

3D Non-LTE radiation transfer: theory and applications to stars, exoplanets, and kilonovae

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Abstract

Most of the physical information about astrophysical objects is obtained via the analysis of their electromagnetic spectra. Observed data coupled with radiation transfer models in physical conditions representative of stars, planets, kilonovae, and ISM, yield constraints on their physical structure, gas flow dynamics at the surface, mass loss, and detailed chemical composition of the systems. All these core astrophysical parameters are just as reliable as the physical quality of the models that are employed for simulations of radiation transfer. Recent advances in multi-D transfer modelling with Non-Local Thermodynamic Equilibrium (NLTE) in inhomogeneous time-dependent systems revealed systematic shortcomings of canonical models. Owing to major complexities of solving coupled multi-frequency RT equations in 3D geometry, a number of approximations have been introduced. This review presents an overview of the physical problem, standard solutions, and recent methodological advances. We also provide an overview of main results in the area of 3D NLTE radiation transfer and its applications to modelling diverse astrophysical environments, including FGKM type- and OBA-type stars, multi-epoch spectra of kilonovae, and atmospheres of rocky and gaseous exoplanets.

Keywords: Radiative transfer, Numerical methods, Stellar abundances, Stellar atmospheres

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1 Introduction

Physical modeling of the emergent radiation field of stars and their companions is one of the main pillars of astrophysics. These calculations can be used to generate models of emergent fluxes and spatially-resolved surface intensities, which are used in nearly every area of research, to address scientific questions ranging from exoplanets to Galaxy structure. Among diverse applications, models of stellar spectra are used to determine the metal content of the Sun (e.g. [Grevesse and Sauval 1998](#); [Asplund et al. 2009](#); [Caffau et al. 2011](#); [Magg et al. 2022](#)) and detailed chemical composition of stars (e.g. [Kudritzki and Hummer 1990](#); [Frebel 2018](#); [Nissen and Gustafsson 2018](#); [Jofré et al. 2019](#)). Models of the angular dependence of stellar intensities are used as inputs for limb darkening profiles, e.g., for modelling light-curves and radial velocity (RV) curves during planet transits ([Ohta et al. 2005](#); [Howarth 2011](#); [Espinoza and Jordán 2016](#)) and exoplanet transmission spectroscopy (e.g. [Morello et al. 2017](#); [Coulombe et al. 2024](#)), for the interpretation of interferometric visibilities ([Kervella et al. 2017](#)), and studies of binaries and multiplicity ([Prša et al. 2016](#); [El-Badry et al. 2018](#)) in the context of stellar physics. Photometric magnitudes are main by-products of the synthetic spectral energy distributions and are needed to convert the observed photometry in different narrow- and broad-band filters into absolute stellar magnitudes and luminosities (e.g. [Casagrande and VandenBerg 2018](#)). Stellar fluxes are also required in the calculations of stellar population synthesis and integrated light spectroscopy of star clusters and galaxies (e.g. [Maraston and Strömbäck 2011](#); [Bastian and Lardo 2018](#); [Maiolino and Mannucci 2019](#); [Larsen et al. 2022](#)). More recently, radiation transfer methods used in stellar astrophysics were adapted for electromagnetic studies of kilonovae events, one of the electromagnetic counterparts of compact binary mergers (e.g. [Watson et al. 2019](#)). The objects latter also commonly use the methods adopted from studies of RT in expanding shells of supernovae (e.g. [Noebauer and Sim 2019](#)). Finally, RT methods in exoplanet atmospheres are becoming important.

Determination of the emitted radiation field from an astronomical object is a highly complex numerical problem that requires inputs from atomic and molecular physics and it relies on physical processes and relationships known from hydrodynamics, statistical mechanics, and energy transport. Generally, the problem, regardless of whether one refers to stellar or planetary atmospheres, or expanding ‘atmospheres’ of post-merger systems, is a boundary condition problem (Auer and Mihalas 1969; Mihalas 1988). The interaction between the gas and photons in the form of radiatively and collisionally-induced excitation, ionisation, charge transfer, and dissociation (e.g. Kubát 2014), can only be modelled using a framework that combines radiation transfer and hydrodynamics.

Technically 3-dimensional (3D) radiation transfer (RT) is not different from a 1D solution. The same 1D RT equation is solved in both cases. *However, physically there is a major difference, as the solution is done in different types of physical systems.* It has become common in the astronomy community to associate 3D RT with formal solutions of the 1D radiation transfer equation in non-stationary multi-D models of atmospheres. For stars, these are 3D radiation-hydrodynamics simulations of sub-surface convection (Nordlund et al. 2009; Kupka and Muthsam 2017; Leenaarts 2020; Chiavassa et al. 2024). For exoplanets, these are externally-irradiated 3D MHD models with global circulation (e.g. Parmentier et al. 2021; Christie et al. 2021), including prescriptions for formation of dust and clouds (e.g. Helling and Fomins 2013; Lines et al. 2018), that resemble the approaches used in modelling very cool Asymptotic Giant Branch stars (Höfner and Olofsson 2018). Kilonovae are typically represented as 1D spherically-symmetric expanding systems (e.g. Kerzendorf and Sim 2014; Jerkstrand 2011) similar to stars with winds. These physical models are vastly different in complexity and computational burden, and may include magnetic fields and different types of scattering and dust formation.

Regarding the physical state of matter, in which RT is solved, there are two possibilities. One is to assume that matter — and consequently the radiation field — is in Local Thermodynamic Equilibrium (LTE). In LTE, it is typically assumed – often without justification – that collisional rates between particles dominate over radiative transition rates caused by the radiation field in all cases. Hence, the number densities of particles and, in particular, their distribution with respect to the internal energy states (ionisation, excitation, chemical equilibrium) can be described by the Saha–Boltzmann equilibrium statistics.

The other option is **not** to assume this equilibrium. In the latter case, — known as NLTE — the full rate questions, which are also known as (in time-independent case) the equations of statistical equilibrium, must be solved (e.g. Kubát 2014). NLTE is, therefore, not an assumption (in contrast to claims in many literature studies), but - due to physically comprehensive treatment of the interaction between the radiation and the gas — a physically realistic approach. To make the point more clear, we would like to re-cite Mihalas and Athay (1973) directly: “*Departures from LTE occur simply because stars have a boundary through which photons escape into space*” which obviously applies to any other astronomic system, such as atmospheres of exoplanets or kilonovae. Further, sub-surface convection in stars occurs **because** stars loose energy at the surface through radiation. This implies that a major part of physics of stellar

interior is controlled by the properties of radiation propagation and loss from stellar atmospheres.

None of the physical effects are, strictly speaking novel. However, the computational demands of 3D NLTE modelling are so high that such calculations for the vast majority of astrophysical applications have been become feasible only very recently. It has since been shown that 3D and NLTE modelling is relevant in studies of ISM (e.g. Juvela 1997; van der Tak et al. 2007), exoplanet atmospheres (Fossati et al. 2021; Young et al. 2024, e.g.), hot stars (e.g. Dreizler and Werner 1993; Puls et al. 2005; Aschenbrenner et al. 2023), polarisation of circumstellar discs (Bjorkman and Carciofi 2005), dusty emission from galaxy discs (Baes et al. 2011), solar spectro-polarimetry (Socas-Navarro et al. 2015; de la Cruz Rodríguez et al. 2019) and solar prominences (Labrosse et al. 2010), accretion discs in AGN (Hubeny et al. 2001), and Type Ia supernovae (e.g. Lentz et al. 2000; Kromer and Sim 2009; Botyánszki and Kasen 2017). Full 3D NLTE radiation transfer has primarily found its applications in recent studies of the Sun and chemical composition and fundamental parameters of FGK-type¹ stars, where the effects of 3D NLTE physics play a non-negligible role. This progress has been, to a various extent covered in recent reviews by Jofré et al. (2019), Nissen and Gustafsson (2018), and Lind and Amarsi (2024).

In this review, the primary emphasis is on the radiative transfer problem within the NLTE framework in 1D hydrostatic and 3D inhomogeneous atmospheres. For academic clarity, we begin with conceptual discussion of RT in 1D and LTE, and progressively move to more complex geometric and physical setups throughout the text. We devote a substantial space to the methods of numerical integration and interpolation in various quantities, focusing primarily on iterative RT techniques. The two related topics — Monte-Carlo RT and 3D RHD models — were subjects of a comprehensive review in other contributions (Höfner and Olofsson 2018; Noebauer and Sim 2019; Chiavassa et al. 2024), therefore we do not aim to address these topics here. We will summarise the recent 1D and 3D NLTE calculations and their key results. We also devote attention to the present limitations of the models and highlight the aspects of the field where progress still needs to be made from the numerical, physical, and observational perspective.

2 Motivation

2.1 Stellar spectra and line bisectors

Studies of convective blueshifts in stellar spectra are fundamentally limited by the capabilities of the present-day astronomical instrumentation and the wavelength calibration. For the Sun, resolving power in excess of 200 000 is possible with Fourier Transform Spectroscopy (FTS) facilities. However, only very few instruments, like ESPRESSO at the Very Large Telescope (VLT), yield the data quality that can be used to trace the detailed signatures of stellar convection through the studies of convective blue- and red-shifts and bisectors. In this context, a major value of 3D

¹Throughout this paper, for convenience we follow the spectral type classification presented by Eric Mamajec at https://www.pas.rochester.edu/~emamajek/EEM_dwarf_UBVIJHK_colors_Teff.txt

radiation transfer approach is in its ability to provide predictions for the time- and spatially-dependent properties of absorption lines.

This can be done, if 3D (magneto)radiation-convection (M-RHD) simulations are used as a basis to provide the distributions of velocities in stellar photospheres. Convective motions lead to a preferential type of asymmetries in the spectroscopic line shapes, which are known as C-shaped profiles (e.g. [Dravins et al. 1981](#); [Dravins 1982](#); [Dravins and Nordlund 1990a,b](#); [Asplund et al. 2000](#); [Dravins 2008](#); [Allende Prieto et al. 2002b](#); [Bergemann et al. 2019](#); [Dravins et al. 2021](#)), although also inverse C-shape have been reported. The asymmetries, and consequently the C-shape bisectors, are due to the line formation dominated by the up-flows ([Beeck et al. 2013](#)), which occupy about two thirds of the area across the stellar disc (here, FGK type). Figures 1, 2, 3, and 4 demonstrate how the line asymmetry arises owing to granulation and correlated motions in stellar atmospheres.

Among the earlier studies, [Allende Prieto and Garcia Lopez \(1998\)](#) and [Allende Prieto et al. \(2002a\)](#) investigated the effects of convection in the Fe I lines in the very high-resolution spectrum of the Sun and of an F-type star Procyon, see Fig. 5. They showed that 3D RHD models yield a much improved description of observed line bisectors compared to hydrostatic 1D model atmosphere models. 3D models predict the bisectors to a precision of 50 m/s, except the strongest lines with the EWs in excess of 100 mÅ, for which a small systematic offset at the level of a few 100 m/s between models and data was detected. The origin of the offset is presently unclear and it could possibly be caused by NLTE or effect of magnetic fields.

The systematic variation of convective shifts and bisectors in the solar data has also been explored in [Dravins \(2008\)](#) and [Ellwarth et al. \(2023\)](#). Early papers included a comparison of observed solar line shifts and those from 3D models for a small number of diagnostic features, however, although satisfactory agreement was demonstrated for weak lines ([Asplund et al. 2000](#); [Allende Prieto et al. 2009](#)), systematically increasing differences between data and solar models were reported for stronger lines with equivalent widths (EWs) above $\sim 60\text{--}80$ mÅ ([González Hernández et al. 2020](#)). Figure 6 compares the RV shifts in the solar spectrum with predictions of a 3D RHD models.

Convective bisectors are also seen in the observed positions of lines in the high-resolution spectra of other main-sequence stars ([Frutiger et al. 2005](#); [Sheminova 2020](#)), and red giants, such as the F-type Procyon ([Allende Prieto et al. 2002b](#); [Dravins 2008](#)) and K-type metal-poor red giant branch star α Boo ([Allende Prieto et al. 2002a](#)). [Meunier et al. \(2017\)](#) found systematically stronger convective blueshifts of Ti and Fe lines in the observed spectra of more metal-poor stars, with an amplitude that is larger compared to the predictions of 3D RHD simulations. Analysis of intensity spectra of exoplanet host stars, obtained through spectral reconstruction during the planet’s transit, confirms that the spectral lines are redshifted and generally shallower at the limb compared to the disc centre ([Dravins et al. 2017a,b, 2021](#)). This finding is qualitatively consistent with predictions of 3D radiative transfer models.

In summary, however, most of the knowledge on the convective variability of spectral line profiles is currently of an empirical nature. Spectra based on 3D radiation transfer models are indispensable to further understand the nature and amplitude of the variability. 3D RHD simulations support the large (to ~ -600 m/s) blueshifts of

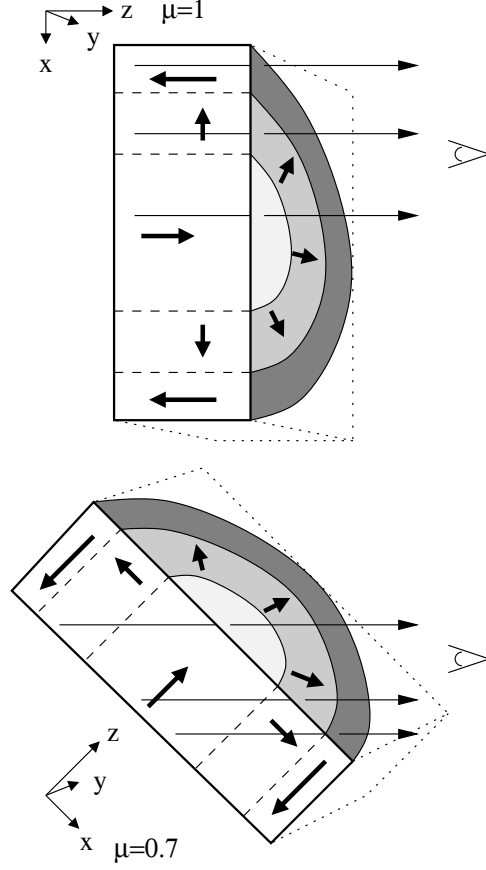


Fig. 1 Figure illustrates the critical effect of line-of-sight geometry in the presence of granulation, that is upflows (granules, which occupy most of the stellar surface) and downflows (inter-granular lanes). Here one granule is schematically shown at $\mu = 1$ and 0.7 . The consequence of this effect is that as the disc centre mostly vertical (longitudinal) flows contribute to intensities, whereas closer to the stellar limb the contribution of horizontal (transveral) motions dominates the emitted radiation field. Image reproduced with permission from [Frutiger et al. \(2005\)](#), copyright by ESO.

weaker lines ([Allende Prieto and Garcia Lopez 1998](#); [Reiners et al. 2016](#)), and these models also predict substantial average RV shifts of up to 0.3 km s^{-1} for different types of stars ([Allende Prieto et al. 2013](#)). Explaining the RV shifts quantitatively may require more refined 3D convective models of stellar atmospheres possibly taking into account magnetic fields.

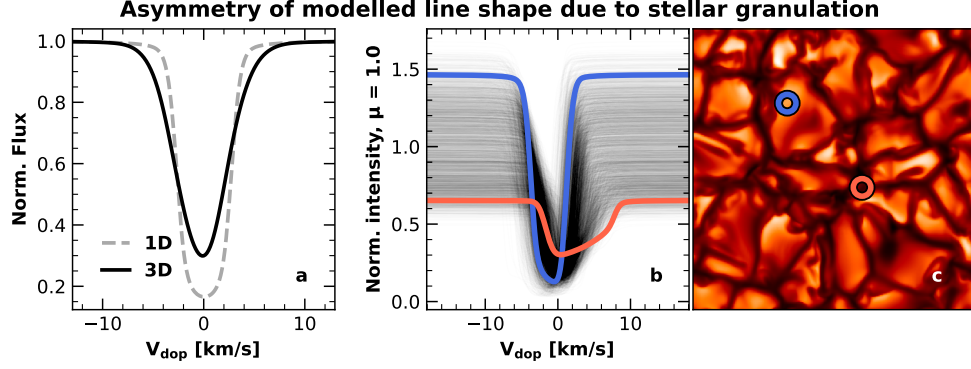


Fig. 2 Left panel: Line shape of $\bar{\text{A}}$ Mn I line. 1D line computed using a solar MARCS model atmosphere vs. 3D line shape from solar STAGGER snapshot. Middle panel: Variation of 3D line shape across the solar granulation pattern. Wavelengths on the x-axis have been converted to corresponding Doppler shift velocities. Right panel: Continuum intensity at 5000 $\bar{\text{A}}$ as a function of surface position. The overplotted circles mark the corresponding position of the highlighted profiles in the middle panel. Convection cells produce blue shifted line profiles. Intergranular lanes produce redshifted line profiles.

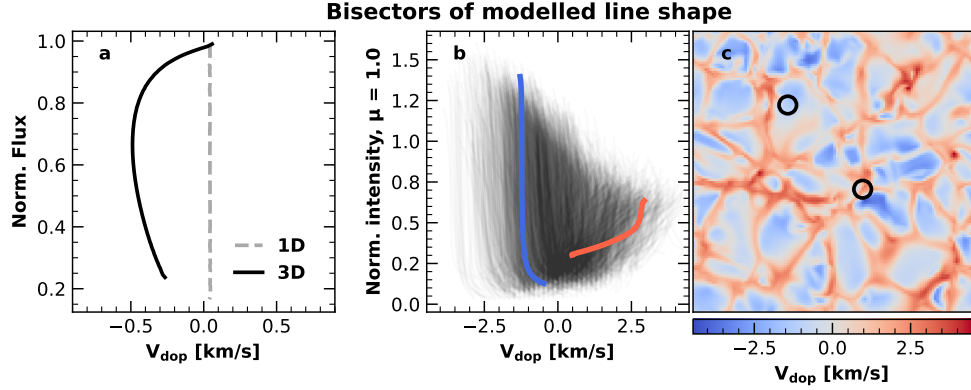


Fig. 3 Left and middle panel: Same as Fig. 2 but showing only line-bisectors instead of line profile. Right most panel: Doppler shift at half maximum of line-bisectors across solar granulation pattern.

2.2 Centre-to-limb variation in lines

Another important observational effect associated with 3D NLTE radiation transfer is the behaviour of spectral lines across the stellar disc, also known as the CLV.

Different studies explored the centre-to-limb variation (CLV) of lines with the primary aim to test the quality of models for abundance retrievals of the solar atmosphere, in particular for iron (Lind et al. 2017) and oxygen (Pereira et al. 2009; Steffen et al. 2015), the latter being a critical element for the solar structure (Serenelli et al.

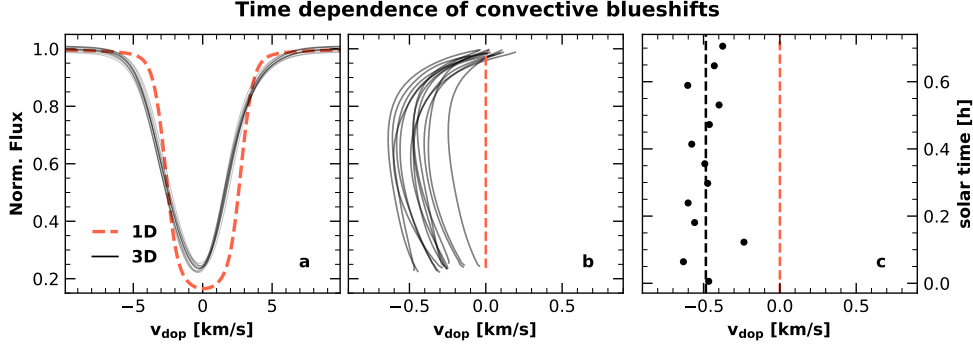


Fig. 4 Left panel: Line profiles of the 4502.2 Å Mn I line computed from 13 different STAGGER snapshots. Middle panel: corresponding line bisectors. Right panel: convective blueshift variation over simulation time. Each dot represents one snapshot. The black dashed line shows the average convective blueshift of all 13 snapshots.

2009; Vinyoles et al. 2017). Bergemann et al. (2021) and Pietrow et al. (2023) combined the new solar data from the SST facility and 3D NLTE radiation transfer to test the ability of the models to describe the variation of line shapes across the solar disc. They found, from the analysis of the line shapes of the O I line at 7772 Å, that 1D LTE models tend to massively under-predict the strength of the line at the solar limb, thereby over-estimating the chemical abundance of the element by 0.6 dex (a factor 4) compared to the measurements carried out at the disc centre. Fig. 7 demonstrates the applications of the CLV test to the solar O abundance

Other recent investigations address the Rossiter–Maclaughlin effect (see Ohta et al. 2005, and references therein) with 1D LTE, 1D NLTE, and full 3D RHD models of synthetic solar spectra (Reiners et al. 2023). This effect is the systematic and functionally well-defined distortion of the RV shifts of stellar spectral lines as a function of time, that is caused by the planet transit in the system, where the orbital axis of the planet and the spin of the host star are approximately aligned (Rossiter 1924; McLaughlin 1924). A detailed analysis suggests that solar 3D RHD models (in LTE) do not yield a better description of the Rossiter–Maclaughlin effect in the lines of Na I, Ca I, Mg I, and Fe I compared to 1D models (Reiners et al. 2023). In fact, 1D NLTE models or even 1D LTE models provide a better description of the observed RV signal (Fig. 8). A similar study using 3D NLTE (Canocchi et al. 2024) indicated an improvement in the Rossiter–Maclaughlin diagnostics using the solar Na I D and K I lines. Other stellar spectral features, which are relevant for exoplanet diagnostics, however, still remain to be fully explored using 3D NLTE models.

2.3 Limb darkening of the continuum

Observations of the solar surface in narrow-band photometric filters can be carried out with different solar telescopes, such as SST. These can be directly compared to predictions of 3D solar RT simulations. Figure 10 shows the surface intensities at 500

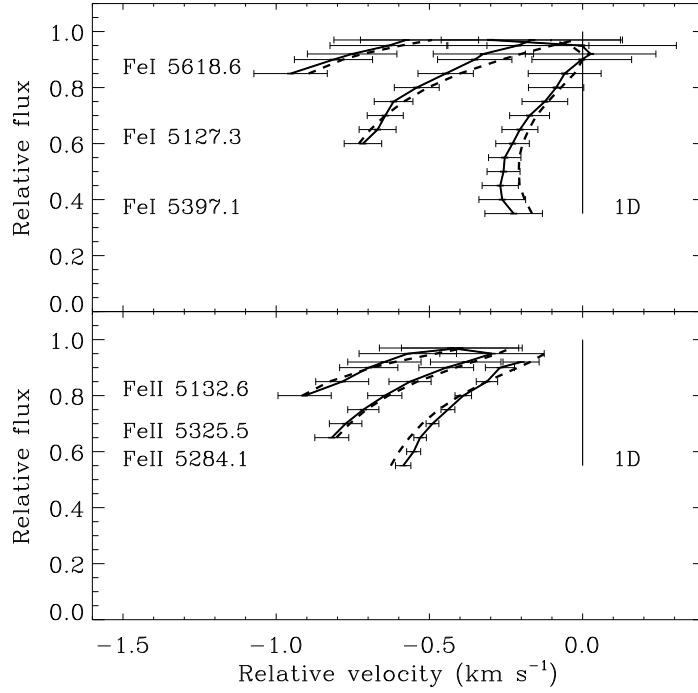


Fig. 5 Convective bisectors observed in high-resolution solar (top) and stellar (bottom) spectra in comparison with bisectors obtained from the 3D LTE radiation transfer models. Here the data are shown with solid lines and error bars. The 3D synthetic spectral models are shown with dashed lines. Image reproduced with permission from [Allende Prieto et al. \(2002a\)](#), copyright by AAS.

nm computed in LTE using the **Stagger** 3D RHD solar model for different viewing angles.

Comparative theoretical studies of the differences between 1D and 3D radiation transfer effects in the broad-band continuum of the Sun were carried out by [Beeck et al. \(2012\)](#), [Pereira et al. \(2013\)](#), and [Eitner et al. \(2024\)](#). These studies suggest that 3D models yield a good agreement in the optical and near-IR CLV continua with the observed solar data. The good agreement is also seen when comparing intensities computed using the small-scale-dynamo (SSD) 3D RHD solar models ([Kostogryz et al. 2024](#)), see Fig. 11. An important unresolved question is the observed continuum brightening in the near-UV. 3D RT models under-estimate the continuum intensities at $\lesssim 400$ nm, especially at the limb.

Taking magnetic fields into account ([Pereira et al. 2013](#); [Kostogryz et al. 2024](#)), yields systematically brighter intensities at all wavelengths and all limb angles. The effect is shown in Fig. 11, where the initial uniform magnetic field of 100 to 300 gauss was applied to the SSD models. The difference with the observed solar data is not a limitation of models, but could also be explained by the observational effect: the solar CLV data were obtained for the quiet Sun, avoiding magnetic concentrations. Indeed, the 10 milli-Tesla (100 gauss) 3D MHD model, which is of the order of the mean magnetic field of the quiet Sun ([Trujillo Bueno et al. 2006](#)), describes the IR solar

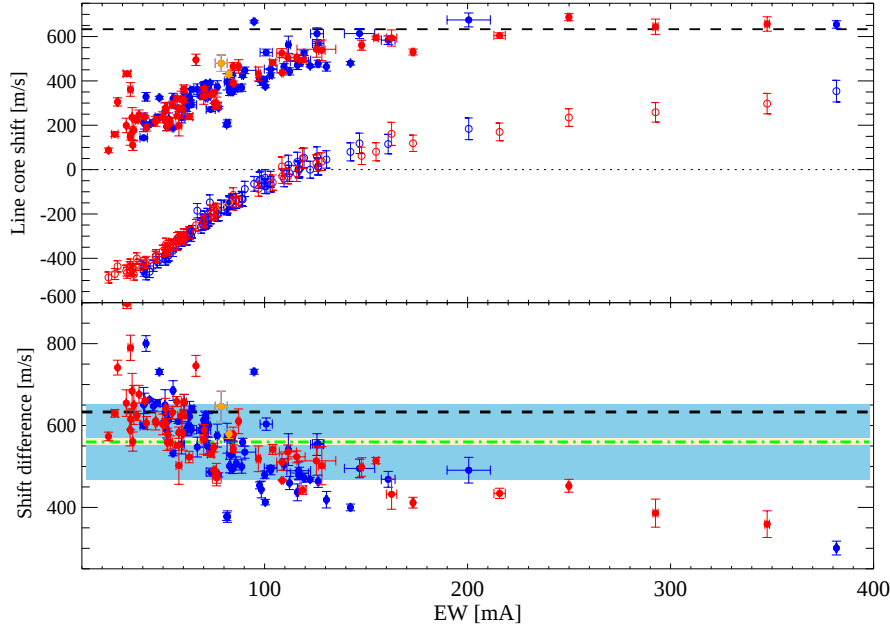


Fig. 6 Observed radial velocity shifts obtained from the cores of over 140 Fe I lines in the solar spectrum (here the spectrum of the Moon), compared to the RV shifts computed in LTE using the solar 3D RHD CO⁵BOLD model. The theoretical solar gravitational redshift 633 m s^{-1} (Einstein) is shown with the black line. Image reproduced with permission from [González Hernández et al. \(2020\)](#), copyright by ESO.

observations better compared to a non-magnetic 3D RHD model ([Pereira et al. 2013](#)). The magnetized 3D model is slightly hotter in the photospheric line formation regions, by up to $\sim +100 \text{ K}$, compared to a non-magnetic RHD model ([Fabbian et al. 2010](#), their Fig. 3). As seen in Fig. 12, the improvement due to MHD effects is also visible in some of the observed solar Fe I lines ([Fabbian et al. 2010](#)). Hence, it still remains to be explored what is the cause of the puzzling mismatch between the observed solar ultra-violet CLV data and the models.

With the availability of TESS lightcurves, it has become possible to place observational constraints on limb darkening of other stars ([Maxted 2018, 2023](#)). Comparison of the data with spatially resolved intensities derived from 1D and 3D model atmospheres suggests that the latter provide an improved agreement with the data for main-sequence stars ([Maxted 2023](#)) compared to 1D LTE hydrostatic models. However, it is also possible to mimic the effects of stellar sub-surface convection by tuning the free parameters, such as those associated with simplified theories describing convecting overshoot and mixing length, in 1D LTE model atmospheres (e.g. [Kostogryz et al. 2022](#)).

Spectral synthesis using 3D MHD simulations further helps to improve the accuracy of the CLV predictions for Sun-like stars. [Ludwig et al. \(2023\)](#) explored 3D MHD models in the context of reproducing stellar optical observations obtained within the Kepler space mission. The principal physical effect is the relative brightening of the

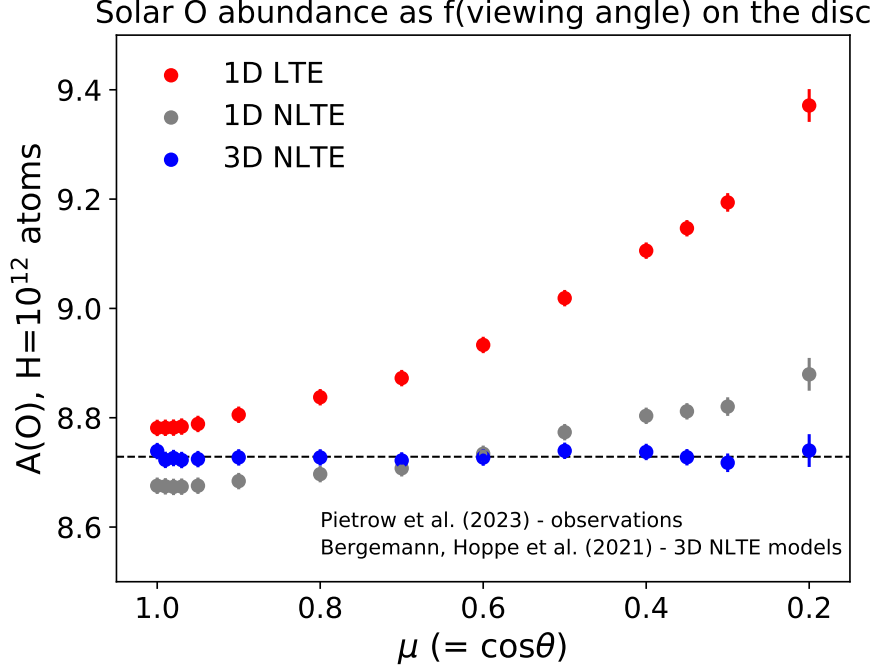


Fig. 7 The centre-to-limb variation of the solar oxygen abundance, computed using 1D LTE, 1D NLTE, and 3D NLTE models. The NLTE models for O and the SST data are from [Bergemann et al. \(2021\)](#) and [Pietrow et al. \(2023\)](#).

limb due to magnetic fields (see the discussion in [Nordlund et al. 2009](#)). A 3D model with 200 to 400 gauss can be up to 200 K warmer at the optical surface compared to the analogous non-magnetic 3D model with the same T_{eff} , $\log g$, and $[\text{Fe}/\text{H}]$ ([Ludwig et al. 2023](#)). However, at larger values of $\langle B_z \rangle \gtrsim 1$ kG a drastic cooling of the entire structure due to suppressed convective motions occurs, leading to the photospheric temperatures drop by almost 1000 K. Also the temperature fluctuations generally increase with increasing $\langle B_z \rangle$.

As a consequence, stellar intensities change substantially when 3D MHD models are used in the calculations of stellar limb darkening (Fig. 13). Specifically, in the optical wavelength range from 450 nm to approximately 900 nm, the relative continuum intensities at $\mu = \cos(\theta) = 2/3$ ($\theta = 48^\circ$) are about 10% higher in 3D MHD models with magnetic fields of around 1 kG than at the disc centre (denoted here as h'_1 ; see Eq. 5 in [Ludwig et al. 2023](#)). Moreover, the intensities at the limb ($\mu = \cos(\theta) = 1/3$, $\theta = 70.5^\circ$) are another 10% brighter compared to that at 50 deg. The sensitivity of intensities to magnetic effects at the level of 0.5 kG is comparable to that of the change in T_{eff} by nearly 1000 K.

In summary, the relative brightening of the limb due to magnetic fields is well-established (e.g. [Ludwig et al. 2023](#); [Kostogryz et al. 2024](#)), but it remains to be explored to which extent do these differences influence studies of stellar activity based on light-curves. Current 3D MHD models for late-type stars consistently under-predict

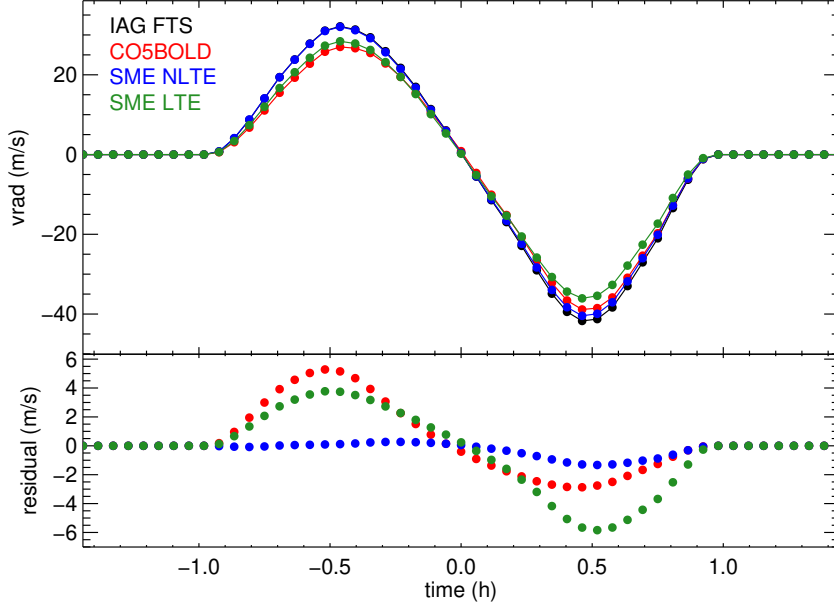


Fig. 8 Comparison of the predicted Rossiter–MaLaughlin RV signals in the cores of the Na I D lines as computed using different 1D and 3D LTE / NLTE radiation transfer models. The curves simulate the transit of a hot Jupiter HD 189733b across a star similar to the Sun. Image reproduced with permission from [Reiners et al. \(2023\)](#), copyright by the author(s).

the limb brightening compared to Kepler light-curve data ([Maxted 2018](#)), which may be attributed to a more complex morphology and distribution of magnetically active regions at the stellar surface ([Ludwig et al. 2023](#)).

