Atomic astrophysics with 3D non-LTE stellar spectroscopy

Anish Amarsi (Uppsala University)
The solar chemical composition

- Thanks to improved atomic data, composition of the Sun was apparently well-constrained at the end of the 20th century
  - Grevesse & Noels 1993: $Z=1.72\%$
  - Grevesse & Sauval 1998: $Z=1.69\%$
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Atomic Data and the Spectrum of the Solar Photosphere

N. Grevesse and A. Noels

Institut d’Astrophysique, Université de Liège, 5, avenue de Cointe, B-4000 Liege, Belgium

Received October 14, 1992; accepted in revised form February 12, 1993
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Much smaller line-by-line scatter when they used improved oscillator strengths.
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(In this plot: Blackwell et al. 1987)
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The revised solar chemical composition

- However, 1990’s analyses were based on simple 1D LTE models:
  - Grevesse & Sauval 1998, Z=1.69%
- Reality: stellar atmospheres are 3D non-LTE
Observations
(Swedish solar telescope)

Simulations
(Stagger code)
Simulated granulation across the HR diagram [Y. Zhou, Aarhus]
1D models need various fudge parameters to try to account for 3D effects and hide important physics e.g.
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- Macroturbulence
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- Microturbulence
- Macro turbulence
- Mixing length parameters
1D models need various *fudge parameters* to try to account for 3D effects and hide important physics e.g.:

- Microturbulence
- Macroturbulence
- Mixing length parameters
- Convective blueshift
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- Microturbulence
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- Mixing length parameters
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- Line asymmetries
1D models need various fudge parameters to try to account for 3D effects and hide important physics e.g.:

- Microturbulence
- Macroturbulence
- Mixing length parameters
- Convective blueshift
- Line asymmetries
- Line strengthening/weakening
LTE versus non-LTE

\[ n_1 \propto \exp\left(-\frac{E_1}{k_bT}\right) \]
**LTE versus non-LTE**

\[ n_1 \propto \exp\left(-\frac{E_1}{k_b T}\right) \]

\[ n_i \sum_j P_{i \rightarrow j} = \sum_j n_j P_{j \rightarrow i} \]

\[ \frac{dI_\nu}{d\tau_\nu} = S_\nu - I_\nu \]

**Figure 1:**
- **Left:** Term diagram illustrating transitions between energy levels \( E_1 \) and \( E_2 \) with the quantum transition \( h\nu \).
- **Right:** Grotrian diagram for neutral nitrogen [Amarsi+ 2020].
Lithium 671nm line in a metal-poor subgiant [Lind+ 2013]

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Grotrian diagram for neutral nitrogen [Amarsi+ 2020]

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Grotrian diagram for neutral nitrogen [Amarsi+ 2020]

3D LTE with 50% smaller A(Li)… also line shape is different

3D LTE versus non-LTE

Normalized flux

Energy / eV

Normalized

Length [Å]
Atomic data needs

Amount of data

Accuracy

Fig. 6. Symbols as in Fig. 7.

[Na, Si, Fe], [Ca/Fe], [Cr, Fe], and [Ni]

References

collision rates

I shall describe the successes, as well as their limitations, and thereby try to make the case for

This information sheds light on the structure and evolution of the stars themselves, as well as

Stars leave their signatures on the light they emit from their atmospheres, in particular their chemical compositions.

By comparing with model stellar spectra, we can decode these lines. By studying the absorption and emission lines, we gain insights into the chemical composition and internal conditions of stars.

Theoretical Astrophysics, Uppsala University, Sweden

P. S. Barklem, A&A

A. M. Amarsi, S. Liljegren, P. E. Nissen, A&A

A. M. Amarsi, P. E. Nissen and W. J. Schuster: Two distinct halo populations in the solar neighborhood

516, 751 20, Uppsala, Sweden

N. Grevesse

M. Amarsi

A&ARv, 36 (2016)

J. Grumer, F. Green, T. Walton, and J. T. Horbury: New estimate of the solar iron abundance

A&A, 554 (2022)

50 (2016)
Atomic data needs

3D RHD simulations: opacities, partition functions (EOS)

Amount of data

Accuracy

Fig. 5. Symbols as in Fig.

