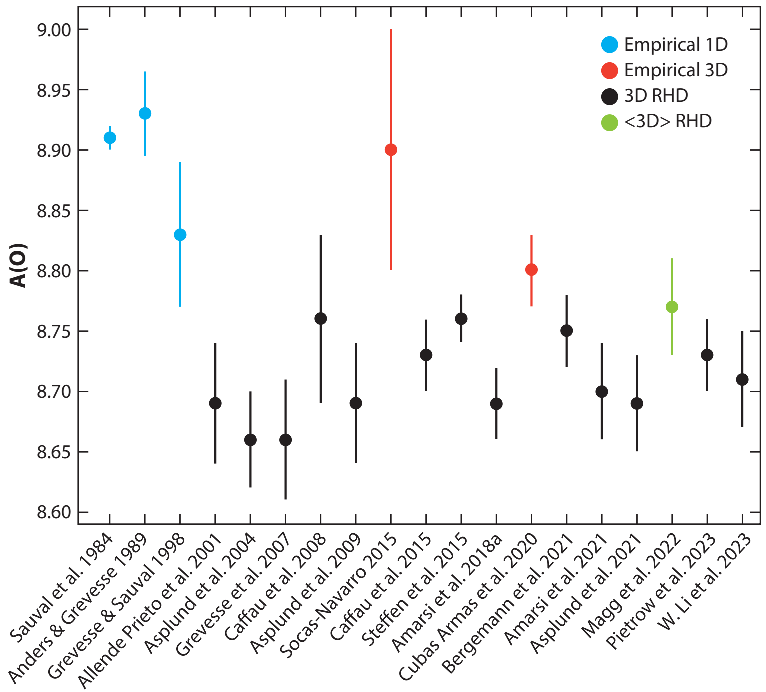
STELLAR SPECTROSCOPY: BEYOND THE CLASSICS

OBSERVATIONS: MULTI-OBJECT SPECTROSCOPY

- BUT: studies of individual stars with single-object spectrographs still relevant!
  - Analysis of atmospheric structures, non-stationary phenomena, high-precision abundances

Solar oxygen abundance

Lind & Amarsi 2024, ARAA, 62, 475



STELLAR SPECTROSCOPY: BEYOND THE CLASSICS

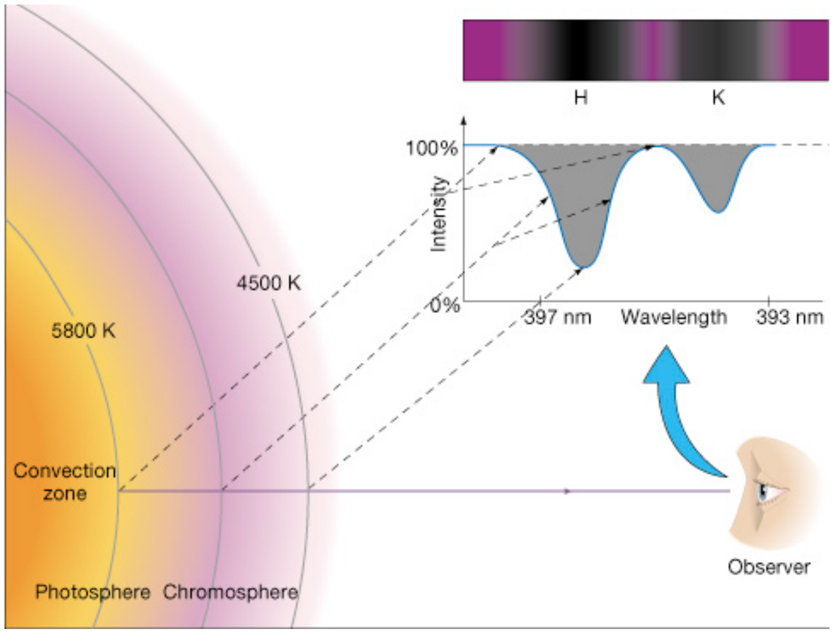
THEORY: WHAT ARE THE OPTIONS BEYOND THE CLASSICS?

- 3D hydrodynamical model atmospheres
- Non-LTE (NLTE) spectral line synthesis
- Ability to apply to a large number of stars!

STELLAR MODEL ATMOSPHERES AND LINE SYNTHESIS

WHAT IS NEEDED TO COMPUTE A SPECTRUM OF THE STAR?

(1) Model atmosphere: theoretical model of the upper (outer) stellar layers
(2) Spectrum synthesis tool(s) for computing spectral line profiles



STELLAR MODEL ATMOSPHERES AND LINE SYNTHESIS

(1) HOW TO COMPUTE A STELLAR MODEL ATMOSPHERE?

Ingredients

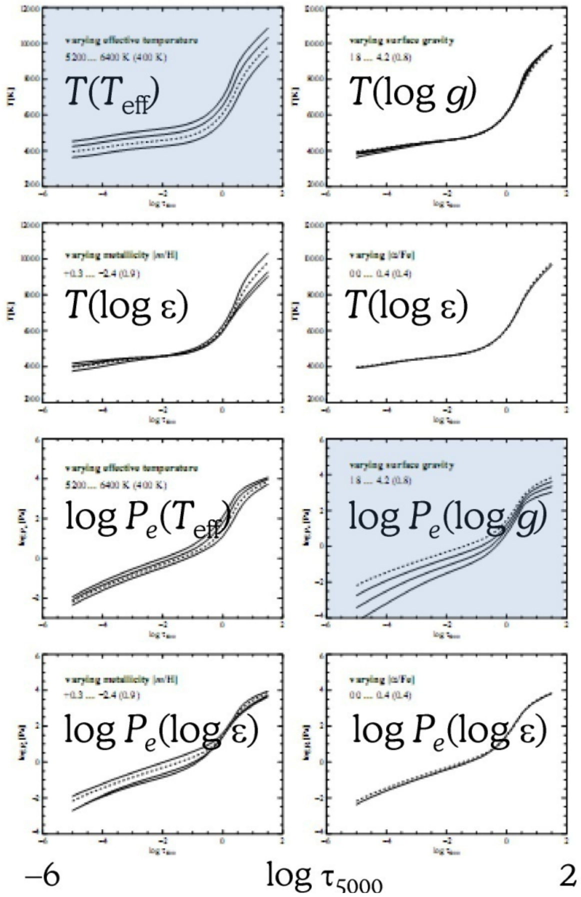
- Stellar structure equations:
  - Equations of gravitational equilibrium, energy transfer, etc.:
    system of differential + algebraic equations
- Equation of radiative transfer
  - A “simplified” version
- Auxiliary data:
  - Opacities, equation of state (EOS)
- Stellar parameters to characterize the star:
  - effective temperature, gravitational acceleration (surface gravity), chemical composition, etc.
    (spherical models: stellar mass)

STELLAR MODEL ATMOSPHERES AND LINE SYNTHESIS

(1) HOW TO COMPUTE A STELLAR MODEL ATMOSPHERE?

Output

- Model atmosphere of a given star:
  - dependence of temperature, gas and electron pressure, density, ... , on the depth in stellar atmosphere (optical depth, mass or geometrical coordinate)
- No stellar spectrum is produced!



Examples of temperature and electron pressure profiles in stellar atmospheres and their dependence on various stellar parameters

STELLAR MODEL ATMOSPHERES AND LINE SYNTHESIS

(1) HOW TO COMPUTE A STELLAR MODEL ATMOSPHERE?

1D STELLAR MODEL ATMOSPHERES

- 1D hydrostatic – mainstream:
  - ATLAS: Kurucz (1970, 1993)
  - MARCS: Gustafsson et al. (1975, 2008)
  - PHOENIX: Hauschildt et al. (1999)
- Various semi-empirical approaches:
  - 1D Holweger-Muller solar model: Holweger & Müller (1974)

STELLAR MODEL ATMOSPHERES AND LINE SYNTHESIS

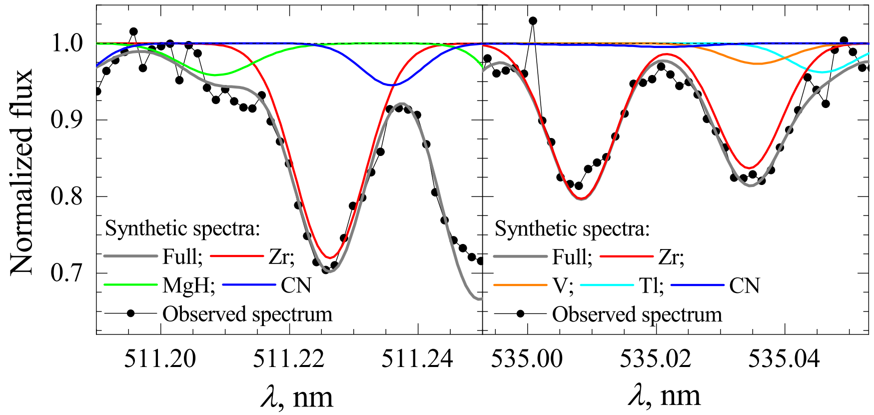
(2) HOW TO COMPUTE A STELLAR SPECTRUM?

Spectrum synthesis tools

- Solves the radiative transfer equation to characterise the wavelength-dependent radiative field in the given stellar model atmosphere:
  - This is how the spectral line profiles are produced!
- Ingredients:
  - Model atmosphere of a given star, chemical composition, opacities, equation of state, atomic parameters of spectral lines to be studied (wavelengths, oscillator strengths), etc.
- Output: stellar spectrum in a selected wavelength range

Zr II lines, star #20885 in 47 Tuc

Kolomiecas et al. 2022, A&A, 660, A46



STELLAR MODEL ATMOSPHERES AND LINE SYNTHESIS

(2) HOW TO COMPUTE A STELLAR SPECTRUM?