2.4 Atmospheric dynamics

Signatures of atmospheric dynamics are also seen in the spectra of red supergiants. The nearby asymptotic giant branch (AGB) star S Ori and red supergiant Betelgeuse have been, in particular, placed in the focus of spatially-resolved studies of atmospheric dynamics with 3D models ([Kravchenko et al. 2019, 2020, 2021](#)). Photocenter variability of Betelgeuse as seen in Gaia were furthermore attributed to large-scale granulation and giant convective cells ([Chiavassa et al. 2020, 2022](#)), although other studies ([Kochanek 2023](#)) find that the instrumental noise is too large to claim the detection of surface sub-structure on RSGs with current facilities like Gaia.

Recently, 3D simulations of red supergiants were carried out in spherical-symmetry using the Athena++ code ([Goldberg et al. 2022](#)). Such 3D star-in-a-box models are essential to map the connection between stellar pulsations, atmospheric dynamics, and mass ejection ([MacLeod et al. 2023](#)), and these models have paved the way to understand interesting observations such as the ‘Great Dimming’ event of Betelgeuse ([Montargès et al. 2021; Dupree et al. 2022](#)) and similar extragalactic events reported in the literature (e.g. [Jencson et al. 2022](#)).

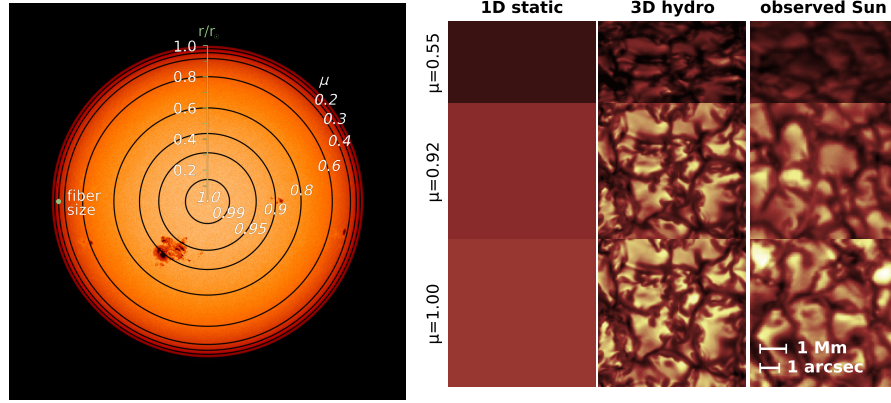


Fig. 9 Left: A view of the solar disk by the Helioseismic and Magnetic Imager (copyright by NASA’s Scientific Visualization Studio). We overplot the concentric rings to illustrate the viewing positions of constant μ -angle and the corresponding radii. The point shows the fiber size of 32.5 arcsec of the IAG instrument. Right: Comparison observed solar G-band intensity at ~ 400 nm with the predictions of 1D hydrostatic and 3D RHD solar model atmospheres at different positions across the solar disc. Both figures from Hoppe et al. submitted.

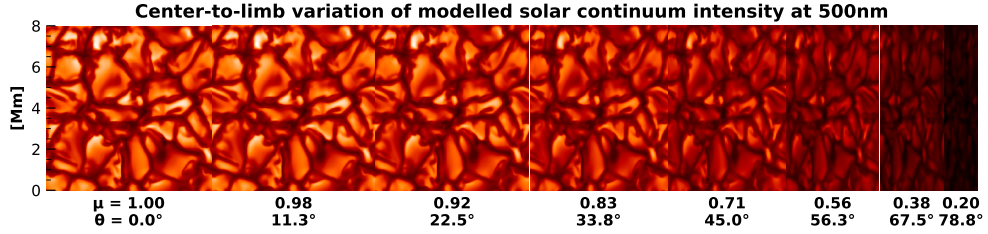


Fig. 10 Continuum intensity at 500 nm as a function of surface position and viewing angle. The employed atmosphere model is a solar STAGGER snapshot.

2.5 Exoplanets and kilonovae

Whereas 3D and NLTE RT in the context of modelling of these two type of objects will be a subject of this review, there are currently no direct spatially-resolved astronomical observations that allow to test the relevance of 3D hydrodynamics and NLTE modelling in their photospheres. Here we adopt the definition that the photosphere is the outer region of the object, where the radiation becomes optically thin and is lost from the object into the interstellar matter, which of course depends on the wavelength.

It, however, is obvious that the main reason for including the effects of geometry and appropriate representation of space and time is primarily the fact that all objects are three-dimensional in nature and conditions in the photospheres of these objects favour deviations from hydrostatic equilibrium and local thermodynamic equilibrium.

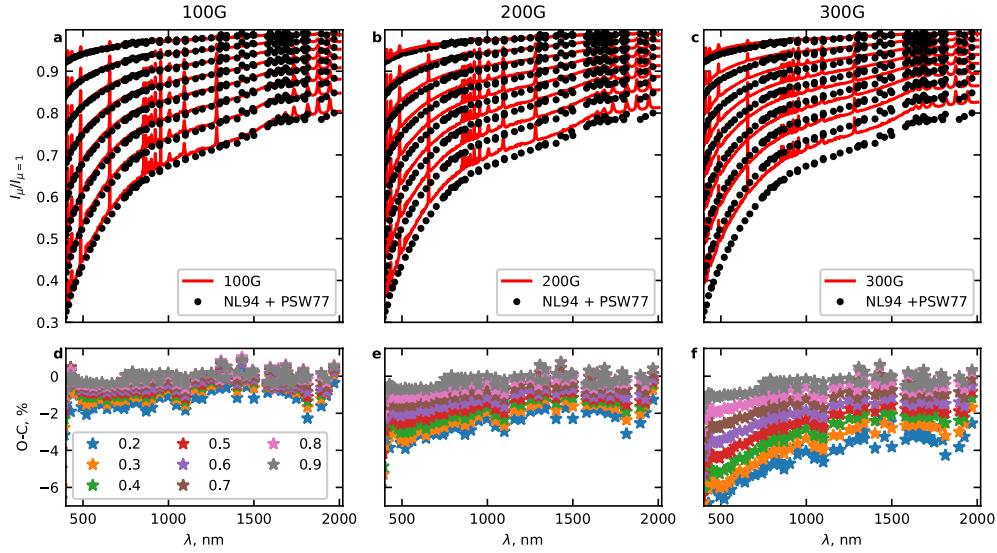


Fig. 11 Comparison of the observed solar center-to-limb variation of intensities with the predictions of 3D SSD models. The models assume different levels of the initial vertical magnetic field (see inset). Image reproduced with permission from [Kostogryz et al. \(2024\)](#), copyright by the author(s).

3 Basic inputs

3.1 Model atmospheres

In order to perform 3D NLTE radiative transfer, pre-computed 3D RHD stellar model atmospheres are typically used. Different codes are available and can be used to generate 3D radiation-hydrodynamics models (RHD), with codes such as MURaM ([Vögler et al. 2004, 2005](#)), CO⁵BOLD ([Freytag et al. 2012](#)), Stagger ([Magic et al. 2013a](#)) and M3DIS ([Eitner et al. 2024](#)). In this review, we only provide a brief summary of the models and techniques, and we refer to other excellent reviews dedicated to solar and stellar convection, and 3D M(RHD) ([Nordlund et al. 2009](#); [Kupka and Muthsam 2017](#); [Leenaarts 2020](#); [Chiavassa et al. 2024](#)).

All 3D RHD models that have so far been used for detailed quantitative studies of the outer stellar convection assume LTE in the calculations of opacity and source function of lines and continua. Approximate treatment of scattering in the lines and/or continuum can be included ([Hayek et al. 2010, 2011](#)), primarily in the framework of coherent and isotropic scattering, representing Rayleigh scattering in the continuum. Comparative analysis of the basic thermodynamic properties of these models suggest excellent agreement in the deeper adiabatic layers ([Beeck et al. 2012](#); [Eitner et al. 2024](#)), where radiative transfer is in the diffusive approximation. But slightly larger deviations between the models are seen in the outer layers, which are sensitive to the detailed micro-physics of line blanketing ([Beeck et al. 2012](#)). Figure 14 illustrates the effect of line opacities in molecular bands of TiO and VO on the radiative energy term Q in the energy equation. The analysis of the influence of opacity binning on the

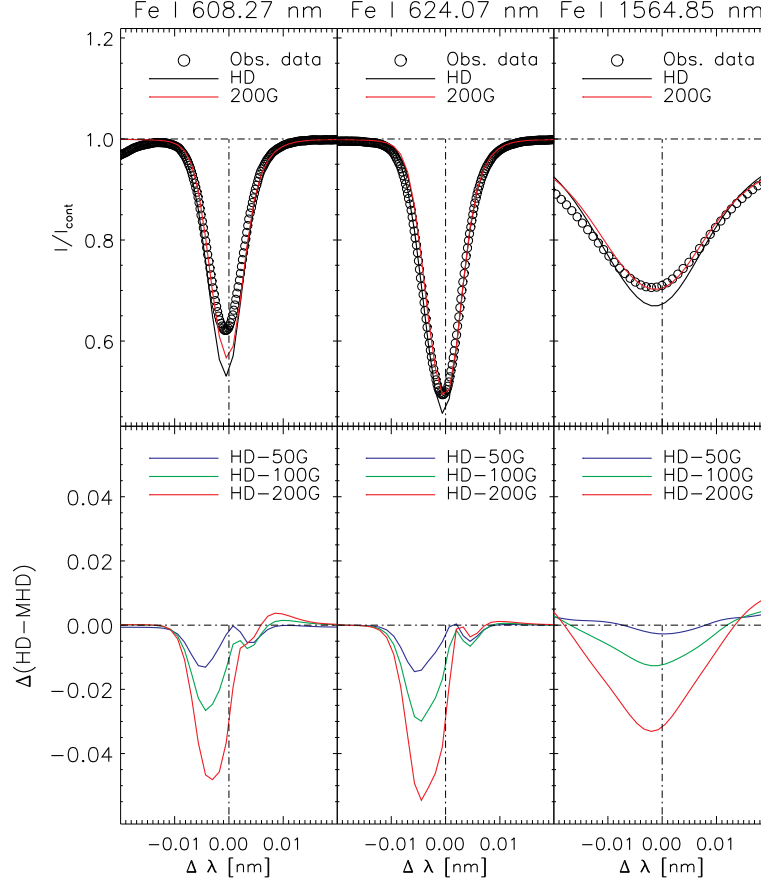


Fig. 12 Comparison of the observed solar Fe I lines with the predictions of 3D MHD solar *stagger* models. The models assume different levels of the initial vertical magnetic field (see inset). Image reproduced with permission from [Fabbian et al. \(2010\)](#), copyright by AAS.

model structure was the subject of [Ludwig \(1992\)](#) and is also extensively investigated in [Perdomo García et al. \(2023\)](#).

Some of the afore-mentioned codes were used successfully to generate grids of 3D models for entire parameter space of FGK-type stars ([Ludwig et al. 2009a](#); [Magic et al. 2013a,c](#); [Bonifacio et al. 2018](#); [Kučinskas et al. 2018](#)). Each model within the grid typically comprises of selected time-slices, that is 3D snapshots, of stellar atmospheres that tabulate temperature T , density ρ , and velocities in the x , y , and z directions v_x, v_y, v_z on a spatial grid consisting of $(n_x \times n_y \times n_z)$ points. For detailed spectroscopy, number densities (or partial pressures) of all species (atoms, molecules) are usually computed from T and ρ within the post-processing NLTE and spectrum synthesis codes. Figure 15 shows the *Stagger*, the 3D *CIFIST*, and *MPIA* grid of 3D RHD models. The coverage is large enough to enable a complete exploitation of 3D RHD structures over the cool part of the HRD, covering the domain of FGKM type stars.

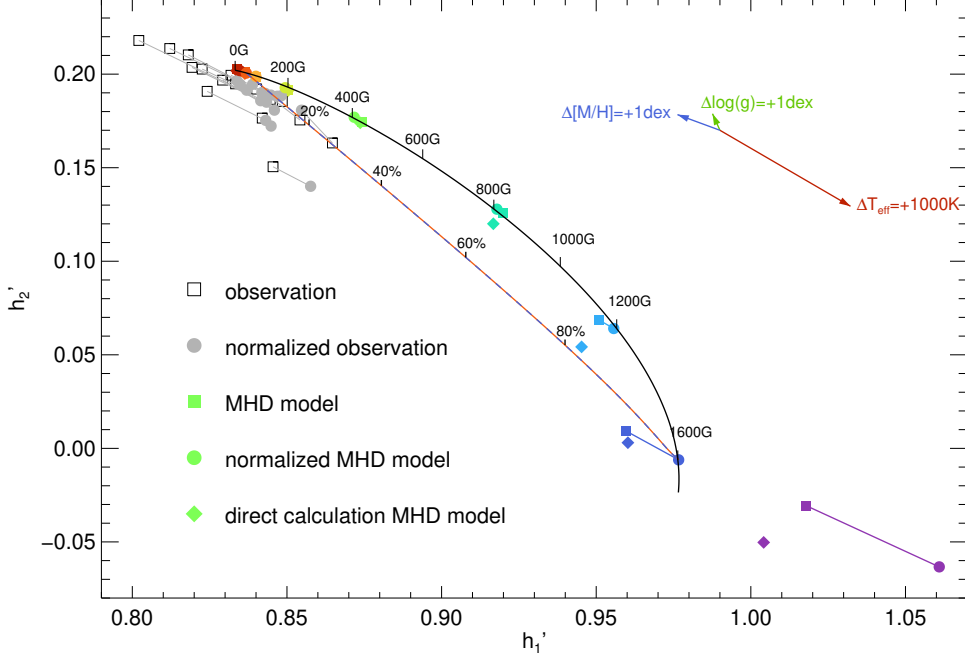


Fig. 13 Comparison of intensity parameters (h_1, h_2) predicted by 3D MHD models with the observed data obtained from Kepler light-curves. See text. Image reproduced with permission from [Ludwig et al. \(2023\)](#), copyright by the authors(s).

3D RHD simulations require a certain minimum spatial resolution and a surface area in order to produce realistic convective patterns and accurate thermodynamic (temperature, pressure, velocity) structures, and to ensure that the radiative balance is captured accurately at all depths. The surface area has to be large enough to contain a representative number of convection cells. Usually, 10 to 20 convection cells are viewed as sufficient to capture the statistical properties of the atmosphere, and such setup is typically used in spectroscopic studies (e.g. [Collet et al. 2007](#); [Bergemann et al. 2012c](#); [Magic et al. 2013a](#); [Amarsi and Asplund 2017](#)). The vertical resolution typically lies around 10 km between adjacent voxels². However, the spatial discretization can vary substantially depending on the desired application ([Eitner et al. 2024](#), their Tab. 2), and on the types of stars ([Rodríguez Díaz et al. 2024](#), their Fig. 3). The vertical step size ranges from δz of ~ 10 km around the optical surface to $\delta z \approx 3$ Mm at the bottom of the simulation for a typical red giant (total size of the 3D box over 250 Mm). [Eitner et al. \(subm.\)](#) furthermore show that a major improvement in the accuracy of the RT solution, and hence a substantial gain in computational efficiency, can be obtained by using a conservative RT solver. That is, in the calculations using short-characteristics

²This is a term that comes from the discipline of computer graphics and may not be taught in physics academic curricula. Here we provide the definition of the term as provided by Wikipedia: “Voxel is a three-dimensional analogue of a pixel; a volume element representing some numerical quantity of a point in a 3D space”

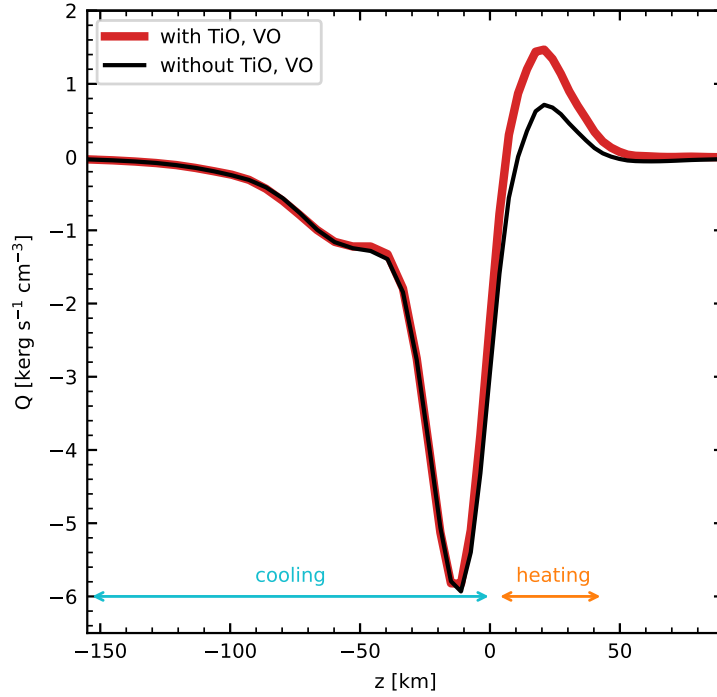


Fig. 14 Effect of line opacities in molecular bands of TiO and VO on the radiative energy term Q in the energy equation. The figure shows the data for a 3D RHD simulation of an M dwarf (Perdomo García et al. 2023).

solver, the intensities are computed at cell interfaces, not in cell centers. This approach conserves energy and allows to reduce the vertical resolution by a factor of 2 to 3.

RT is then carried out in the quasi-stationary setup, using the so-called 3D cubes of physical quantities extracted using regular time steps, typically minutes to hours, depending on whether a main-sequence or an RGB star is analysed. These cubes are commonly referred to as “snapshots”. In Fig. 3.1, we show the surface temperature structure at optical depth unity for 3 types of stars, a typical M dwarf and a red giant branch star. We note that the boxes are very small compared to the total size of the star, and for a more intuitive understanding we additionally show in Fig. 3.1 how the 3D RHD box-in-a-star cubes fit into the stellar sphere (here an red giant) in physical units.

Synthetic stellar spectra computed for different snapshots are then averaged in time (e.g. Bergemann et al. 2019; Gallagher et al. 2020), applying the Ergodic hypothesis (credited to Ludwig Boltzmann, Boltzmann et al. 1964), which postulates — for long time series and large volumes — the equivalence of averaging in time and in space.

The horizontal and vertical resolution of the 3D cubes in the (x, y, z) space is relevant in the context of asymmetries of spectral lines. The detailed line properties are sensitive to the statistics of convective up- and down-flows, and hence usually

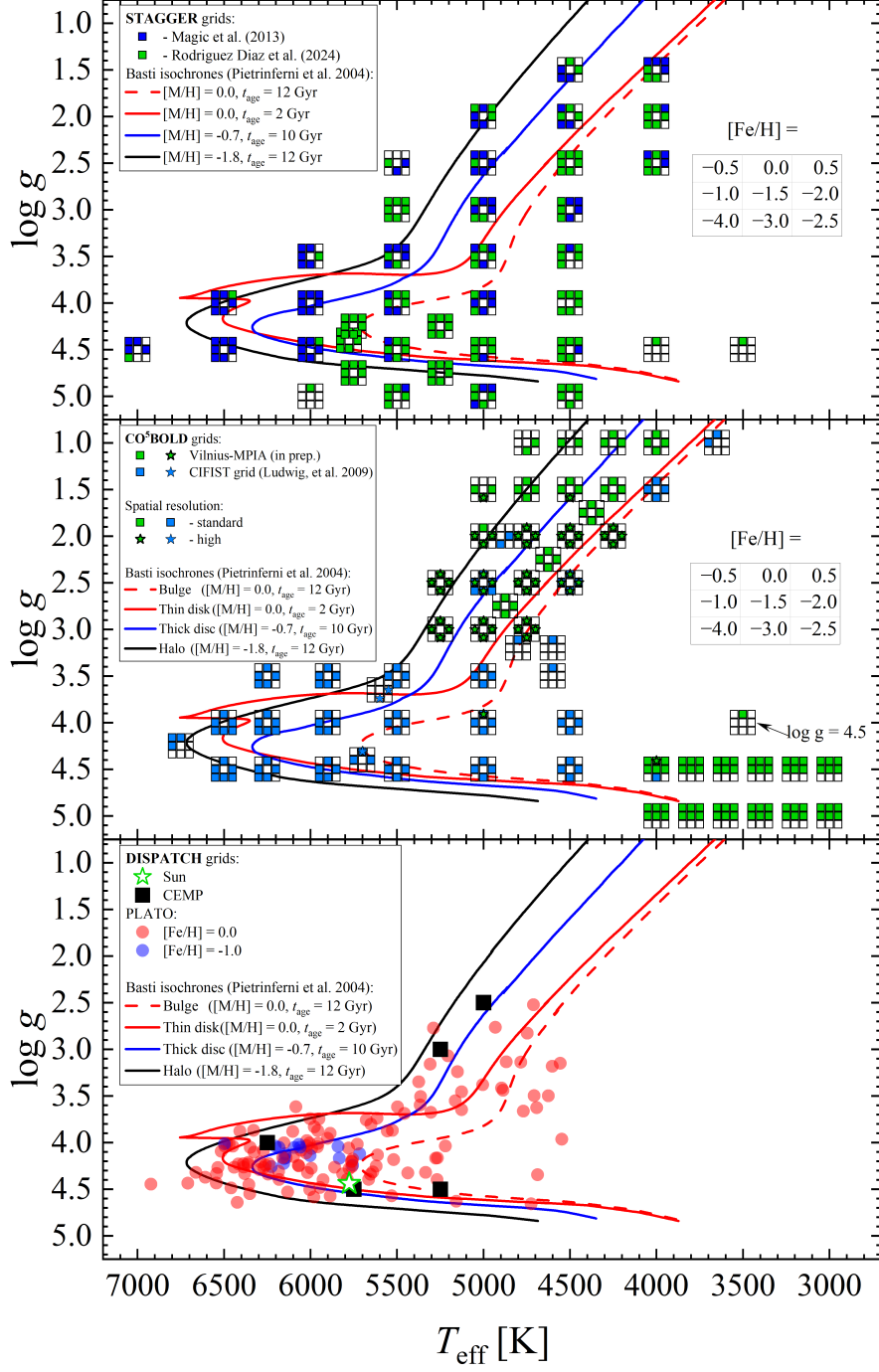


Fig. 15 The Stagger, 3D CIFIST (Co5BOLD), MPIA (M3DIS at Dispatch) grid of 3D RHD models. Image courtesy of Jonas Klevas

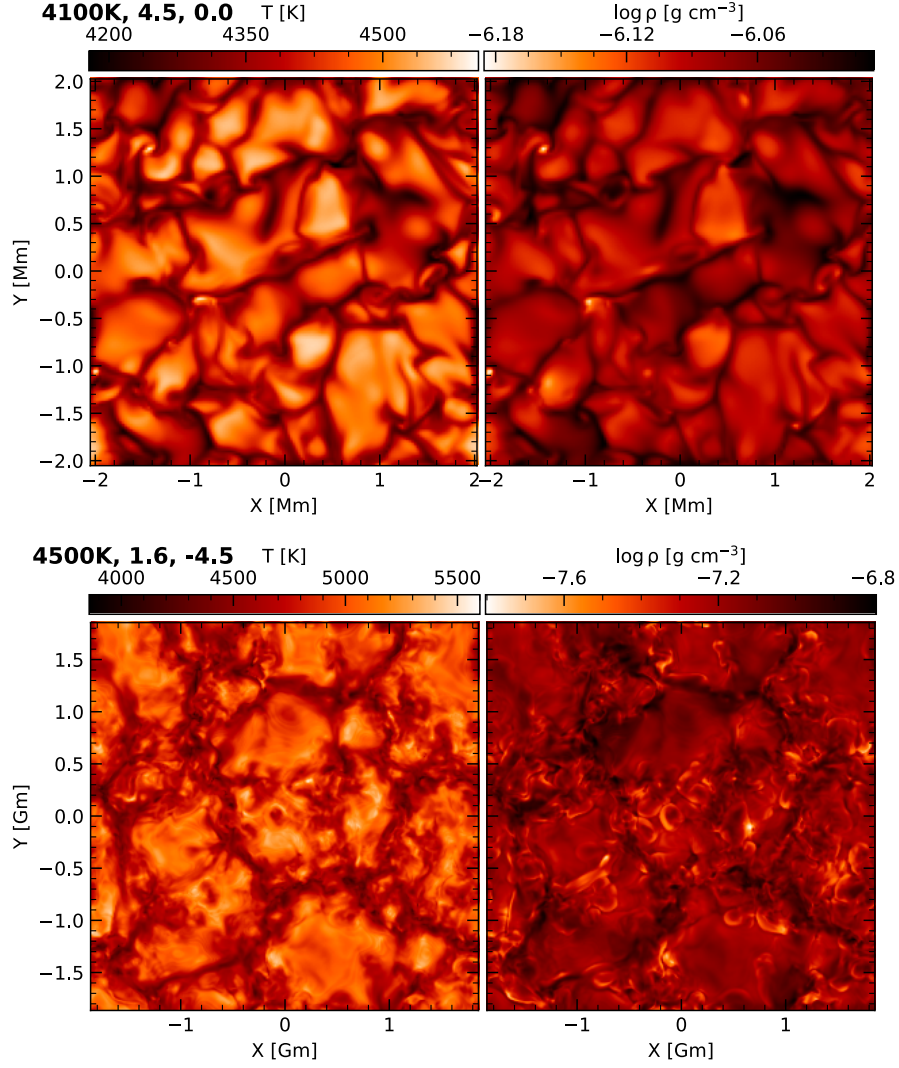


Fig. 16 Surface temperature structure at optical depth unity for two types of stars, a typical M dwarf and a M-type red giant. Note the difference in spatial scales of the simulation boxes, ranging from a few Mm to Gm for a red giant. The M dwarf 3D model adopts the solar metallicity, whereas the red giant 3D RHD model is a CEMP model computed using $[\text{Fe}/\text{H}] = -4$. Images courtesy of Philipp Eitner, see [Eitner et al. \(2024\)](#) for details.

careful tests by down-sampling of the 3D RHD models are performed ([Magic et al. 2013b](#); [Steffen et al. 2015](#); [Nordlander and Lind 2017](#)). For example, [Rodríguez Díaz et al. \(2024\)](#) showed that in LTE, the error introduced by down-sampling the 3D cubes depends on stellar parameters, but for weaker lines (reduced $\log \text{EW} < -5$) is typically within 0.02 dex to 0.03 dex at a vertical resolution of 120 grid points for both turnoff stars and red giants. On the other hand, these asymmetries have a minimal

$T_{\text{eff}} = 3640 \text{ K}$, $\log g = 1.0 \text{ [cgs]}$, $[\text{Fe}/\text{H}] = 0$,
 $1.8 M_{\odot}$ star, continuum at 500 nm

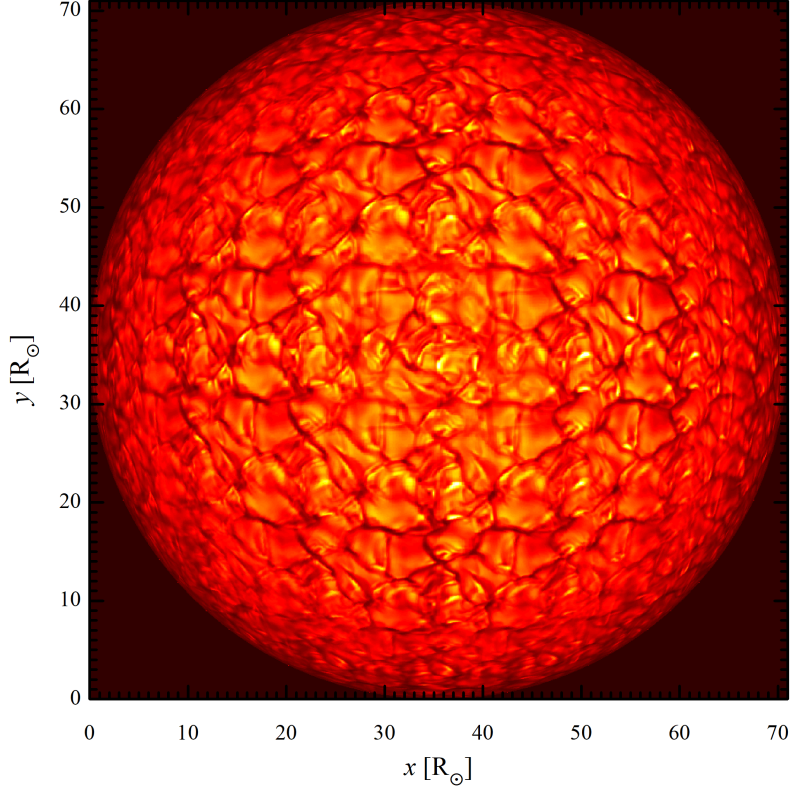


Fig. 17 Radiation field at 500 nm computed using a 3D RHD model of a red giant with parameters indicated in the figure header. The 3D RHD cube (box-in-a-star) was used to fill the entire sphere using the radius of $70 R_{\odot}$ for a mass of $1.8 M_{\odot}$, and tiled to account for the limb darkening. Image courtesy Jonas Klevas.

effect on the integrated radiative rates in the SE calculations. Therefore, it is possible to compute the determine departure coefficients using drastically downsampled 3D snapshots, e.g., at horizontal resolution of $(x, y) = (30, 30)$ (Bergemann et al. 2019). These can then be interpolated and applied to the full-sized 3D snapshot to perform the spectrum synthesis. While this approach applies to the horizontal resolution, it does not necessarily apply to the vertical resolution of the boxes. The steep drop in opacity

in the photosphere (caused by the continuum H^- cooling in FGK-type stars) has to be resolved as well as possible, therefore it is best not to reduce the vertical resolution of the snapshot in the vertical. Potentially one can also utilise static mesh refinement, which keeps the layers of the photosphere at maximum detail, but interpolates the layers at large optical depths onto a coarse grid as the temperature structure becomes more and more homogeneous deeper in the atmosphere.

3.2 The equation of gas state

The Equation of State (EoS) defines the relationship between various state variables, which describe the properties of a plasma, gas or more generally, any kind of medium. These state variables include temperature, density, pressure, internal energy and more, therefore the EoS is not strictly a single equation. While the formal solution of the RT equation is reasonably similar in all types of astrophysical media, the choice of the EoS defines the applicability of a numerical code to a certain temperature-density regime, since it plays a central role when determining the radiative opacities and hence stability with respect to convective energy transport (Cox and Stewart 1965; Mihalas et al. 1978; Hummer and Mihalas 1988). The most widely-used and simplest EoS is the ideal gas law

$$P = nk_B T, \quad (1)$$

where P is the gas pressure, $n \equiv N/V$ is the number density of particles in the gas (per unit volume), k_B is the Boltzmann-constant, and T is the gas (also known as kinetic) temperature. This relation appears simple enough, but hides the fact, that n has a number of dependencies, including a strong temperature dependence. The gas contains many different particles

$$n = n_e + n_{\text{ions}} + n_{\text{molecules}}, \quad (2)$$

where n_e is the number density of free electrons, n_{ions} the number densities of atoms in different ionization stages (neutral, singly-ionized, etc), and $n_{\text{molecules}}$ the number density of molecules.

The number densities of the various ions and molecules depend on temperature, chemical composition of the gas, and other quantities. Different particles can combine in one way or another, which does not conserve the quantity n . When the gas is in thermo-dynamic equilibrium, the chemical equilibrium constant K may be used. These constants yield the ratios of particles from a given process of dissociation or attachment, $A + B \rightleftharpoons AB$.

$$K_{A+B} = \left[\frac{n_A n_B}{n_{AB}} \right]_{\text{LTE}} \quad (3)$$

Generally the relative number of particles are given by

$$\left[\frac{n_A n_B}{n_{AB}} \right]_{\text{LTE}} = \frac{U_A U_B}{U_{AB}} \left(\frac{2\pi k_B T}{h^2} \right)^{3/2} \left(\frac{m_A m_B}{m_{AB}} \right)^{3/2} e^{-E_D/k_B T}, \quad (4)$$

where U are the temperature dependent partition functions of the respective species, m are their masses, E_D is the dissociation energy of the compound specie, and the rest of the constants have their usual meanings.

For ionizing reactions between free electrons and atoms in different ionization stages I , there is the equivalent Saha equation:

$$\left[\frac{n_e n_{I+1}}{n_I} \right]_{\text{LTE}} = \frac{2U_{I+1}}{U_I} \left(\frac{2\pi m_e k_B T}{h^2} \right)^{3/2} e^{-E_I/k_B T}, \quad (5)$$

where E_I is the ionisation threshold energy.

Given estimates of K_{A+B} for the most frequent interactions, one can assemble a system of non-linear equations and solve it iteratively to obtain the number densities of the different particles. This system of equations is closed through particle conservation. The number of free electrons changes due to ionisation of atoms, and thus n_e is obtained by summing the number of ionised particles multiplied by their corresponding ionization stage. To determine an electron number density that is consistent with T and ρ , an iterative process is used, starting with an initial guess for n_e , since it is also required in the Saha equation.

The fundamental Boltzmann equation relating the ratio of bound energy states (states within the same ionization stage) is:

$$\left[\frac{n_j}{n_i} \right] = \frac{g_j}{g_i} e^{-(E_j - E_i)/k_B T}, \quad (6)$$

where E_i is the excitation energy of the level i and E_j is the excitation energy of the level j , and g_i are the statistical weights of both levels, respectively.