[Si/Fe], [Cr/Fe], and [Ti/Fe] as a function of [Fe].

References

I shall describe the function for the N I 668.34 nm line in a vertical slice of a snapshot of a 3D non-LTE modelling of N I lines in the solar atmosphere. This information sheds light on the structure and evolution of the stars themselves, as well as on the low- and high-density regimes. From Fig. 8, we can decode these functions (EOS) and thermal parameters.

Left: UVES spectra of two stars with nearly the same atmospheric parameters.

Right: Two distinct halo populations in the solar neighborhood.

Fig. 7. The same symbols as in Fig.

Fig. 6. The same symbols as in Fig.

Theoretical Astrophysics, Department of Physics and Astronomy, Uppsala University, Box 516, 751 20, Uppsala, Sweden.


A&ARv, 26, 516, 751 (2022).

5624 K, log g = 4.37, [Fe/H] = 0.12) is shown with a red line and that of the high-density regime with a green line.
Atomic data needs

3D RHD simulations: opacities, partition functions (EOS)

Non-LTE models:
Radiative/collisional BB and BF transition rates

Amount of data

Accuracy
Atomic data needs

Amount of data

Non-LTE models:
Radiative/collisional BB and BF transition rates

High precision spectroscopy:
wavelength; BB transition rate; broadening parameters; HFS

3D RHD simulations:
opacities, partition functions (EOS)

Accuracy
Atomic data needs

- Amount of data
- Non-LTE models: Radiative/collisional BB and BF transition rates
- 3D RHD simulations: opacities, partition functions (EOS)
- High precision spectroscopy: wavelength; BB transition rate; broadening parameters; HFS

Accuracy
Databases (not exhaustive):

- NIST

**Atomic data needs**

Amount of data

Accuracy
Atomic data needs

- Amount of data
- Accuracy

Databases (not exhaustive):
- NIST
- OP/IP

I shall describe the function for the $\text{NI}_{2668.34\text{nm}}$ line in a vertical slice of a snapshot of Figure 1:

This information sheds light on the structure and evolution of the stars themselves, as well as on the low-$\alpha$ stars, in particular their chemical compositions.

- UVES spectra of two stars with nearly the same atmospheric parameters: $T=5524\ \text{K}$, $\log g=4.55$, [Fe/H] = -0.2.

- The spectrum of the low-$\alpha$ star G 159-45 is compared with the spectrum of a high-$\alpha$ star.

- The observations are explained in terms of thermodynamic equilibrium (non-LTE) and hydrodynamics, taking into account statistical equilibrium, inelastic processes, collision-induced absorption, and quantum mechanical corrections.

- The model spectra are analyzed by comparing with model stellar atmospheres, in particular their chemical compositions.

- The same symbols as in Figures 5, 6, and 7 are used.

- References:
  - P. E. Nissen and W. J. Schuster: Two distinct halo populations in the solar neighborhood

- Databases (not exhaustive):
  - NIST
  - OP/IP

- Theoretical Astrophysics, Uppsala University

- Planets, and even the Galaxy as a whole... provided that the model spectra are sufficiently realistic.
Atomic data needs

Databases (not exhaustive):
- NIST
- OP/IP
- Kurucz

Amount of data

Accuracy
**Atomic data needs**

- NIST
- OP/IP
- Kurucz
- VALD

Databases (not exhaustive):

Amount of data

Accuracy

---

**Fig. 5.**

Symbols as in Fig.

**Fig. 6.**

Symbols as in Fig.