Spectrum synthesis tools

- Abundances of chemical elements:
  - Strengths of spectral lines depend on the abundance of a given chemical element
  - By adjusting abundance, one may produce lines of different strengths and choose the one that best fits the observed profile
  - Abundance of the chemical element = abundance that was used to compute the best-fitting synthetic line profile
- Methods to determine abundances:
  - Synthetic spectrum method

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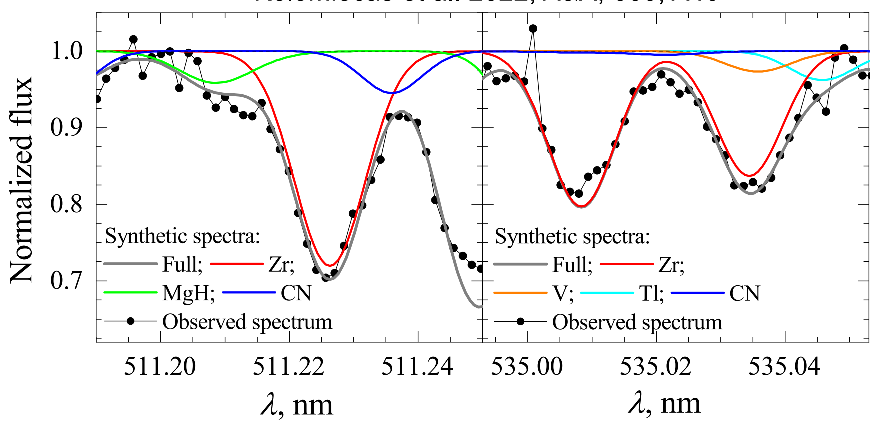

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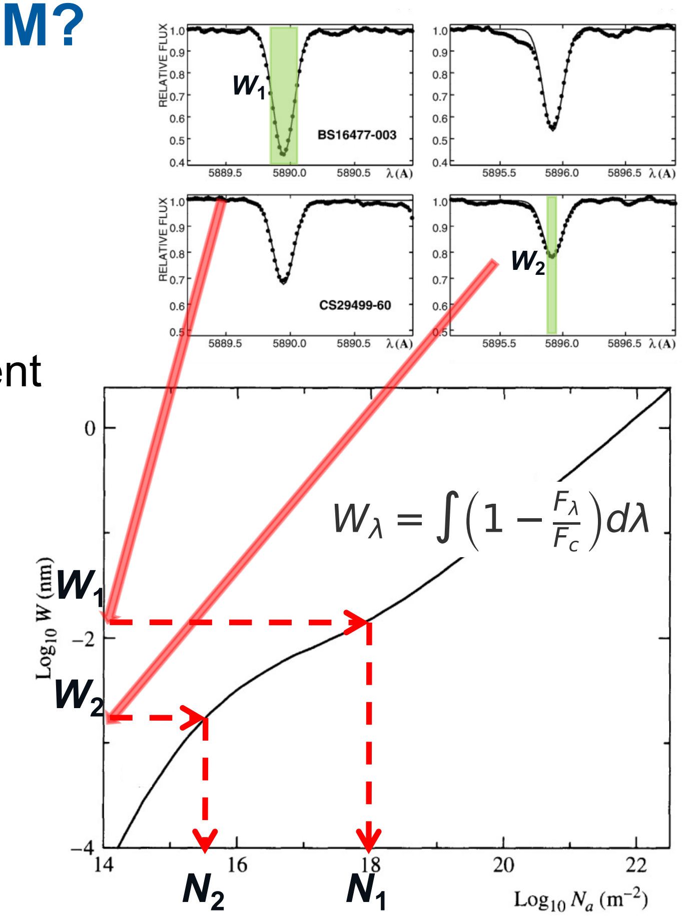
- Methods to determine abundances:
  - Synthetic spectrum method
  - Equivalent width model

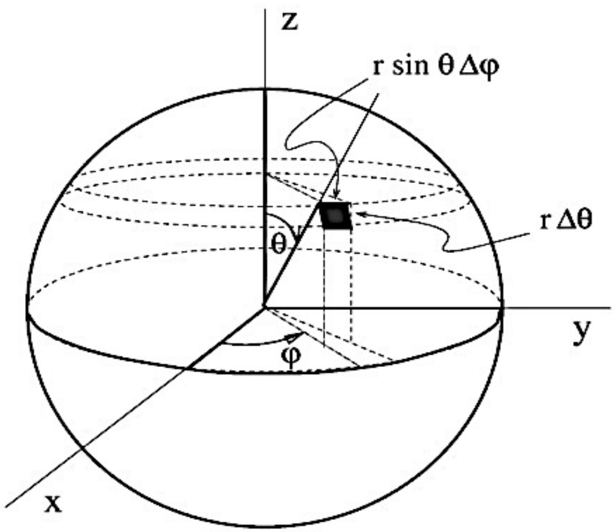


Determination of abundances of chemical elements in stellar atmospheres using the method of curves of growth.

3D HYDRODYNAMICAL STELLAR MODEL ATMOSPHERES

LIMITATIONS OF 1D HYDROSTATIC MODEL ATMOSPHERES

- 1D dimensional – symmetry and homogeneity in all directions!
- Hydrostatic – nothing moves!
- Convection is parametrized, not modelled!
- BUT – fast and easy to compute; extensive grids are available



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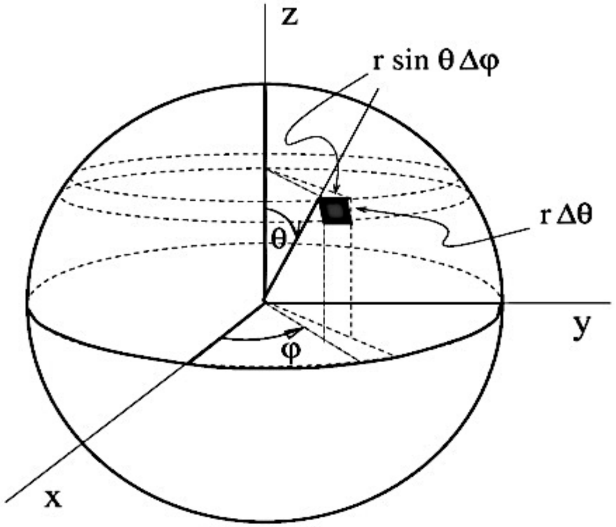
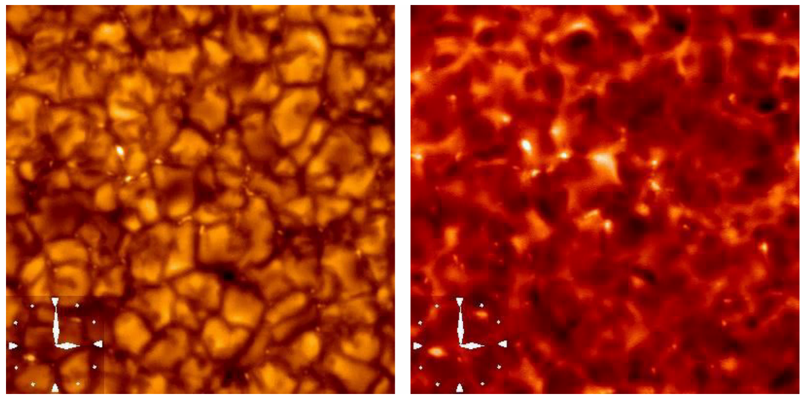




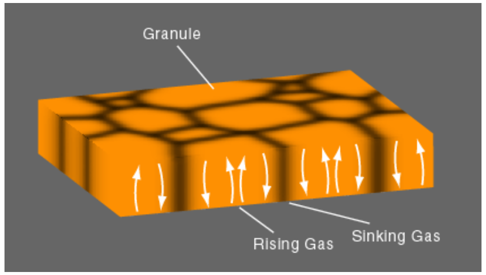
Quiet Sun: in the G-band (430 nm, left) and Ca II H band (397 nm, right; SOT/HINODE).

3D HYDRODYNAMICAL STELLAR MODEL ATMOSPHERES

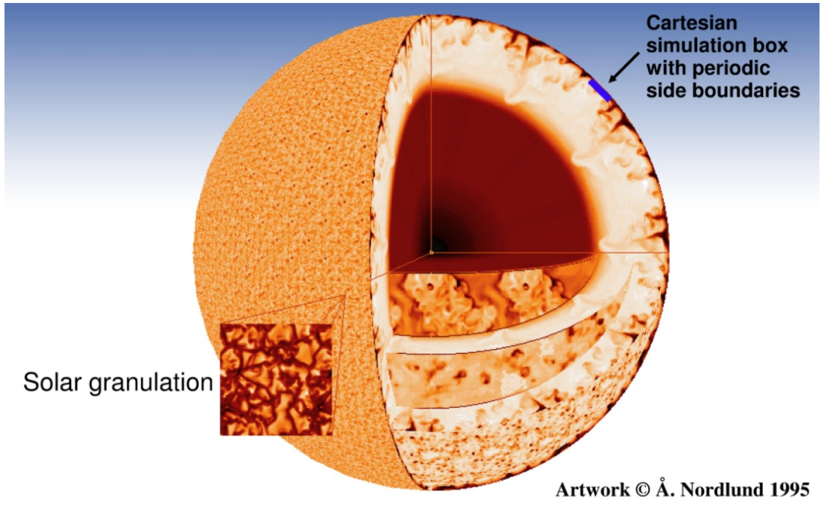
BEYOND THE CLASSICAL 1D HYDROSTATIC MODEL ATMOSPHERES

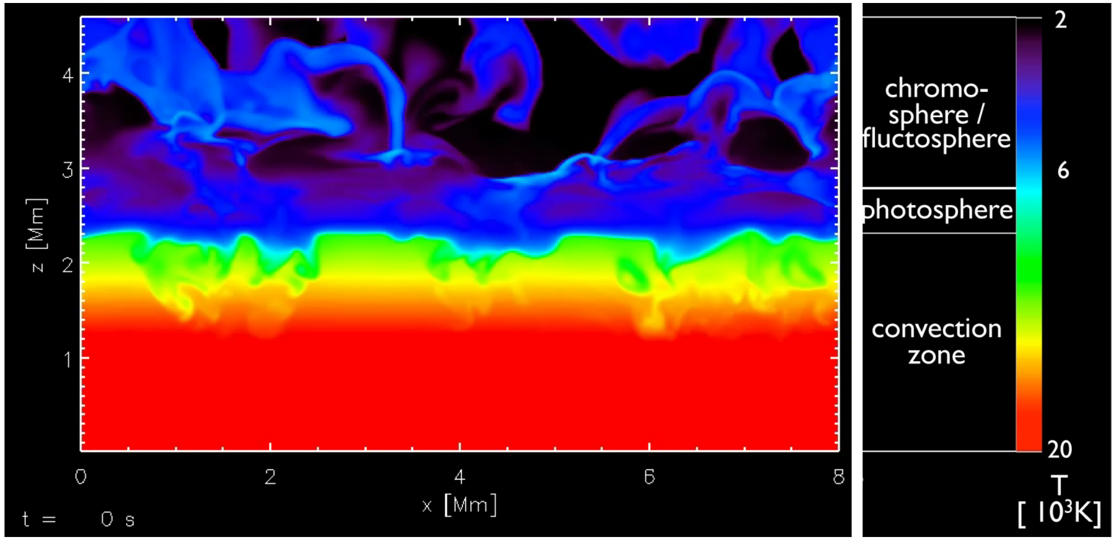
3D hydrodynamical model atmospheres

- Realistic representation of the surface convection
- Tools to compute 3D hydrodynamical models available
- Tools to do 3D spectral line synthesis available



3D HYDRO MODEL ATMOSPHERES





3D HYDRODYNAMICAL STELLAR MODEL ATMOSPHERES

HOW TO COMPUTE A 3D HYDRODYNAMICAL MODEL ATMOSPHERE?