The choice of partition functions U_I of the ions has an impact on the EoS (Graboske et al. 1969). They influence the state variables through Eq. (5) and they enter the opacities when computing the number densities of individual atomic energy states in LTE. The partition function of the ionization stage I of an ion is give by the sum:

$$U_I = \sum_i g_i e^{-(E_i - \Delta E)/k_B T}, \quad (7)$$

here, the ΔE term is introduced since ionisation and excitation energies are effectively altered by the presence of charged particles in the surrounding medium. Increasing electron number density lowers the ionisation threshold and some highly excited energy states might become unbound. This phenomenon is known as Debye shielding, Debye screening or pressure ionisation. Without this depression in the ionisation potential one would face infinite partition functions as Eq. (7) diverges when leaving out ΔE and including more and more excited energy states. The radius of the atoms would become larger than the mean distance to the neighbouring atoms, which is obviously not the case in reality. Debye shielding can be treated to various degrees of physical realism and is mostly important in the interiors of stars.

The atomic partition function calculations by Irwin (1981) for example use a static value $\Delta E = 0.1 \text{ eV}$. This means they truncate the sum in Eq. (7) to only include

energy levels with $E_i < E_I - \Delta E$. The high-energy states were given lower weights when fitting polynomials to their calculations though. Therefore, the effective value of ΔE in the published polynomial expressions of the partition functions might vary. [Irwin \(1981\)](#) also states that many of the atomic partition functions used by [Kurucz \(1970\)](#) are based on tables by [Drawin and Felenbok \(1965\)](#), which also employ $\Delta E = 0.1 \text{ eV}$. Some of the other partition functions by [Kurucz \(1970\)](#) were calculated using values for ΔE based on the Debye–Hückel theory

$$\Delta E = Z \frac{q_e^2}{r_D}, \quad r_D = \sqrt{\frac{k_B T}{4\pi q_e^2}} \left[n_e + \sum_i Z_i^2 n_i \right]^{-1/2}, \quad (8)$$

where Z is the ionisation stage, so $Z = 0, 1, 2$ for neutral, singly ionised and doubly ionised species respectively, r_D is the Debye length and $q_e^2 = e^2/(4\pi\epsilon_0)$, with the electron charge e . If there are only singly ionised species or hydrogen is by far the most dominant ion, then $n_e + \sum Z_i^2 n_i \approx 2n_e$, therefore

$$r_D \approx \sqrt{\frac{k_B T}{8\pi q_e^2 n_e}} \quad \text{and} \quad \Delta E \approx Z \sqrt{\frac{8\pi n_e}{k_B T}} q_e^3, \quad (9)$$

The latter approximation is employed by [Griem \(1964\)](#), whose formulation has been widely adopted in the stellar atmospheres community, especially those codes descendent from the Uppsala opacity package ([Gustafsson et al. 1975](#)), such as MARCS and STAGGER.

Using this depression in the ionisation potential results in a thermodynamically inconsistent EOS however, as the populations are corrected, but the same does not necessarily apply for partition functions, internal energies and gas pressures. The abrupt switching between bound and free states also introduces undesirable discontinuities in the thermodynamic as well as optical properties of the medium ([Hummer and Mihalas 1988](#)).

A more accurate treatment of the shielding effect is done in the occupation probability formalism developed by [Hummer and Mihalas \(1988\)](#); [Mihalas \(1988\)](#); [Daeppen et al. \(1988\)](#), also known as the MHD (Mihalas–Hummer–Däppen) EoS. In this formalism the energy shift ΔE is interpreted as the occupation probability w_i of a given state and the partition function is reformulated as

$$U_I = \sum_i w_i g_i e^{-E_i/k_B T}. \quad (10)$$

w_i describes the complement probability of the event that an energy level is disrupted by interactions with other particles in the medium and an electron becomes unbound. The occupation probability drops rapidly close to the ionisation threshold and allows for a smooth transition between bound and free states. Equations (7) and (10) are mathematically equivalent, so reformulating the partition function is not the reason, why the MHD formalism is more accurate. Unfortunately, w_i depends on the number densities of particles, which act as potential collision partners. This means U_i

depends on the chemical composition of the medium and its computation becomes significantly more involved. In all cases the quality of the partition functions depends on the available atomic data, such as values for g_i and E_i .

Recent values of partition functions and dissociation constants for vast number of molecules and all stable atoms are provided by [Barklem and Collet \(2016\)](#). With the intention to provide chemical composition independent partition functions they neglect the effects of pressure ionisation though. Their Fig. 8 shows that uncertainties in the partition function of neutral atoms due to pressure ionisation are $> 1\%$ above 6000 K and $> 10\%$ above 8000 K.

In summary, astrophysical equations of state can be divided into two groups. Firstly, composition dependent EOSs used in spectrum synthesis codes, which typically neglect or approximate high-density effects like pressure ionisation. Secondly, EOSs used in structure modelling, which are usually precomputed for specific chemical compositions for reasons of efficiency. It should not be forgotten, however, that our knowledge of astrophysical structures and spectra is codependent. Therefore, we would like to point out, that the differences between the two types of EOSs need to be bridged for the consistent spectroscopic study of chemically peculiar environments.

3.3 Models of atoms and molecules

LTE and NLTE calculations rely on atomic and molecular structure. Here we provide a brief overview of sources that are typically used in calculations of radiation transfer in conditions of stellar and planetary atmospheres, as well in conditions of expanding shells, such as, e.g. kilonovae.

In LTE, the required inputs are vastly simpler compared to NLTE, as only a few parameters are required to describe the radiation field in a given transition. These are: wavelengths of transitions, energies and statistical weights of their lower and upper energy states, and the corresponding transition probabilities. For LTE radiation transfer, all required information is usually provided in public databases, such as:

- NIST (National Institute of Standard and Technology, at the time of submission of this review, Standard Reference Database 78) includes ionization energies, levels, and lines for all elements from H to U <https://physics.nist.gov/PhysRefData/ASD/lines.form.html>
- VALD (The Vienna Atomic Line Database) includes linelists for atoms and di-, tri-atomic molecules, also hyperfine structure and isotopic shifts <http://vald.astro.uu.se/>
- Exomol (High temperature molecular line lists for modelling exoplanet atmospheres) includes linelists for <https://www.exomol.com/>
- Kurucz database includes energy states, linelists, hyperfine and isotopic structure for neutral, singly-ionized atoms of most chemical elements, as well as some data for higher-ionized atomic species, and selected di- and tri-atomic molecules <http://kurucz.harvard.edu/>
- DREAM (Database on Rare Earths At Mons University) includes atomic data for lanthanides ($Z= 57$ to 71 in up to three ionization stages) <https://agif.umons.ac.be/databases/dream.html> ([Quinet and Palmeri 2020](#))

- VAMDC (Virtual Atomic and Molecular Data Center) includes TBC <https://species.vamdc.org>
- MOOG (linemake) (Atomic and Molecular Line List Generator for the MOOG spectrum synthesis code) includes critically-reviewed atomic and molecular linelists for neutral and singly-ionised atoms of most chemical elements <https://github.com/vmplacco/linemake> (Placco et al. 2021)
- HITRAN (high-resolution transmission molecular absorption database) (Gordon et al. 2022). <https://hitran.org/home/>.

The following compilations may also serve as a useful and critical resource of atomic and molecular data: MOOG data <https://www.as.utexas.edu/~chris/lab.html> and the Carsus package <https://github.com/tardis-sn/carsus>.

In NLTE, in contrast, much more sophisticated atomic or molecular data are required. These, in addition to the parameters described above, include detailed wavelength-dependent photo-ionization cross-sections for each energy state, collisional rate coefficients for excitation, charge-transfer, and ionising reactions, photo-dissociation cross-sections, and possibly other types of processes, such as di-electronic and three-body recombination. Some examples of NLTE atomic models are shown in Fig. 18.

Recently, sophisticated quantum mechanical calculations of collision induced inelastic processes have become available for many atoms (Barklem 2016). These include transitions in neutral and singly-ionized atoms of Li I, Na I, O I, Fe I, Ni I, Y I (e.g. Belyaev and Barklem 2003; Barklem et al. 1998; Barklem 2007; Belyaev et al. 2010; Barklem 2018; Voronov et al. 2022; Wang et al. 2024), but also effects in transitions involving different isotopes $^6\text{Li}/+H/D/T^7\text{Li}$ (Belyaev and Voronov 2021). These rely on methods of nuclear dynamics, such as probability currents and multichannel linear combination of atomic orbitals (LCAO), which involves different levels of treatment of non-adiabatic regions (in the simplest case, ion-covalent interactions only). But also more sophisticated approaches are available that consider large and small inter-nuclear distances (Landau–Zener approach, Belyaev et al. 2014). Also potential energy surfaces for interim states (quasi-molecule) are needed, which are typically obtained via quantum chemistry calculations. In addition, the recipe by Kaulakys (1991, 1992) can be used for very high-excitation (above ~ 5 eV) Rydberg states. In certain instances, e.g. Li and Na, validation on experimental data has been carried out (Barklem et al. 2003, 2021).

NLTE atomic models have been publicly released as part of several NLTE RT codes. These include the Tlusty database: (Lanz and Hubeny 2003) and Turbospectrum v20. database <https://keeper.mpg.de/d/6eacbf95b88448f98a4/> (Gerber et al. 2023).

4 Numerical 3D radiative transfer

4.1 Motivation and equations

The development of astrophysical 3D RT solvers has been tightly coupled to the development of 3D RHD models of stellar sub-surface convection and of model stellar

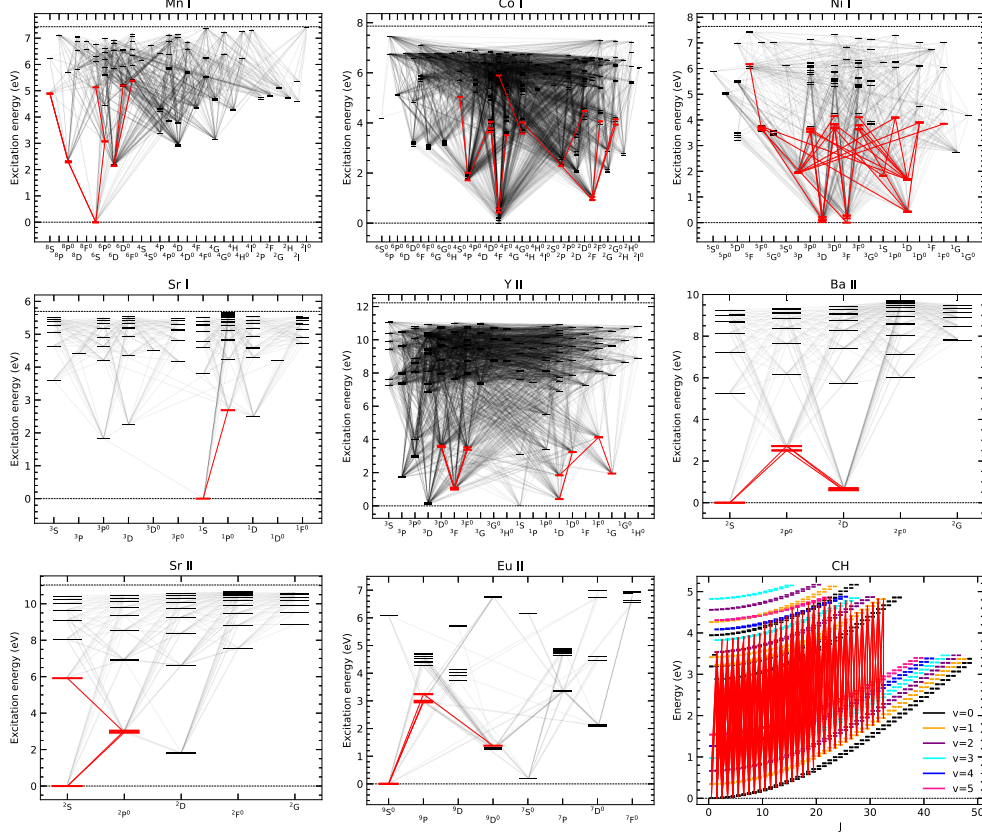


Fig. 18 NLTE model atoms for selected atoms and molecules (see figure insets). Figure reprinted with permission from [Storm et al. \(2025\)](#), copyright by the author(s).

spectra. The latter can be used to determine fundamental stellar parameters and chemical composition by comparing synthetic observables with the observed data (spectra, broad-band photometry, light-curves, etc).

In the following section, we limit ourselves to 3D RT codes and methods, which found application in stellar diagnostic spectroscopy and 3D NLTE radiative transfer. We thus, do not cover comprehensively the RT methods that have been developed as components of RHD solvers. The latter usually employ a simplified treatment of RT equations, because these dominate the computational cost when progressing the RHD solvers by one timestep (e.g. [Nordlund 2019](#)).

We note that commonly radiative transfer is assumed to be *quasi-static*, that is, the time derivative is neglected. This is a good approximation when the photon propagation time is much shorter than the fluid motion time ([Mihalas 1988](#)). Light is assumed to propagate instantly through the system.

4.2 Time-independent formal solution

Standard textbooks and papers, including [Mihalas et al. \(1978\)](#), [Carlsson \(2008\)](#), [Crivellari et al. \(2020\)](#), give an excellent overview of numerical approaches in one- and multi-dimensional radiative transfer. A compact overview of the history of radiation transfer and its basis can be found in [Shore \(2002\)](#).

The main work in 3D radiative transfer consists of solving the time-independent monochromatic equation of radiative transfer along the path of the photons, which is essentially the same problem as in the 1D case.

$$\frac{dI}{d\tau} = I - S, \quad (11)$$

where I is the specific intensity [usually in units of $\text{erg}/\text{cm}^2/\text{s}/\text{\AA}/\text{ster}$] and S is the source function defined as $S \equiv \eta/\chi$, the ratio of the emissivity η [$\text{erg}/\text{cm}^3/\text{s}/\text{\AA}/\text{ster}$] and the extinction coefficient χ [cm^{-1}]. The formal solution is obtained by integrating the optical depth τ and source function along the direction of propagation.

$$\tau(s) = \tau_0 - \int_0^s \chi ds \quad (12)$$

$$I(\tau) = I_0 e^{-\tau} + \int_0^\tau S(\tau') e^{-(\tau-\tau')} d\tau'. \quad (13)$$

Since there are usually no analytical expressions of χ and S along the ray, we have to discretise the integrals above to match the spacing of points on the simulation grid. Then we can use simple functions to estimate how χ and S vary between the grid points, ie. interpolation. These simple functions can be integrated analytically and give us an approximation of the original integral. [Janett et al. \(2017\)](#) point out that the accuracy of the conversion to optical depth in Eq. (12) is as important as for the interpolation of the source function in Eq. (13).

In order to minimise the computational cost, one has to strike a balance between fine grid spacing with simple interpolation techniques or a coarser grid with higher-order interpolation methods. The latter usually inhibits efficient vectorisation of the radiative transfer solver and increases the amount of communication in parallelised codes, which divide the simulation grid between multiple MPI ranks. Increasing the number of grid points, on the other hand, increases memory requirements and overall execution time (including opacity and possibly non-LTE calculations).

4.3 1.5D RT approach

We begin with the so-called “1.5D” RT approach ([Kiselman and Nordlund 1995](#)), which is a very convenient method that circumvents most of the problems of full angle-coupled 3D RT in a 3D data cube. In the 1.5D approximation, every vertical column in the 3D cube from the 3D RHD simulation is treated as a separate 1D atmosphere, however, with realistic physical T - P_{gas} -velocity structure from the 3D RHD simulations. This way there is no interpolation of local matter quantities between the columns and no cross-talk of the radiation field either. The emerging radiation

fluxes computed for each column are then averaged at the top plane of the atmosphere to represent the flux of the full 3D RT solution.

The 1.5D approximation yields a major speed up in the 3D RT computation, if the interpolation of off-grid quantities is the main bottleneck. We note, however, that for larger NLTE statistical equilibrium problems, this interpolation is just one of many computationally expensive operations. The 1.5D approach is used, for example, in NLTE codes `RH1.5D` (Pereira and Uitenbroek 2015) and `Nicole` (Socas-Navarro et al. 2015). The consequences of this approximation are not easily predicted and are best checked for each individual application. Socas-Navarro et al. (2015) suggest that it works well in LTE and also for strong lines in NLTE, where the mean free path is small. Kislman and Nordlund (1995) find that it has little influence on the NLTE source function of the 777 nm oxygen triplet in the Sun, but one should still use full 3D radiative transfer when computing the line profiles. Amarsi et al. (2016) repeat this test with multiple FGK-type stars and show that the approximation yields an error of 0.01 dex in the oxygen abundance where the 777 nm triplet forms higher in the atmosphere, typically solar-metallicity turn-off stars. Bergemann et al. (2019) compare 3D and 1.5D for Mn and find that both yield very similar line profiles suggesting that 1.5D NLTE is fully sufficient for spectroscopic diagnostics of late-type stars.

Since continuum emission in FGKM-type stellar atmospheres is fairly isotropic, the 1.5D RT method produces reasonable estimates of mean (angle-averaged) intensities J_ν even when integrated over only a few number of angles. This implies that 1.5D approach can be safely used in NLTE SE calculations, where only J_ν (usually integrated over large frequency ranges) are required for the integrals of radiative rates.

4.4 Interpolation of extinction, source function and intensity to the photon path

The main complexity of multi-D radiative transfer in inhomogeneous atmospheres (in contrast to 1D plane-parallel RT) is that all quantities appearing in the radiative transfer equation must be mapped to the path of the photons.

This mapping is necessary before one can perform the formal solution of the radiative transfer equation in the same way as is done in the 1D case. For this purpose one has to choose which rays to follow through the simulation domain. The methods of *long-characteristics* and *short-characteristics* have proven dominant for this purpose in the context of stellar atmospheres (e.g. Carlsson 2008). In the context of both schemes, it is useful to introduce the concept of *upstream*, or “*U*” and *downstream*, or “*D*” directions. In this analogy, the flow of photons resembles a stream, with quantities positioned either upstream (the direction from which the photons come) or downstream (the direction they flow in). Both of these methods are illustrated in Fig. 19 and will be described below.

The method of long-characteristics (LC), also known as full characteristics, involves following a ray of light from a fixed boundary condition through the entire simulation box until it exits the atmosphere at the top (Jones and Skumanich 1973; Jones 1973). One has to interpolate χ and S between the grid-points, but one can reuse I from the upstream ray since the rays connect. However, if the value of I is needed on the grid points, one would either have to trace as many rays through the entire box as there

are grid points, which is very costly, or one would have interpolate I after all and map it back onto the grid-points (e.g. Skartlien 2000).

A widely-used alternative is the method of short-characteristics (SC) (Mihalas et al. 1978; Kunasz and Auer 1988), also presented in Fig. 19. In this approach, one follows disconnected rays, which only extend from one layer to the next. The basic quantities χ , S and I , are interpolated between the grid points of the upstream plane. This leads to I being blurred between each layer and strong sources of intensity can be diffused outwards horizontally, which can be demonstrated in searchlight beam tests (Hayek et al. 2010; Ibgui et al. 2013). For a more detailed description of the SC method in three dimensions see V  th (1994). SC and LC are equivalent for plane-parallel atmospheres or if the rays cross a grid point in each horizontal layer, i.e. when there is no need for horizontal interpolation.

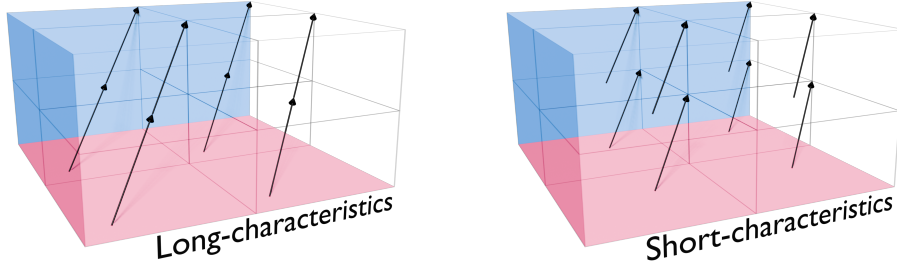


Fig. 19 Methods of long and short-characteristics. In the case of short-characteristics (right-hand side panel) the upstream intensity I_+ is interpolated at the base of each ray, whereas in the case of long-characteristics (left-hand side panel) the resulting intensity has to be interpolated on the grid points.

The MAGRITTE code (De Ceuster et al. 2020) uses a classic LC scheme, as it traces rays upstream until hitting the boundary condition for each grid point in the simulation grid. Also MULTI3D (Leenaarts and Carlsson 2009), SCATE Hayek et al. (2011) and BALDER (Amarsi et al. 2018) use LC when computing the flux emerging at the top of a stellar atmosphere. LC is the method of choice, when high-precision spectral line profile are desired as it is the least diffusive way of transferring radiation through the atmosphere.

The SC method is favoured, if the mean intensity on the grid points is required. This is for example the case when the scattering problem or the NLTE problem are tackled. All scattering codes listed in table 1, except for PHOENIX/3D Hauschildt and Baron (2006) and NLTE3D (Steffen et al. 2015), use the SC method to compute the mean intensity J at each grid point. This requires repeated usage of the SC method for multiple directions. The resulting intensities at the grid points can be integrated via a weighted sum to yield J , see section 4.6. The value of J has an impact on S of each grid point and radiative transfer can be repeated with updated S values. Coherent and isotropic scattering is additionally sometimes included in the continuum (e.g. Cayrel et al. 2004), therefore the diffusion of spectral line shapes is often no great concern. The SC method is more easily vectorised than the LC method, especially on regular grids.

Hauschildt and Baron (2006) have shown that for strongly scattering atmospheres, the method of LC outperforms SC noticeably in terms of accuracy in *J.* Baron and Hauschildt (2007) point out that SC might make up for this with an increased grid resolution, since their SC implementation has lower memory requirements. The NLTE3D code (Steffen et al. 2015) used to compute the NLTE statistical equilibrium uses the LC scheme.

In either case, SC or LC, one has to choose a suitable interpolation scheme to map χ , S and potentially I to the photon path. In order to minimise the number of interpolations, most codes interpolate these quantities at the positions where the rays intersect the XY, XZ or YZ planes. This reduces the problem to 2D interpolation. An exception here is “subgridding”, discussed in section 5, when one has to perform a 3D interpolation. While linear interpolation is an obvious and robust choice, higher-order methods are also used in the stellar atmospheres community, as their accuracy improves much faster with increased resolution compared to linear interpolation. The drawback of more complex interpolation schemes, like parabolic and higher-order methods, is that they can introduce spurious extrema in the interpolated quantity between the grid points. In the worst case, this can result in negative values in the interpolated quantity (e.g., this sometimes leads to *negative opacities*) even when the underlying datasets are monotonically varying (in one of the dimensions) and strictly positive. For example, Auer and Paletou (1994) show that parabolic interpolation can lead to negative intensities near sharp beam edges, which is clearly non-physical.

A number of different interpolation methods exist which avoid any additional extrema in the interpolant. Steffen (1990) introduced a strictly monotonic interpolation scheme for the use in numerical hydrodynamics. Similar methods were brought to the attention of the wider astrophysical community by Auer (2003). We refer the reader therein for an introduction to piecewise monotonic interpolation.

While n data points can be used to construct a unique Lagrange polynomial of the order $n - 1$, one can also construct higher-order polynomials by fixing the derivatives at the data points. Constructing an interpolant polynomial by making use of fixed derivatives is known as Hermite interpolation. One can use parabolic or cubic interpolation between two points i and $i + 1$ by fixing the derivatives at either a single or both points respectively. By supplying suitable estimates of these derivatives one can easily avoid spurious extrema in the interpolant.

Bézier interpolation between two points, on the other hand, is essentially recursive linear interpolation. By introducing a number of control points one can construct a curve between the two anchor points i and $i + 1$. Bézier curves cannot necessarily be expressed as polynomials, unless one places the x-positions of the control points uniformly between the two anchor points. In this case the gradient at the anchor points is given by the gradient of the line connecting the anchor and the adjacent control point. Therefore the polynomial type of Bézier curve can also be rewritten as a Hermite polynomial. Bézier curves have the nice property, that they never leave the bounding box spanned by the control and anchor points. This makes it incredibly easy to suppress under or overshoots in the interpolant. If there is no over or undershoot, however, the position of the control point is determined from the gradients at the data points, in which case one might as well use a Hermite scheme. Differences between the

properties of Hermite and Bézier interpolants are discussed in further detail in [Ibgui et al. \(2013\)](#).

Besides Bézier/Hermite methods also other higher-order interpolation schemes have been proposed for radiative transfer, but to our knowledge they have not found any use in the 3D community yet. [Janett et al. \(2019\)](#) point out that strictly monotonic schemes sacrifice accuracy when enforcing monotonicity, which can degenerate to linear interpolation near smooth extrema of the interpolated function. Therefore they argue for the use of weighted, essentially non-oscillatory (WENO) techniques, which do not suffer from this loss in accuracy while still suppressing oscillations near discontinuities. The fourth-order WENO interpolation proposed by [Janett et al. \(2019\)](#) has been implemented in the 1D NLTE code LIGHTWEAVER ([Osborne and Milić 2021](#)), which can be found on Github.

The Bézier/Hermite interpolation techniques discussed in the literature vary mostly in how the derivatives at the data points are estimated. Here we discuss some common choices. Considering the three consecutive points $i - 1$, i and $i + 1$, we can derive the two interval spacings s_- and s_+

$$s_- = x_i - x_{i-1}, \quad s_+ = x_{i+1} - x_i, \quad (14)$$

as well as the *backward difference* d_- and *forward difference* d_+

$$d_- = \frac{y_i - y_{i-1}}{s_-}, \quad d_+ = \frac{y_{i+1} - y_i}{s_+}. \quad (15)$$

For the following discussion we will introduce a few approximate derivatives for the central point i . A simple approximation is the *central difference*, which is simply the gradient between the two surrounding points to i .

$$d_c = \frac{y_{i+1} - y_{i-1}}{x_{i+1} - x_{i-1}} = \frac{s_- d_- + s_+ d_+}{s_- + s_+} \quad (16)$$

The gradient at point i , when fitting the Lagrangian parabola through the 3 points is given by

$$d_p = \frac{s_- d_+ + s_+ d_-}{s_- + s_+}. \quad (17)$$

We note that (16) and (17) are identical in the equidistant case, where $s_- = s_+$. The central difference d_c and the parabola gradient d_p are essentially weighted means of d_- and d_+

$$d_w = \alpha d_- + (1 - \alpha) d_+, \quad (18)$$

which only differ in their choice of α . Alternatively one can use the weighted harmonic mean of d_- and d_+

$$d_h = \begin{cases} \left(\frac{\alpha}{d_-} + \frac{1-\alpha}{d_+} \right)^{-1}, & \text{if } d_+ d_- > 0, \\ 0, & \text{if } d_+ d_- \leq 0, \end{cases} \quad (19)$$

where [Brodie \(1980\)](#) and [Fritsch and Butland \(1984\)](#) suggest the following weight α to minimise suspicious wiggles in the interpolant

$$\alpha = \frac{1}{3} \left(1 + \frac{s_+}{s_- + s_+} \right). \quad (20)$$

The weighted harmonic mean has the interesting property that d_h approaches zero if either d_- or d_+ approach zero. Therefore there is a smooth transition between the 2 cases of Eq. (19). Finally, [Steffen \(1990\)](#) propose yet another approximation of the gradient:

$$d_{p^*} = (\text{sign}(d_-) + \text{sign}(d_+)) \min(|d_-|, |d_+|, |d_p/2|), \quad (21)$$

where $\text{sign}(d_-)$ is -1 for negative d_- and +1 if it is positive. This incredibly dense statement has intriguing consequences. If d_- and d_+ have opposite signs, the result is zero as for d_h . If the absolute values of d_- or d_+ are smaller than $|d_p/2|$, this means an extremum will be present in the backward or forward interval if one fitted a parabola through the three points. If this is not the case d_{p^*} is simply equal to d_p . As for Eq. (19) the resulting cases of d_{p^*} transition smoothly. Geometric representations of d_c , d_p , d_w and d_h are shown in Fig. 20.

Reviewing the interpolation techniques used in 3D radiative transfer codes proved to be quite challenging. Out of the following codes only the **MAGRITTE** code is public. For the other codes, we had to rely mostly on the papers where they were used for the first time, which are not always concerned with the technical details of the codes. Most of the papers are rather old, and they likely do not represent the current status of the codes.

The **MAGRITTE** code uses the simplest approach. They assume χ and S to be constant within their grid cells, so they avoid any interpolation. This is because the code operates on a Voronoi grid, which makes multi-D interpolation rather difficult.

OPTIM3D ([Chiavassa et al. 2009](#)) prefer speed over precision by choosing bilinear interpolation in $\ln \chi$. It is not specified whether they interpolate in S or if they interpolate in T and use $S = B(T)$, where B is the Planck function as it is an LTE code. **IRIS** ([Ibgui et al. 2013](#)) use bicubic Hermite interpolation, using d_h to estimate the slope at the grid points, which results in an always monotonic interpolant as shown in the top surface in Fig. 21. [Koesterke et al. \(2008\)](#) state that **ASSeT** relies on monotonic cubic Bézier polynomials for interpolation, but they do not discuss their choice of control points. In **PORTA** ([Štěpán and Trujillo Bueno 2013](#)) one can choose between bilinear and biquadratic interpolation. The authors state that bilinear is sufficient, if one uses the original grids of the MHD models.

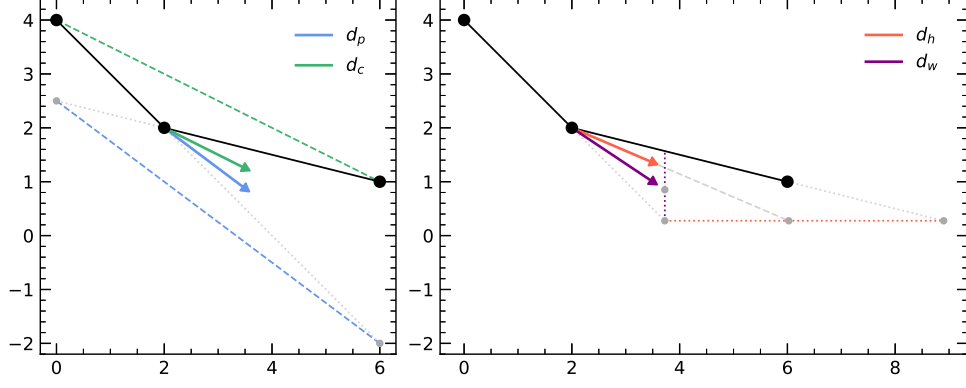


Fig. 20 This figure shows geometric interpretations of commonly used gradients, when interpolating piecewise between discrete data points. Data points are shown as black circles connected by lines resembling linear interpolation. The left panel shows the difference between the central difference d_c and the parabola gradient d_p . The plotted arrows are parallel to the dashed lines of the same colour. The right panel shows the weighted mean d_w and the weighted harmonic mean d_h , both evaluated using the weight α proposed by [Fritsch and Butland \(1984\)](#). α determines the positioning of the small grey points along the coloured dotted lines, which define the direction the arrows point in.

The 3D SC code by [Hennicker et al. \(2020\)](#) for 3D scattering problems in the winds of hot stars uses a quadratic Bézier scheme. Since a quadratic scheme requires an odd number of known points, the points used in constructing the interpolant are asymmetrically positioned around the interpolation interval. They choose to always use data from the points positioned to the left and below of the interpolation interval as shown in Fig. 1 of their Appendix C. Their choice of control points corresponds to Hermite interpolation employing d_w , where they limit the weight α to enforce monotonicity. This yields the same result as limiting the gradient in d_{p*} , but only accounting for under or overshoots in the interpolation interval and not in both backward and forward interval.

MULTI3D ([Leenaarts and Carlsson 2009](#)) and BALDER ([Amarsi et al. 2018](#)) mention the use of cubic convolution when interpolating the upstream quantities. This does not describe the method of interpolation, but rather how the interpolation is carried out. Both codes use the bicubic Hermite interpolation as well, but with the node derivatives approximated by the central difference d_c at the 4 corner points of the face which is intersected by the ray. Since the central difference can be expressed as a linear combination of y_{i-1}, y_i and y_{i+1} , one can precompute a 4×4 convolution kernel, which performs the bicubic interpolation efficiently when applied to the entire upstream plane. This is not possible when d_h is chosen, since it depends non-linearly on the y-values of the grid points which are not known in advance. This does not necessarily yield monotonic interpolation as one can see some overshoots close to steep drops in the right surface in Fig. 21. In order to suppress undershoots and to avoid negative values in the intensity, MULTI3D and BALDER check the minimum value of the 4 corner grid points and if any interpolated values fall below, they are replaced by this minimum. This was also taken into account in Fig. 21 where this clipping is clearly

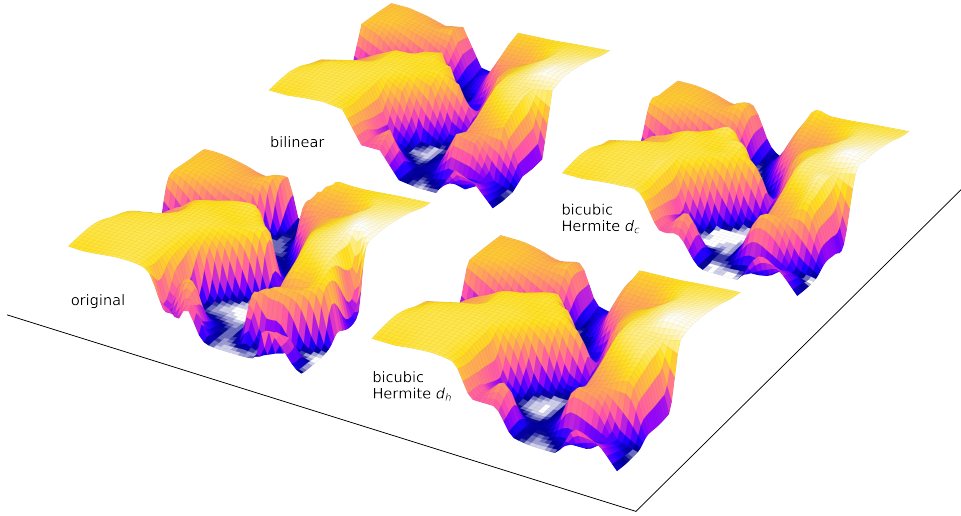


Fig. 21 Presentation of different 2d interpolation schemes. The height of the surface as well as its colour show the extinction coefficient χ at a random horizontal slice close to the optical surface in a solar atmosphere model. *original* refers to the original resolution of the radiation-hydrodynamics snapshot. The other three surfaces were obtained by sampling every 4th point in x and y respectively and interpolating back to the original resolution. Undershoots in *bicubic Hermite d_c* have been corrected by limiting the interpolant to the minimum of the 4-corner points of the face in which the interpolation occurs.

visible in the valley floors. In the LC solver MULTI3D uses a bilinear interpolation. Amarsi et al. (2018) also adopt a monotonic cubic interpolation scheme in the LC solver, but it was not explained how the monotonicity is enforced.