- \([\text{Na}]/\text{Fe}\]
- \([\text{Si}]/\text{Fe}\]
- \([\text{Cr}]/\text{Fe}\]
- \([\text{Ti}]*\]

---

**References**

This information sheds light on the structure and evolution of the stars themselves, as well as their atmospheres, in particular their chemical compositions. By comparing with model stellar spectra, we can decode these signatures to reveal the physical properties of stars, in particular their chemical compositions. To achieve this, it is necessary to determine the collision rates for stars with \([\text{Fe}]/\text{H}\]. The same model spectra are used.

**Fig. 7.**

**Fig. 8.**

- \([\alpha = 0.31) \text{ with a} \]
- \([\alpha = 4.55, [\text{Fe}]]\]
- \([\alpha = 93, [\text{Fe}]]\]
- \([\alpha = 120, [\text{Fe}]]\]

**Fig. 9.**

- \([\alpha = 50 (\text{green line. The Fe lines have the same strength in the two spectra, but}]]\)
- \([\alpha = 516, 751 20, \text{Uppsala, Sweden}]]\)

Further information on the form of absorption and emission lines. By comparing with model stellar spectra, we can decode these signatures to reveal the physical properties of stars, in particular their chemical compositions. Such successes, as well as their limitations, and thereby try to make the case for thermodynamic equilibrium (non-LTE) modelling of N I lines in the solar atmosphere.

**Fig. 10.**

- \([\text{Fe}]/\text{H}\]
- \([\text{Fe}]/\text{H}\]
- \([\text{Fe}]/\text{H}\]
- \([\text{Fe}]/\text{H}\]

**Fig. 11.**

- \([\text{Fe}]/\text{H}\]
- \([\text{Fe}]/\text{H}\]
- \([\text{Fe}]/\text{H}\]
- \([\text{Fe}]/\text{H}\]

**Fig. 12.**

- \([\text{Fe}]/\text{H}\]
- \([\text{Fe}]/\text{H}\]
- \([\text{Fe}]/\text{H}\]
- \([\text{Fe}]/\text{H}\]

**Fig. 13.**

- \([\text{Fe}]/\text{H}\]
- \([\text{Fe}]/\text{H}\]
- \([\text{Fe}]/\text{H}\]
- \([\text{Fe}]/\text{H}\]

**Fig. 14.**

- \([\text{Fe}]/\text{H}\]
- \([\text{Fe}]/\text{H}\]
- \([\text{Fe}]/\text{H}\]
- \([\text{Fe}]/\text{H}\]

**Fig. 15.**

- \([\text{Fe}]/\text{H}\]
- \([\text{Fe}]/\text{H}\]
- \([\text{Fe}]/\text{H}\]
- \([\text{Fe}]/\text{H}\]
Atomic data needs

Databases (not exhaustive):
- NIST
- OP/IP
- Kurucz
- VALD
- CHIANTI

Amount of data

Accuracy

Fig. 5. Symbols as in Fig. 1.

This information sheds light on absorption and emission lines. By comparing with model stellar spectra, we can decode these signatures on the light emitted from stars, in their atmospheres, in low-\(\alpha\) and high-\(\alpha\) stars. The UVES spectra of two stars with nearly the same atmospheric parameters are shown. For stars with \([\text{Fe}/\text{H}]=-0.12\), the spectrum of the low-\(\alpha\) star is shown with a red line and that of the high-\(\alpha\) star with a blue line.
Atomic data needs

- Amount of data
- Accuracy

Databases (not exhaustive):
- NIST
- OP/IP
- Kurucz
- VALD
- CHIANTI

(Plus data found scattered in the literature, including those produced by people here)
The revised solar chemical composition

• However, 1990’s analyses were based on simple 1D LTE models:
  - Grevesse & Sauval 1998, Z=1.69%

• Reality: stellar atmospheres are 3D non-LTE
The revised solar chemical composition

• However, 1990’s analyses were based on simple 1D LTE models:
  - Grevesse & Sauval 1998, Z=1.69%