Assumptions about the physics

- Hydrodynamical equations:
  - Equations of the conservation of mass, momentum, energy transfer, etc.: system of differential + algebraic equations
- Equation of radiative transfer
  - A “simplified” version
- Auxiliary data:
  - Opacities, equation of state (EOS)
- Stellar parameters to characterize the star:
  - effective temperature, gravitational acceleration (surface gravity), chemical composition, etc. (spherical models: stellar mass)

3D HYDRODYNAMICAL STELLAR MODEL ATMOSPHERES

HOW TO COMPUTE A 3D HYDRODYNAMICAL MODEL ATMOSPHERE?

Assumptions about the numerics

- Choice of the physical model size – the computational box:
  - How big must the computational box be to capture all important effects?
  - Example: fine-structure of the Sun: at least a few granules in each horizontal direction
- Discretization:
  - Solution of the physical equations on discrete grid locations (or on grid cells)
  - Numerical grid:
    - Box in a star? Star in a box?
    - How many grid points?
- Etc., etc., etc., …

3D HYDRODYNAMICAL STELLAR MODEL ATMOSPHERES

HOW TO COMPUTE A 3D HYDRODYNAMICAL MODEL ATMOSPHERE?

Coding, debugging, coding, debugging, …, repeat!

$$\rho,\ \rho v1, \rho v2, \rho v3,\ \rho eikg$$
$$\rho,\ v1, v2, v3,\ ei$$

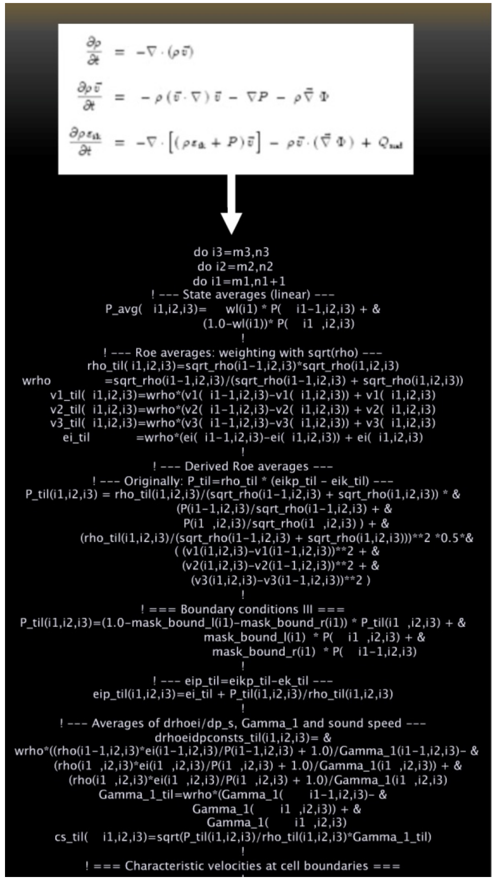
$$\frac{\partial \rho}{\partial t} + \frac{\partial\, \rho\, v1}{\partial x1} + \frac{\partial\, \rho\, v2}{\partial x2} + \frac{\partial\, \rho\, v3}{\partial x3} = 0$$

$$\frac{\partial}{\partial t}\begin{pmatrix} \rho v1 \\ \rho v2 \\ \rho v3 \end{pmatrix} + \frac{\partial}{\partial x1}\begin{pmatrix} \rho v1\ v1 + P \\ \rho v2\ v1 \\ \rho v3\ v1 \end{pmatrix} + \frac{\partial}{\partial x2}\begin{pmatrix} \rho v1\ v2 \\ \rho v2\ v2 + P \\ \rho v3\ v2 \end{pmatrix} + \frac{\partial}{\partial x3}\begin{pmatrix} \rho v1\ v3 \\ \rho v2\ v3 \\ \rho v3\ v3 + P \end{pmatrix} = \begin{pmatrix} \rho\ g1 \\ \rho\ g2 \\ \rho\ g3 \end{pmatrix}$$

$$\frac{\partial \rho eik}{\partial t} + \frac{\partial\,(\rho eik + P)\ v1}{\partial x1} + \frac{\partial\,(\rho eik + P)\ v2}{\partial x2} + \frac{\partial\,(\rho eik + P)\ v3}{\partial x3} = \rho\ (g1\ v1 + g2\ v2 + g3\ v3) + Q_{\mathrm{rad}}$$

$$P = P(\rho, ei)\ .$$

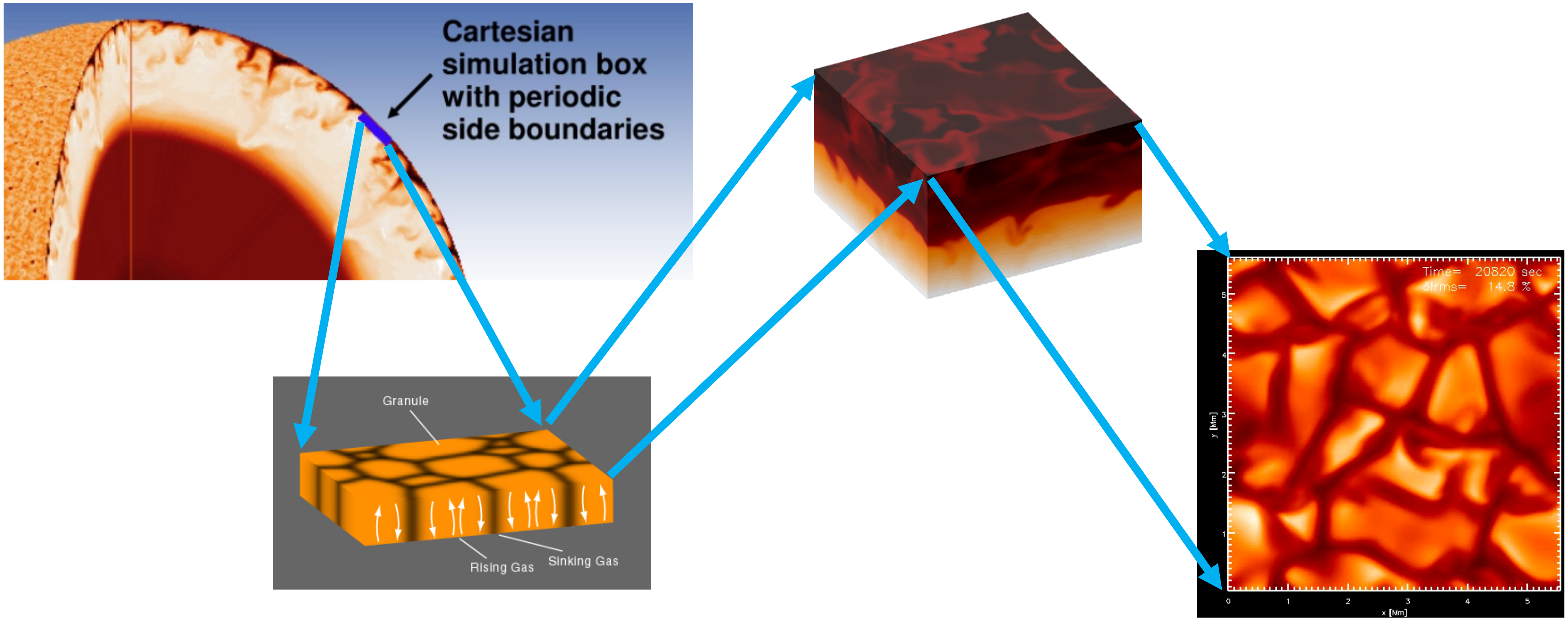
$$\vec{g} = \begin{pmatrix} g1 \\ g2 \\ g3 \end{pmatrix} = -\begin{pmatrix} \frac{\partial}{\partial x1} \\ \frac{\partial}{\partial x2} \\ \frac{\partial}{\partial x3} \end{pmatrix} \Phi$$



3D HYDRODYNAMICAL STELLAR MODEL ATMOSPHERES

HOW TO COMPUTE 3D HYDRODYNAMICAL MODEL ATMOSPHERE?

3D HYDRO MODEL ATMOSPHERE: BOX-IN-A-STAR



3D HYDRODYNAMICAL STELLAR MODEL ATMOSPHERES

HOW TO COMPUTE 3D HYDRODYNAMICAL MODEL ATMOSPHERE?