The SCATE code (Hayek et al. 2010, 2011) combines two schemes to maximise efficiency and accuracy. It uses bicubic Hermite interpolation with d_h in its SC solver when iterating the source function in the presence of scattering. Its LC solver, however, interpolates the atmosphere, i.e. temperature, density and velocities, onto a tilted grid which aligns with the direction of the ray for each angle. This minimises horizontal diffusion in the emerging intensity as is shown in Fig. 3 in Peck et al. (2017). Furthermore, it massively reduces the number of interpolations as no frequency dependent data has to be interpolated. The tilting itself is done with local cubic logarithmic interpolation, the details of which are not specified. Linfor3D (priv. comm. M. Steffen) uses a similar approach, where only frequency independent data is interpolated onto the ray using Lagrangian bicubic interpolation, not correcting for any over or undershoots. Afterwards the frequency dependent and velocity shifted χ and S values are calculated for each ray independently.

It is unclear how the mean intensity J is calculated in the LC solvers in PHOENIX/3D and NLTE3D and whether this involves interpolations of I between the rays and the grid points. We were unable to find an explanation whether the scattering part of the

source function or the departure coefficients are determined on the rays or the grid points and if there are further interpolations involved.

Peck et al. (2017) emphasize that enforced monotonicity in interpolation also results in the nonconservation of the radiative energy, however, both Hayek et al. (2010) and Ibgui et al. (2013) suggest that their monotonic cubic Hermite schemes conserves the photon count in their searchlight beam tests.

In summary, each 3D RT code has a unique way of determining opacity, source function and intensity values along the photon path. Another question left unanswered is what quantities are best interpolated. Should one interpolate for example in χ or $\ln \chi$ or only in frequency independent variables? Clearly, the range of techniques in use likely reflects the pros and cons of each in application to a given science question at hand. The proprietary nature of the majority of these codes prevents meaningful comparisons of the accuracy and efficiency of the different implementations. Comprehensive tests of this kind are welcome, along with performance benchmarks, in order to identify reliable as well as efficient interpolation methods.

4.5 Interpolation of opacity and source function along the photon path

The Feautrier methods (Feautrier 1964), which are popular amongst 1D codes (Carlson 1986; Uitenbroek 2001; Hubeny and Lanz 2017b), requires big matrix inversions and storing all values of χ and S along the entire photon path (Fabiani Bendicho 2003). This is incompatible with many 3D codes as they are often domain decomposed and only pass information between a limited number of neighbouring grid points. An exception to this is the 3D Non-LTE code MAGRITTE (De Ceuster et al. 2020), which assumes shared-memory across the entire domain and uses a second-order Feautrier scheme. Also the 3D NLTE departure coefficient determination code NLTE3D relies on a Feautrier scheme, but little detail on this is given in Steffen et al. (2015) and it is not clear whether this code is parallelised at all. Unfortunately, we were not able to find any information on the numerical details of the radiative transfer solver in the widely used Cloudy code (Ferland et al. 2017). This might be due to the fact, that the references to older papers on the code have been linked to the online documentation of the code. This documentation focuses on guiding the user rather than giving insights on the technical details however.

All codes discussed below are time-independent radiative transfer codes, used for post-processing 3D hydrodynamical simulations. They all rely on a 3-point scheme, which considers for each point i exactly one upstream point $i - 1$ and one downstream point $i + 1$ when constructing the polynomial that approximates the interval between $i - 1$ and i . This reflects the importance of minimising the amount of communication between ranks in MPI parallelised programs. Auer and Paletou (1994) state that parabolic or higher order interpolation between S_{i-1} and S_i is important to recover the diffusion approximation in the optically thick regime.

- Linfor3D uses a monotonic quadratic Hermite scheme, where the gradient at point i is taken to be d_{p*} .

- The 3D non-LTE code **PORTA** (Štěpán and Trujillo Bueno 2013), for polarized radiative transfer, uses a monotonic parabolic Bézier scheme, which results in the same gradient at i when the direction of the ray is flipped. It turns out that the resulting gradient is *exactly* d_{p^*} as implemented by Steffen (1990). Therefore this Bézier scheme is equivalent to the Hermite scheme used in **Linfor3D**.
- **PHOENIX/3D** code (Hauschildt and Baron 2006) linearly interpolates in χ and S and only moves to ordinary parabolic interpolation in the source function in the optically thick regime, while the interpolation in χ is linear. For these kind of adaptive schemes, Holzreuter and Solanki (2012) point out that changes in the source function values can result in switching interpolation techniques between iterations when one solves for the source function in non-LTE. These “flip-flop” situations are non-linear and can lead to oscillations which prevent convergence.
- The 3D SC code by Hennicker et al. (2020) for 3D scattering problems in the winds of hot stars smoothly transitions from a quadratic Bézier scheme, equivalent to the one used in **Linfor3D**, to linear interpolation in the source function in order to ensure convergence. From their discussion it appears that even a smooth transition between Lagrangian and monotonic quadratic interpolation can introduce convergence preventing oscillations in an iterative scheme.
- **OPTIM3D** (Chiavassa et al. 2009) uses linear interpolation in $\ln(\chi)$ to convert to optical depth and linear interpolation in S on the $\ln(\tau)$ scale. To our knowledge this is the only code using ln-linear integration of the opacity.
- **SCATE** (Hayek et al. 2010) and **RH** (Uitenbroek 2006) as updated by Holzreuter and Solanki (2012) employ the monotonic parabolic Bézier scheme proposed by Auer (2003). This corresponds to Hermite interpolation with d_{p^*} , but neglecting the forward difference d_+ in the $\min()$ function, allowing for under or overshoots in the $[i, i+1]$ interval.
- **IRIS** (Ibgui et al. 2013) favour a monotonic cubic Hermite scheme by fixing the gradient at point $i - 1$ as well as i . The gradient at $i - 1$ is taken to be d_- , whereas the gradient at i is taken to be d_h with α given by Eq. (20). Štěpán and Trujillo Bueno (2013) claim that fixing the gradient at point $i - 1$ to d_- may cause loss in accuracy of the formal solver.
- The 3D LTE code **ASS ϵ T** uses a monotonic cubic Bézier scheme, but they do not specify their choice of control points.
- **MULTI3D** and **BALDER** offer linear interpolation of the source function as well as the interpolation schemes used in **SCATE** and **IRIS**.
- Though not a 3D code, we note that Auer (2003) approximate the optical depth integral by linearly integrating the logarithmic density $\ln \rho$ and multiplying it with $(\kappa_i + \kappa_{i-1})/2$, where $\kappa = \chi/\rho$.

The **IRIS** and **PORTA/Linfor3D** implementations are shown in Fig. 22. A concise list of proposed solvers for polarized radiative transfer is found in Table 1 of Janett et al. (2017).

Summary: The needs for a given interpolation scheme — just as any other ingredient in 3D NLTE RT — can and shall be judged with respect to a given astrophysical problem. Codes that are used for atmospheres of FGKM-type stars, such as **PHOENIX/3D**, **OPTIM3D**, **SCATE**, **MULTI3D**, **BALDER** and **Linfor3D**, are tailored to specific

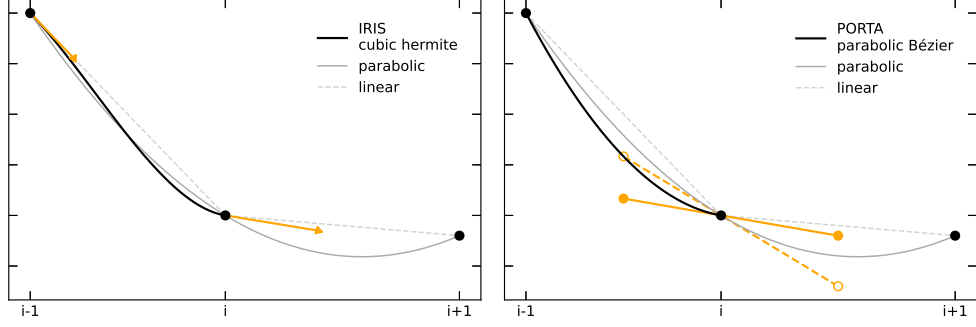


Fig. 22 Piecewise monotonic interpolation methods used in the formal radiative transfer solvers in the IRIS and PORTA codes. Linear and parabolic interpolation is overplotted for comparison. The derivatives at the grid points are shown as orange arrows for the hermite interpolation in the left panel. The linear gradient is used at the $i - 1$ position, while the weighted harmonic mean is used at i . In the right panel the control points of the Bézier curves are plotted as orange points. The unfilled points are the default control points, which yield the Lagrangian parabolic curve. Even though the parabolic curve does not undershoot in the interval $[i - 1, i]$, the control points are corrected. The filled points are the control points after overshoot correction, since the control point at $i + 1/2$ is outside the bounding box spanned by the three points.

physical conditions and therefore are only used in a very restricted range of **astro-physical** applications. Other codes, such as **Cloudy** and **MAGRITTE**, deal with a very different temperature-density regime and appear to use much more basic methods. We trust the authors that their interpolation schemes are sufficient in their particular regimes, even though it would be better to see this proven and published. Unfortunately, it seems that the community has a preference to develop a new code every time a new PhD thesis begins, which likely reflects the progress in computer sciences and availability (or progressive phase-out) of different compilers. Therefore we cannot recommend an all-purpose interpolation scheme, which is efficient and sufficiently accurate for all applications. However, we note that linear interpolation is still widely used as it remains the most efficient and robust method. We certainly doubt that the scientific gain from using cubic interpolation over quadratic interpolation in the source function justifies the increased computational cost involved.

4.6 Angle quadrature

Radiative transfer codes based on the methods of long or short-characteristics solve the radiative transfer equation for a discrete set of geometric rays, see Fig. 23. The *angle quadrature* defines which rays have been chosen and how they are weighted when integrating intensities. For NLTE, for example, the mean intensity J_ν is the quantity that is needed in order to solve the rate equations. The value of J_ν is the integral of the directed intensities over the unit sphere

$$J_\nu = \frac{1}{4\pi} \int I_\nu d\Omega = \frac{1}{4\pi} \int_0^{2\pi} \int_0^\pi I_\nu \sin \theta d\theta d\phi \quad (22)$$

$$= \frac{1}{4\pi} \int_0^{2\pi} \int_{-1}^1 I_\nu d\mu d\phi \quad (23)$$

where we introduced $\mu = \cos \theta$ for convenience. The resulting monochromatic net flux from an astronomical object F_ν is defined as:

$$F_\nu = \int I_\nu \mu d\Omega = \int_0^{2\pi} \int_{-1}^1 I_\nu \mu d\mu d\phi \quad (24)$$

and the emerging flux is given by integration over the interval where μ is positive, therefore:

$$F_\nu^+ = \int_0^{2\pi} \int_0^1 I_\nu \mu d\mu d\phi \quad (25)$$

For efficient evaluation of the integrals we discretise the intervals and replace the integrals by a weighted sum

$$J_\nu \approx \sum_i^n w_i I_\nu, \quad (26)$$

where n is the number of discrete rays and w_i are their respective weights. As the computational cost of any radiative transfer application scales nearly linearly with n , it is essential to strike an optimal balance between the accuracy of the integral and the number of rays. However, even for a given n , it is not trivial to find the set of rays and weights, which yields optimal accuracy. For one dimensional integration it is pretty clear that Gaussian quadratures and its variants yield supreme accuracy and it hardly matters, which one is picked. Therefore 1D radiative transfer codes are using Gaussian quadratures for approximating J_ν (e.g. [Hubeny and Lanz 2017c](#)). For plane parallel atmospheres, we can write

$$J = \frac{1}{2} \int_{-1}^1 I(\mu) d\mu \approx \frac{1}{2} \sum_i^n w_i I(\mu_i) \quad (27)$$

$$\approx \frac{1}{2} (w_1 I(\mu_1) + w_2 I(\mu_2) + \dots + w_n I(\mu_n)), \quad (28)$$

where we have dropped the frequency index for clarity. Gaussian quadratures yield the values for w_i and μ_i , which approximate $I(\mu)$ exactly if it was a polynomial of order $2n - 1$ or lower. This is because Eq. (28) has $2n$ unknowns, namely $w_1, w_2, \dots, w_n$ and $\mu_1, \mu_2, \dots, \mu_n$, assuming that we are free to evaluate $I(\mu)$ at any μ we like. For the case of $n=2$ we have 4 unknowns and we can set up the following system of 4 equations:

$$\begin{aligned} \int_{-1}^1 \mu^0 d\mu &= w_1 + w_2 \\ \int_{-1}^1 \mu^1 d\mu &= w_1 \mu_1 + w_2 \mu_2 \\ \int_{-1}^1 \mu^2 d\mu &= w_1 \mu_1^2 + w_2 \mu_2^2 \\ \int_{-1}^1 \mu^3 d\mu &= w_1 \mu_1^3 + w_2 \mu_2^3 \end{aligned} \quad (29)$$

where we have approximated $I(\mu)$ by simple polynomials of up to third order in μ . Solving this system yields the Gauss–Legendre quadrature weights and abscissas for $n=2$ points. One common variant is the Gauss–Lobatto quadrature which fixes the endpoints to $\mu_1=-1$ and $\mu_n=1$, i.e. the vertical rays. Considering an isotropic radiation field we expect $J_\nu = I_\nu$, $F_\nu = 0$ and $F_\nu^+ = I_\nu/2$. The construction of any quadrature scheme for radiative transfer is motivated by meeting the following criteria:

$$\sum_i^n w_i = 2, \quad \sum_i^n w_i \mu_i = 0, \quad \sum_i^n w_i \mu_i^2 = \frac{2}{3} \quad (30)$$

Equation (27) is only fulfilled when the first criterion holds. The second criterion demands that F_ν^+ and F_ν^- cancel each other, i.e. $F_\nu = 0$. The third criterion is derived from conservation of the third moment of the intensity K_ν , which is related to radiative pressure, in isotropic radiation. The case $F_\nu^+ = I_\nu/2$ is not reproduced when using Gaussian quadratures in the μ interval $[-1, 1]$, which is clearly a strong limitation of these schemes. A simple solution to this issue has been found by Sykes (1951), who propose to use double-Gaussian quadratures. They map the μ -values and their weights to the μ interval $[0, 1]$ and simply “mirror” them for the interval $[-1, 0]$. For the Gauss–Lobatto quadrature this has the inconvenient result of including $\mu = 0$, which is problematic in the 3D case if one has periodic boundary conditions in the horizontal. An alternative can be found in the double-Gauss–Radau quadrature, which only fixes one end-point, i.e. $\mu = 1$, and results in two fixed endpoints $\mu_1 = -1$ and $\mu_n = 1$ after the mirroring. Unfortunately, many authors do not specify, whether they are using Gaussian quadratures in the interval $[-1, 1]$ or the mentioned double-Gaussian quadratures.

Thus, in 1D we can integrate the intensity efficiently with high order accuracy using only a few rays. This is clearly superior to integration using the trapezoidal or Simpson’s rule, which require significantly more points for the same accuracy. Unfortunately, Gaussian quadratures do not generalise to higher dimensions. Therefore the choice of rays in 3D radiative transfer is significantly less straight forward and quite diverse angle quadratures are used in the literature.

One popular strategy to obtain a discretised set of rays was proposed by Carlson (1963), also see Bruls et al. (1999) for a more recent derivation. The so-called *Carlson A* quadratures are defined in a single octant and are invariant under rotations of 90° along the x,y and z axis. Furthermore, the Carlson A rays are equidistant in μ^2 , although only within one octant and not across octant boundaries. μ_1 is therefore a free parameter and related to the spacing $\Delta\mu$. The ϕ angles follow from the invariance under 90° rotation. This gives rise to the triangular patterns in the octants of panels 2a and 2b in Fig. 23. This scheme has been implemented in many radiative transfer codes including MULTI3D, SCATE, BALDER and IRIS.

Another approach is to split the 2D integral in Eq. (23) into two 1D integrals. The codes PORTA and ASSεT use a Gauss–Legendre quadrature for the integration in μ and trapezoidal integration in ϕ . We suspect that they employ the double-Gauss–Legendre quadrature mentioned above. The integration weights for each ray are therefore the

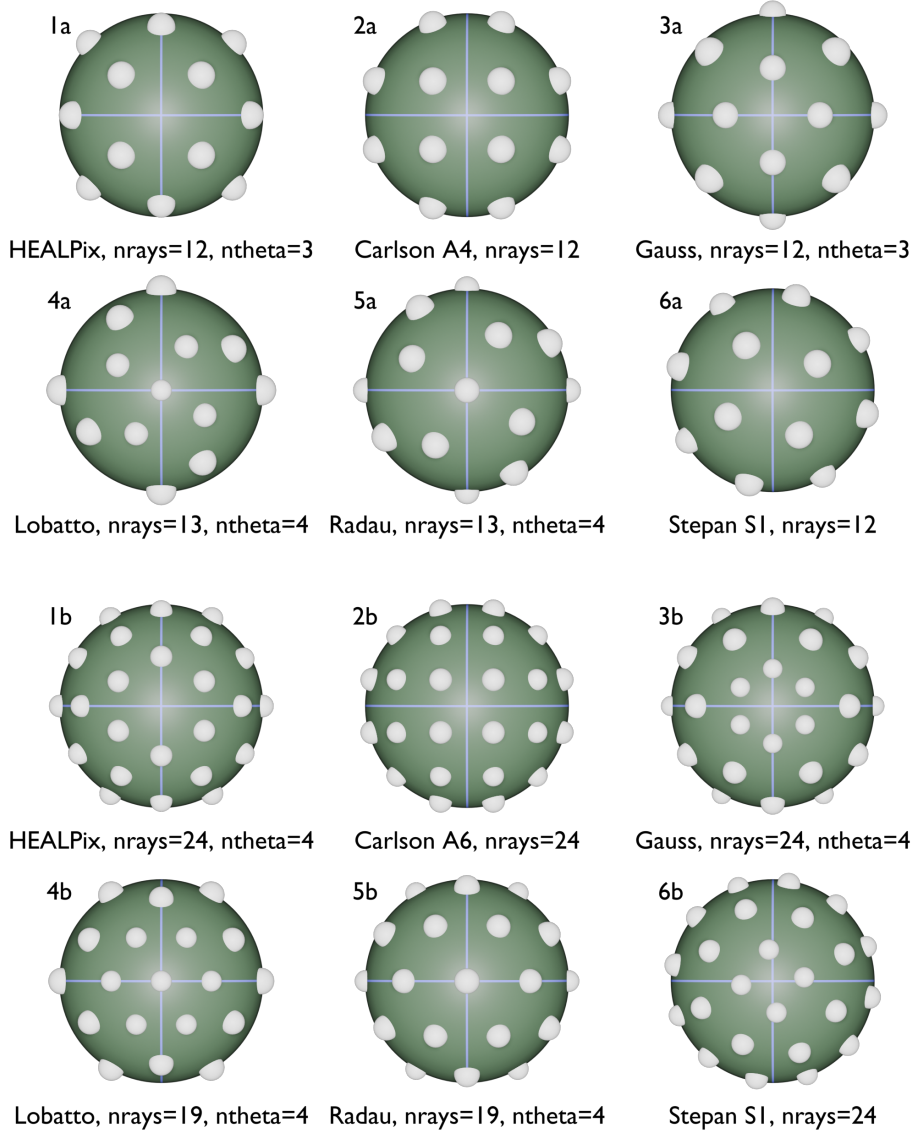


Fig. 23 Visualisations of popular angle quadratures used for 3D radiative transfer. Here we only show the top hemisphere, i.e. only “up” pointing rays. “Down” pointing rays are simply mirrored version of the “up” rays. The number of upward rays n_{rays} and theta angles n_{θ} have been chosen in order to highlight the differences between the quadrature schemes. They do not necessarily represent the most commonly used choices of n_{rays} and n_{θ} . The white spheres represent the discretised set of angles, i.e. rays, for which the radiative transfer equation is solved. The volume of each white sphere is proportional to the weight given to that particular ray. The blue lines mark the position of the x and y axes. Neighbouring rings of constant θ have been offset by $90^{\circ}/(n_{\theta} - 1)$ with respect to one another in the case of the Gauss, Lobatto and Radau quadratures.

tensor-product of the 1D quadrature weights. Double-Gauss–Legendre quadratures are presented in panels 3a and 3b of Fig. 23. For better comparison with the other schemes we have taken the liberty to rotate rings of constant μ by $90^\circ/(n_\mu - 1)$ with respect to their neighbours. BALDER implemented a similar quadrature, only that they choose a Gauss–Lobatto quadrature in μ , which includes the vertical rays (Amarsi and Asplund 2017). Their quadrature choice is shown in panel 4a of Fig. 23, although their particular quadrature is rotated by another $\pi/12$, probably in order to avoid the alignment of the rays with the x and y axes. Unfortunately, they do not quantify the gain from using this quadrature instead of the Carlson quadratures used in their previous studies. Štěpán et al. (2020) propose another type of quadrature which is based on spherical harmonics. Employing their quadrature schemes, two of which are presented in panels 6a and 6b, they find similarly accurate results using up to 30% less rays compared to the tensor product approach of Gauss–Legendre and trapezoidal integration. It should be noted, that their scheme, however, does not satisfy the $F_\nu^+ = I_\nu/2$ condition in an isotropic radiation field.

The previously mentioned double-Gauss–Radau quadrature is used in the MHD codes STAGGER, BIFROST and DISPATCH (Trampedach et al. 2013) and is also available in Linfor3D. It is shown in panels 5a and 5b of Fig. 23.

The MAGRITTE code uses the HEALPix discretisation of the sphere (Górski et al. 2005), shown in panels 1a and 1b of Fig. 23. This quadrature is equally spaced in μ and ϕ , however every second ring of constant μ is rotated by π/n_ϕ . This has the result that all rays are equally weighted.

The current state of the literature does not allow to utter a definite recommendation for which angle quadrature is the most accurate. There appears to be some agreement, that the Gauss–Legendre tensor product quadratures are sub-optimal (Ibgui et al. 2013; Štěpán et al. 2020; Jaume Bestard et al. 2021) and that the double-Gauss–Radau quadrature is an improvement over the Carlson quadratures for the case of stellar atmospheres (Amarsi and Asplund 2017). Naturally, it would be good to see a comparison of the double-Gauss–Radau quadrature and the “near optimal” quadratures proposed by Štěpán et al. (2020) and Jaume Bestard et al. (2021). Furthermore it would be interesting to see how Sobolev–Lebedev quadratures as those proposed by Ahrens and Beylkin (2009), which are invariant under the icosahedral rotation group, perform in comparison.

Generally, it seems like one needs relatively few rays to approximate J_ν to sufficient accuracy, when calculating the impact of the radiation field on the source function. Significantly more rays are recommended for the calculation of spectral lines in F_ν^+ in order to reproduce the centre-to-limb variation and therefore fluxes from stellar atmospheres. Bergemann et al. (2019) use the Carlson A4 quadrature, so 12 rays per hemisphere, for the statistical equilibrium calculation of Mn. Using BALDER Wang et al. (2021) state the use of 26 rays for the statistical equilibrium, i.e. J_ν , calculation of atomic Li. This corresponds to the 13 rays on the hemisphere in panel 4a. However, for the emerging fluxes they use a total of 57 rays distributed over a hemisphere. For the considerably more complex atoms Fe and K, they revert to 5 rays on the hemisphere for J_ν and 29 rays for F_ν^+ in Wang et al. (2022). Many angles for the J_ν calculation are used in Koesterke et al. (2008), which use 24 rays on the hemisphere ($n_\mu=3$, $n_\phi=8$).

For the flux calculation they use essentially the same quadrature but reduce n_ϕ to 4 for the angles with the lowest μ value. This saves them 4 rays and yields 20 rays in total. Štěpán and Trujillo Bueno (2013) do a benchmark J_ν calculation with 80 rays on the hemisphere, but do not explain why they deem this high number of angles necessary.

4.7 Escape probability

For completeness, we should state that there is an approximate way of obtaining angle-dependent intensities, which avoids solution of the RTE. The emergent intensity along a given ray is

$$I_\nu(\tau_\nu = 0) = \int_0^\infty S_\nu e^{-\tau_\nu} d\tau_\nu \quad (31)$$

$$= \int_0^\infty S_\nu p_\nu d\tau_\nu, \quad (32)$$

where we have introduced the probability of a photon escaping the medium along this ray

$$p_\nu = e^{-\tau_\nu}. \quad (33)$$

At the same time it follows from simply integrating Eq. (11):

$$I_\nu(\tau_\nu = 0) = \int_0^\infty (S_\nu - I_\nu) d\tau_\nu. \quad (34)$$

Equating both expressions for the emergent intensity we obtain an expression for the intensity at τ :

$$\int_0^\infty S_\nu p_\nu d\tau_\nu = \int_0^\infty (S_\nu - I_\nu) d\tau_\nu, \quad (35)$$

$$I_\nu \approx S_\nu(1 - p_\nu) \quad (36)$$

While (35) is exact, the latter is only an approximation as it does not have to hold for each point in the atmosphere individually, unless S_ν is constant throughout the atmosphere. If there is a significant external source of intensity I_ν^{ext} , this expression can be easily adjusted

$$I_\nu \approx S_\nu(1 - p_\nu) + p_\nu I_\nu^{\text{ext}}. \quad (37)$$

When $I_\nu^{\text{ext}} \gg S_\nu$, as is the case in irradiated planetary atmospheres, this is a reasonable approximation. This way, one does not have to worry about integrating S_ν along the ray, but one still has to integrate the optical depth τ_ν numerically. The `CLOUDY` code uses Eq. (36) alongside further approximations to calculate the mean intensity for each spectral line at each point in the model.

4.8 Boundary conditions

The boundary conditions of the formal solution generally depend on the astrophysical application. Box-in-a-star simulations of stellar sub-surface convection employ periodic boundary conditions in the horizontal direction (that is perpendicular to the radial direction). Therefore these boundary conditions are adopted for the radiative transfer calculations in 3D boxes of stellar atmospheres as well. This allows one to track the origin of each ray to either the top or bottom boundary. In the end, the boundary condition at the start of each ray does not differ from the boundaries applied in 1D radiative transfer codes. If the ray starts in the optically thick regime (bottom boundary), the starting intensity is assumed to be the Planck function at the bottom boundary temperature of the model radiation (e.g. Mihalas and Athay 1973; Rutten 2003; Ibgui et al. 2013), i.e. $I_\nu = S_\nu = B_\nu$. For the top boundary, when the ray starts in empty space, one can for example assume that the stellar atmosphere is non-irradiated, i.e. the incoming intensity at the top is zero. Alternatively, incoming radiation from a binary companion, from the host star of an exoplanet, or even the chromosphere and corona can be modelled by adjusting the incoming intensity at the upper boundary. Extrapolations of I_ν and χ are also possible and sometimes necessary when smooth gradients in J_ν are needed. This is for example the case, when calculating heating or cooling rates for 3D RHD applications.

4.9 Opacities and emissivities

As is clear from Eq. (11), radiation transfer depends highly on opacities and emissivities, which are the two critical parameters that describe the local state of matter at each point in the atmospheres. For convenience, different definitions of opacities are used in the literature, which all depend simply on the expression of *monochromatic extinction coefficient* representing the cross-section σ_ν in cm^2 per particle, but it can be given (or tabulated) either per unit volume, per unit mass, or per unit length.

Here, following Rutten (2003, Section 2.1.2) we use the following definitions:

- monochromatic extinction coefficient per gram of material, also referred to as *opacity* κ_ν , given in cm^2/g ;
- monochromatic extinction coefficient per unit volume α_ν is defined as $\alpha_\nu = \kappa_\nu \times \rho$, with α given in cm^{-1} ;
- monochromatic extinction coefficient per unit length α , equivalent to the one above;

Definitions equivalent to the above can also be given for emissivities. We note that the notation of the geometric mean free path of the photon l follows from the assumption of the photon propagation in a homogeneous gas without emission, and it represents the mean optical depth of unity ($\langle \tau_\nu \rangle = 1$), hence $l = 1/\alpha_\nu = 1/(\kappa_\nu \rho)$. Opacities and emissivities (as well as, of course, the source function defined as their ratio, that is, $S_\nu = j_\nu/\alpha_\nu$), depend on local kinetic temperature, gas density (and pressure), detailed chemical abundances, atomic and molecular data, and, in the case of NLTE, also on the radiation field.

The coupling between the atomic/molecular parameters and the properties of the gas are rather simple, for their derivation of this quantity, we refer to the aforementioned book by [Rutten \(2003\)](#). Assuming the Maxwell velocity distribution for particles involved, the following relations for *opacity and emissivity due to bound-bound radiative transitions* between a lower energy state i and a higher energy state j hold:

$$j_{ij,\nu} = \frac{h\nu}{4\pi} A_{ji} n_j \psi \quad (38)$$

$$\alpha_{ij,\nu} = \frac{h\nu}{4\pi} (n_i B_{ij} \varphi - n_j B_{ji} \chi) \quad (39)$$

$$S_{ij,\nu} = j_{ij,\nu} / \alpha_{ij,\nu} = \frac{A_{ji} n_j \psi}{(n_i B_{ij} \varphi - n_j B_{ji} \chi)} = \frac{2h\nu^3}{c^2} \frac{\psi / \varphi}{(g_j n_i / g_i n_j) - \chi / \varphi}, \quad (40)$$

where A_{ji}, B_{ij}, B_{ji} are the Einstein coefficients and φ, χ, ψ are the profile functions for absorption, stimulated emission and spontaneous emission, respectively. The latter equation for the source function reduces to the Planck function ($S_\nu = B_\nu$), if the level populations n_i and n_j are LTE.

If the assumption of complete redistribution (CRD) is used, all profile functions are assumed to be equal $\varphi = \chi = \psi$. With the application of relationships between Einstein coefficients ($g_i B_{ij} = g_j B_{ji}$ and a similar expression for A_{ji}), the Eqs. (38) and (39) in NLTE then simplify to the commonly used form in CRD:

$$\alpha_{ij,\nu} = \frac{h\nu}{4\pi} \varphi B_{ij} n_i (1 - g_i n_j / g_j n_i) \quad (41)$$

$$= \sigma_\nu^l n_i (1 - g_i n_j / g_j n_i) \quad (42)$$

$$= \sigma_\nu^l n_i^{\text{LTE}} (b_i - \frac{g_i}{g_j} \frac{n_j^{\text{LTE}}}{n_i^{\text{LTE}}} b_j) \quad (43)$$

$$= \sigma_\nu^l n_i^{\text{LTE}} (b_i - b_j \exp(-h\nu / k_B T)) \quad (44)$$

$$= \alpha_{ij,\nu}^{\text{LTE}} b_i (1 - \frac{b_j}{b_i} \exp(-h\nu / k_B T)) / (1 - \exp(-h\nu / k_B T)) \quad (45)$$

$$(46)$$

where, the LTE extinction coefficient is defined as $\alpha_{ij,\nu}^{\text{LTE}}$. For a bound-bound radiative transition, its numerical value at a given frequency ν (note that in codes wavelength units are often used) is simply:

$$\alpha_{ij,\nu}^{\text{LTE}} = \sigma_\nu^l n_i^{\text{LTE}} (1 - \exp(-h\nu / k_B T)) \quad (47)$$

$$= \frac{\pi e^2}{mc} f_{ij} \varphi(\nu - \nu_0) (1 - \exp(-h\nu_0 / k_B T)) \quad (48)$$

Correspondingly, the emissivity and the source function are written as:

$$j_{ij,\nu} = \frac{h\nu}{4\pi} \varphi A_{ji} n_j \quad (49)$$

$$= \sigma_\nu^l n_j \frac{2h\nu^3}{c^2} \frac{g_i}{g_j} \quad (50)$$

$$S_{ij,\nu} = \frac{2h\nu^3}{c^2} \frac{1}{(g_j n_i / g_i n_j) - 1} \quad (51)$$

$$= \frac{2h\nu^3}{c^2} \frac{1}{\exp(h\nu/k_B T) b_i / b_j - 1} \quad (52)$$

$$= B_\nu \frac{(\exp(h\nu/k_B T) - 1)}{\exp(h\nu/k_B T) b_i / b_j - 1} \quad (53)$$

$$(54)$$

where B_ν is the Planck function and σ_ν^l is the already introduced monochromatic extinction coefficient per particle for a frequency point within the line ($\sigma^l = \frac{h\nu}{4\pi} B_{ij} = \frac{\pi e^2}{mc} f_{ij}$, with f_{ij} being the oscillator strength). The relationships are very powerful, as they can be conveniently employed to convert an LTE spectrum synthesis code into a NLTE code, as long as the departure coefficients b_i and b_j are available from NLTE statistical equilibrium codes. These relations, or numerically simplified re-formulations thereof (as only α and S are used), are therefore used in post-processing 1D NLTE spectrum synthesis codes, such as SIU (Reetz 1999), Turbospectrum v20 (Gerber et al. 2023), and PySME (Piskunov and Valenti 2017). A comparison of NLTE synthetic profiles computed with such scaling relations and with direct NLTE RT codes can be found, e.g. in Wehrhahn et al. (2023). NLTE departure coefficients computed with different codes are compared, e.g. in (Bergemann et al. 2019). These relationships in principle allow the application of NLTE departure coefficients in 3D NLTE codes, but we are currently not aware of such implementations in any of the codes described in Sect. 7.