• Reality: stellar atmospheres are 3D non-LTE

• More realistic 3D/non-LTE modelling presented in 2005, refined in 2009, 2015, and most recently in 2021:
  - Asplund, Amarsi, Grevesse 2021, Z=1.39%
The solar modelling problem

- **3D/non-LTE modelling**: downwards revision of solar metallicity
  - Grevesse & Sauval 1998: $Z=1.7\%$
  - Asplund, Amarsi, Grevesse 2021: $Z=1.4\%$
- Revealed a severe discrepancy between solar interior structure models and helioseismic inferences
- Worrying broader implications for (stellar) astrophysics
The solar modelling problem

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![Error in the predicted interior sound speed](Stasińka+ 2012)
A problem with 3D non-LTE models?

- Unlikely, because **direct inversions** of helioseismic data also suggest 
  \( Z \approx 1.4\% \) consistent with 3D non-LTE models (Buldgen et al. submitted)

![Graph showing direct helioseismic inference vs. high and low Z models](image)

Best estimate of \( Z \) directly from helioseismic data [Buldgen+ submitted]
A problem of missing opacity?

- A possible contributing factor to the solar problem is the treatment of interior opacities
  - Temperatures of around 2 million kelvin
  - Larger abundances or larger opacities = similar impact on solar models
- (Also see talk #4 on Monday; poster #26)
A problem of missing opacity?

- “The measured wavelength-dependent opacity is 30–400 per cent higher than predicted. This represents roughly half the change in the mean opacity needed to resolve the solar discrepancy, even though iron is only one of many elements that contribute to opacity” [Bailey+ 2015]

Higher-than-predicted measured opacities [Bailey+ 2015]
Atomic-astrophysics connections

- The solar problem is a good illustration of the **connections** between atomic physics and astrophysics

- Atomic → Astro
  - Improved log gf’s = well-constrained 1D LTE composition (e.g. 1990’s)

Evolution of solar iron abundance with improving log gf data [Grevesse & Noels 1993]
Atomic-astrophysics connections

- The solar problem is a good illustration of the connections between atomic physics and astrophysics.
  - Atomic → Astro
    - Improved log gf’s = well-constrained 1D LTE composition (e.g. 1990’s)
  - Astro → Atomic
    - More realistic 3D/non-LTE models in the 2000’s helped motivate a deeper look into theoretical opacities.

Higher-than-predicted measured opacities [Bailey+ 2015]
The message of this talk

• Rapid progress in developing 3D non-LTE model stellar spectra, with increasing sophistication and accuracy

• Cause/caused by stronger connections between atomic/astrophysics

• Atomic → Astro
  - Improved atomic data improve the models
  - Reveal new astrophysics

• Astro → Atomic
  - Use Sun/stars for complementary tests of atomic data?
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Imprints of solar system formation

- The solar abundances are reaching precision/accuracy to resolve possibly intrinsic differences with pristine meteorites
- Trend with condensation temperature at ~2 sigma

Sun - meteoritic abundances versus condensation temperature [Asplund+ 2021]
Imprints of solar system formation

- The solar abundances are reaching precision/accuracy to resolve possibly intrinsic differences with pristine meteorites
- Trend with condensation temperature at ~2 sigma
- Amplitude of signature ~ 25%
- Precision (for one element) ~ 10-25%
Imprints of solar system formation

- The solar abundances are reaching precision/accuracy to resolve possibly intrinsic differences with pristine meteorites
- Trend with condensation temperature at ~2 sigma
- Amplitude of signature ~ 25%
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Similar signature found in the solar wind via Genesis (Jurewicz, Burnett+ in prep.)
Stars with and without planets

- Look at **carbon to oxygen abundance ratios** in different stars
  - X-axis is a proxy for cosmic time

![Graph showing carbon to oxygen abundance ratios](image-url)
Stars with and without planets

- Look at carbon to oxygen abundance ratios in different stars
  - X-axis is a proxy for cosmic time
- Separation between stars with and without planets
- Amplitude of signature ~ 10-20%
- Precision (for one star) ~ 10%