SELECTED 3D STELLAR MODEL ATMOSPHERE CODES

- CO^5BOLD: Freytag et al. 2012, J. Comp. Phys., 231, 919
- Stagger: Magic et al. 2013, A&A, 557, A26
- MURAM: Vögler et al. 2005, A&A, 429, 335

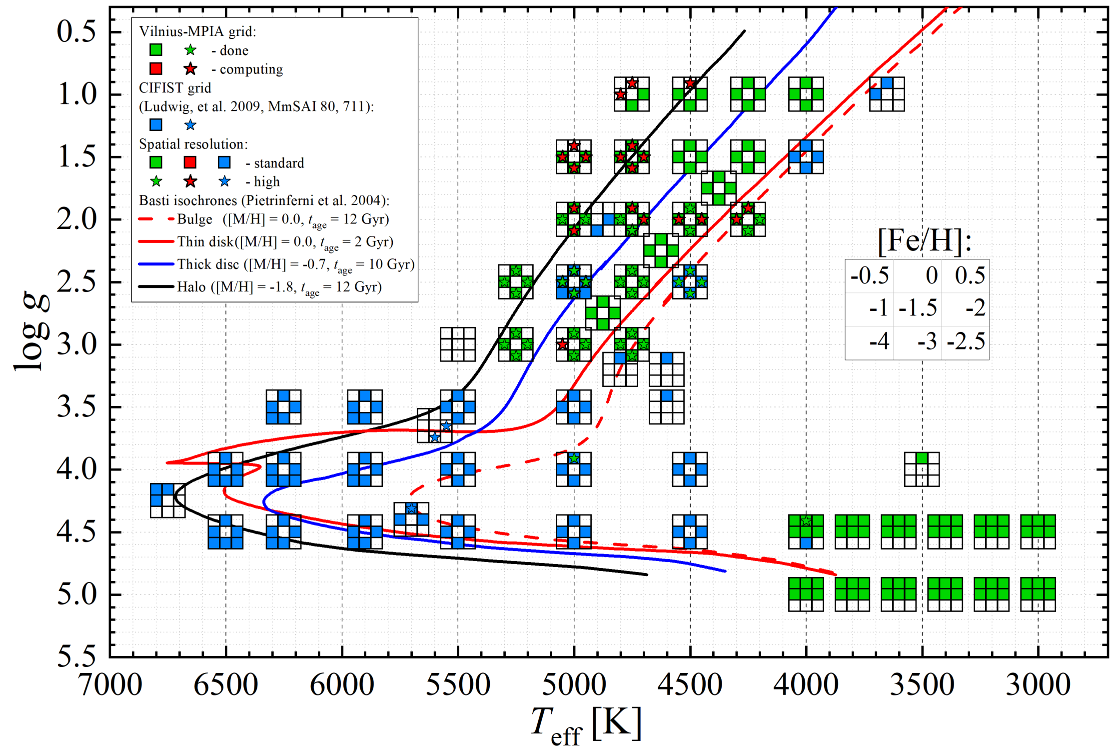
3D HYDRODYNAMICAL STELLAR MODEL ATMOSPHERES

GRIDS OF 3D HYDRODYNAMICAL MODEL ATMOSPHERES

CO⁵BOLD 3D MODEL ATMOSPHERE GRID

- Cartesian geometry, box-in-a-star
- 240x240x240 (*xyz*) grid points per model
- T_{eff} = 4000 – 6500 K, ΔT_{eff} = 250 K
- log g = 1.0 – 5.0, Δlog g = 0.5
- [Fe/H] = – 3.0, –2.0, –1.0, 0.0

Klevas et al., in prep.



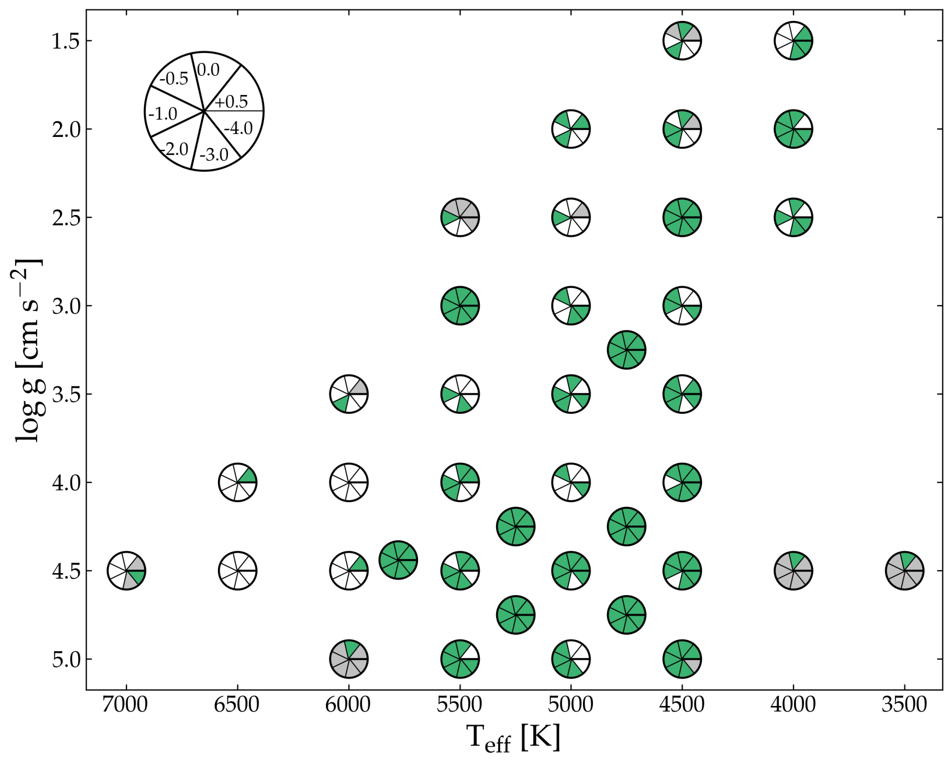
3D HYDRODYNAMICAL STELLAR MODEL ATMOSPHERES

GRIDS OF 3D HYDRODYNAMICAL MODEL ATMOSPHERES

STAGGER 3D MODEL ATMOSPHERE GRID

- Cartesian geometry, box-in-a-star
- 240x240x240 (*xyz*) grid points per model
- T_{eff} = 4000 – 6500 K, ΔT_{eff} = 250 K
- log g = 1.5 – 5.0, Δlog g = 0.5
- [Fe/H] = – 4.0 to +0.5, Δ[Fe/H] = 0.5

Rodrigues Diaz et al. 2024, A&A, 688, A212



3D HYDRODYNAMICAL STELLAR MODEL ATMOSPHERES

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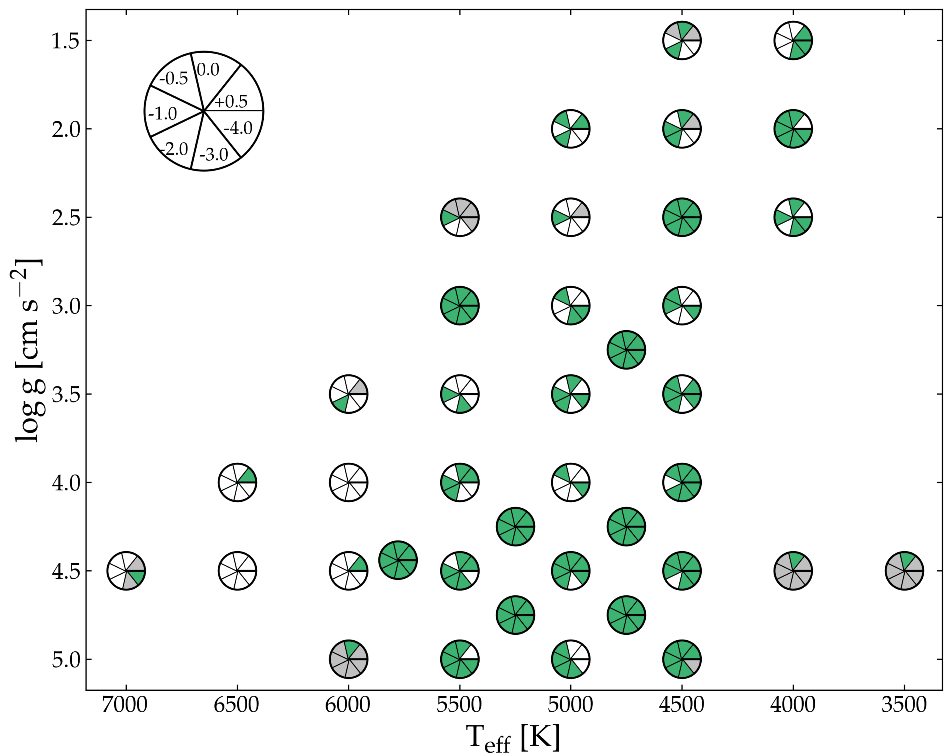
- log *g* = 1.5 – 5.0, Δlog *g* = 0.5
- [Fe/H] = – 4.0 to +0.5, Δ[Fe/H] = 0.5

3D MODEL GRIDS AVAILABLE; HOWEVER, COVERAGE IN STELLAR PARAMETER SPACE IS SPARSE!

Rodrigues Diaz et al. 2024, A&A, 688, A212



3D HYDRODYNAMICAL STELLAR MODEL ATMOSPHERES

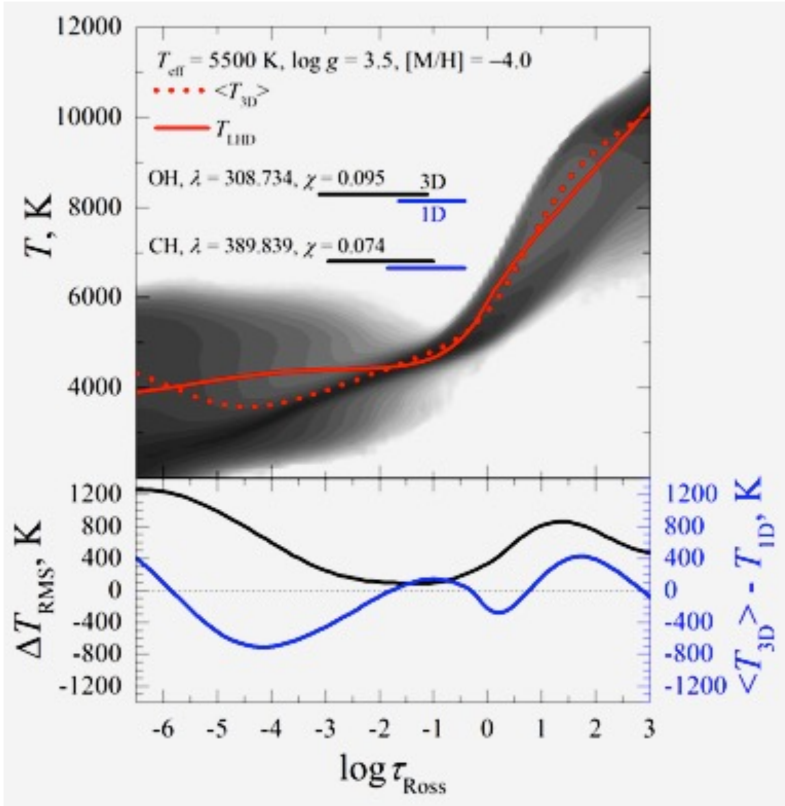
3D HYDRODYNAMICAL MODEL ATMOSPHERES: WHY BOTHER??

The influence of non-stationary phenomena on:

- The atmospheric structure

Metal-poor subgiant BD+44493

Kolomiecas et al., in prep.



3D HYDRODYNAMICAL STELLAR MODEL ATMOSPHERES

3D HYDRODYNAMICAL MODEL ATMOSPHERES: WHY BOTHER??