For the interpretation of NLTE effects for the near-UV and optical diagnostic lines, it has become convenient to re-write the equations 45 and 53 as follows (since $h\nu > k_B T$, which holds in the optical):

$$\alpha_{ij,\nu}^{\text{NLTE}} \approx \alpha_{ij,\nu}^{\text{LTE}} b_i \quad (55)$$

$$S_{ij} \approx \frac{b_j}{b_i} B_\nu \quad (56)$$

The assumption of complete redistribution physically means that the probability to emit a photon somewhere with a spectral line is not correlated with the probability to absorb there, so the source function is defined for a line and is assumed to be independent of frequency. The CRD is a reliable assumption if the collisions are frequent enough to ensure a random redistribution of the frequency of the scattered photon. However, this approximation may break down for the strongest chromospheric spectral features, such as the Na D lines, Mg II H & K, Ca II H & K, the core of H $_\alpha$, which require partial re-distribution (Leenaarts et al. 2009, 2010, 2013a,b; Pereira et al. 2015; de la Cruz Rodríguez et al. 2019; Moe et al. 2024) and we refer the reader to Linsky (2017) for a review of PRD-sensitive diagnostic lines in stellar atmospheres.

The distinction between continuum and line opacities has classically relied on the underlying physical process at hand. The continuum opacities are typically defined as due to bound-free or free-free transitions in interaction between the radiation field and different types of gas particles. These can be of various types (Gustafsson et al. 2008, their table 1), including photo-ionization reactions in atoms (Bautista 1997; Nahar and Pradhan 1997; Nahar 2015; Bautista et al. 2017; Smyth et al. 2019), photo-dissociation and photo-ionization reactions in molecules (Heays et al. 2017; Hrodmarsson and van Dishoeck 2023), and their reverse reactions (recombination and photo-induced attachment), but also free-free transitions in various species, e.g. negative ions of atoms, such as H^- , C^- , N^- , O^- (e.g. John 1975b,a; Bell et al. 1988; Ramsbottom et al. 1992), negative ions of molecules CO^- , H_2O^- . For stellar atmospheres of FGK-type stars, the most important source of continuum opacity are the H^- bound-free transitions, for which new cross-sections were recently published by McLaughlin et al. (2017). Also other physical processes, such as CIA (collisionally-induced absorption) between H I atoms or H_2 molecules (Doyle 1968; Borysow et al. 2001) may lead to a quasi-continuum type absorption. Finally, isotropic scattering representing Rayleigh scattering on H I, He I, H_2 , and on free electrons, is typically included. The latter is coherent isotropic scattering, and it is only relevant in the UV spectrum of extremely metal-poor RGB stars (Gustafsson et al. 1975; Cayrel et al. 2004; Sobeck et al. 2011), but in this wavelength regime there are additional complexities due to the chromosphere (Avrett and Loeser 2008; Dupree et al. 2016) and these effects make it hardly possible (and barely reasonable) to study such types of coherent isotropic scattering in any detail.

The continuum absorption is usually wide-band, covering a huge range of frequencies and, for most of the afore-mentioned reactions can be triggered by any photon, as long as its frequency is greater than the threshold (minimum) energy value $\nu_{\text{threshold}}$. However, for practical computational reasons, especially in 3D NLTE, it is normally not possible, neither feasible, to include the semi-infinite range of corresponding cross-sections. Hence for the background continuum, a fixed grid is typically adopted, which covers fully the dominant range of stellar fluxes for a given type of stars. For example the DETAIL code for FGK-type ($T_{\text{eff}} \sim 4000$ to 7000 K) stars covers the frequency range from 6×10^{15} Hz ($500 \text{ \AA}$) to 10^{11} Hz ($3000 \mu\text{m} = 3 \text{ mm}$) for the continuum with a mesh, which is non-equidistant in the wavelength space and has a dense sampling of 3 to $5 \text{ \AA}$ in the optical and IR, but very coarse sampling at higher wavelengths. MULTI, in contrast, defines the continuum mesh directly by the properties of individual bound-free transitions provided in the model atom, which are usually taken from published datasets of atomic physics calculations. For example, for Mn I the photo-ionization cross-sections are sampled at 5000 evenly-spaced energy points between zero and 0.8 Ryd above the first ionisation threshold, followed by 250 points from 0.8 Ryd to 2.0 Ryd (Bergemann et al. 2019). Figure 24 shows examples of cross-sections for two Mn I states obtained from theoretical quantum mechanical calculations. In other codes, such as Cloudy which is mostly used for planetary atmospheres or very hot environments, the wavelength coverage as offered by linelists and continuum opacities extends to much greater ranges from $\sim 1 \text{ \AA}$ to over 3 meters (Ferland et al. 2013). However, for the vast majority of neutral and singly-ionized atoms of astrophysical interest (except

a few core species like H I, He I, and recent update to Fe II in [Chatzikos et al. 2023](#)), no detailed quantum-mechanical photo-ionization cross-sections are available in `Cloudy` ([Ferland et al. 2017](#)).

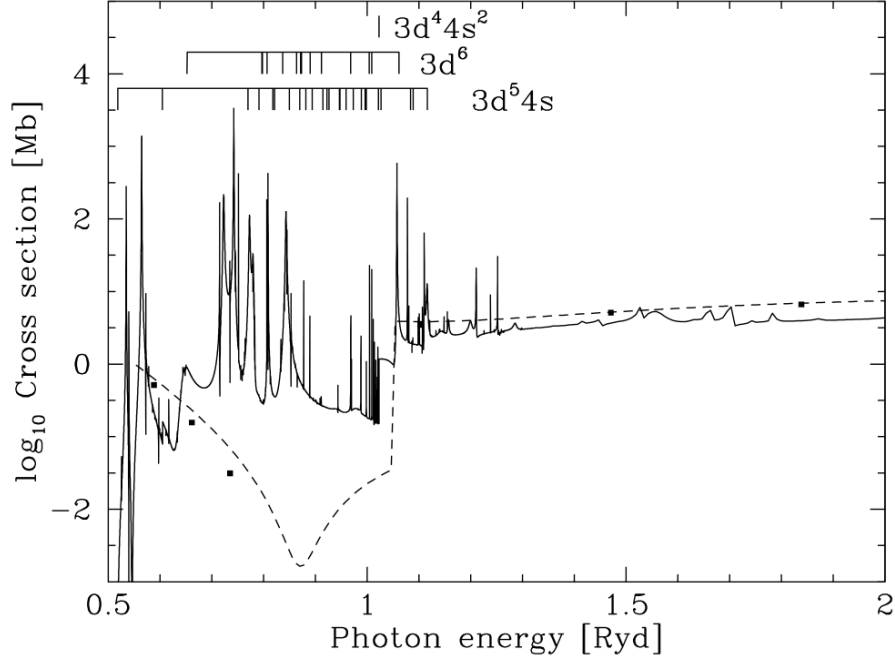


Fig. 24 Detailed photo-ionization cross-section for the ground state of neutral manganese. The data shown with the solid line were computed using the R-matrix. We also show the data computed using the central-field approximation by [Verner and Yakovlev \(1995\)](#) and [Reilman and Manson \(1979\)](#). Image reproduced with permission from [Bergemann et al. \(2019\)](#), copyright by the author(s).

In bound-bound transitions, it is only the transition probability f_{ij} that matters, which enters the equations together with the statistical weight g_{ij} of the energy state, its degeneracy. The values of f_{ij} for atoms and molecules can be calculated using theory or measured via experiment by combining the level lifetimes and branching fractions. Large-scale spectroscopic surveys like APOGEE or Gaia-ESO devote a substantial effort to compile accurate datasets to describe the stellar spectra taken within the survey programs ([Shetrone et al. 2015](#); [Heiter et al. 2021](#)). For atoms, the statistical weight depends only on the orbital angular momentum quantum number of each energy level. For molecules, however, one has to take into account the nuclear spin degeneracy g_{nuc} ([Demtröder 2010](#)):

$$\text{atoms} \quad g_{ij} = (2J + 1) \quad (57)$$

$$\text{molecules} \quad g_{ij} = g_{\text{nuc}}(2J + 1), \quad (58)$$

where g_{nuc} depends on several properties of molecules. One of them is the nuclear spin I of the individual atoms within the molecule. The other is the molecular point

symmetry group. For example, diatomic heteronuclear molecules, such as CN and CO, have the symmetry term of unity (Ochkin 2009). The main isotopes of C and O (^{12}C , ^{16}O) have $I = 0$ and hence for the main isotope $^{12}\text{C}^{16}\text{O}$, $g_{\text{nuc}} = 1$. For N (^{14}N), $I = 1$, as a consequence for the $^{12}\text{C}^{14}\text{N}$ isotopologue, $g_{\text{nuc}} = 3$ (product of g_{nuc} for ^{12}C and ^{14}N). There are more complexities for non-linear poly-atomic molecules, such as H_2O . These differences are significant and shall be accounted for, when computing the molecular opacities for applications in stellar and planetary atmospheres.

4.10 Broadening

The absorption and emission lines in spectra of astronomical objects are not infinitely narrow, but represent a characteristic shape reflecting different broadening processes. The broadening processes can be broadly classified into intrinsic (internal to the physical system) and extrinsic (external). The former represent the natural broadening, thermal broadening due to motion of particles (usually according to Maxwellian distribution), and pressure broadening. The pressure broadening arises due to elastic collisions between different kinds of particles. The natural broadening is the consequence of the Heisenberg uncertainty principle and the finite lifetime of energy states. External broadening mechanisms include, but are not limited to, stellar rotation and broadening of the intensity due to the finite slit width (instrumental).

The profile function ϕ is usually defined by the Voigt profile, i.e. the convolution of profiles due to different broadening processes:

$$\psi(\nu - \nu_0) = \phi(\nu - \nu_0) = \frac{H(a, v)}{\sqrt{\pi}\Delta\nu_D} \quad (59)$$

with

$$a = \frac{\gamma_R + \gamma_3 + \gamma_4 + \gamma_6}{4\pi\Delta\nu_D} \quad v = \frac{\nu - \nu_0}{\Delta\nu_D} \quad (60)$$

where γ_R for natural damping and γ_n for pressure broadening, n being the impact parameter. The Doppler broadening is due to the thermal and non-thermal (microturbulence) motions of atoms:

$$\Delta\nu_D \equiv \frac{\nu_0}{c} \sqrt{\frac{2kT}{m} + v_{\text{mic}}^2} \quad (61)$$

with m the mass of the atom under consideration. The parameter v_{mic} is the microturbulence velocity, which is defined as the parameter describing qualitatively random motions on scales *smaller* than the photon mean free path. Doppler broadening arises because the observer sees the integrated radiation from particles moving with different velocities along the *line-of-sight*. It is described by a Gaussian profile:

$$\psi(\nu - \nu_0) = \frac{1}{\Delta\nu_D\sqrt{\pi}} e^{[(\nu - \nu_0)/\Delta\nu_D]^2} \quad (62)$$

The Voigt profile, i.e., the convolution of a Gaussian and a Lorentzian profile is described as:

$$\phi(q, q_D, \gamma) = \frac{e^{-q^2/q_D^2}}{\sqrt{\pi}q_D} * \frac{\gamma}{\pi(q^2 + \gamma^2)} \quad (63)$$

$$\phi(u, a) = \frac{e^{-u^2}}{\sqrt{\pi}} * \frac{a}{\pi(u^2 + a^2)}, \quad (64)$$

where $q = \nu/\nu_0 - 1$, $q_D = \Delta\nu_D/\nu_0$, and (in 1D static model atmospheres, for 3D RT in convective models see below) $u = q/q_D$, and $a = \gamma/q_D$.

In 3D RT calculations, a critical difference in the calculations of profile and hence, opacity and emissivity, arises because of the 3D velocity fields and hence the requirement to project the real velocity vectors (gas velocities) on the direction of photon propagation (see also [Ibgui et al. 2013](#), section 8.3). In this case, the u parameter that enters the exponent in the numerator and the denominator in Eq. (64) changes its form to a slightly more sophisticated expression:

$$u = \frac{(\nu/\nu_0 - 1 - v_{\text{proj}}/c)}{\sqrt{2kT/mc^2}} = \frac{(\nu - \nu_0(1 + v_{\text{proj}}/c))}{\frac{\nu_0}{c}\sqrt{2kT/m}} = \frac{q - v_{\text{proj}}/c}{q_D} \quad (65)$$

where v_{proj} is the projection of the velocity vector on the ray. It is exactly this exponential dependence on the velocity that leads to drastic differences in the line formation between 1D and 3D RT methods.

The Voigt function can be computed using different recipes. For example, in the *Cloudy* code ([Ferland et al. 2017](#)), the expression based on [Wells \(1999\)](#) is used. Other techniques include [Kuntz \(1997\)](#); [Letchworth and Benner \(2007\)](#); [Zaghloul \(2007\)](#); [Ngo et al. \(2013\)](#); [Tran et al. \(2013\)](#). We are not aware of dedicated tests of the profile implementation within the astrophysical domain of the objects we are dealing with in this review. However, the following study deserves to be mentioned. [von Clarmann et al. \(2002\)](#) present a comparative analysis of LTE and NLTE line profiles computed with different RT codes under conditions of the Earth's middle atmosphere. Their results suggest that despite the vast differences in the underlying micro-physics and numerical recipes, the agreement between the synthetic observables is very good and is usually better than 0.5 percent, in some cases up to a few percent. For exoplanet or stellar applications, such effects are of no relevance, except when extremely small astrophysical signatures are sought for. These are, for example, when arbitrary fits using a Voigt profile are needed to determine *the line shifts* in the observed spectra for the purpose of studies of the variability of the fine structure constant $\Delta\alpha/\alpha$ ([Murphy et al. 2001](#); [Griest et al. 2010](#); [Murphy et al. 2022](#)).

Regarding the damping coefficient, the general expression for the damping constant γ is as follows:

$$\gamma_n = N \int_{-\infty}^{\infty} v f(v) \sigma_n(v) dv \quad (66)$$

where N and $f(v)$ are the number density and velocity distribution of perturbing particles, σ_n is the broadening cross-section and this physical quantity can be obtained from theoretical calculations for transitions between different energy states of different ions. Depending on the type of perturbers, the impact parameter n may take different values. Resonance broadening, $n = 3$, represents interaction between two hydrogen atoms. The Quadratic Stark effect, $n = 4$, causes broadening due to the interaction of an atom with a charged particle, e.g. free electrons or protons. A rather special case is the van der Waals broadening, $n = 6$, describing the interactions in collisions of atoms or molecules with neutral H atoms. The latter is formulated using the ABO theory (Anstee and O'Mara 1991, 1995; Barklem et al. 1998, 2000), which is based on the full interaction potential between an atom and a hydrogen particle, avoiding series expansion in $1/r$. Line broadening cross-sections $\sigma_6(v_0)$ for a relative collision speed $v_0 = 10 \text{ km s}^{-1}$ are tabulated as a function of effective principal quantum numbers for the upper and lower level of a transition. Damping constants are then calculated as:

$$\gamma_6 = N_H \left(\frac{4}{\pi} \right)^{\alpha/2} \Gamma \left(\frac{4 - \alpha}{2} \right) \left(\frac{v}{v_0} \right)^{-\alpha} v \sigma_6(v_0) \quad (67)$$

with Γ the gamma function, v the relative velocity of an atom and a perturber, and α the velocity exponent. For a comprehensive review of the broadening cross-sections for different types of perturbers, we refer to the reader to Barklem and Collet (2016).

Finally, high-resolution synthetic spectra are then be convolved with a the instrumental profile (see Gray (1992)) in order to compare with observations with a given spectral resolution of R . The instrumental broadening is treated like macroturbulence, by a Gaussian with the full width at half maximum $c/2\sqrt{\ln 2}R_{\text{sp}}$. Here, $R_{\text{sp}} = \lambda/\delta\lambda$ is the resolution of a spectrograph.

4.11 Frequency quadrature

The primary objective of 3D NLTE radiative transfer is to output detailed synthetic spectra for comparison with spectroscopic observations. The accuracy of the resulting spectra and the computational cost of the calculation are directly impacted by the number and choice of frequencies for which the monochromatic radiative transfer equation is solved. One has to choose a frequency grid, which captures all the relevant features in the spectral region to be modelled, while keeping the computational cost at a reasonable level. The outputs of radiative transfer codes have infinite spectral resolution. When comparing to observations with low spectral resolution, it is therefore not enough to use the same frequency discretisation as employed in the observations.

In LTE one can compute a spectrum in a wavelength range of choice, while neglecting all other wavelengths without a change in precision. Even when taking coherent scattering into account (such as Thomson and Rayleigh scattering), photons are only scattered into different directions, but never change wavelength. In NLTE this is not the case, since photons can be absorbed in one spectral line and be emitted in another at a different wavelength. In principle one has to model the entire spectrum even if one is only interested in the intensity of a single spectral line. This makes NLTE line formation significantly more complex than line formation under the assumption of

LTE and is the main reason why it is computationally a lot more costly. In NLTE one should differentiate between the frequencies used when integrating the radiative rates and when printing the emerging flux. The latter has the same frequency requirements as LTE spectrum synthesis, while the former requires an adequate discretisation of the $\sigma_{ij}J_\nu$ term. Here the J_ν factor usually truncates the spectrum which has to be modelled in a certain astronomical environment.

A popular way to setup a frequency grid is to define a wavelength range between $\lambda_{\min}$ and $\lambda_{\max}$ and to distribute NF points between them with a constant wavelength step (e.g. [de Laverny et al. 2012](#)) or constant spectral resolution $\lambda/\Delta\lambda$ (e.g. [Plez 2008](#); [Chiavassa et al. 2018](#)). For codes, which work on the frequency scale, one then has to convert wavelengths into frequencies via $\nu = c/\lambda$. This scheme is reasonable for LTE as well as the NLTE flux calculations, since one usually wants to compare to observations with a given $\lambda_{\min}$ and $\lambda_{\max}$. In principle one can construct an equally accurate frequency grid with fewer points, by placing the points exactly where strong gradients in the intensity with wavelength are expected. The problem is that the frequency grid has to be defined before any intensities are calculated and one can only guess where $dI/d\nu$ is strong before having a look at the actual spectrum.

One attempt to improve the efficiency is to distribute the frequencies on a line by line basis. This idea was adopted from older RT codes, which were not able to deal with overlapping lines. Therefore there was no single frequency grid, but each line had its own frequency grid. If one assumes a nearly Gaussian line profile, it is clear that more frequency points are needed near the core of the line, while fewer points are needed where the wings fade into the continuum. Furthermore one has to specify $\Delta\lambda_{\max} = \lambda_{\max} - \lambda_0$ for each line. Choosing a reasonable $\Delta\lambda_{\max}$ alone is not trivial as it depends on the modelled environment and is often adjusted manually in practice. One can combine this multitude of grids into a single frequency set by concatenation and subsequent sorting of frequencies. This approach is used in many NLTE applications when defining a frequency grid for the integration of the radiative rates. The spectral resolution is secondary when performing this integration, since the uncertainty in atomic data, such as oscillator strength, for example, easily surpasses the uncertainty that results from using a frequency quadrature that is relatively coarse compared to the spectrum synthesis resolution.

As a result, the frequency resolution of the lambda-iteration may be much lower than the final spectrum synthesis resolution. Nevertheless, this does not imply that the total number of frequencies utilised is lower. Bound-free transitions play a crucial role in establishing statistical equilibrium, even though their absorption features may hardly be visible in a spectrum. Since bound-free transitions are “active” over a wide frequency range, we must include a sufficient number of frequencies from these ranges to ensure the $\sigma_{ij}J_\nu$ term is probed sufficiently.

Photo-ionisation cross-sections, either computed ([Cunto et al. 1993](#); [Badnell et al. 2005](#)) or measured ([Shafique et al. 2022](#)), are typically on a very detailed frequency grid, since σ_{ij} has a very complex dependence on energy owing to strong resonances in the cross-sections ([Nahar and Pradhan 1997](#); [Bautista et al. 2017](#)). Some of which are so insignificant to the statistical equilibrium that they can be omitted entirely.

A rather coarse frequency discretisation of spectral line is usually enough to obtain a reasonable estimate of the radiative rates. Weak spectral lines with low $\log(gf)$ are more likely to be insignificant, but this cannot be guaranteed in advance, and it must be validated by repeated calculation with and without them. [Bergemann et al. \(2019\)](#) employ 13 frequency points per line in the rate integrals, which was sufficient to obtain reliable level populations of Mn. [Gallagher et al. \(2020\)](#) use only 9 frequency points per line, arguing that a refined frequency resolution did not affect their diagnostic Ba II lines. [Lind et al. \(2017\)](#) use less than 5 frequency points per line on average to make calculations of their Fe NLTE model feasible in 3D. Employing the same Fe NLTE model, [Asplund et al. \(2021\)](#), use roughly 10 frequency points per line. The references above dealt with FGK-type stars, where velocity gradients are small enough that convective broadening only has a minor impact on $\lambda_{\min}$ and $\lambda_{\max}$ chosen for each line. For applications in hot stars with winds, where radiative transfer is usually carried out in the comoving frame, the situation is slightly more complicated. Strong velocity gradients shift the line profiles in the observer’s frame far away from their rest position. Therefore $\Delta\lambda_{\max} \gg \text{FWHM}$ of the line if we define $\lambda_{\max}$ as the wavelength where the line profile “ends”. The radiative rates can be integrated in the comoving frame, however, and only has to be evaluated where the intrinsic line profile without any Doppler shifts is non-zero. Even though the P Cygni line profiles are represented by 100 frequency points in [Lobel and Blomme \(2008\)](#), the rate integral is only performed over 3 frequency points. [Hennicker et al. \(2018\)](#) state that their frequency discretisation is comparatively much finer and the rate integral covers 15 frequency points per line.

5 Velocities

Microscopic thermal motion of particles as well as macroscopic convective motions of the gas lead to observable broadening of spectral features. Typically, at conditions of atmospheres of FGKM-type stars, the Doppler shifts are of the order a $\sim$ few 100 meter to a few km/s ([Sheminova 2020](#)). For the solar spectral lines, for example, Doppler shifts of up to 800 m/s are observed ([Allende Prieto and Garcia Lopez 1998](#); [Allende Prieto et al. 2002a](#); [Reiners et al. 2016](#)). This implies a wavelength shift of a 0.1 Å to few milli-Å. Therefore continuum opacities can be considered as fairly isotropic, i.e., independent of the apparent motion of the gas. However, the velocity shifts may be significant in spectral lines, and these may interfere with other effects, like hyperfine splitting, isotopic structure, or planetary motion.

In RT calculations in 1D plane-parallel (or spherically-symmetric) homogeneous atmospheres, the only source of microscopic broadening is the thermal broadening due to random isotropic motions of particles. However, this thermal broadening is not sufficient, and it is common in all 1D RT calculations ([Kurucz 1970](#); [Gustafsson et al. 2008](#)) to adopt an additional non-thermal component to ‘correct’ the Doppler width for the *absence of turbulence and convection* (see eq. 61). This component is known as microturbulence v_{mic} . Typically, v_{mic} is either a free parameters, or it solved iteratively together with the determination of stellar abundances and metallicities ([Bergemann et al. 2012c](#)). In some cases, e.g., in large spectroscopic surveys like Gaia-ESO ([Smiljanic et al. 2014](#)) and GALAH ([Buder et al. 2021](#)), functional forms for v_{mic}

are assumed. For the Gaia-ESO survey, in particular, we (M. Bergemann and V. Hill; ref. v2, 2013) developed the following v_{mic} velocity parametrisation using the fits to the spectroscopic measurements of v_{mic} obtained from the literature.

The following relations for microturbulence velocity v_{mic} (in km s^{-1}) are valid for:

$$4000 < T_{\text{eff}} < 7000, \quad 0 < \log g < 5, \quad -4.5 < [\text{Fe}/\text{H}] < +1$$

Let:

$$t_0 = 5500 \text{ K}, \quad g_0 = 4.0, \quad t = T_{\text{eff}}, \quad g = \log g, \quad m = [\text{Fe}/\text{H}].$$

- **Main sequence and subgiants** ($T_{\text{eff}} \geq 5000 \text{ K}$, $\log g \geq 3.5$):

$$v_{\text{mic}} = 1.05 + 2.51 \times 10^{-4}(t - t_0) + 1.5 \times 10^{-7}(t - t_0)^2 - 0.14(g - g_0) - 0.005(g - g_0)^2 + 0.05m + 0.01m^2$$

- **Main sequence stars** ($T_{\text{eff}} < 5000 \text{ K}$, $\log g \geq 3.5$):

$$v_{\text{mic}} = 1.05 + 2.51 \times 10^{-4}(5000 - t_0) + 1.5 \times 10^{-7}(5000 - t_0)^2 - 0.14(g - g_0) - 0.005(g - g_0)^2 + 0.05m + 0.01m^2$$

- **Giants** ($\log g < 3.5$):

$$v_{\text{mic}} = 1.25 + 4.01 \times 10^{-4}(t - t_0) + 3.1 \times 10^{-7}(t - t_0)^2 - 0.14(g - g_0) - 0.005(g - g_0)^2 + 0.05m + 0.01m^2$$

This formula is based on fitting the following datasets: [Bensby et al. \(2003, 2005\)](#); [Bruntt et al. \(2012\)](#); [Barklem et al. \(2005\)](#); [Bonifacio et al. \(2009\)](#); [François et al. \(2007\)](#); [Allende Prieto et al. \(2004\)](#); [Takeda et al. \(2005\)](#); [Johnson \(2002\)](#); [Ghezzi et al. \(2010\)](#); [Yong et al. \(2008\)](#), and [Ruchti et al. \(2013\)](#).

We remind that v_{mic} is a free parameter which does not have a physical basis in 1D calculations and cannot be derived from first principles. Since v_{mic} enters the equation for the line opacity, the resulting line profile is strongly correlated with the assumed v_{mic} ([Bergemann et al. 2012b](#); [Takeda 2022](#)). Such that for the spectral lines with EWs $> 80 \text{ mÅ}$, a 0.1 km s^{-1} increase in v_{mic} leads to a 0.05 dex lower abundances, and vice versa ([Takeda 2022](#)). Hence adopting a v_{mic} of 0.2 km s^{-1} only may change abundances by 0.1 dex (see also the discussion in [Bergemann et al. 2019](#)).

6 Non-Local Thermodynamic Equilibrium

6.1 Kinetic equilibrium or rate equations

The assumption of radiation in local equilibrium with the gas violates any object which has an outer transmitting boundary.

The most computationally expensive part of NLTE is the calculation of the number density n_i of the particles which occupy different internal energy states, i . In scientific literature, n_i is also known as the level population or occupation number of the level i . Depending on the physical context, the concept of the level varies, and may refer to, e.g. the excitation state of an atom or a molecule, which may either refer to a hyperfine structure level, a fine structure level, a term (in the notation of NIST handbook), or even a “hyper-state” which is a statistical representation of hundreds of terms.

In NLTE, the level populations directly depend on the radiation field, that is, on the mean specific intensity of radiation J_ν at different frequencies ν . Extensive summaries on the determination of occupation numbers in NLTE have been presented elsewhere (e.g. [Auer and Mihalas 1969](#); [Mihalas 1988](#); [Rybicki and Hummer 1991, 1992](#); [Kubát 2014](#)), and we refer the reader to these papers. Below we briefly outline the basic aspects of the coupled radiation transfer and SE solution.

Following [Mihalas and Athay \(1973\)](#) and [Rutten \(2003\)](#), we define the probability P_{ij} of a particle to transition from the energy state i to j as given by the sum of all collision-induced transition rates C_{ij} and the radiation-induced transition rates R_{ij} :

$$P_{ij} = C_{ij} + R_{ij}, \quad (68)$$

where the individual rate coefficients are defined as:

$$R_{ij} = \int_0^\infty \frac{4\pi}{h\nu} \sigma_{ij} J_\nu d\nu \quad (69)$$

$$R_{ji} = \int_0^\infty \frac{4\pi}{h\nu} \sigma_{ij} G_{ij} \left(J_\nu + \frac{2h\nu^3}{c^2} \right) d\nu \quad (70)$$

with

$$G_{ij} = \left[\frac{n_i}{n_j} \right]_{\text{LTE}} e^{-h\nu/kT} \quad (71)$$

where the first equation represent excitation or ionisation by photons, and the second equation represents the inverse process of radiative de-excitation or recombination. For molecular NLTE, these equations may also be used to represent, in a simplified expression, photo-dissociation processes ([Popa et al. 2023](#)). We note that in a molecule both kinds of processes, photo-ionizations and photo-dissociations may take place simultaneously. The cross-sections for all radiative transitions are typically computed with quantum-mechanical methods or are obtained via experimental methods (see Sect. 3.3).

For collision-induced reactions, including excitations and ionization, the rates of transitions are calculated as follows, with the detailed balance assumed for reverse reactions:

$$C_{ij} = n_e \int_{v_0}^\infty \sigma_{ij}(v) v f(v) dv \quad (72)$$

where $\sigma_{ij}(v)$ is the electron collision cross-section, $f(v)$ is the Maxwellian velocity distribution, v_0 is the threshold velocity with $mv_0^2/2 = h\nu_0$.

$$C_{ij} = \left[\frac{n_i}{n_j} \right]_{\text{LTE}} C_{ji} \quad (73)$$

Statistical equilibrium, that is, the time dependence and advection terms are neglected, is then formulated as:

$$n_i \sum_{j \neq i} P_{ij} = \sum_{j \neq i} n_j P_{ji} \quad (74)$$

In contrast, the rate equations including the time dependence and advection:

$$\frac{\delta N_i}{\delta t} + \frac{\delta v N_i}{\delta z} = \sum_j N_j P_{ji} - N_i \sum_j P_{ij} \quad (75)$$

The equilibrium populations n can be computed once the $(K \times K)$ transition matrix P is known. The equilibrium distribution is defined as the eigenvector of the transition matrix with eigenvalue unity.

$$P(n - 1) = 0 \quad (76)$$

The set of equations is closed by the particle conservation equation:

$$\sum_{i,c} n_{i,c} = \frac{\alpha_{\text{el}}}{\alpha_{\text{H}}} \left(\sum_i n_{i,\text{H}} + n_p \right) \quad (77)$$

where $\alpha_{\text{el}}/\alpha_{\text{H}}$ is the fraction of all atoms and ions of an element relative to that of H atoms, $n_{i,\text{H}}$ are the hydrogen level populations and n_p is the number of ionised hydrogen atoms (free protons).

6.2 Lambda iterations

For a given J_ν we can fill the entries of the transition matrix P (Eq. (68)) and predict how many atoms occupy each energy state of a species i.e. the level populations numbers n . Unfortunately, J_ν , the total incident radiation on a local point arriving from all directions, depends on the population numbers in the entire physical system.

Solving radiation transfer and the equations of statistical equilibrium simultaneously is an overwhelming task, which is extremely time-consuming in a multi-D system with correlated motions within. It is more reasonable to estimate J_ν based on some initial level populations n^0 in order to predict new level populations n , which allow us to recompute J_ν in turn. This method results in iteratively updating J_ν and n and has been shown to converge to the correct solution after a sufficiently large number of iterations. This is the method of Λ -iterations, which is schematically illustrated in Fig. 25.

Here Lambda, Λ_ν , is the so-called *operator*, or - more precisely - a method used to predict J_ν from the source function S_ν . Λ_ν can be expressed as a $\text{NP} \times \text{NP}$ matrix, where NP is the number of discrete points in the atmosphere model. The matrix element $\Lambda_{\nu,ij}$ then contains the contribution weight of S_ν from point j to J_ν at point i .

$$J_\nu = \Lambda_\nu S_\nu \quad (78)$$

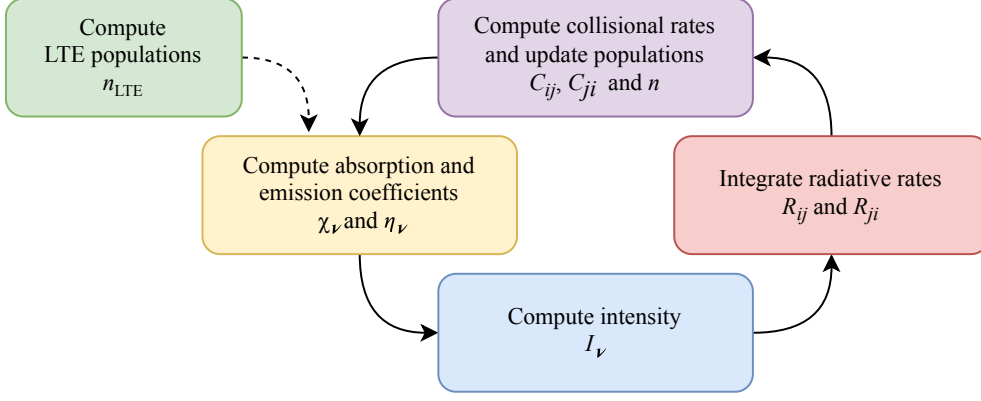


Fig. 25 The four conceptual steps of lambda iterations.

Theoretically there is a non-zero chance of a photon arriving at point i from any point in the atmosphere including i itself, therefore $\mathbf{\Lambda}_\nu$ is a dense matrix with no zeros. The value of $\Lambda_{\nu,ij}$ mainly depends on the optical depth $\Delta\tau_\nu$ between points i and j , but one should not forget about the angle-dependence of $\Delta\tau_\nu$ introduced by velocity fields.

In practice, this matrix is never constructed in 3D NLTE RT codes, not only because $\text{NP} \times \text{NP}$ is a very large number, but also because the matrix elements are not completely uncorrelated. This becomes more obvious when splitting $\mathbf{\Lambda}_\nu$ into its contributions from a discrete set of μ -angles $\Lambda_{\mu\nu}$.

$$J_\nu = \sum_{\mu} w_{\mu} \Lambda_{\mu\nu} S_{\mu\nu}, \quad (79)$$

where w_{μ} is the angle integration weight and $S_{\mu\nu}$ is the angle dependent source function. Consider a vertical ray travelling from the bottom of the atmosphere to the top. Firstly, all matrix elements $\Lambda_{\mu\nu,ij}$ for $\mu = 1$ are zero if point j is above point i in the atmosphere. Secondly, if point i and j are not directly connected by a vertical line, $\Lambda_{\mu\nu,ij}$ should also be zero. Here it also becomes clear how important the angular quadrature is during the lambda-iterations.

How lambda iterations are carried out in practice without the explicit construction of the Lambda-operator is discussed in Sect. 6.2.

6.3 Accelerated Lambda Iteration

A very common method to solve the statistical equilibrium and radiative transfer equations is the method of Accelerated Lambda Iteration) [Rybicki and Hummer \(1991, 1992\)](#), which is employed in vast majority of modern astronomy codes, including `Cloudy`, `Multi`, `MULTI3D`, `DETAIL`, `MAGRITTE`, etc. This method builds upon the fundamental realisation of unsatisfactory convergence properties of Λ -iteration that seeded the development of operator-splitting techniques ([Scharmer 1981](#); [Scharmer and Carlsson 1985](#); [Olson and Kunasz 1987](#); [Rybicki and Hummer 1991](#)).