Carbon and oxygen abundances in dwarfs [Amarsi+ 2019]
Stars with and without planets

- Look at **carbon to oxygen abundance ratios** in different stars
  - X-axis is a proxy for cosmic time
- Separation between stars **with** and **without** planets
- Amplitude of signature ~ **10-20%**
- Precision (for one star) ~ **10%**
- Signature washed away in 1D LTE

![Graph showing separation between stars with and without planets. Labels indicate different star conditions with [Fe/H] > -0.4, without planets, and with planets of maximum mass M_max < 0.8M_J or M_max > 0.8M_J.](image)

Carbon and oxygen abundances in dwarfs [Amarsi+ 2019]
Stars with and without planets

- Look at carbon to oxygen abundance ratios in different stars
  - X-axis is a proxy for cosmic time
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Planet signature only seen thanks to improved atomic data for 3D non-LTE modelling

Carbon and oxygen abundances in dwarfs [Amarsi+ 2019]
The message of this talk

- Rapid progress in developing **3D non-LTE model stellar spectra**, with increasing sophistication and accuracy
- Cause/caused by stronger connections between **atomic/astrophysics**
- **Atomic → Astro**
  - Improved atomic data *improve the models*
  - Reveal *new astrophysics*
- **Astro → Atomic**
  - Use Sun/stars for *complementary tests of atomic data*?
Astrophysical tests of atomic data

- **Oscillator strengths**
  - Examine scatter and trends in line-by-line analyses of standard stars using different data sets
Astrophysical tests of atomic data

- **Oscillator strengths**
  - Examine scatter and trends in line-by-line analyses of standard stars using different data sets

**Figure**: Comparison of oscillator strengths for different data sets. The graph shows log $\epsilon_c$ (carbon abundance) against $\lambda_{air}$ (air wavelength). Different markers represent different data sets, with error bars indicating uncertainties. The title of the graph is "Astrophysical tests of C I oscillator strengths [Li et al. 2021]."
Astrophysical tests of atomic data

- Oscillator strengths
  - Examine scatter and trends in line-by-line analyses of standard stars using different data sets

- Broadening parameters
  - Examine detailed line shapes

Validation of hydrogen collisional broadening data [Barklem 2016]
Astrophysical tests of atomic data

• Oscillator strengths
  - Examine scatter and trends in line-by-line analyses of standard stars using different data sets

• Broadening parameters
  - Examine detailed line shapes

• Inelastic collisions
  - Examine centre-to-limb variations
Astrophysical tests of atomic data

- Oscillator strengths
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- Broadening parameters
  - Examine detailed line shapes

- Inelastic collisions
  - Examine centre-to-limb variations

Testing inelastic hydrogen collisions using the O I 777nm [Amarsi+ 2018]
Astrophysical tests of atomic data

- Oscillator strengths
  - Examine scatter and trends in line-by-line analyses of standard stars using different data sets
- Broadening parameters
  - Examine detailed line shapes
- Inelastic collisions
  - Examine centre-to-limb variations
Astrophysical tests of atomic data

- Oscillator strengths
- Broadening parameters
- Inelastic collisions
- More ideas are welcome
  - Increasing potential to use stars as lab benches as 3D non-LTE models continue to improve in sophistication

Error in the predicted interior sound speed [Stasińska+ 2012]
Conclusion

• Rapid progress in developing 3D non-LTE model stellar spectra, with increasing sophistication and accuracy

• Cause/caused by stronger connections between atomic/astrophysics

• Atomic → Astro
  - Improved atomic data improve the models
  - Reveal new astrophysics

• Astro → Atomic
  - Use Sun/stars for complementary tests of atomic data?
A(Fe) <3D> non-LTE, Fe1, AAG21
A(Fe) <3D> non-LTE, Fe2, AAG21
A(Fe) <3D> non-LTE, Fe1, Magg+
A(Fe) <3D> non-LTE, Fe2, Magg+