The influence of non-stationary phenomena on:

- The atmospheric structure
- Spectral line formation properties and line strengths

Metal-poor subgiant BD+44493

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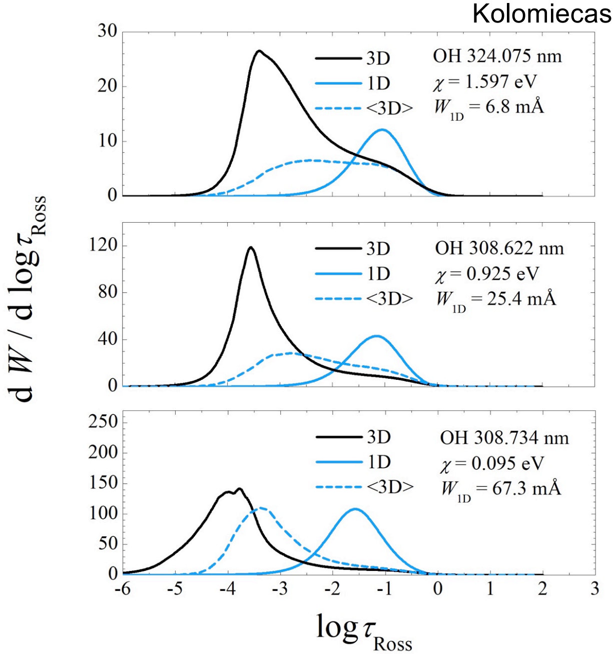

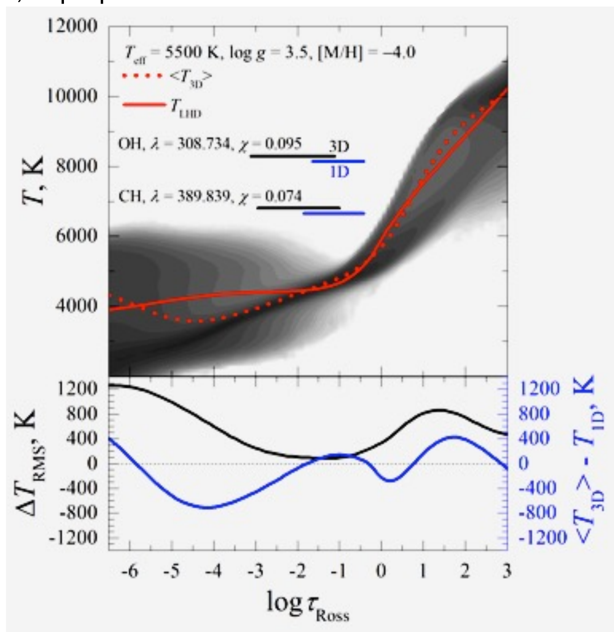

3D HYDRODYNAMICAL STELLAR MODEL ATMOSPHERES

3D HYDRODYNAMICAL MODEL ATMOSPHERES: WHY BOTHER??

The influence of non-stationary phenomena on:

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- Differences between the 3D and 1D abundances

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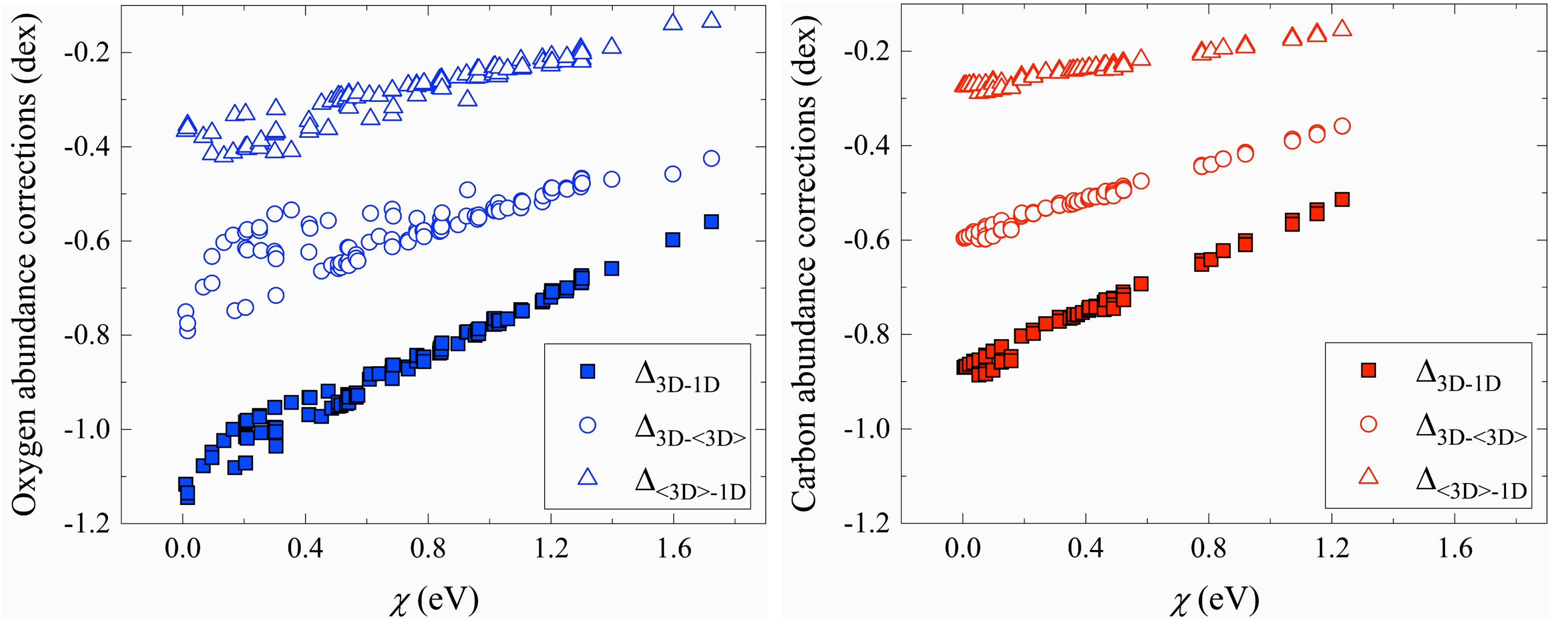
Kolomiecas et al., in prep.



3D HYDRODYNAMICAL STELLAR MODEL ATMOSPHERES

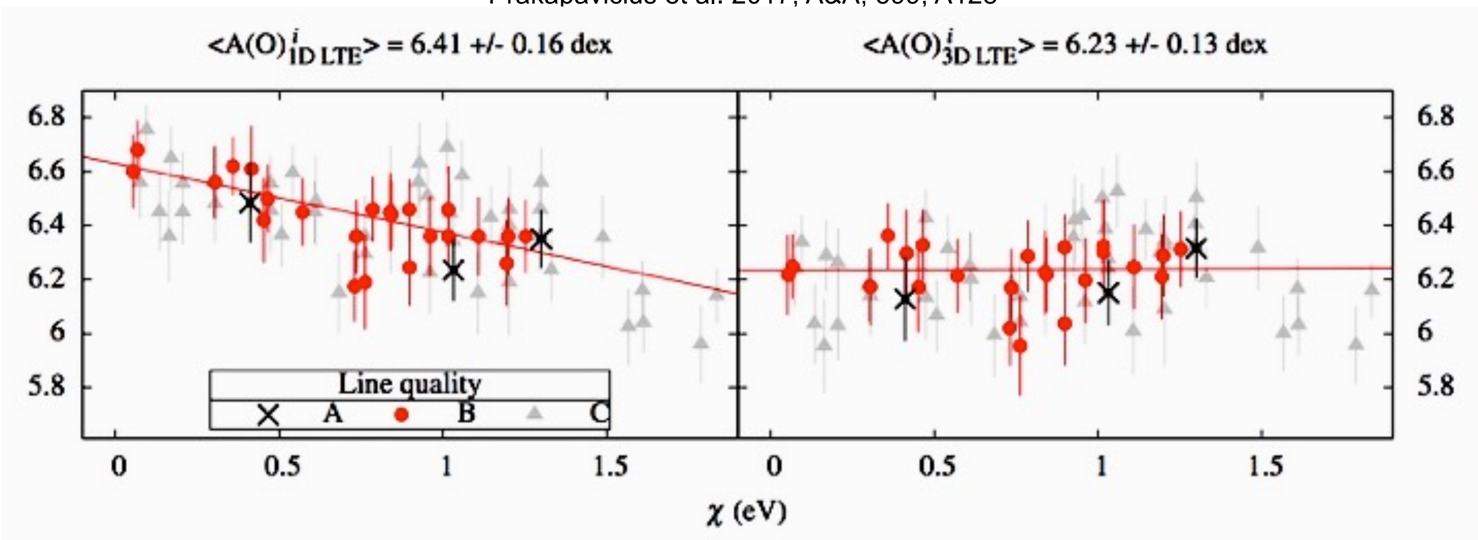
3D HYDRODYNAMICAL MODEL ATMOSPHERES: WHY BOTHER??

The influence of non-stationary phenomena on:

- The atmospheric structure
- Spectral line formation properties and line strengths
- Differences between the 3D and 1D abundances

Oxygen abundance from OH lines in the metal-poor giant HD+122563

Prakapavicius et al. 2017, A&A, 599, A128



3D HYDRODYNAMICAL STELLAR MODEL ATMOSPHERES

3D HYDRODYNAMICAL MODEL ATMOSPHERES: WHY BOTHER??

3D STELLAR MODEL ATMOSPHERES FOR STELLAR SPECTROSCOPY

- **PROS:**
  - Higher physical realism
  - Possibility to study non-stationary phenomena
  - (Large) differences in the line formation properties in 3D and 1D

3D HYDRODYNAMICAL STELLAR MODEL ATMOSPHERES

3D HYDRODYNAMICAL MODEL ATMOSPHERES: WHY BOTHER??