In this, the radiative transfer equation is solved approximately with a simplified operator (see [Hubeny 2003](#), for an overview). The exact operator is written as $\hat{\Lambda}_\nu = \hat{\Lambda}_\nu^* + (\hat{\Lambda}_\nu - \hat{\Lambda}_\nu^*)$, where $\hat{\Lambda}_\nu^*[S_\nu]$ is the *approximate* operator. The formula (78) is expanded to:

$$J_\nu^{(n)} = \hat{\Lambda}_\nu^*[S_\nu^{(n)}] + (\hat{\Lambda}_\nu - \hat{\Lambda}_\nu^*)[S_\nu^{(n-1)}] \quad (80)$$

where $S^{(n-1)}$ is the source function from the previous iteration. The approximate operator acts on the new estimate of the source function, whereas the difference between the exact and approximate operator, $\hat{\Lambda}_\nu - \hat{\Lambda}_\nu^*$, operates on the previous known source function. The latter can be found from the formal solution. Then the new estimate is found from the inversion of $\hat{\Lambda}_\nu^*$. This inverted approximate operator acts as an accelerating factor that ensures fast convergence.

Equation (80) must be solved for all frequencies ν that are related to the transitions in the atom under consideration and for all depth points τ_d in the model atmosphere. However, because the lambda-operator is integrated over all depths, the mean intensity for a certain depth point requires knowledge of source functions at all other depths. One could take into account the depth-dependency for both exact and approximate operators, but this is costly in the computational sense. The solution is to choose the special form of the approximate operator $\hat{\Lambda}_\nu^*$, so that it is local for the first term in the right-hand side of the Eq. (80). In this case, only the source function at one depth point k is considered. This term can be written as $\hat{\Lambda}_\nu^*[S_{\nu,k}^{(n)}]$, whereas the dependency on other depth points k' is taken into account only in the second term of the Eq. (80). This is called the diagonal operator, because the matrix Λ^* contains terms corresponding to the specified depth point d diagonally. Using the diagonal operator results in a Jacobi iterative scheme ([Olson et al. 1986](#)). In the context of radiative transfer this means the following execution of tasks:

1. Start from an initial guess of the source function at each point in the atmosphere $S_\nu^{(0)}$
2. Solve the RTE by propagating the intensities I from one boundary to the other. This can be done in arbitrary order or even in parallel.
3. Integrate I over all angles to get J . Compute an effective mean intensity J_{eff} , which excludes the contribution of the local source function at each point.
4. Plug this J_{eff} into the rate equations to determine the radiative rates of each transition.
5. Solve the statistical equilibrium and obtain a new set of source functions $S_\nu^{(n+1)}$.
6. If the global update has not met the convergence criterion then jump to step 2 and repeat.

The Jacobi method ensures the fastest execution of a single iteration step. A common alternative to this are the Gauss–Seidel (GS) method and its extension the successive over-relaxation (SOR) method. When iteratively solving a system of equations, these methods update the vector $S_\nu^{(n)}$ in-situ, meaning that one overwrites the source function results from the previous iteration as soon as new values can be obtained. Since the vector $S_\nu^{(n)}$ is updated element by element, one takes $i - 1$ already updated elements into account, when updating the element i . The GS and SOR methods represent a lower triangular operator as an alternative to the diagonal operator of

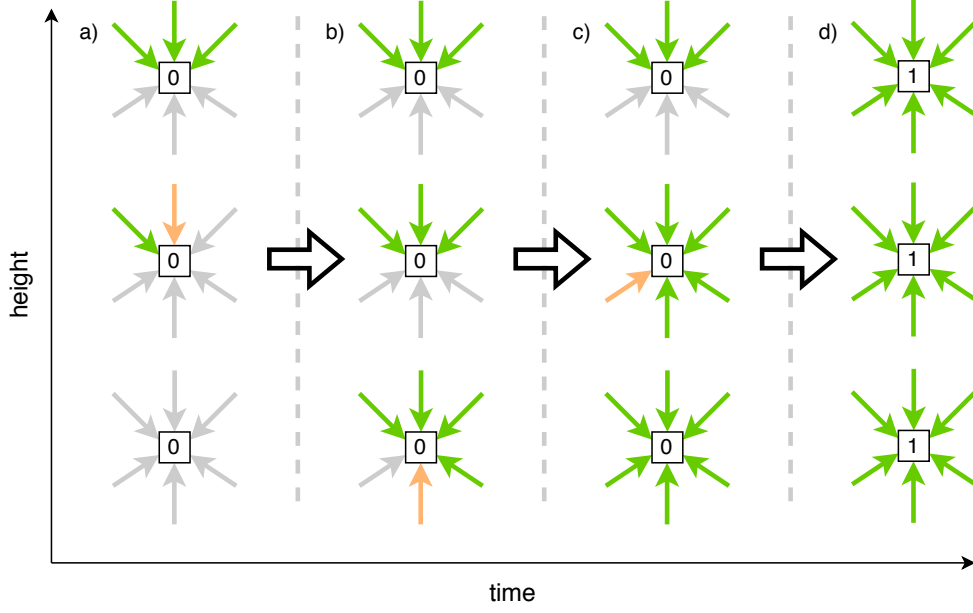


Fig. 26 Jacobi iterations visualised in 4 steps (a, b, c and d) for a one-dimensional atmosphere consisting of 3 points. The squares mark the grid points with the number showing the number of times the source function has been updated. The grey arrows mark the intensities that have yet to be computed, the green arrows mark those that have already been computed and the orange arrow marks the intensity that is computed in the current step. Most notably, the source function of all grid points is updated in the last step.

the Jacobi method. In order to implement such a scheme for radiative transfer think of J as being made of an up and down part $J = J^+ + J^-$, where J^+ contains contributions from all angles with $\mu > 0$. Now let's update the scheme from above in the following way, where we have dropped the frequency index for clarity:

1. Start from an initial guess of the source function at each point in the atmosphere $S^{(0)}$
2. Sweep the atmosphere from the top boundary to the bottom while calculating and storing all values of J^- on the way. Now we start from layer $k=1$ (counting from the bottom) where we can make use of the bottom boundary condition.
3. Compute J_k^+ and J_k^- . Compute $J_{\text{eff},k}$ and plug it into the rate equations. Update element $S_k^{(n+1)}$.
4. In case of a 3-point formal solver, which makes use of the downwind source function, one then has to correct J_{k+1}^- as well as J_k^+ using $S_k^{(n+1)}$, since both originally had contributions from $S_k^{(n)}$.
5. Increment k by 1 and repeat step 3 until reaching the other boundary.
6. If the global update has not met the convergence criterion then jump to step 2 and repeat.

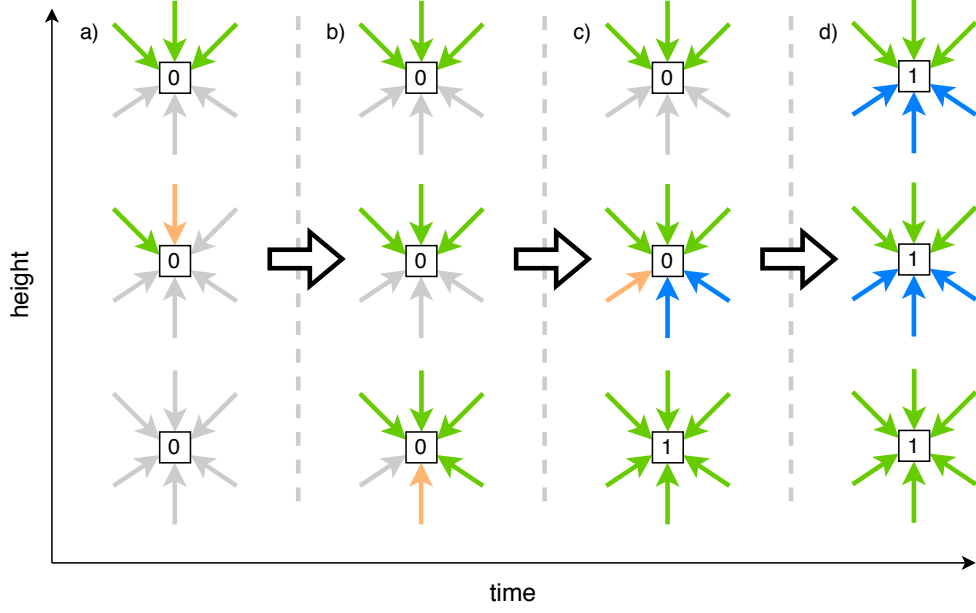


Fig. 27 Same as Fig. 26, but for Gauss-Seidel iterations. While steps a) and b) are the same, the source function at the bottom of the atmosphere is already updated in step c). The intensities including the updated source function from this point already are coloured in blue.

For a more detailed description see [Trujillo Bueno and Fabiani Bendicho \(1995\)](#), who were the first to propose this scheme in the context of non-LTE radiative transfer. See [Trujillo Bueno and Manso Sainz \(1999\)](#) for an application to polarized line transfer. The SOR method differs from the GS method in the way that it calculates the source function update as

$$S_k^{(n+1)} = S_k^{(n)} + \omega \Delta S_k^{\text{GS}}, \quad \Delta S_k^{\text{GS}} = \left[S_k^{(n+1)} - S_k^{(n)} \right]_{\text{GS}} \quad (81)$$

where $1 < \omega < 2$. One has some freedom in choosing the parameter ω , but the optimum value is the one which leads to the highest rate of convergence. Mathematically, this corresponds to the value of ω which minimises the spectral radius (the largest absolute eigenvalue) of the approximate operator $\hat{\Lambda}_\nu^*$.

The original GS and SOR methods proposed in [Trujillo Bueno and Fabiani Bendicho \(1995\)](#) only consider using the partially updated source functions during the upward sweep. [Trujillo Bueno \(2003\)](#) introduces the possibility to apply the procedure stated in step 3 also to the downward sweep, which the author called symmetric-SOR (SSOR).

The Jacobi method requires twice as many iterations as the one-sided GS method ([Trujillo Bueno and Fabiani Bendicho 1995](#)). The symmetric-GS method improves convergence by another factor of 2, so it requires only a quarter of the iterations needed by the Jacobi method ([Fabiani Bendicho 2003](#)). The SOR and SSOR methods

accelerate convergence even further with the factor depending on the choice of ω . The SSOR method was found to be generally less sensitive to the exact choice of ω (Trujillo Bueno 2003). Theoretically, an implementation of a GS or SOR iteration does not need to perform many more operations than a Jacobi iteration. In practice, this acceleration comes at a cost, however, as the in-situ updates of the source functions requires alternating solutions of the SE and the RTE for each point in the domain. This requires a more complex implementation which prohibits efficient parallelisation and vectorisation Štěpán and Trujillo Bueno (2013). This is a well known drawback of GS like schemes (Bertsekas and Tsitsiklis 1988) and for this reason the Jacobi method, i.e. the diagonal operator, remains the method of choice for parallelised NLTE applications such as PORTA, Nicole, MULTI3D and BALDER.

Otherwise, one can take into account the interdependence of $S_\nu^{(n)}$ between nearby grid points. For example, in 1D calculations one can account for changes in the upstream and downstream points, S_{k-1} and S_{k+1} , yielding a tridiagonal operator. In multidimensional setups the contributions from the neighbouring points of a cell result in a sparse matrix operator, which is no longer tridiagonal. The inversion of so-called multi-band or non-local operators requires sparse matrix inversions at each grid point instead of a single simple division in the case of a diagonal operator. The multi-band operators can improve the performance of the ALI despite this additional computational effort, since they converge in less iterations. Hauschildt et al. (1994) define the optimum bandwidth as the one, which minimises the total CPU time needed for the solution of a particular radiative transfer problem. They find that the number of iterations required for convergence drops rapidly with increased bandwidth, but the optimum bandwidth strongly depends on the vectorising capabilities of the CPU and the number of frequency points N_ν and angles N_μ considered. The formal radiative transfer solver vectorises well, but its cost scales linearly with N_ν and N_μ . The inversion of the matrix operator vectorises poorly, but this is done after the radiative rates have been integrated over angle and frequency, so its cost does not increase with an increase in N_ν or N_μ . For multidimensional applications Hauschildt and Baron (2006) point out that the memory requirements of non-local operators prevent employment of large bandwidths. Considering the interaction of a point with its direct neighbours requires the storage of 3^3 matrix elements times the number of grid points. Large bandwidth setups, going beyond the nearest neighbour interactions, already require much more memory and the authors only consider them useful for highly complex problems. Interestingly, it was also observed that Ng acceleration works better for narrower bandwidths and deteriorates when increasing the bandwidth. Hennicker et al. (2020) developed a nearest neighbours non-local operator for spherical geometries and confirm its fast convergence behaviour.

The convergence rate of operator splitting methods generally depends on the resolution of the mesh and convergence is obtained much faster when working on relatively coarse grids. Auer et al. (1994) give an intuitive explanation: *By taking larger optical depth steps we reduce the influence of the off-diagonal terms, make the diagonal approximate operator more accurate, and accordingly speed the convergence.* More precisely, the low-frequency oscillations around the solution are suppressed very effectively on coarser meshes. This leads to rapid initial convergence, but the converged

solution might still be far from the true, analytic solution. The analytic solution can be defined as the converged solution on a mesh with infinite resolution. Simulations with a higher resolution therefore get closer to the true result, but take more iterations to converge which is multiplied with the increased computational cost needed to solve each single iteration. Multi-grid methods have been developed in order to achieve quick convergence independent of the mesh resolution (Steiner 1991; Auer et al. 1994; Fabiani Bendicho et al. 1997; Bjørgen and Leenaarts 2017).

The basic idea is to solve the NLTE problem using multiple mesh resolutions. One interesting result of changing mesh resolution is that one can estimate the uncertainty in the calculation through the change in convergence speed between the different grid resolutions. Auer et al. (1994) developed a method which refines the mesh resolution once the relative change between iterations R_e falls below the approximated true error T_e . They are defined as

$$R_e(I, L) = \text{Max} \left[\frac{|n(I, L) - n(I - 1, L)|}{n(I, L)} \right] \quad (82)$$

$$T_e(I, L) = \text{Max} \left[\frac{|n(I, L) - n(\infty, \infty)|}{n(\infty, \infty)} \right] \quad (83)$$

where $n(I, L)$ is the set of level populations at iteration I and refinement level L (higher L meaning finer resolution). T_e basically describes how far the populations are from the analytical solution $n(\infty, \infty)$. There is no point in iterating further than $R_e < T_e$, since there is no more gain in accuracy. The analytical solution is of course unknown, but T_e can still be roughly approximated, which allows the definition of a convergence criterion resulting in a solution with the desired T_e . For how T_e is approximated in detail, we refer the reader to Auer and Paletou (1994).

Fabiani Bendicho et al. (1997) generalise the grid refinement method further and develop a nested multi-grid method. Their method is based on iterating on grids of different refinement levels, where the refinement is always a factor of 2 in the grid spacing. The solutions are interpolated back and forth between the multiple levels ensuring rapid decay of the low-frequency error oscillations as well as the high-frequency error oscillations. In contrast to the method by Auer et al. (1994), they do not only go from low to high-resolution, but they also go from high to low-resolution iterations. This is called a V-cycle (see figure 1. of Bjørgen and Leenaarts (2017)). The complex setup comes with an overhead, however, which only pays off over the classic Jacobi method when interested in particularly fine resolutions. For 1D applications the break-even point is reached approximately at $\Delta z \approx 10$ km. For multidimensional applications the break-even point is reached at much coarser resolution, since the computational cost is dominated by solving the formal solution on the finest grids only (Fabiani Bendicho 2003). Assuming the resolution is doubled between refinement levels, the finest grid already has 8 times as many points as the next coarser grid.

Štěpán and Trujillo Bueno (2013) implemented a multi-grid method for radiative transfer in 3D and tested its efficiency compared to the standard Jacobi method. From their figure 15 it is clear that the multi-grid method is at least an order of magnitude faster, with the exact numbers depending on the desired convergence criterion. Their

test bed, however, was not a true 3D hydrodynamical simulation, but based on a plane-parallel 1D atmosphere with smooth, artificial perturbations in the horizontal directions.

Björge and Leenaarts (2017) showed that when using real MHD snapshots of stellar atmospheres, the multi-grid method does not converge as quickly as previously thought, but still gives a speed up with a factor of 3 to 6 compared to the Jacobi method. Furthermore there was no single setup of V-cycle parameters that provided optimal convergence in all tested atmospheres. One for example has to decide how many iterations are performed at each refinement level. This number is largest for the finest mesh, while only few iterations are needed on the other meshes, but finding the optimal values required manual fine tuning of each simulation. When applying coarse grid corrections to the populations numbers on the finer grids, unfortunately, negative population numbers may arise, which is not possible in the Jacobi method. This demands additional alertness from the side of the user.

In a proof-of-concept paper Arramy et al. (2024) recently presented a NLTE solver, which is not based on the operator splitting method. Alternatively they explore a Jacobian-Free Newton–Krylov (JFNK) method. Another radically different approach was explored by Panos and Milic (2025), who tackle the 2-level atom NLTE problem using Soft Actor-Critic Reinforcement Learning. This ”Approximate-Lambda-Operator-Free” method requires a pre-trained agent to predict the source function (or potentially level populations) to be used in the next lambda iteration. While it is not surprising, that a well-trained agent could potentially achieve rapid convergence, it remains to be shown how such an agent may be trained in order to generalise to unseen environments. Also the computational cost of the training phase should not be neglecting when benchmarking performances of pre-trained operators against classical methods.

6.4 The diagonal operator

Here we would like to look at the diagonal approximate lambda iterator in more detail. The diagonal elements are determined by the choice of formal solver (see section 4.5). Defining Λ_{kk}^* means defining the impact of the local source function S_k on the local mean intensity J_k (here we have dropped the frequency indices). The angle-dependent intensity at point k can be expressed in a multitude of ways, but here we list the most commonly used expressions:

$$I_k = I_{k-1}e^{\Delta\tau} + \alpha_L S_{k-1} + \beta_L S_k, \quad \text{linear} \quad (84)$$

$$I_k = I_{k-1}e^{\Delta\tau} + \alpha_Q S_{k-1} + \beta_Q S_k + \gamma_Q S_{k+1}, \quad \text{quadratic} \quad (85)$$

$$I_k = I_{k-1}e^{\Delta\tau} + \alpha_B S_{k-1} + \beta_B S_k + \gamma'_B C_B, \quad \text{quadratic Bezier} \quad (86)$$

$$I_k = I_{k-1}e^{\Delta\tau} + \alpha_H S_{k-1} + \beta_H S_k + \beta'_H \frac{dS_k}{d\tau}, \quad \text{quadratic Hermite} \quad (87)$$

$$I_k = I_{k-1}e^{\Delta\tau} + \alpha_C S_{k-1} + \beta_C S_k + \alpha'_C \frac{dS_{k-1}}{d\tau} + \beta'_C \frac{dS_k}{d\tau}, \quad \text{cubic Hermite} \quad (88)$$

where we would also like to remind that for quadratic Bézier polynomials C_B is commonly defined as

$$C_B = S_k - \frac{\Delta\tau}{2} \frac{dS_k}{d\tau}. \quad (89)$$

The α and β factors are unique for each formal solver and depend on the exact details of the interpolation of the source function between k and the upstream point $k - 1$. Let us define the local angular contribution Λ_μ^* to Λ_{kk}^* such that

$$\Lambda_{kk}^* = \sum_{\mu}^{N_\mu} w_\mu \Lambda_\mu^*. \quad (90)$$

Λ_μ^* is the contribution of S_k to I_k . For the linear case (Eq. (84)) it is clear that $\Lambda_\mu^* = \beta_L$. For higher order interpolation the choice of Λ_μ^* is more ambiguous and depends on the way $dS/d\tau$ is defined.

Olson and Kunasz (1987) suggest to determine Λ_μ^* by using the equation for I_k but setting I_{k-1} and $S_{k\pm 1}$ to zero and setting $S_k = 1$. This eliminates contributions from the α and γ terms, but not necessarily from the terms including α', β' or γ' . Monotonicity preserving solvers enforce $dS_k/d\tau = 0$ if S_k is a local maximum, as is the case when $S_k = 1$ and $S_{k\pm 1} = 0$. When choosing the Hermite methods, this results in no contributions from the β' term, but in the Bézier formulation $\Lambda_\mu^* = \beta_B + \gamma'_B$, since $C_B = S_k = 1$. Hayek et al. (2010) decide to reformulate their quadratic Bézier solver to resemble Eq. (85), i.e. using $\Lambda_\mu^* = \beta_Q$ in the case when there are no overshoots in the source function interpolant. Socas-Navarro et al. (2015) claim that there is no reason to split the gradients $dS/d\tau$ into the individual contributions from S_k and $S_{k\pm 1}$. By direct comparison, they find that $\Lambda_\mu^* = \beta_B + \gamma'_B$ achieves convergence in fewer iterations than $\Lambda_\mu^* = \beta_Q$. The cubic Hermite implementation in MULTI3D employs $\Lambda_\mu^* = \beta_C$.

6.5 Preconditioning the radiative rates

The discretised radiative rates are given by:

$$R_{ij} = \sum_{\mu}^{N_\mu} \sum_{\nu}^{N_\nu} w_\mu w_\nu \frac{4\pi}{h\nu} \sigma_{ij} I_\nu, \quad (91)$$

$$R_{ji} = \sum_{\mu}^{N_\mu} \sum_{\nu}^{N_\nu} w_\mu w_\nu \frac{4\pi}{h\nu} G_{ij} \sigma_{ij} \left(I_\nu + \frac{2h\nu^3}{c^2} \right), \quad (92)$$

where we have replaced the integrals by weighted sums using the angle and frequency quadrature weights w_μ and w_ν .

These expressions can be modified to reduce the feedback between the local source function and the local mean intensity. This is also known as preconditioning the rate equations. Here the approximate lambda operator comes into play.

Rybicki and Hummer (1992) derive the *full-preconditioning* strategy for multi-level atoms, which can handle overlaps between multiple transitions. Their recipe was

implemented in the RH code (Uitenbroek 2001), which got its name from this seminal paper. Its implementation was subsequently adopted by MULTI3D and its off-spring BALDER. However, Rybicki and Hummer (1992) state that in many situations the full treatment is most likely an overkill and preconditioning the rate equations by only considering interactions of a transition with itself is probably more efficient. This scheme, we call *auto-preconditioning*, appears to gain popularity in radiative transfer codes Hubeny and Lanz (2017a); Amarsi et al. (2020a); Osborne and Milić (2021). In the auto-preconditioning scheme the preconditioned radiative rates are given by

$$R'_{ij} = \sum_{\mu}^{N_{\mu}} \sum_{\nu}^{N_{\nu}} w_{\mu} w_{\nu} \frac{4\pi}{h\nu} \frac{2h\nu^3}{c^2} \sigma_{ij} \left(\mathcal{I}_{\nu} - \frac{\Lambda_{\mu\nu}^*}{\chi_{\text{tot}}} G_{ij} \sigma_{ij} n_j \right) \quad (93)$$

$$R'_{ji} = \sum_{\mu}^{N_{\mu}} \sum_{\nu}^{N_{\nu}} w_{\mu} w_{\nu} \frac{4\pi}{h\nu} \frac{2h\nu^3}{c^2} G_{ij} \sigma_{ij} \left(\mathcal{I}_{\nu} - \frac{\Lambda_{\mu\nu}^*}{\chi_{\text{tot}}} \sigma_{ij} n_i + 1 \right) \quad (94)$$

where we have introduced the dimensionless intensity $\mathcal{I}_{\nu}$, also known as the photon occupation number

$$\mathcal{I}_{\nu} \equiv \left[\frac{2h\nu^3}{c^2} \right]^{-1} I_{\nu} \quad (95)$$

Using $\mathcal{I}_{\nu}$ has the advantage that the factors $4\pi/h\nu$ and $2h\nu^3/c^2$ can be included in w_{ν} which is usually computed and stored during initialisation and does not change between iterations. In contrast to the full-preconditioning, the auto-preconditioning scheme allows for computing the rates on a line-by-line basis, rather than on a frequency-by-frequency basis, since no information has to be shared between transitions. The $\Lambda_{\mu\nu}^*/\chi_{\text{tot}}$ factor is also referred to as the $\Psi_{\mu\nu}^*$ operator, where the Psi-operator acts on the emissivity η rather than the source function, i.e., $J = \Psi[\eta]$.

6.6 Complete linearisation

Another method to solve the NLTE problem is known as complete linearization. In this method, the statistical equilibrium equations and the radiative transfer equation are solved simultaneously by expanding them in a Taylor series, dropping 2nd and higher order terms, and solving the resulting linear system. However, the system is coupled over all depths (through radiative transfer) and all frequencies (statistical equilibrium). The system is huge and only small atomic models can be handled with this approach. Complete linearization still can be used for numerical testing, because the method is very efficient and stable, and it can deal with very complicated multilevel cases on line formation problems. A combination of ALI and CL is used, for example, in the Cloudy NLTE RT code (Ferland et al. 2017).

6.7 Scattering and two-level (coronal) approximation

Following Ferland et al. (2017), we distinguish between the full NLTE RT solution (the collisional-radiative model) and simplified NLTE approaches, which, for example, neglect either the internal level structure of the system (atoms or molecules) or neglect

everything, except the ground and first excited level of the ion. The former approach is commonly used in studies of the ISM (Spitzer 1978; Osterbrock and Ferland 2006). The latter approach is used, e.g. in the calculations of the solar corona (e.g. Gudiksen et al. 2011) and modelling winds of massive stars (e.g. Hennicker et al. 2020).

In the two-level approximation (Crivellari et al. 2020, their Chapter 1 for derivation and references), the radiation intensities are computed using the line or continuum source function of the following form:

$$S_{l,c} = \epsilon B(T) + (1 - \epsilon) J_{\Phi}, \quad (96)$$

where J_{Φ} is the integral of mean intensity over the frequencies sampled by the line and ϵ is the so-called *photon destruction probability (by inelastic collisions)* and $(1 - \epsilon)$ is photon creation probability (here by spontaneous de-excitation in the transition between two states). The parameter is unity in LTE, but can range from 0.1 to express the “moderate scattering” to 10^{-6} to express “strong scattering” (Gudiksen et al. 2011).

Physically, the assumption is that the NLTE effects are driven by radiation and collisions in the transition between two energy states only, and all other effects (that may normally change the populations) play a negligible role. This assumption, for example, quantitatively holds in very strong resonance lines of species that have a rather special atomic structure (such as Li). Yet, generally this approach holds primarily the academic value allowing a convenient method to explore qualitatively the influence of scattering on the structure of the model (e.g., for 3D applications). In stellar atmospheres, the value of ϵ about 10^{-7} . For example, the form of Eq. (96) for the continuum was used in Hayek et al. (2011) to explore the influence of coherent isotropic scattering due to free e^- scattering and Rayleigh scattering on H in the atmospheres of metal-poor red giants. A similar formalism, assuming either the coherent continuum scattering or the two-level approach for a spectral line, is used in studies of 3D RT in expanding atmospheres of hot stars with winds (Hennicker et al. 2020).

Another form of a two-level approximation, as used e.g. in Cloudy (Ferland et al. 2017) is the representation of the number densities of ions through the ionization-recombination balance. In this approximation, it is assumed that the populations of ions are determined solely by photo-ionisations and/or recombinations followed by (instantaneous) suction to the ground state, hence the following expressions are used:

$$\frac{n_{i+1}}{n_i} = \frac{\int F_{\nu} \times \sigma_{\nu} d\nu}{\alpha(i+1)n_e}, \quad (97)$$

and

$$\frac{n_{i+1}}{n_i} = \frac{q(i)}{\alpha(i+1)} \quad (98)$$

where α is the total recombination rate coefficient for an ion $(i+1)$ and F_{ν} the radiative flux, and σ_{ν} the photoionization cross-sections. The former equation is used for systems with photo-ionization equilibrium, and the latter for systems with recombination equilibrium (e.g., for the solar corona).

7 3D and/or NLTE radiative transfer codes

In this section, we provide a brief description of 3D LTE, 1D NLTE, and 3D NLTE codes that are used for spectral modelling and diagnostics of exoplanets, hot stars, and cool stars. For more details and specific applications, such as kilonovae, which share much of the numerical approach with SNe modelling, we refer the reader to the next section. Table 1 presents a compact overview of some of the commonly-used codes in different communities.

Table 1 Comparison of available 3D RT codes. Recent interest in inversion codes has revived forward modelling codes. **RH** (STIC), **NICOLE**, **SNAPI** and **PORTA** are used in inversion codes. **Balder** is a branch of the original code **MULTI3D** and is listed in the same row. Cool stars are defined as those with T_{eff} below 8000 K (following [Gustafsson et al. 2008](#)). **MC stands for Monte-Carlo radiation transfer**.

Code	open access	dim.	physics	reference
SNe, Kilonovae				
SUMO (Supernova Modeling, MC)	no	1D / Sobolev	NLTE	Jerkstrand (2011) ; Pognan et al. (2023)
EXTRASS	no	3D / Sobolev	NLTE	van Baal et al. (2023)
TARDIS	yes	1D / Sobolev	LTE/NLTE approx.	Kerzendorf and Sim (2014)
ARTIS	yes	3D / Sobolev	NLTE	Kromer and Sim (2009) ; Shingles et al. (2023)
Exoplanet atmospheres				
Cloudy	yes	1D	NLTE	Ferland et al. (2017, 2013)
Hot stars				
PHOENIX/3D	no	3D	NLTE	Hauschildt and Baron (2006, 2014)
Fastwind	no	1D	NLTE	Puls et al. (2005)
Tlusty	yes	1D	NLTE	Hubeny and Lanz (2017a)
CMFGEN	yes	1D	NLTE	Hillier and Miller (1998) , also SNe
T Tauri stars, YSO				
MCFOST-art	no	1D/3D	NLTE	Pinte et al. (2009) ; Tessore et al. (2021)
FGKM stars				
Magritte	yes	3D	NLTE, winds	De Ceuster et al. (2022)
RH	yes	1.5D	NLTE/polarized	Uitenbroek (2006) ; Pereira and Uitenbroek (2015)
Nicole	yes	1.5D	NLTE/polarized	Socas-Navarro et al. (2015)
Optim3D	no	3D	LTE	Chiavassa et al. (2009)
Iris	no	3D	LTE	Ibgui et al. (2013)
Porta	no	3D	NLTE/polarized	Štěpán and Trujillo Bueno (2013)
Scate	no	3D	LTE/scattering	Hayek et al. (2010)
Linfor3D, NLTE3D	no	3D	LTE / NLTE	Cayrel et al. (2007) ; Steffen et al. (2015)
Multi3D/Dispatch, Balder	no	3D	NLTE	Leenaarts and Carlsson (2009) ; Amarsi et al. (2018) ; Eitner et al. (2024)

7.1 Exoplanets

Different physical codes are available for exoplanet atmosphere and synthetic spectral modelling. `petitRADTRANS` is among the most widely used codes for 1D LTE modelling of exoplanet spectra, both in transmission and in emission (Mollière et al. 2019). For NLTE RT, the most commonly-used code is `Cloudy` (<https://trac.nublado.org/>).

Although originally intended for modelling and diagnostics of emission spectra from externally irradiated molecular clouds (Ferland 1983; Ferland et al. 1998) and referred to as `HAZY`, this iterative NLTE RT code has over decades become a general-purpose software and it is presently broadly applicable to modelling diverse astrophysical environments with temperatures in the range from ~ 3 K to 10^{10} K (Ferland et al. 2013, 2017). The code is more restrictive in terms of density owing to prescriptions used to compute the heating and cooling rates, hence the applicability is limited to densities $\rho \lesssim 10^{15} \text{ cm}^{-3}$. For more details, we refer the reader to Chatzikos et al. (2023), and details on microphysics and numerical relevant to exoplanet atmospheres are further provided in Turner et al. (2016).

In the latest public version (Gunasekera et al. 2023), the code includes available atomic data from diverse databases (NIST, LAMDA, STOUT, CHIANTI) for chemical elements with atomic numbers up to zinc (Zn), as well as selected molecular data permitting chemical equilibrium calculations for some of the key species for planet atmospheres like carbon monoxide CO, water H₂O, molecular hydrogen H₂, methane CH₄, and carbon dioxide (Madhusudhan 2012). For the H and He-like iso-electronic sequence atoms (e.g. He I, Li II, Be III, etc) and diatomic molecules, full coupled equations of SE and RT are solved. For other species, however, simpler approaches, e.g. within the framework of the two-level (also known as ‘coronal’ approximation, see Sect. 6.7) are used. Comparative examples of H number densities computed the two limiting cases (LTE and the coronal), compared to the full comprehensive NLTE solution, can be found in Ferland et al. (2013).

7.2 Hot stars

In contrast to cool stars, LTE approximation in the analysis of spectra of hot OBA-type stars was abandoned very early (Auer and Mihalas 1969; Kudritzki and Hummer 1990) and powerful NLTE RT methods were employed not only for spectrum synthesis, but also for atmospheric structure calculations (see Sect. 8.3). The specific development progressively implied that most groups have directly relied on NLTE solvers for various diagnostic problems, circumventing the phase of individual analysis and determination of NLTE abundance corrections. Here we provide only a brief summary of recent work in modelling NLTE atmospheres of hot stars.

Among several powerful numerical codes, there are the `Kiel` code (Dreizler and Werner 1996) and `Tlusty` (Hubeny and Lanz 1992, 1995, 2017a), which are commonly-used iterative codes to compute NLTE model atmospheres in 1D and hydrostatic equilibrium with detailed handling of line blanketing due to metals and multi-element NLTE calculations. `Tlusty` operates in a hybrid framework both using the complete linearisation (Auer and Mihalas 1969) and ALI methods and it includes detailed

atomic and molecular linelists permitting physically comprehensive treatment of physical conditions from a few tens of K to $\sim 10^8$ (Hubeny and Lanz 2017a). The lower temperature limit reflects the availability of molecular data, whereas at $T \gtrsim 10^8$ the need to include more complex atomic processes, such as relativistic Compton scattering and inner-shell electronic structure restricts the applicability of the code. Similar restrictions apply for densities in excess of 10^{20} cm^{-3} , requiring a more accurate handling of line broadening and non-ideal effects (Hubeny and Lanz 2017a).