3D STELLAR MODEL ATMOSPHERES FOR STELLAR SPECTROSCOPY

- **PROS:**
  - Higher physical realism
  - Possibility to study non-stationary phenomena
  - (Large) differences in the line formation properties in 3D and 1D
- **CONS:**
  - Computations time consuming
  - Model grids are sparse
  - Ideally, should be used with NLTE line synthesis – too complex/time-consuming yet

NLTE SPECTRAL LINE FORMATION

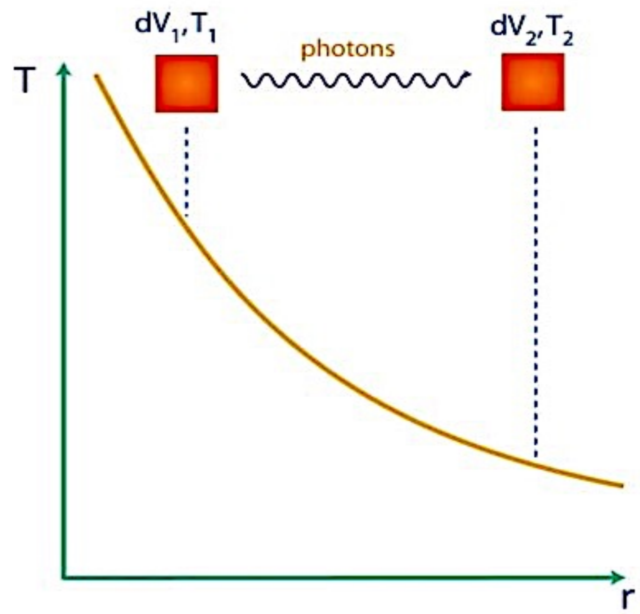
NLTE VERSUS LTE

- Requirement for the local thermodynamic equilibrium LTE assumption to be valid:
  - *T* scale height >> mean free path of the photon!

  E.g. the mean free path of the gas particle in the solar photosphere is ~10^{-4} m; temperature scale height

$$H_T \equiv \frac{T}{|dT/dr|} \approx 670 \quad \text{km}$$

→ LTE assumption applicable!



NLTE SPECTRAL LINE FORMATION

NLTE VERSUS LTE

- Under the assumption of LTE:
  - Particle velocities: Maxwellian distribution

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

  - Level populations of atoms/ions: Boltzmann equation

$$\frac{N_n}{g_n} = \frac{N_m}{g_m} \exp\left(-\frac{E_n - E_m}{kT}\right)$$

  - Particle number density in different ionization degrees: Saha equation

$$\frac{N_{r+1}}{N_r} N_e = \frac{U_{r+1}}{U_r} \frac{2\left(2\pi mkT\right)^{3/2}}{h^3} \exp\left(-\frac{\chi_r}{kT}\right)$$

NLTE SPECTRAL LINE FORMATION

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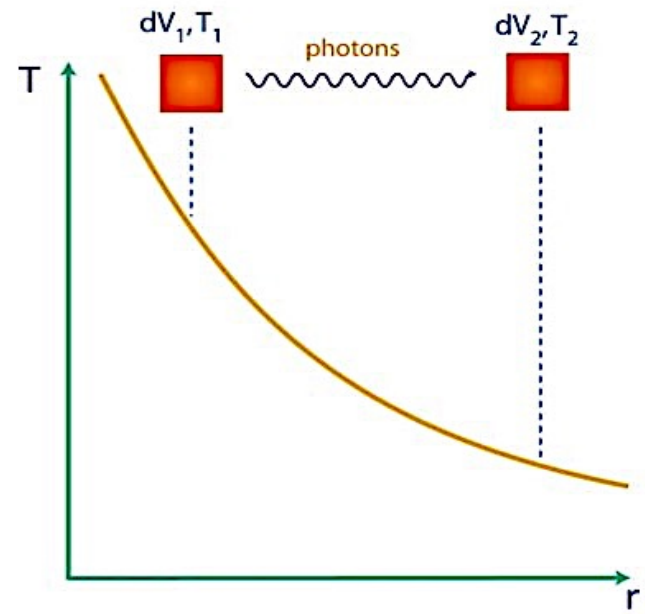
Local temperature defines local thermodynamic properties!

NLTE SPECTRAL LINE FORMATION

NLTE VERSUS LTE

- Real situation in stellar atmospheres:
  - Narrow layers of stellar atmosphere are in (local) thermodynamic equilibrium, despite the fact that *T* varies with depth
  - Deviations from LTE in the outer atmospheric layers!

NLTE approach is needed to account for deviations from the LTE!



NLTE SPECTRAL LINE FORMATION

NLTE SPECTRAL SYNTHESIS INSTEAD OF LTE

- Radiative transfer equation, emission and absorption coefficients – as in LTE

$$\frac{dI_\nu}{ds} = j_\nu - \kappa_\nu I_\nu \qquad \text{or} \qquad \frac{dI_\nu}{\kappa_\nu ds} = S_\nu - I_\nu$$

In the presence of emission and absorption:

$$j_\nu^{\text{induced}} = n_{\text{up}} \frac{h\nu_0}{4\pi} B_{\text{ul}} I_\nu \psi(\nu)$$

$$j_\nu^{\text{spontaneous}} = n_{\text{up}} \frac{h\nu_0}{4\pi} A_{\text{ul}} \psi(\nu)$$

$$\kappa_\nu^{\text{abs}}(\nu) = n_{\text{low}} \frac{h\nu_0}{4\pi} B_{\text{lu}} \varphi(\nu)$$

Line broadening mechanisms

How to compute level population numbers??

Quantum-mechanical computations

$$B_{\text{lu}} = \frac{4e^2\pi^2}{mch\nu_0} f_{\text{lu}}$$

$$B_{\text{ul}} = \frac{g_{\text{up}}}{g_{\text{low}}} B_{\text{lu}} = \frac{g_{\text{up}}}{g_{\text{low}}} \frac{4e^2\pi^2}{mch\nu_0} f_{\text{lu}}$$

$$A_{\text{ul}} = \frac{2h\nu_0^3}{c^2} B_{\text{ul}} = \frac{g_{\text{up}}}{g_{\text{low}}} \frac{8e^2\nu_0^2\pi^2}{mc^3} f_{\text{lu}} =$$

$$= 3\gamma_{\text{ul}} \frac{g_{\text{up}}}{g_{\text{low}}} f_{\text{lu}}$$

NLTE SPECTRAL LINE FORMATION

NLTE SPECTRAL SYNTHESIS INSTEAD OF LTE

- Radiative transfer equation, emission and absorption coefficients – as in LTE
- **Level populations of atoms/ions – from statistical equilibrium equation**

$$\sum_{j\neq i}\Big(\underbrace{n_i(R_{ij}+C_{ij})}_{\text{lines}}+\underbrace{n_i(R_{ik}+C_{ik})}_{\text{ionisation}}\Big)=\sum_{j\neq i}\Big(\underbrace{n_j(R_{ji}+C_{ji})}_{\text{lines}}+\underbrace{n_k(R_{ki}+C_{ki})}_{\text{recombination}}\Big)$$

Additional atomic data needed!

where $R_{ij/ji}$ are radiative transitions,
$C_{ij/ji}$ – collisional transitions.

- Particle density n_i in level i remains const

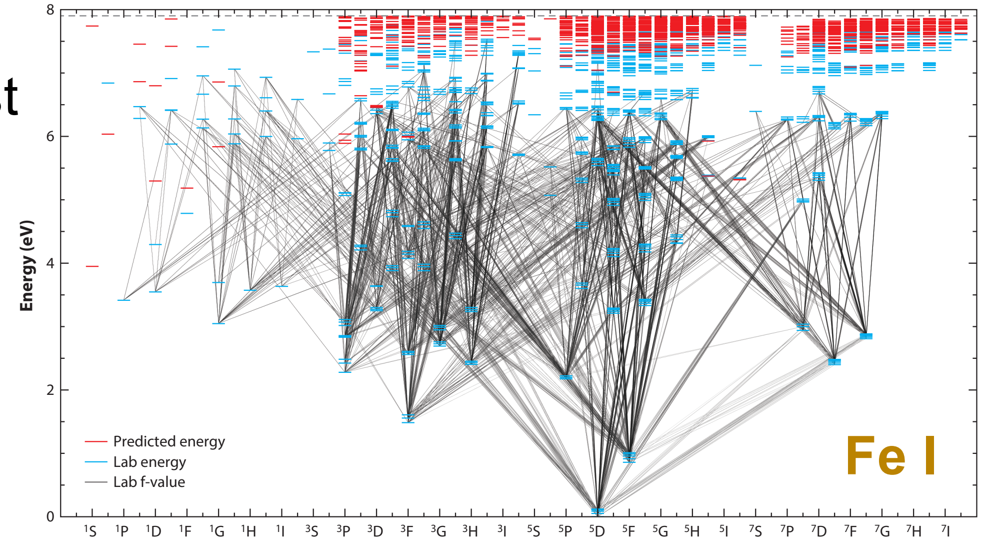
$$dn_i / dt = 0$$

i.e., the number of transitions **from** and **to** level i are equal

rate out = rate in

$$n_i \sum_{j\neq i} P_{ij} = \sum_{j\neq i} n_j P_{ji}$$

Lind & Amarsi 2024, ARAA, 62, 475



3D NLTE LINE FORMATION

3D NLTE SPECTRAL SYNTHESIS: WHY BOTHER?

NLTE–LTE differences in the departure coefficients, b_i

$\Rightarrow$ Significant differences between the NLTE and LTE line profiles
$\Rightarrow$ Differences in NLTE and LTE abundances
$\Rightarrow$ 3D plays a role, too!

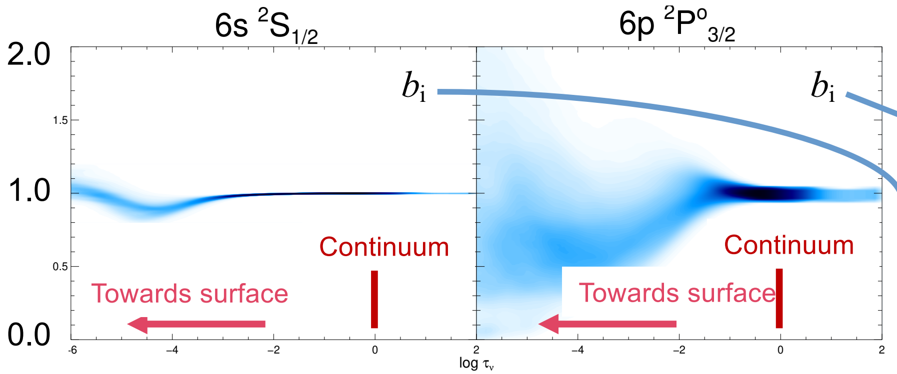
Atomic levels

LTE: Boltzmann equation $\frac{n_i}{n_j} = \frac{g_i}{g_j} e^{-E_{ij}/kT}$

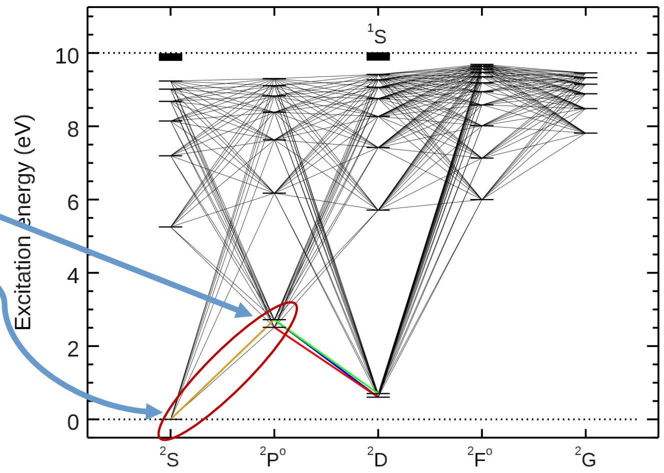
NLTE: departure coefficients $b_i = \frac{n_i^{NLTE}}{n_i^{LTE}}$

EXAMPLE: Ba II model atom

Gallagher, Steffen et al., in prep.