Another widely-used code for modelling OB-type expanding stellar atmospheres is *Fastwind* based on the ALI scheme. The code has similar physical capabilities to *Tlusty*, however, it also permits comprehensive treatment of stellar winds (Santolaya-Rey et al. 1997; Puls et al. 2005; Herrero et al. 2002). The code is suitable for calculations of hot stars with T_{eff} greater than roughly 8500 K and for all $\log g$ and mass loss values.

7.3 Cool stars

The 1D NLTE and 3D NLTE codes used in RT calculations for cool stars were extensively described in Sect. 4. Here we provide only a small selection of studies that were seminal either by introducing a new mathematical or numerical framework, and/or introducing a new code, which found applications in many subsequent studies. We caution that this list is not complete.

- Rybicki and Hummer (1992): This paper is the first to derive the preconditioned statistical equilibrium equations for overlapping transitions. Including overlapping transitions requires the use of the Psi operator which operates on the emissivity rather than on the source function. A recipe for full-preconditioning is given as well as a recipe for self-preconditioning of single transitions is given. Preconditioning accelerates convergence, because it removes the self-interaction of transitions.
- Trujillo Bueno and Fabiani Bendicho (1995) The MUGA code uses Gauss–Seidel iterations, a multi-grid scheme. The RH code is mentioned for its partial-redistribution scheme, but it has seen little application in 3D.
- Auer (2003): This paper describes the translation from observer’s frame to comoving frame quantities and also describes the monotonic cubic Hermite interpolation scheme, which was later implemented in the IRIS code and after that in the MULTI3D code.
- Carlsson (2009) and Leenaarts and Carlsson (2009): The MULTI3D codes applies a linearization of the statistical equilibrium equations following (Scharmer and Carlsson 1985) and the approximate operator of Rybicki and Hummer (1991). The code was adapted to a full preconditioning scheme from Rybicki and Hummer (1992) similar to RH.
- Ibgui et al. (2013): This paper showcases the 3D RT code IRIS, which was purely LTE at the time and not MPI parallelised. The main contribution of this paper was a very efficient piecewise cubic, locally monotonic, interpolation technique, that considerably reduces the numerical diffusion effects of the short-characteristics method. This technique was also adapted in the MULTI3D code as the “hermite” Sinterpol

option. It is mentioned that IRIS is to be fused with the NLTE code TLUSTY in order to provide a 3D NLTE RT code.

- [Hauschildt and Baron \(2014\)](#) The 3D version of Phoenix is using a long-characteristics scheme and has been parallelised using the MPI library making it the most scalable code at the time. The conclusion in this paper is that there are many mature 3D NLTE RT codes, but too few realistic 3D RHD simulations and high resolution observations to test them on.
- [Janett et al. \(2019\)](#): A novel fourth-order WENO interpolation technique. A possible new tool designed for radiative transfer; discussion of advantages r.t. Hermite and other more sophisticated approaches.

8 Main results and applications

8.1 Physical domains and 3D NLTE codes

We begin with summarising the physical conditions, that correspond to atmospheres of different astronomical objects, in which 3D geometry and/or NLTE radiation effects become relevant in Fig. 28. With this figure, we are responding (indirectly) to the critical comment by [Ivanov \(1979\)](#) made in response to the textbook on Stellar Atmospheres by [Mihalas et al. \(1978\)](#). Precisely, the comment by [Ivanov \(1979\)](#) is:

Even the most diligent student will, after working through Mihalas’s book, remain fully in the dark about the chemical composition of stellar atmospheres and the accuracy with which it has been determined, as well as the diverse range of problems which astrophysics today links with differences in the composition of stellar atmospheres. Moreover, he (NB: she) will not even gain an idea of what order of magnitude the density is in the atmospheres of various types of stars: [...] Mihalas [...] has not thought it necessary to provide his readers with numerical data on how temperature and density are distributed with depth in the atmospheres of various stars.

Therefore in this paper, we provide such an overview of physical conditions, but we include also other systems, which are better aligned with the landscape of modern astronomy and astrophysics research.

This figure shows the gas density versus gas temperature in different domains, including the atmospheres of hot O-type (TLUSTY OSTAR2002 model with $T_{\text{eff}} = 55\,000$ K, $\log g = 4.0$, and solar Z from [Lanz and Hubeny 2003](#)) and cool G- and M-type (the Sun, red supergiant Betelgeuse) stars, the expanding atmosphere of a high-energy lanthanide-rich kilonova for two different epochs (5 and 20 days after the merger of two neutron stars, from [Pognan et al. 2023](#), $Y_e = 0.15$ and $M_{\text{ej}} = 0.05 M_{\odot}$), the atmospheres of an exoplanet (hot Jupiter, (c) Paul Molliere, $T_{\text{eff}} = 2200$ K³, $\log g = 3.00$, and solar metallicity Z) and of the Earth (the standard ISA 1976 model), and — for comparison — the parameter space probed by an AGN torus from [Matsumoto et al. \(2023\)](#) based on ([Wada et al. 2016](#)), where NLTE effects are common and have to be included in line transfer. For guidance, we also show the parameter space covered by the interior structure of the Sun (model adopted from [Herrera and Serenelli 2023](#)

³Here, the T_{eff} of the planet refers to the following definition $T_{\text{eff}} = (T_{\text{int}}^4 + T_{\text{equilibrium}}^4)^{1/4}$, where $T_{\text{equilibrium}}$ is the temperature of a body (here the exoplanet), which is in a radiative equilibrium given the external radiation (stellar radiation) and its internal heat (planet emission).

Table 2 3D and/or NLTE studies of elements in different astrophysical regimes. For stellar conditions, only papers, where NLTE model atoms or comprehensive multi-element NLTE modelling is presented are listed below. We do not distinguish here between 1D NLTE, 1.5D NLTE, or 3D NLTE, but when all kinds of results are available, we give a preference to the latter (3D NLTE) obtained with comprehensive micro-physics and atomic/molecular models.

Element, ion	Applications	NLTE (ref)
<i>Stars</i>		
Li I	cosmology, Spite plateau	Wang et al. (2021)
C (C I)	Sun, star-planet connection	Amarsi et al. (2019a)
C (CH)	Sun, red giants	Popa et al. (2023)
N I	[C/N] ratio, CNO cycle and the RGB	Amarsi et al. (2020a)
O I	standard solar model, interior	Amarsi et al. (2018) ; Bergemann et al. (2021)
Na I	globular clusters, multiple populations	Bergemann et al. (2017)
Mg I,II	α -enhancement proxy for stars	Nordlander and Lind (2017)
Al I	globular clusters, anomalies	Amarsi et al. (2018)
Fe I,II	metallicity proxy for stars	Bergemann et al. (2019)
Mn I, II	Fe-peak, SN Ia progenitors	Gallagher et al. (2020)
Ba II	s-process, 1st-peak	Storm et al. (2024)
Y I, II	s-process, 1st-peak	Storm et al. (2024)
Eu II	r-process	Storm et al. (2024)
<i>Exoplanets</i>		
H α	dynamics	Fossati et al. (2023)
He I	1083 nm, atmospheric escape	Oklopčić and Hirata (2018) ; Young et al. (2020)
Na I	Na D (589 nm), winds, clouds	Barman et al. (2002) ; Fisher and Heng (2019) ; Canocchi et al. (2024)
K I	atmospheres	Canocchi et al. (2024)
Ca II	850 nm, heating, dynamics	Deibert et al. (2021)
Mg I,II	285,280 nm, opacity	Young et al. (2020)
Mg I, Fe I, II	broad-band, atmospheric heating	Fossati et al. (2021) ; Young et al. (2024)
<i>Kilonovae</i>		
He I	1.08 μ m, spectral modelling, LC evolution	Tarumi et al. (2023)
Sr II	1.037 μ m, r-process nucleosynthesis	Perego et al. (2022)
Ce II, Pt III	opacity	Pognan et al. (2022b)

based on the calculations of [Vinyoles et al. 2017](#)). The distinction between different NLTE domains is based on reported published evidence of the sensitivity of different species (ions, atoms, molecules, dust) to NLTE effects.

The physical basis of 3D and NLTE effects on radiation transfer is described in detail in subsequent sessions, which discuss the recent literature addressing the topic.

8.2 Overview of NLTE effects

In the astronomical literature, it has become common to refer to the qualitative influence of NLTE on line profiles as NLTE effects, whereas the quantitative influence that can be quantified via the effect of the departures from LTE on the line EW or the

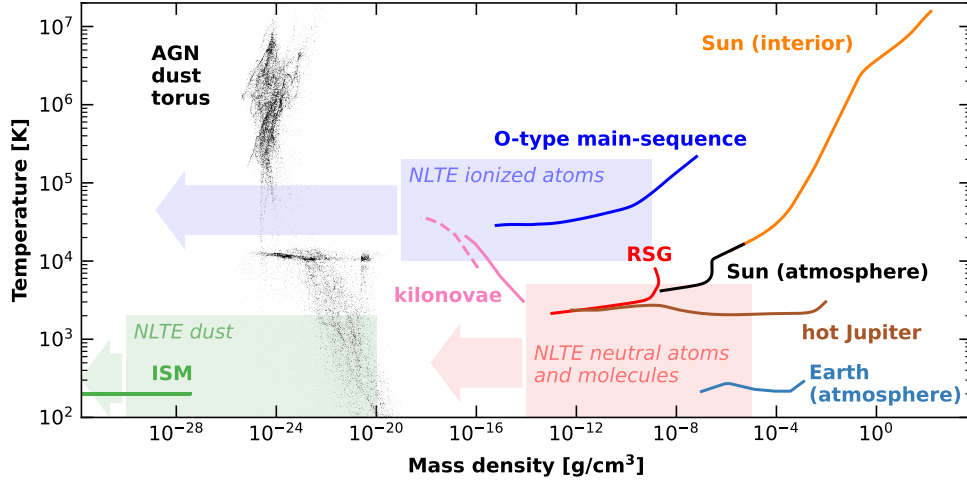


Fig. 28 Gas density versus gas temperature in different astrophysical domains. See text.

chemical abundance of an element derived from a given line is referred to as “NLTE abundance correction”. In what follows, we first briefly address the physical mechanisms behind NLTE effects in stellar atmosphere. An overview of Non-LTE effects in spectral lines can be found in [Asplund \(2005\)](#), [Bergemann and Nordlander \(2014\)](#), and [Lind and Amarsi \(2024\)](#) for cool stars. We note that such classification has not been adopted in other areas of research, e.g., in exoplanet research or kilonovae. Spectra of the latter objects are vastly more complex, as all absorption and emission features overlap and hence individual de-compositions into atomic and molecular diagnostic features caused by transitions in individual chemical species are difficult.

Generally, since the NLTE conditions are driven by the radiation field, the effects are generally larger in physical conditions that lead to stronger, that is, more intense, radiation fields. These are the conditions in hotter stars (F-type), more metal-poor stars, or stars with lower density rarefied atmospheres (red giants or red supergiants). These conditions are illustrated in Fig. 28. The NLTE effects can be divided into two classes, radiation-driven and collision-driven ([Gehren et al. 2001](#); [Bergemann and Nordlander 2014](#)). In case of radiation-driven species, the NLTE effects are primarily caused by the over-ionisation due to super-thermal radiation, $J_\nu > B_\nu$ (exceeding the Planck function) in the UV ([Rutten 2003](#); [Bergemann et al. 2012c](#)). These conditions are, physically, the consequence of radiation propagation in an RE model atmospheres with no incoming radiation from outside, that is the weighting of the source function by the E1 kernel, which represents the exponential behaviour of the opacity with depth. In the Rayleigh–Jeans regime, where the depth gradient of the source function is steep (for a given radiative equilibrium T gradient), equation 18 leads to $J_\nu > S_\nu$, and thus super-thermal radiation field. In the Wien regime (IR), the gradient of the source function is much shallower (flatter) and $J_\nu < S_\nu$, so the radiation field is sub-thermal. The latter situation favours recombination over over-ionisation.

The type of NLTE effect also depends on the structure of the atom or molecule and on its abundance in the atmosphere. Atoms like, e.g. Mg I, Ca I, Ti I, Mn I, Fe I, Cr I, and Sr I have large ionization cross-sections in the near-UV and blue wavelength regime (a few electron-Volt), and therefore in physical conditions of cool stars are typically over-ionised (e.g. Korn et al. 2003; Gehren et al. 2004; Bergemann et al. 2010; Mashonkina et al. 2011; Bergemann 2011; Bergemann et al. 2012c,b; Lind et al. 2012; Amarsi et al. 2018; Mallinson et al. 2022). The atomic level populations of these neutral ions are thus all systematically smaller compared to LTE populations. A similar process, but acting in bound-bound transitions, is referred to as a super-thermal over-excitation, and this process may also contribute to the depletion of the number densities of low-excitation states in the system.

In contrast, the energy levels system of species like Na I and K I is much less complex (Baumueller and Gehren 1997; Zhao et al. 1998; Baumueller et al. 1998; Mashonkina et al. 2000; Gehren et al. 2004; Zhang et al. 2006; Reggiani et al. 2019; Lind et al. 2022). The NLTE effects in these species are driven by over-recombination coupled with photon losses in the wings of strong spectral lines. Photon loss describes the following microscopic physical process. As energy is redistributed in the spectral line, a fraction of energy is lost through the line wings, which become optically thin in deeper atmospheric layers. As a consequence of this redistribution, some photons from the line core leak and escape through the wings, which leads to brighter (weaker) wings and fainter (stronger) cores in NLTE conditions (see Mashonkina et al. 2000; Gehren et al. 2004, for example). Similar NLTE effects are found for singly-ionised species of trans-Fe-group elements, such as Nd II, Ba II, Sr II, and Eu II (e.g. Mashonkina and Gehren 2000; Mashonkina et al. 2005; Bergemann et al. 2012b; Gallagher et al. 2020; Storm et al. 2024). Finally, certain ions, such as Li I and O I, are mixed-type ions that may behave similar to either collision- or to radiation-driven species, depending on physical conditions or the diagnostic lines under consideration (e.g. Carlsson et al. 1994; Lind et al. 2009; Amarsi et al. 2019b).

In 3D NLTE radiative transfer, the effects are qualitatively similar. Yet, so far, only selected species have been subject to a thorough analysis. In 3D NLTE modelling, overall, the tendency of certain species to be over-ionized is amplified, so that positive NLTE effects on line profiles become even larger. This is due to the prevalence of up-flows over down-flows in 3D convective models. The up-flows are characterised by steeper temperature gradients and thereby enhance the inequality between J_ν and the local value of B_ν . For a more detailed discussion of the differences between 3D NLTE and other approaches, we refer the reader to Sect. 8.5.

8.3 OBA and FGK model structures

Standard calculations of NLTE radiation transfer in the context of stellar atmospheres are currently routinely performed for OB-type stars. Physical conditions of these hot systems with $T_{\text{eff}} \gtrsim 10\,000$ K are such that strong departures from NLTE arise owing to extreme radiation field in the UV, and radiation pressure on lines is also the main driver of stellar winds (e.g. Mihalas and Auer 1970; Auer and Mihalas 1972; Kudritzki and Simon 1978; Kudritzki and Hummer 1990; Kudritzki and Puls 2000). Whereas both self-consistent NLTE calculations for the model structure and spectrum synthesis

have been explored, more recent work progressively relies on a hybrid approach, where LTE and 1D are adopted for structure of the atmospheres, where multi-element NLTE RT is performed for the key diagnostic elements, such as H I, He I and He I, O II, C II and C III, Si III (Nieva and Przybilla 2007, 2012, 2014; Aschenbrenner et al. 2023).

Multiple grids of NLTE model atmospheres and NLTE synthetic spectra for OBA-type stars exist. They are publicly available to the community, including but not limited to the following databases:

- OB-type and early A-type stars: **Fastwind** / WM grid (Puls et al. 2005; Bestenlehner et al. 2024). Following the definition in Puls et al. (2005), the code is to be written *not* in capital letters. This grid covers the domain of T_{eff} in the range from 17.8 to 56.2 kK and $\log g$ from 2 to 4.5, as well as variable He abundance and metallicity;
- early B-type stars: the **Tlusty** grid (Lanz and Hubeny 2007). This grid covers T_{eff} in the range from 15 to 30 kK, $\log g$ from 1.75 to 4.75, and v_{mic} of 2 km s⁻¹;
- O-type **METUJE** (Krtićka and Kubát 2010, 2018);
- hot B- and O-type sub-dwarfs (T_{eff} from 30 to 50 kK, $\log g$ from 4 to 8) (Kudritzki 1976; Przybilla et al. 2006), see also Heber (2009) for an overview of the relevance of NLTE on the surface structure of these stars;
- **Phoenix** Nextgen grid (Hauschildt et al. 1999a,b) for T_{eff} from 2000 to 10 000 and $\log g$ from 0.0 to 5.5 (separate grids for RGB and MS stars, the latter computed using spherically-symmetric radiation transfer);
- A-type - there are no A-type NLTE or 3D grids. Perhaps because there has not been enough motivation for this work, or due to evidence that NLTE effects in A-type stars are not critical and can be ignored (Przybilla et al. 2011).

A comprehensive comparison of OBA type model atmospheres, synthetic energy distributions, and individual spectral lines in LTE and NLTE can be found in Przybilla et al. (2011). This study also found that the structures of LTE and NLTE model atmospheres are very similar for stars with $15\,000 \lesssim T_{\text{eff}} \lesssim 35\,000$, including both dwarfs and giants. This justifies the use of the hybrid approach (LTE atmospheres, NLTE line profiles) in spectral diagnostics of B to late-O type stars. A rather novel approach in massive star atmosphere modeling is to use insights from full 3D simulations to improve the structure of 1D HE atmosphere models. This was done, for example, in González-Torà et al. (2025).

NLTE calculations of stellar model atmospheres for cool late-type (FGKM-type) stars are considerably more complex, owing to a gigantic number (over 500 millions, Hauschildt et al. 1999b) of absorption lines due to line transitions in neutral atoms and molecules across the entire spectrum from the UV to the IR. So far, these calculations have been carried out using the 1D hydrostatic version of the **Phoenix** model atmosphere code, yet with treating the line blanketing with comprehensive atomic and molecular databases, and including the effect of NLTE on the atmospheric structure through changes in the radiative heating and cooling (Hauschildt et al. 1997). For the Sun, the effects of NLTE the model atmosphere structure are marginal and do not exceed about 20 K in the outer layers relevant for line formation (Short and Hauschildt 2005). The study by Haberreiter et al. (2008) took a step further and explored the impact of NLTE on the SEDs and fluxes of the Sun. They showed that using NLTE

opacity distribution functions in the calculations of the solar model atmosphere has a noticeable effect at only far-UV wavelengths shorter than 260 nm (their Fig. 7), although, they did not compare the fluxes computed self-consistently with LTE and NLTE opacity distribution functions. Their calculations also included NLTE effects in H^- continuum opacity. Other studies of NLTE effects on the H^- include [Shapiro et al. \(2010\)](#) and in [Barklem and Amarsi \(2024\)](#). These analyses suggest that the effects for FGKM-type stars are small, at a sub-percent level, although may become more important in the outer layers of the atmospheres of warm and low gravity stars, $\log g \lesssim 2$ and $T_{\text{eff}} \gtrsim 6000$ K ([Barklem and Amarsi 2024](#), their Fig. 7). [Young and Short \(2014\)](#) investigated NLTE model atmospheres for red giants. Also, their work shows that NLTE effects influence the spectral energy distribution in stars with T_{eff} greater than 4000 K only below 400 nm.

8.4 Cool stars: fundamental parameters

The analysis of stellar parameters has so far been primarily limited to 1D models with NLTE included for selected chemical elements, such as Fe (e.g. [Bergemann et al. 2012c](#); [Ruchti et al. 2013](#); [Kovalev et al. 2019](#)), Mg ([Kovalev et al. 2019](#)), and H ([Mashonkina et al. 2008](#); [Amarsi et al. 2018](#), e.g.). Recent studies also addressed the influence of 3D NLTE in the formation of the optical H lines, specifically, H_α and H_β finding non-negligible effects in the line wings and in the cores. This may influence the determination of T_{eff} from the Balmer line wings, e.g. [Giribaldi et al. \(2021\)](#) showed that the effective temperatures derived using 3D NLTE line profiles of H lines tend to be larger, by up to 300 K at low metallicity, $[\text{Fe}/\text{H}] \approx -2$, compared to 1D LTE values. Similar effects are found in 1D NLTE calculations ([Kovalev et al. 2019](#)).

Comparative analyses of the bulk influence of NLTE on synthetic stellar spectra were presented, e.g. in [Bialek et al. \(2020\)](#), who reported a substantial improvement of the estimates of T_{eff} , $\log g$, and metallicity values obtained in NLTE compared to model-independent estimates obtained using the methods of interferometry and/or asteroseismology. Overall, however, substantial differences between 1D and 3D synthetic spectra are expected for different types of stars, and for different wavelength regimes. In Figs. 29 and 30 we compare synthetic spectra computed using 1D hydrostatic and 3D hydrodynamic model atmospheres in the APOGEE H-band window (1.5 to 1.7 μm). Clearly, the difference in the spectral lines are systematic and ubiquitous across the entire 200 nm wavelength range, necessitating 3D RT calculations with RHD models from first principles.

Estimates of 1D and 3D NLTE abundance corrections for the diagnostic lines of Fe I and Fe II are available in different studies and a comprehensive review of those can be found in [Lind and Amarsi \(2024\)](#). Here we only briefly summarise the main effect and demonstrate how these influence stellar metallicities derived from stars of different Galactic populations. For main-sequence stars, the 1D NLTE corrections for Fe I and Fe II lines typically do not exceed +0.02 to 0.15 dex, at least within the $[\text{Fe}/\text{H}]$ range from -3 to solar ([Lind et al. 2012](#); [Ruchti et al. 2013](#); [Kovalev et al. 2019](#); [Larsen et al. 2022](#)). In comparison, 3D NLTE abundance corrections for Fe I lines are of the order -0.2 dex to 0.15 dex for unevolved (main-sequence) stars ([Amarsi et al. 2022](#), their Fig.4, here inverted sign as they adopted the convention of 1D LTE-3D NLTE) at

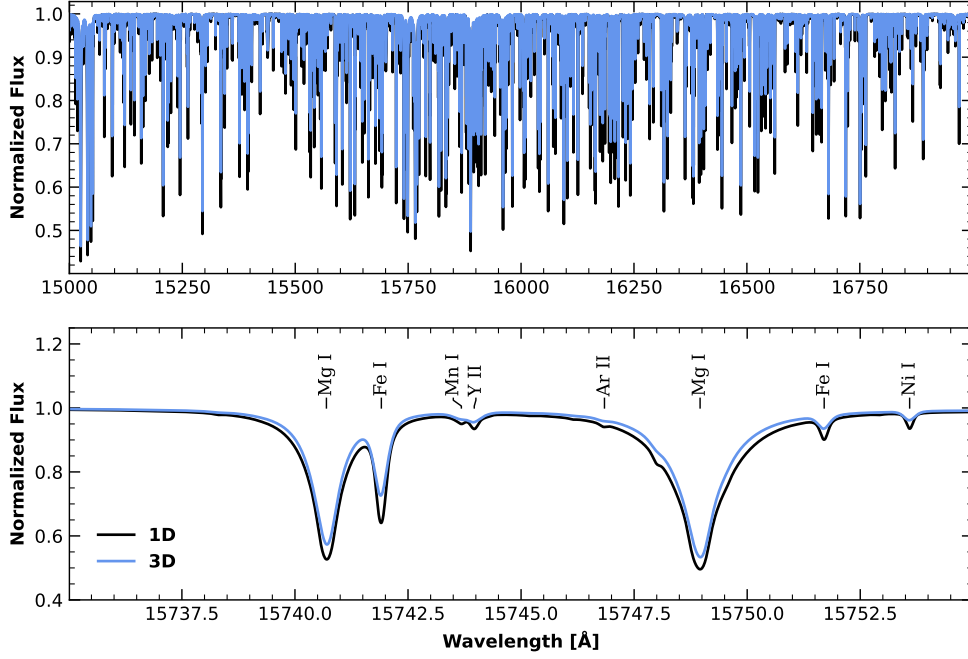


Fig. 29 APOGEE spectral range modelled using a 1D solar MARCS model and a 3D STAGGER snapshot.

solar metallicity. However, for metal-poor ($[\text{Fe}/\text{H}] = -3$) main-sequence and TO stars, the 3D NLTE corrections may exceed 0.5 dex (Amarsi et al. 2022). The lines of Fe II, although not particularly affected by NLTE (Lind et al. 2012), are rather sensitive to the structure of the atmospheric models, especially the horizontal inhomogeneities of temperature and density. Recent detailed estimates, suggest effects of the order 0.05 to 0.15 for weaker Fe II lines (with reduced $\log EW/\lambda$ of $\lesssim 5$), but for stronger Fe II features the 3D NLTE may be both positive and negative. The biases depend, however, on the atomic properties of the line, primarily on the excitation potential and transition probability, and on stellar parameters. For red giants, the effects of 3D NLTE on the Fe I lines are more substantial, at the level of ~ 0.5 dex, at least at very low metallicities $[\text{Fe}/\text{H}] \lesssim -4$ (Lagae et al. 2023). For such stars, however, also 1D NLTE calculations yield comprehensive values of abundances: at $[\text{Fe}/\text{H}]$ of ~ -2.5 , for example, the NLTE abundance corrections for RGB stars reach up to 0.3 dex (Kovalev et al. 2019).

8.5 Cool stars: abundances

Very substantial and tedious work has been carried out already regarding 1D NLTE calculations for vast majority of elements up to and including the post-Fe-group elements (see also Mashonkina 2014, for an overview). This includes the light species (H, He, Li), CNO, α -elements, and Fe-group. We collate these studies in Table 2. Some

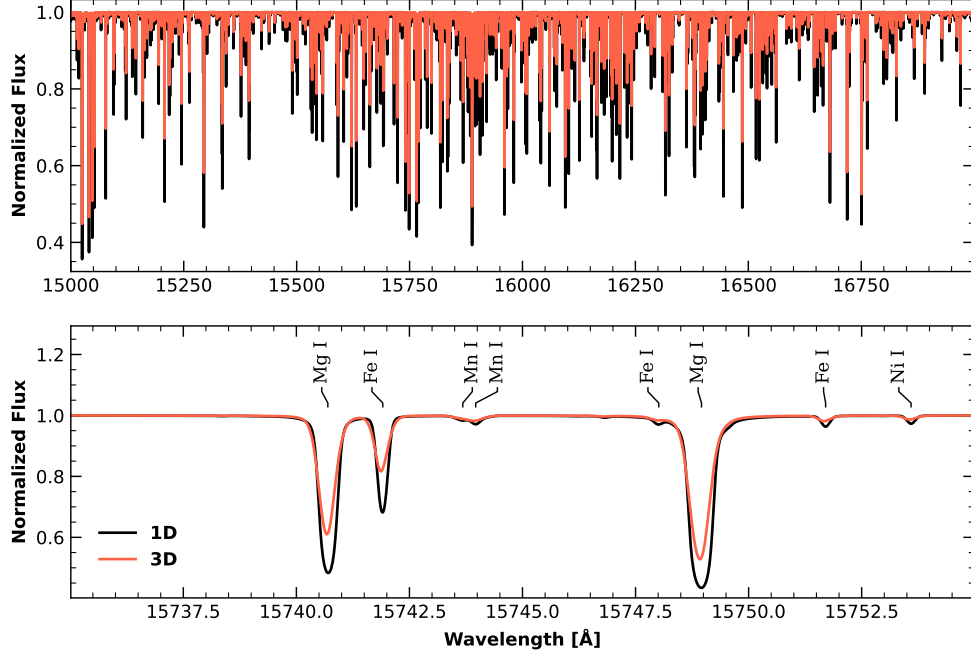


Fig. 30 APOGEE spectral range modelled using a 1D red giant MARCS model ($T_{\text{eff}}=4500$, $\log(g)=2.0$, $[\text{Fe}/\text{H}]=-1.0$) and a 3D STAGGER snapshot.

NLTE abundance corrections computed with 1D and 3D NLTE codes are further presented in Figs. 31 and 32.

For trans-Fe group elements, selected estimates of NLTE effects are available for the 1-st peak s-process elements Rb, Sr, Y, Zr (Korotin 2020; Mashonkina et al. 2007; Bergemann et al. 2012a; Storm and Bergemann 2023; Storm et al. 2024; Velichko et al. 2010), 2nd-peak elements Ba and Pr (Mashonkina and Gehren 2000; Mashonkina et al. 2009), and selected r-process species Eu, Gd, and Nd (Mashonkina 2000; Mashonkina et al. 2005; Storm et al. 2024, 2025). Also estimates of NLTE effects for the heaviest elements of the actinide series (Pb, Th) are available (Mashonkina et al. 2012).

Regarding full 3D NLTE, much of the early work focussed on chemical elements, for which rather simple model atoms (a few tens of energy states) can be used to derive astrophysically relevant results. These, specifically, addressed line formation of Li I (Barklem et al. 2003; Cayrel et al. 2007), O I (Asplund et al. 2004), and H I (Pereira et al. 2013). More recently more complex 3D NLTE calculations for astrophysically relevant atomic lines of Fe-group and trans-Fe neutral elements became possible. As a consequence, estimates of 3D NLTE effects on abundances are now available for the following atoms: H (Amarsi et al. 2018), Li (Wang et al. 2021), C (Amarsi et al. 2019a), N (Amarsi et al. 2020a), O (e.g. Amarsi et al. 2016; Bergemann et al. 2021), Na (Asplund et al. 2021), Mg (Bergemann et al. 2017; Asplund et al. 2021), Al (Nordlander and Lind 2017), Si (Amarsi and Asplund 2017; Asplund et al. 2021), K (Reggiani et al.

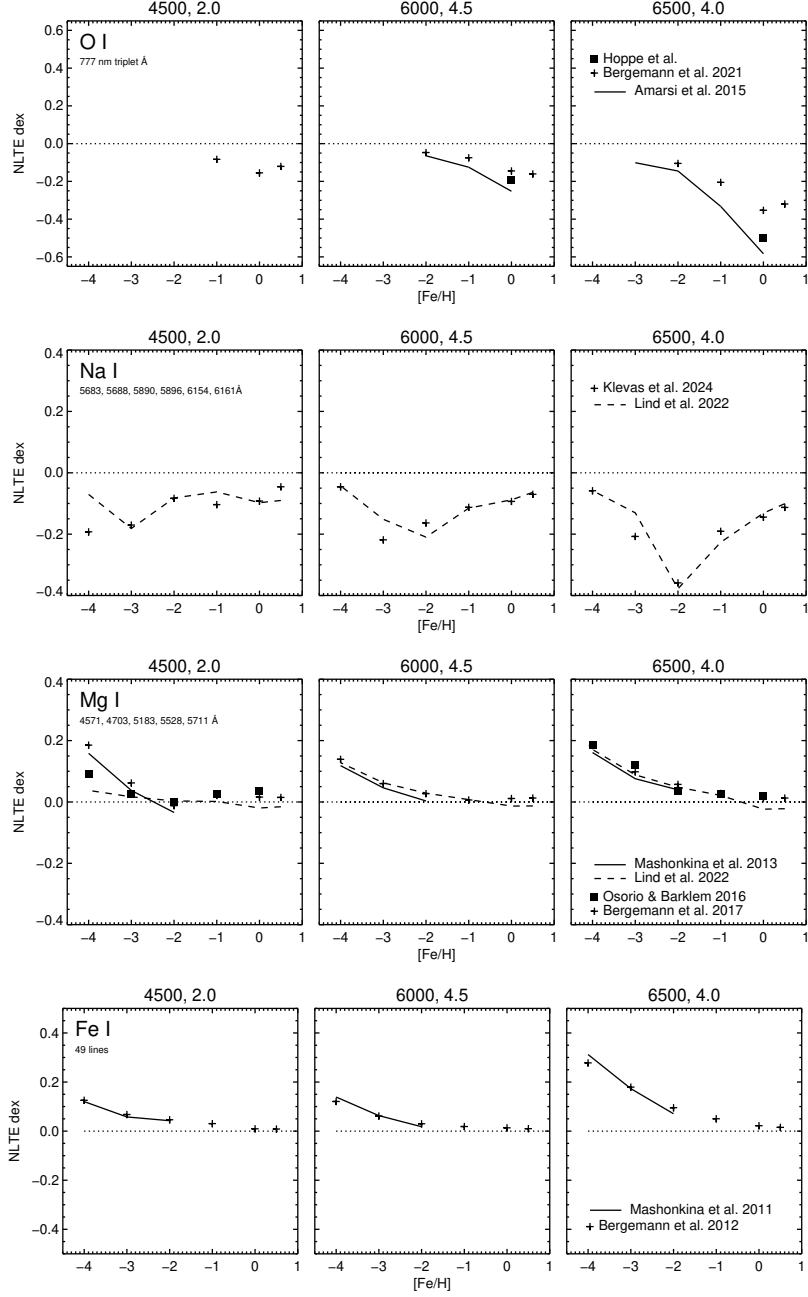


Fig. 31 NLTE effects on abundances of different chemical elements, including O, Mg, Fe, Mn, Sr, Y, and Eu, computed with 1D and 3D hydro-dynamical model atmospheres. See text. The figure highlights that overall the agreement between different independent calculations, based on different model atmospheres, atomic models, and NLTE RT codes (1D and 3D), is excellent. Hence the NLTE effects can be trusted.