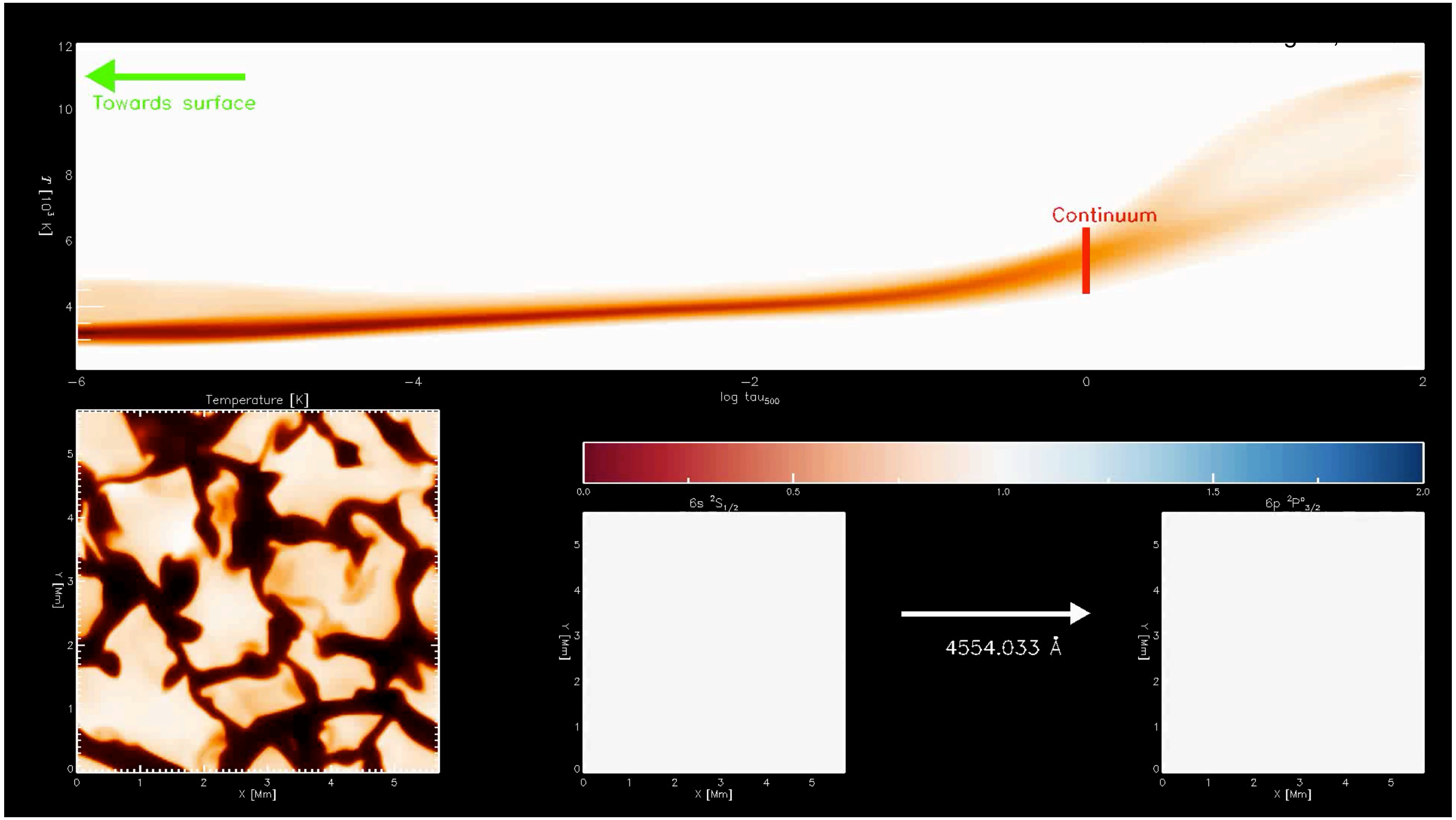
Gallagher et al. 2020, A&A, 634, A55



3D NLTE LINE FORMATION

3D NLTE SPECTRAL SYNTHESIS: WHY BOTHER?

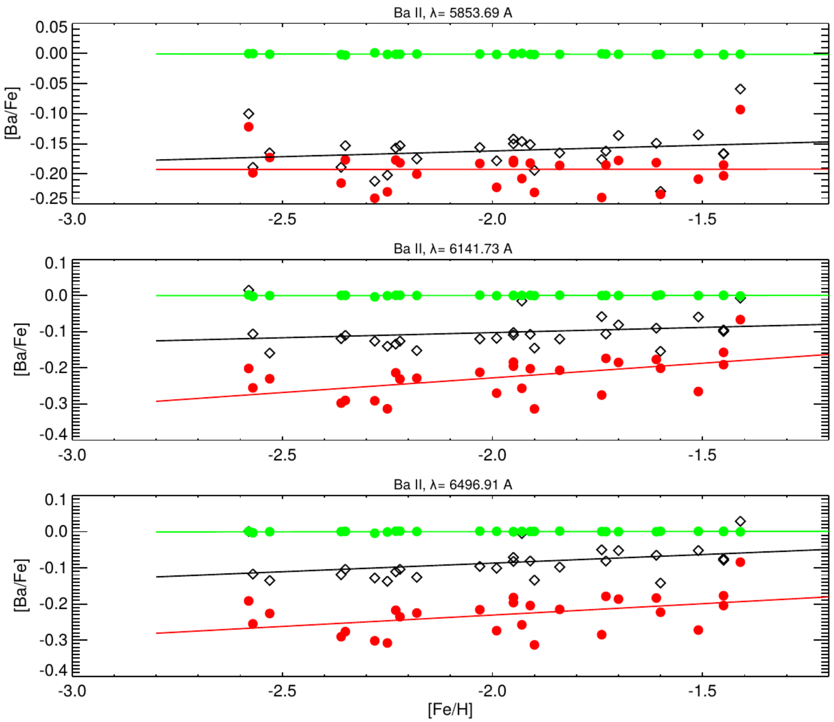
Ba II 455.4033 nm 3D NLTE line formation in the atmosphere of red giant star



3D NLTE LINE FORMATION

3D NLTE SPECTRAL SYNTHESIS: WHY BOTHER?

Ba 1D/3D NLTE ABUNDANCES IN A SAMPLE OF 27 RED GIANT STARS



Gallagher, Steffen et al., in prep.

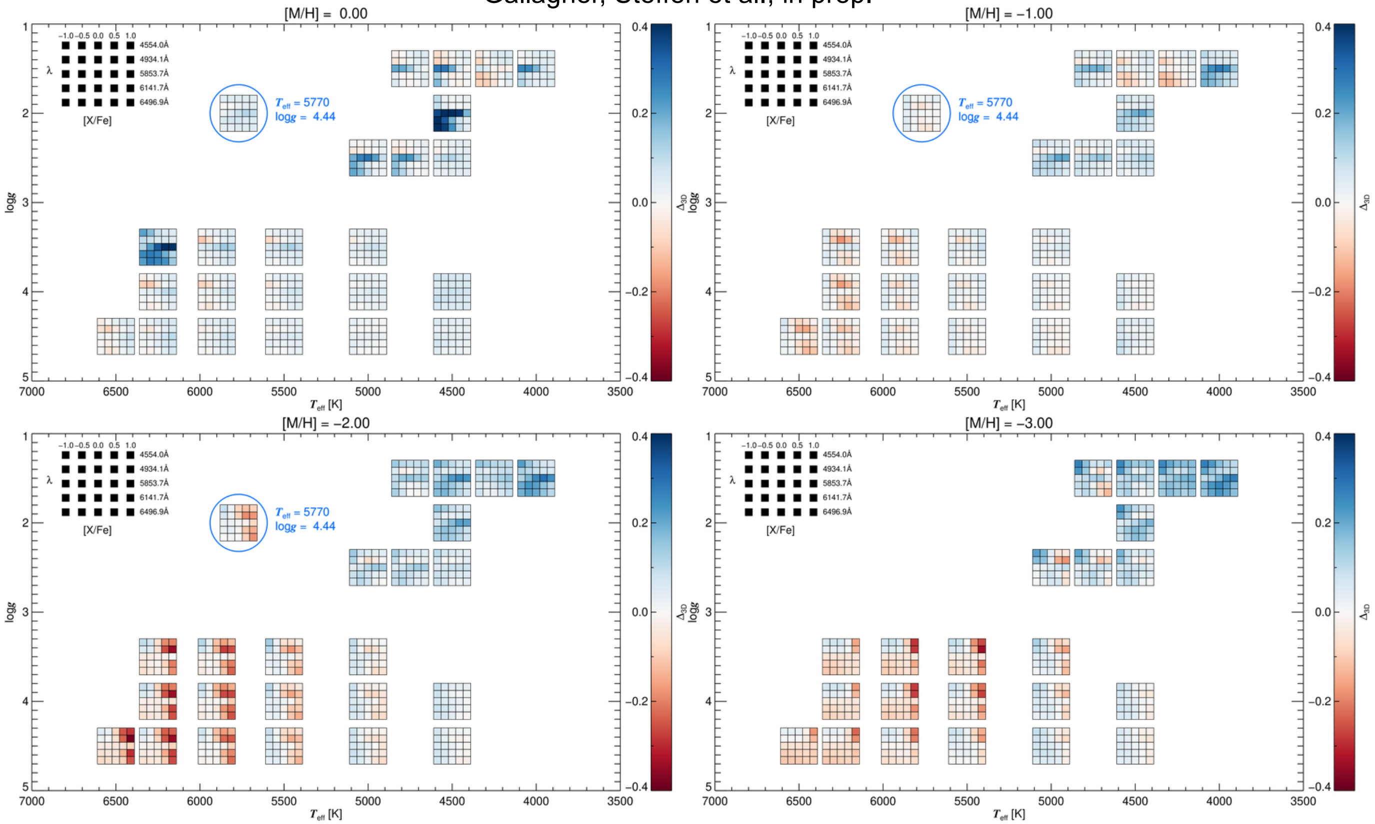
Barium abundance [Ba/Fe] that would be obtained in 1D LTE (black) and 1D non-LTE (red) assuming that the true abundance, as derived by a 3D non-NLTE analysis, is [Ba/Fe]=0 for all stars (green). Ignoring non-LTE effects leads to an underestimation of [Ba/Fe] by-0.05 to -0.20 dex, depending on the considered spectral line. For the 4554 Å line, 1D LTE and 1D non-LTE results are very similar, both showing a spurious trend of [Ba/Fe] with [Fe/H]. In general, the 1D non-LTE corrections exacerbate the LTE results.

3D NLTE LINE FORMATION

3D NLTE SPECTRAL SYNTHESIS: WHY BOTHER?

3D NLTE ABUNDANCE CORRECTIONS FOR Ba II LINES

Gallagher, Steffen et al., in prep.



3D NLTE LINE FORMATION

3D NLTE SPECTRAL SYNTHESIS: WHY BOTHER?

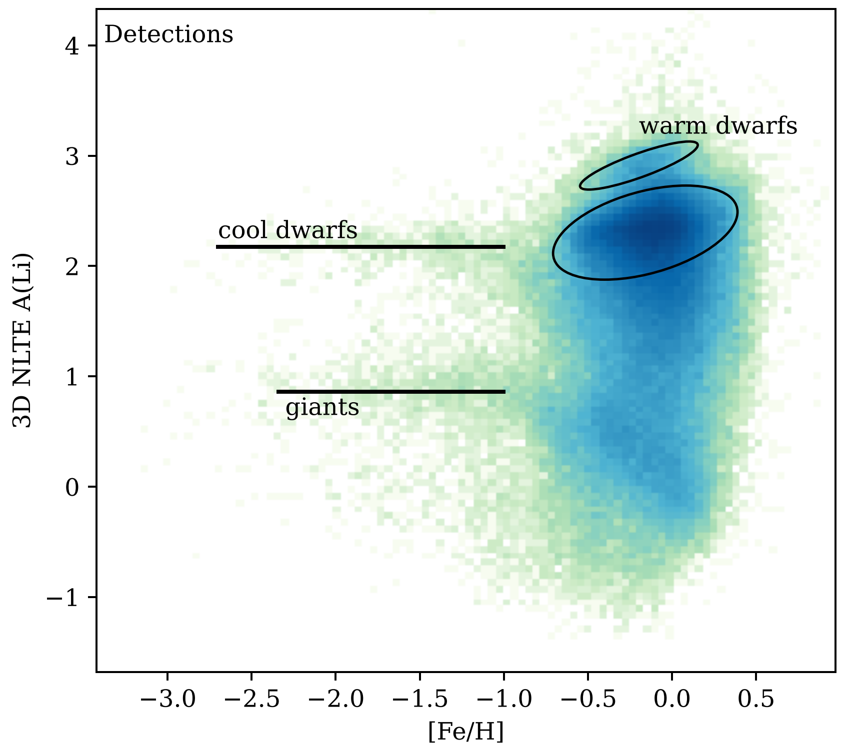
APPLICATION OF 3D NLTE ANALYSIS FOR LARGE STELLAR SAMPLES

MNRAS **528,** 5394–5411 (2024) https://doi.org/10.1093/mnras/stae385
Advance Access publication 2024 February 6

3D NLTE Lithium abundances for late-type stars in GALAH DR3

Ella Xi Wang ,[1,2★] Thomas Nordlander ,[1,2] Sven Buder ,[1,2] Ioana Ciucă,[1,2,3] Alexander Soen,[3,4] Sarah Martell ,[2,5] Melissa Ness,[6,7] Karin Lind,[8] Madeleine McKenzie [1,2] and Dennis Stello[2,5,9,10]

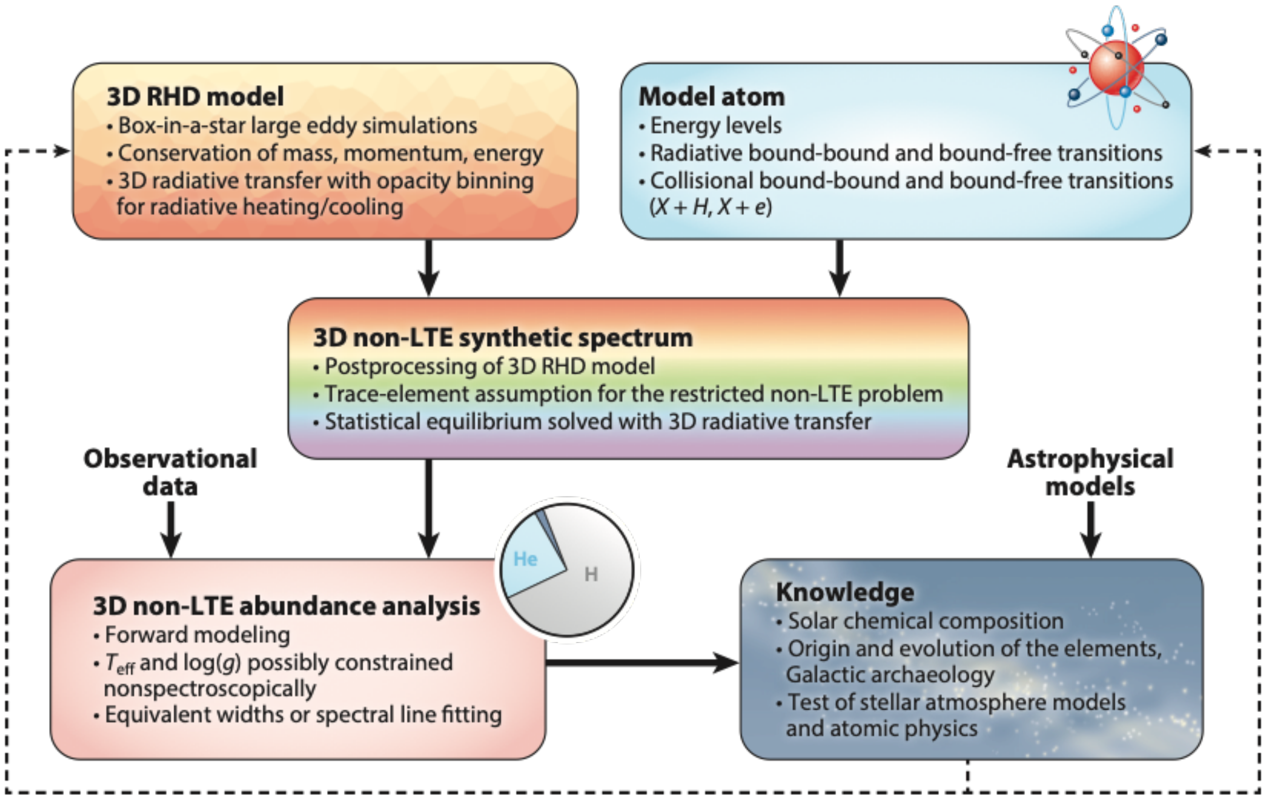
ABSTRACT
Lithium's susceptibility to burning in stellar interiors makes it an invaluable tracer for delineating the evolutionary pathways of stars, offering insights into the processes governing their development. Observationally, the complex Li production and depletion mechanisms in stars manifest themselves as Li plateaus, and as Li-enhanced and Li-depleted regions of the HR diagram. The Li-dip represents a narrow range in effective temperature close to the main-sequence turn-off, where stars have slightly super-solar masses and strongly depleted Li. To study the modification of Li through stellar evolution, we measure 3D non-local thermodynamic equilibrium (NLTE) Li abundance for 581 149 stars released in GALAH DR3. We describe a novel method that fits the observed spectra using a combination of 3D NLTE Li line profiles with blending metal-line strength that are optimized on a star-by-star basis. Furthermore, realistic errors are determined by a Monte Carlo nested sampling algorithm which samples the posterior distribution of the fitted spectral parameters. The method is validated by recovering parameters from a synthetic spectrum and comparing to 26 stars in the Hypatia catalogue. We find 228 613 Li detections, and 352 536 Li upper limits. Our abundance measurements are generally lower than GALAH DR3, with a mean difference of 0.23 dex. For the first time, we trace the evolution of Li-dip stars beyond the main sequence turn-off and up the subgiant branch. This is the first 3D NLTE analysis of Li applied to a large spectroscopic survey, and opens up a new era of precision analysis of abundances for large surveys.



3D NLTE LINE FORMATION

3D NLTE SPECTRAL SYNTHESIS: WHY BOTHER?

3D NLTE ABUNDANCE ANALYSIS: THE WORKFLOW



3D NLTE LINE FORMATION

3D NLTE SPECTRAL SYNTHESIS: WHY BOTHER?

3D NLTE ABUNDANCE ANALYSIS

- Higher physical realism – but still, many simplifying assumptions
- Abundance corrections can be
- Generally, impossible to approximate with 1D NLTE or 3D LTE
- Computations of 3D NLTE abundance corrections extremely time-consuming
- BUT: grids of 3D NLTE abundance corrections becoming available

CONCLUSIONS AND FINAL TAKEAWAYS

YOUR STRATEGY FOR DOING SPECTROSCOPIC STUDIES OF STARS

- A variety of tools available, differing in physical realism, assumptions, etc.
- Determine the most optimal tools to achieve your goals
  - Observations: which telescopes/spectrographs, spectral, ranges, resolution, etc.
  - Analysis: 1D versus 3D, LTE versus NLTE
- Identify colleagues you could team up with; one can not be an expert in everything
- Have a critical look at the tools available (and the team!) versus your goals (and vice versa); the world runs on compromises!
- Take a critical look at the results; any tools/techniques have limitations! Never overinterpret!

THANK YOU!