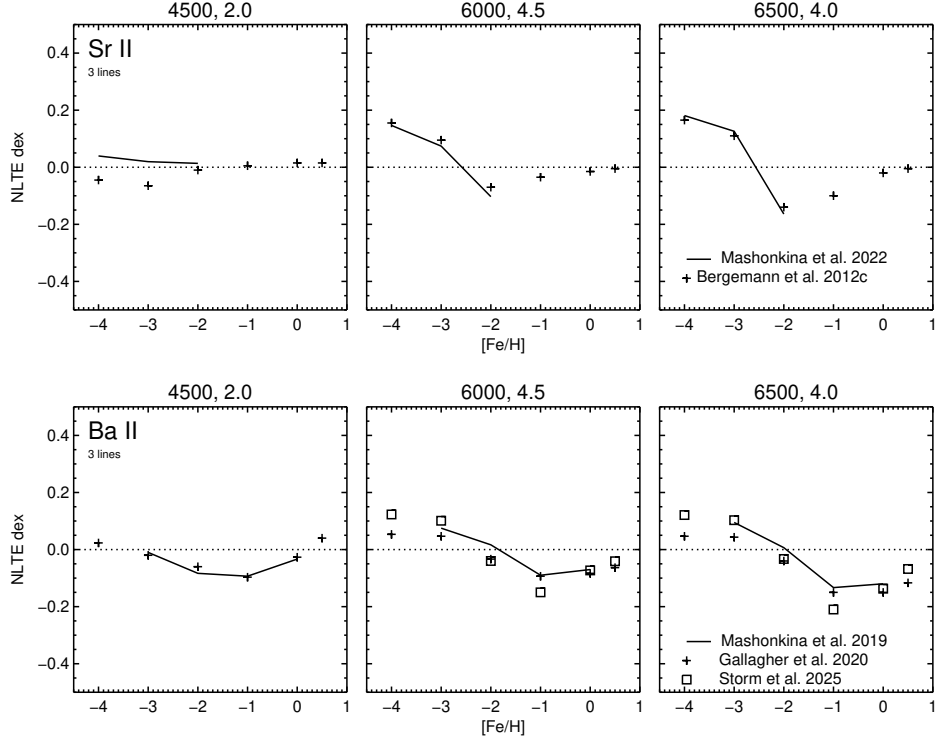


Fig. 32 NLTE effects on abundances of different chemical elements, including Sr, Ba, and Eu, computed with 1D and 3D hydro-dynamical model atmospheres. The label insets are as follows. Crosses: Sr II results based on the model atom from (Bergemann et al. 2012b) updated to QM collisional data in Gerber et al. (2023), computed using MARCS and MULTI2.3. Solid line: NLTE Sr II results from Mashonkina et al. (2022) computed using MAFAGS-OS models and DETAIL. For Ba, the NLTE results computed using the model atom from Gallagher et al. (2020) (MULTI and Turbospectrum) and Mashonkina and Belyaev (2019) (DETAIL and SIU) are presented.

2019), Ca (Asplund et al. 2021; Lagae et al. 2023), Fe (Amarsi et al. 2016; Lind et al. 2017), Mn (Bergemann et al. 2019), Ba (Gallagher et al. 2020), Y (Storm et al. 2024), and Eu (Storm et al. 2024). These studies are typically performed for a small sample of stars with high-quality astrophysical parameters inferred by independent techniques. All these calculations, with a few exceptions, were carried out under the trace element assumption. Also grids of 3D NLTE abundance corrections for selected elements were computed by some groups (e.g. Amarsi et al. 2020b; Storm et al. 2025). In Fig. 33 we show the resulting line profiles for selected chemical elements computed using 1D LTE, 1D NLTE, and 3D NLTE. The corresponding differences in abundance diagnostics are gigantic, and may exceed a factor of 3. The resulting difference in chemical abundances inferred using 1D and 3D NLTE models are furthermore demonstrated in Fig. 34.

Osorio et al. (2020) explored simultaneous multi-element NLTE RT using the *Tlusty* code. They find that the influence of cross-talk of radiation field is very modest,

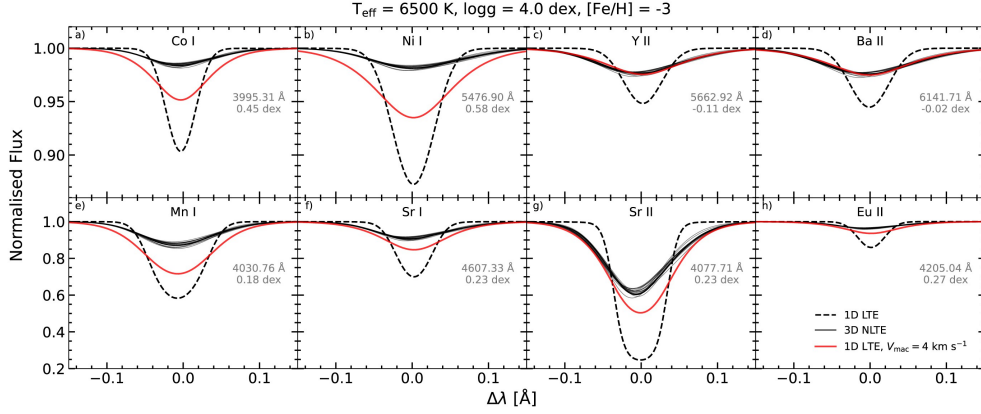


Fig. 33 Figure illustrates the theoretical line profiles computed using 1D LTE and 3D NLTE models using the parameters of a very metal-poor turn-off star with metallicity $[\text{Fe}/\text{H}] = -3$. The same abundances were used. Note that major differences between 3D NLTE and 1D in line profiles for iron-group elements, Co I, Ni I, and Mn I, with 1D LTE over-estimating the line strength and EW by over a factor of two. As a result, the abundances of Co and Ni ($[\text{Co}/\text{Fe}]$ and $[\text{Ni}/\text{Fe}]$) may be erroneous by over 0.5 dex (a factor of 3, panels a and b). Image reproduced with permission from Storm et al. (2025), copyright by ESO.

typically not exceeding 0.01 dex in the abundance space, that is the effects are within (and even significantly smaller) than the physical quality of sub-grid microphysics, for example, cross-sections describing inelastic collisions with hydrogen (Bergemann et al. 2019). However, there are physical conditions, such as metal-poor red giants, where coupling between the radiation field in lines of *different* chemical species becomes important. These are, for example the impact of NLTE on populations involved in formation of the key O I lines through the NLTE radiation in Ly β (Dupree et al. 2016).

8.6 Databases

Public NLTE databases can be used to calculate 1D and 3D NLTE abundance corrections for the key diagnostic elements:

- <https://www.inspect-stars.com/> hosted by University of Stockholm. NLTE corrections are available for Li I, O I, Na I, Mg I, Ti I, Ti II, Fe I, Fe II;
- <https://nlte.mpia.de/> hosted by the Max Planck Institute for Astronomy, Heidelberg. This database offers NLTE corrections for H I, O I, Mg I, Si I, Ca I, Ca II, Ti I, Ti II, Cr I, Mn I, Fe I, Fe II, and Co I;
- <https://spectrum.inasan.ru/nLTE2/> hosted by the Institute for Astronomy of the RAS. This database offers NLTE corrections for Ba II, Ca I, Ca II, Fe I, Mg I, Na I, Sr II, Ti II, Zn I and Zn II.
- NLTE corrections computed withing the ChETEC project <https://www.chetec-infra.eu/3dnlte/abundance-corrections/strontium/> and <https://www.chetec-infra.eu/3dnlte/abundance-corrections/barium/>

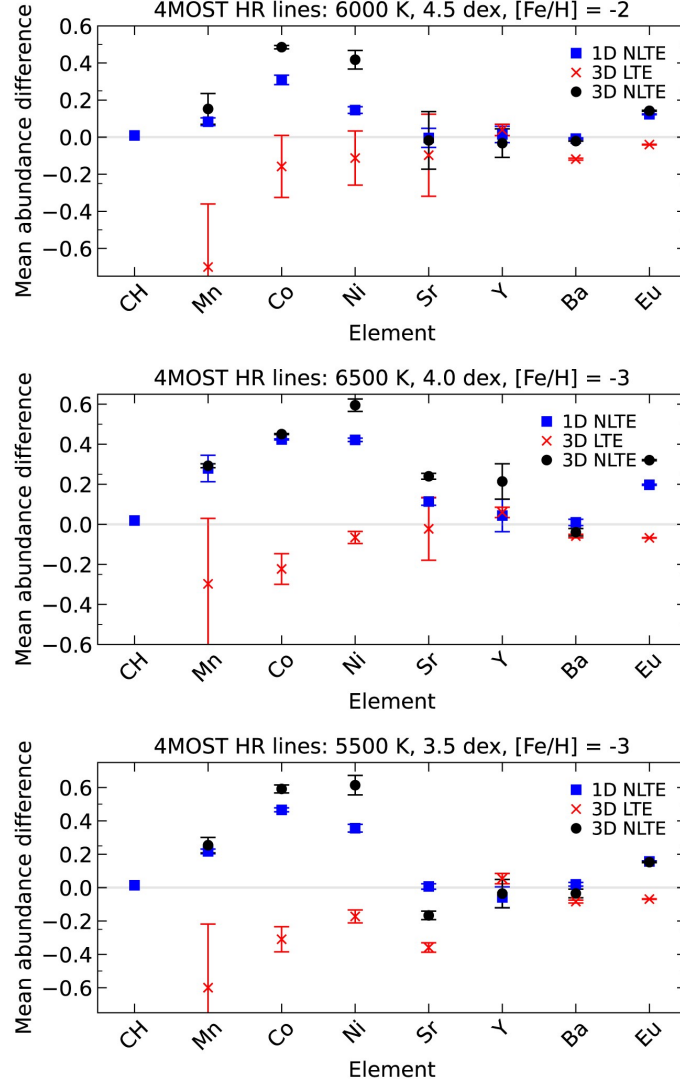


Fig. 34 3D NLTE abundance corrections for different chemical elements computed using very metal-poor 3D model atmospheres, as indicated in the figure titles. Image reproduced with permission from [Storm et al. \(2025\)](#), copyright by ESO.

8.7 M dwarfs and pulsating stars

For M dwarfs and other types of stars, such as Cepheids and RR Lyr, only very limited knowledge of impact of 3D and NLTE effects on structure and diagnostics is available.

Selected studies of statistical equilibrium were carried out for M dwarfs by [Hauschildt et al. \(1997\)](#) on Ti I and by [Schweitzer et al. \(2000\)](#) on CO. For Cepheids, preliminary work on NLTE abundances was carried out using the DETAIL code by

Przybilla et al. (2021) in 1D, and in 2D NLTE by (Vasilyev et al. 2019). The latter study, in particular, found that using 2D pulsating models of Cepheids in combination with NLTE RT for oxygen leads to large impact on oxygen abundance. For the O I triplet lines, in particular, the 2D RHD models with 3- and 9-day pulsation periods yield oxygen abundances lower by up to -1 to -0.25 dex depending on phase, compared to results obtained using standard 1D LTE hydrostatic models. The large order of magnitude difference is particularly prominent for the low- $\log(g)$ model (P9), at the phases of maximum contraction ($\phi = 0.8 \dots 1.2$), when T_{eff} is the range $\sim 6200 - 6700$ K and $1.4 \lesssim \log g \lesssim 2.0$. The effect is primarily due to extremely strong over-population of the O I lower energy states due to photon losses in the lines.

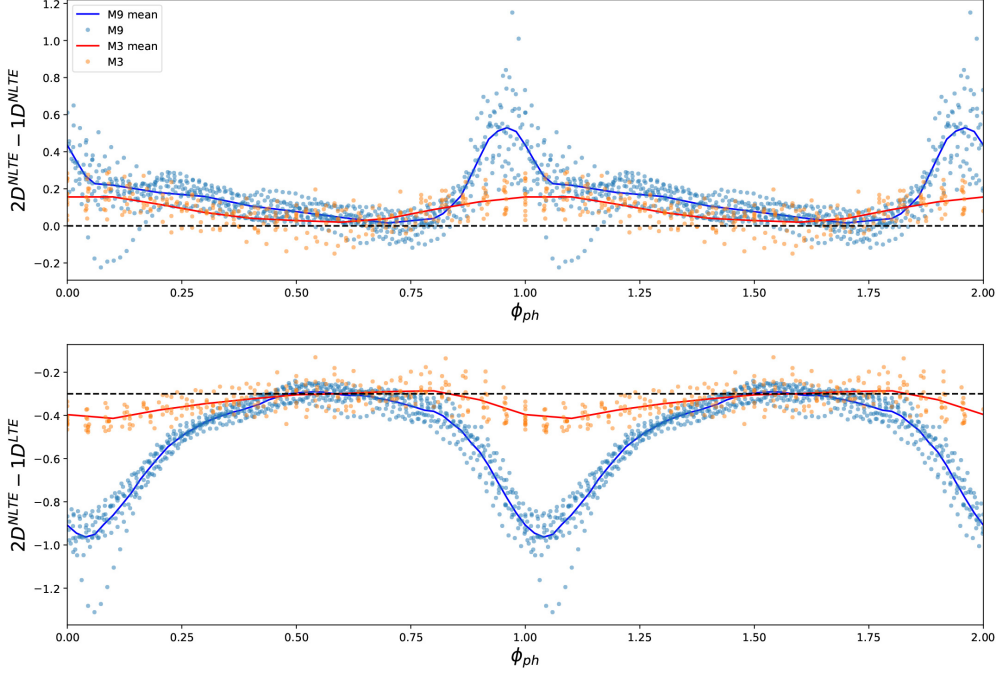


Fig. 35 Figure illustrates the impact of 2D NLTE effects on the analysis of oxygen (O I) abundances from multi-phase spectra of Cepheids. Here two solar-metallicity pulsation-convective RHD models with the pulsation periods of 3 days ($T_{\text{eff}} = 5600$ K, $\log g = 2.0$) and 9 days ($T_{\text{eff}} = 5600$ K, $\log g = 1.5$) are shown, respectively. Image reproduced with permission from Vasilyev et al. (2019), copyright by ESO.

It remains to be explored, with 2D and 3D RHD convective-pulsating model atmospheres, whether similarly large NLTE effects influence the chemical abundance diagnostics of spectra of variable stars.

8.8 Exoplanets

This section is truly inspired by the following statement (Ornes 2017)

“One of the biggest surprises is that driving a system far from equilibrium doesn’t just lead to turbulence. It leads to structure, and the most fascinating one is life.”

Physical conditions in exoplanet atmospheres favour substantial NLTE effects, owing to low gas densities of less than 10^{-7} g cm $^{-3}$ (Fig. 28). Yet at lower gas temperatures, and with an additional source of irradiation from the host star, NLTE conditions are primarily limited to lines of neutral atoms and molecules. We note that in the context of exoplanet atmosphere work, NLTE may have entirely different meaning, depending on the literature source. Here we use the more inclusive definition, which covers different type of NLTE. On the one extreme, there is the very approximate semi-empirical NLTE modelling (Treanor et al. 1968), in which, e.g., population numbers of rotational and vibrational energy states are set by the product of Boltzmann distributions for several temperature values, one of them the kinetic temperature (set to be, T_{rot} for rotational states) and the other being the vibrational temperature, also known as the adjustable “NLTE” parameter, see e.g. (Wright et al. 2022). On the side of more comprehensive physically-based investigations, there are also models that solve coupled RT and SE equations and include a range of atomic and/or molecular processes, such as photo-ionization, ionization by free electrons, charge transfer with H and other atoms and ions (Yelle 2004; Koskinen et al. 2013).

So far, the focus of dedicated NLTE studies (e.g., Barman et al. 2002; Young et al. 2020; Deibert et al. 2021; Fossati et al. 2021, 2023) has been primarily on hot exoplanet environments, with characteristic temperatures higher than 2000 K, and only limited knowledge of conditions in cooler atmospheres is available. In this context, perhaps the only planet that has been extensively studied by means of NLTE calculations is Earth atmosphere (see von Clarmann et al. 2002; Lopez-Puertas and Taylor 2001, and references therein). To a lesser extent, NLTE methods were applied in spectroscopic diagnostics of the atmosphere of Mars (e.g. Read et al. 2015, and references therein) and Titan (Yelle 1991; López-Puertas et al. 2013).

The earliest NLTE studies can be traced back to Appleby (1990) (CH $_4$), Seager and Sasselov (2000) (He), and Barman et al. (2002) (Na). The former study performed NLTE calculations for the He I triplet line at 1083 nm employing the methods developed for Cepheid atmospheres (Sasselov and Lester 1994). The latter focussed on the effects of NLTE in the key diagnostic doublet lines of Na D at 589 nm in atmospheric conditions of a gas giant HD 209458 b. This study, in particular, went into a great detail what concerns the origin of NLTE effects, behaviour of the level departure coefficients, and the influence of collision rates on the NLTE results. The paper is also relevant, as the work that highlighted that even a qualitative interpretation of exoplanet spectra may change depending on physics of NLTE, e.g. misinterpreting the weakness of the Na D feature for low metallicity or presence of high-altitude clouds (Barman et al. 2002).

Over the past years, NLTE RT calculations have become more common and have since been applied to modelling the atmospheric structure and/or diagnostic spectroscopy of warm and hot Neptunes (Kubyskhina et al. 2024), hot and ultra-hot Jupiters Kelt-9 b, Kelt-20 b (Fossati et al. 2021; Borsa et al. 2021; Fossati et al. 2023), HD 209458 b (Oklopčić and Hirata 2018; Lampón et al. 2020; Young et al. 2020), WASP-12 b and WASP-76 b (Wright et al. 2022), WASP-33 b (Wright et al.

2023), WASP-121 b (Young et al. 2024), sub-Neptunes (García Muñoz et al. 2024), and Neptunes (Oklopčić and Hirata 2018). The findings cannot be yet generalised to all conditions relevant to planet atmospheres, as only targeted investigations for individuals models and/or ions are available, and no systematic study across the entire parameter space has been performed. Also, in terms of observations and detection of NLTE effects in exoplanet transmission spectra, one source of complexity is the degeneracy with amount of stellar light blocked by the planet, but also the still poorly understood effects of hydrodynamic outflows (Hoeijmakers et al. 2020). Nonetheless, from the theoretical perspective, the evidence is as follows. Large and negative NLTE effects were reported for similar systems in many others species, including the O I 777 nm triplet (Borsa et al. 2021), H_α lines (Fossati et al. 2021), 1083 nm He I line (Oklopčić and Hirata 2018; Young et al. 2020), and in the strong UV Mg I and Mg II lines at 2852.12 and 2802.7 Å (Young et al. 2020), respectively. For H I lines, we show the results obtained for Kelt-9b in Fig. 36.

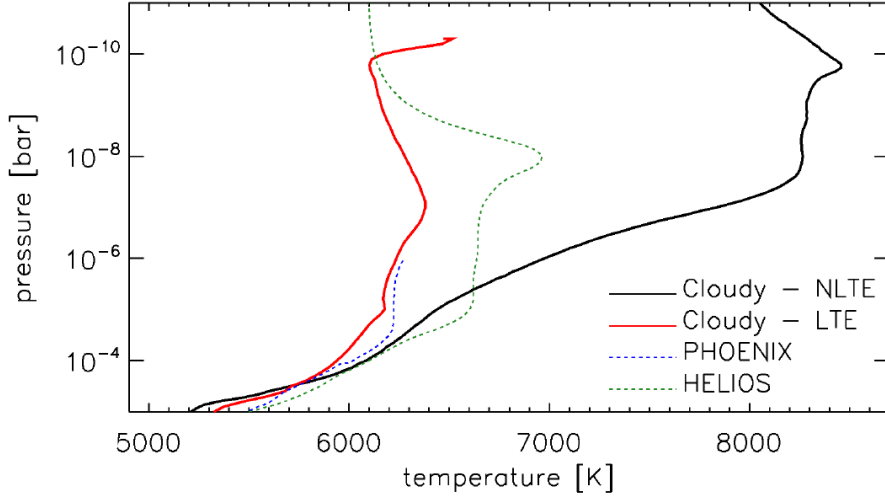


Fig. 36 NLTE and LTE calculations of transmission spectra in the region of hydrogen H_α and H_β lines in the atmosphere of a hot Jupiter Kelt-9b, compared with the observed data. Image reproduced with permission from Fossati et al. (2021), copyright by the author(s).

The NLTE results for diagnostic spectral lines in exoplanet atmospheres are qualitatively similar to NLTE effects reported for FGK-type stars (see Sect. 8.5). In this context, negative NLTE effects imply stronger NLTE absorption features, thus, lower abundances compared to LTE diagnostics. The Na D doublet at 589 nm shows weaker wings, but stronger cores in NLTE (Fisher and Heng 2019; Young et al. 2020), which is, however, opposite to the findings by Barman et al. (2002). The latter work explored irradiated and non-irradiated profiles of the atmospheric structure of HD 209458 b, taking into account collisions with free electrons and molecular hydrogen H_2 , but in both cases their NLTE profiles of the resonance Na D lines were systematically weaker compared to LTE predictions, and even fully reverted to emission when collisions with

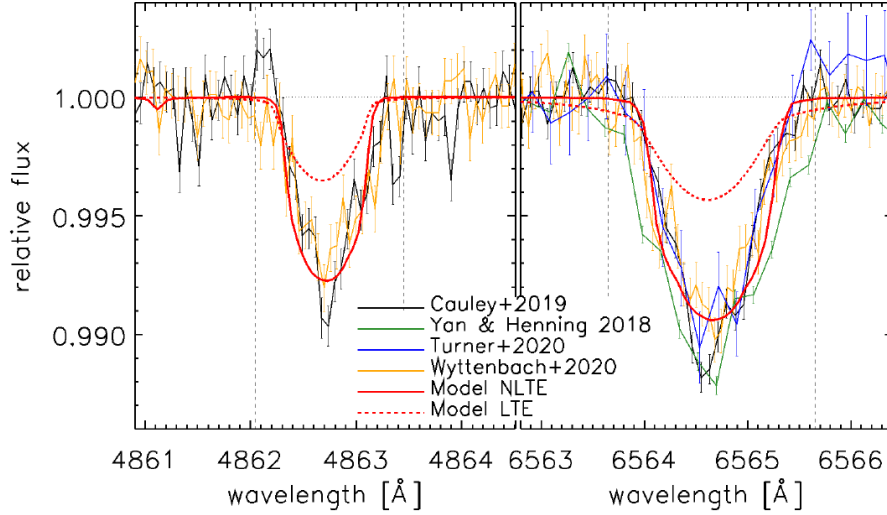


Fig. 37 NLTE and LTE calculations of the atmospheric structure of hot Jupiter Kelt-9b. Image reproduced with permission from [Fossati et al. \(2021\)](#), copyright by the author(s).

H_2 were neglected. Hence according to [Barman et al. \(2002\)](#) work, Na abundance in exoplanet atmospheres is substantially underestimated.

Studies of NLTE or non-equilibrium effects in molecules are currently rather scarce. Among the first, [Swain et al. \(2010\)](#) proposed the possibility of NLTE emission from the methane ν_3 band in the atmosphere of a hot Jupiter HD 189733 b. The relationship between this feature and its possible NLTE origin were further explored in [Waldmann et al. \(2012\)](#). We note, however, that several other studies ([Mandell et al. 2011](#); [Birkby et al. 2013](#)) did not confirm the emission using high-resolution observations of the planet with NIRSPEC and CRIRES, and instead link the signal at $3.25 \mu\text{m}$ to tellurics, specifically to the ν_2 band of the Earth's water vapour. Non-equilibrium chemistry was investigated by means of detailed photo-chemistry calculations in different studies (e.g. [Stevenson et al. 2010](#); [Madhusudhan and Seager 2011](#); [Moses et al. 2011](#); [Knutson et al. 2012](#); [Moses et al. 2013](#); [Baeyens et al. 2024](#)). Photo-chemistry is driven by the radiation field, but also advection (that is, the transport-induced processes) may further have a substantial impact on the population numbers of molecules and, hence, on the composition and structure of atmospheres.

The question typically asked is what is the impact of NLTE on the structure of models. First estimates suggest that the outer thermodynamic structure of hot Jupiters is highly sensitive to the effect of photo-ionization by the stellar radiation. The classical effect is the *re-heating of the outer layers*, leading to the characteristic inversion of the $T(\tau)$ and $T-\rho$ profiles, which was demonstrated in the early detailed calculations by [Yelle \(2004\)](#) and further carefully explored by e.g., [Koskinen et al. \(2013\)](#), [Fossati et al. \(2021\)](#) and [Fossati et al. \(2023\)](#). The main physical process leading to *heating* is the photo-effect reaction, that is, radiatively-driven ionization (by stellar X-UV field) ([Cecchi-Pestellini et al. 2009](#)) and subsequent redistribution of energy of photo-electrons in inelastic collisions. Classical LTE atmospheric models

that do not account for NLTE overionization of H (a continuum process) and NLTE pumping in metal lines are unable to reproduce this interesting physical effect (Fig. 37). Specifically, strong heating in Fe II lines, which constitute the vast majority of over 300 000 transitions (priv. comm. Mitchell Young) and in Mg I lines was reported by Fossati et al. (2021). Also, overionization of Fe I has been shown to influence the temperature-density structure (Young et al. 2024). All these effects lead to significantly hotter upper atmospheres and thus, due to increased pressure scale height, greater radii of hot Jupiters.

Over past years, some effort went into understanding the effects of hydrodynamics in planet atmospheres, especially in the context of mass loss, also known as *hydrodynamic escape*. It is typically argued that the bulk planet atmospheres are nearly in HE, as from the analysis of the Jeans parameter (Fossati et al. 2017) characteristic outflows in the line formation regions are subsonic (Koskinen et al. 2013; Fossati et al. 2023). However, also 1D RHD simulations are now available that solve 1D equations of mass, momentum, and energy (e.g. Yelle 2004; García Muñoz 2007; Koskinen et al. 2013; Erkaev et al. 2016) and may take into account the effects of charge separation and viscosity. Available evidence suggests, however, that hydro-dynamical effects are not large, and the velocities are typically much smaller compared to thermal velocities. Such models be coupled with 1D NLTE codes, such as Cloudy (Salz 2015; Kubyshkina et al. 2024), therefore NLTE effects can be taken into account by including photo-ionisation, recombination, charge transfer, and collision-driven transitions in various atomic species.

With the impact of NLTE on the physical structure of exoplanet atmospheres (Young et al. 2024), we argue that a comprehensive treatment of NLTE is highly desirable for modelling these systems. Whereas the *detectability (presence or absence)* of species may not be substantially affected by the assumption of LTE (but see Barman et al. 2002; Swain et al. 2009, for an interesting discussion), major NLTE effects may show in the spectroscopic diagnostics of the chemical composition. These may show when departures from atomic and especially molecular equilibrium are of a relevance in physics of exoplanet atmospheres.

8.9 Cosmologically relevant elements

Abundances of three elements, Li, Be, and B, are crucial in the context of observational cosmology. Their observed abundances right after the Big Bang Nucleosynthesis (BBN) are typically used to inform, among other constraints, the standard cosmological model (e.g. Boesgaard and Steigman 1985; Yang et al. 1984; Walker et al. 1991; Coc et al. 2012; Coc and Vangioni 2017; Fields et al. 2020).

The observed abundances of these elements are typically determined from the spectra of low-mass low-metallicity stars, which are thought to be born shortly after the BB (e.g. Spite and Spite 1982; Charbonnel and Primas 2005; Bonifacio et al. 2007; Aoki et al. 2009). The measurements are model-dependent, and we are facing a growing body of work on the analysis of 3D and NLTE effects on the abundances of Li. Recent studies (Klevas et al. 2016; Wang et al. 2021) suggest that in full 3D NLTE radiation transfer calculations, surprising cancellation effects occur at low metallicity, such as the abundances of Li in the so-called Spite plateau (Spite and Spite 1982) stars at $[\text{Fe}/\text{H}]$

~ -2 inferred using 1D LTE are nearly identical to those inferred using 3D NLTE modes (see [Klevas et al. 2016](#), their Fig.3, right-handside panel, and [Wang et al. 2021](#), their Fig. 11 bottom panel). Overall, 1D and 3D NLTE effects on Li abundances are also not large, and usually do not exceed 0.1 dex in modulus, except solar-metallicity red giants and cool M-dwarfs ([Klevas et al. 2016](#)). The latter study also emphasised the 1D NLTE and average 3D NLTE modelling approaches yield as reliable abundances of Li, as full 3D NLTE, for most of the parameter space, except low-metallicity red giants, where 3D NLTE effects are slightly larger in amplitude. Finally the effects of NLTE and 3D were quantified in the context of Li isotopic structure, with interesting implications for the $^6\text{Li}/^7\text{Li}$ isotopic ratios ([Harutyunyan et al. 2018](#)).

8.10 Kilonovae

As summarised in Fig. 28, the physical conditions in which NLTE effects are important also include the so-called kilonova events. These events are thought to be, among other extreme systems like gamma-ray bursts (GRB), electromagnetically observed counterparts of compact binary mergers (e.g. [Li and Paczyński 1998](#); [Metzger et al. 2010](#); [Barnes and Kasen 2013](#); [Tanaka and Hotokezaka 2013](#); [Pian et al. 2017](#)). With the development of gravitational wave astronomy following the detection of GWs from mergers of neutron stars (NS) or black hole–neutron star mergers (BH–NS) (e.g. [Abbott et al. 2017b,a,c](#)), it is becoming highly important to model accurately the broad-band fluxes and their time evolution (lightcurves) ([Villar et al. 2017](#); [Watson et al. 2019](#); [Domoto et al. 2021](#); [Perego et al. 2022](#)) including NLTE (e.g. [Hotokezaka et al. 2021](#); [Pognan et al. 2022a](#); [Hotokezaka et al. 2022](#)) in order to constrain physical conditions and nucleosynthesis in these enigmatic astrophysical events.

Different from stellar conditions, the radiation of kilonovae is highly time-dependent. Following the merger, the subsequent time evolution of the optical emission is guided by an extremely rapid expansion of the envelope, at speeds of ~ 0.1 to 0.3 of the light speed, synthesis of neutron-capture elements (specifically, in rapid neutron-capture process) on the timescales of a few seconds, and subsequent radioactive decays and photon losses on longer timescales of up to several months ([Villar et al. 2017](#); [Waxman et al. 2018](#); [Radice et al. 2018](#)). Fission cascades, α – and β –decays of radioactive nuclei produce energetic particles and photons ([Way and Wigner 1948](#)). Overall the evolution represents a transition from a hot and optically-thick system early (in full LTE) to a highly rarefied system owing to rapidly decreasing densities (in full NLTE), with corresponding effective temperatures T_{eff} of a few $\sim 10\,000$ at 0.5 days dropping to a few $1\,000$ K at 3–4 days ([Waxman et al. 2018](#)). While the bulk properties of the SED can be approximated by the Planck function, with heating driven by the β –decays ([Waxman et al. 2018](#); [Hotokezaka and Nakar 2020](#)), the detailed SED structure is primarily set by high opacity in spectral lines due to, e.g., Ca II, Sr II, Y II, Zr II, and lanthanides Ce III, La III (e.g. [Domoto et al. 2022](#); [Pognan et al. 2023](#)), although the identifications are limited by the availability of atomic data ([Flörs et al. 2023](#)). The corresponding statistical equilibrium is dominated by highly ionised species (up to 11th ionization stages) as early as 0.1 days after the merger at characteristic temperatures around $100\,000$ K, but transitions to singly-ionized and neutral species

around 5 000 K (Banerjee et al. 2022). Subsequently approximate or more comprehensive (SE) NLTE treatment is used to compute NLTE populations. Recombination coefficients, accurate photo-ionization cross-sections, and comprehensive treatment of bound-bound radiative transitions are particularly important (e.g. Pognan et al. 2023).

NLTE codes that handle photospheric RT in expanding envelopes (with a steady-state system with a high outflow velocity) include TARDIS (Kerzendorf and Sim 2014) and SUMO (Jerkstrand 2011; Pognan et al. 2023). Both are 1D spectrum synthesis codes employing the Monte Carlo RT approach and allowing for fluorescent emission. TARDIS is based on the photospheric RT in the Schuster–Schwarzschild formalism, whereas SUMO carries out full-domain simulations, and NLTE RT is handled in a more comprehensive approach in the latter. The expansion is assumed to be homologous⁴ ($v = r/t$) and the underlying t/ρ (density) structure follows from the velocity profile and solution of the 1st law of thermodynamics. Profiles like $\rho \sim v^{-4}$ or $\sim v^{-3}$ can be used, however, codes can handle other $\rho - v$ profiles. With various heating and cooling processes are included, such as heat exchange due to atomic line transitions, radioactive heating, and adiabatic cooling, with an assumed electron fraction Y_e . Radiation-hydrodynamic simulations predict diversity of velocity profiles, but overall the effects of dynamics are very small (Wu et al. 2022). Similar to SNe RT modelling, the concept of Sobolev expansion opacity⁵ is usually adopted in the calculations (Sobolev 1957; Karp et al. 1977). However, simplified 1D LTE spectrum synthesis calculations using the stellar atmosphere codes like MOOG (Watson et al. 2019) have also found applications in the context of kilonovae light-curve fitting and diagnostics. In the later paper, specifically the emission was represented by a stellar model atmosphere from Kurucz database with $T_{\text{eff}} = 5\,500$ K, the surface gravity $\log g = 0$.

Recent studies suggest that NLTE effects become critical in the structure of KN after a few (~ 4 to 5 days) after the merger. In terms of thermodynamics, the general effect of NLTE is that it leads to progressively increasing kinetic temperature and ionization fractions with time, opposite to what simplified LTE calculations suggest (e.g. Hotokezaka et al. 2021; Pognan et al. 2022b, 2023). The temperature rise is thought to continue for months to a year, until adiabatic cooling sets in (priv. comm. A. Jerkstrand). Detailed calculations of NLTE opacities and number densities show that only at very early times (1 to 2 days) after the merger, level populations of the key species, such as Ce II and Pt III, are nearly thermalised and the LTE equilibrium is achieved (Pognan et al. 2022a). However, substantial (many orders of magnitude) de-population of upper energy states is achieved at later times ($\gtrsim 5$ days) after the merger due to very low densities, and hence inefficient collisional thermalisation and dominance of spontaneous radiative de-excitations. The LTE opacity can therefore be over-estimated by a factor of 2 (as for Pt III at early epochs) to a factor of $\sim 1\,000$ (as for Ce II 20 days after merger), which is due to a failure of the Saha ionization equilibrium to produce realistic ionization fractions (Pognan et al. 2022a). This major effect

⁴Homologous expansion represents a constant shape of mathematical objects irrespective of time, albeit the size of the shape might scale with, e.g., time. This property is commonly used in astronomy, e.g. in the simulations of supernova explosions (Noebauer and Sim 2019), cosmological expansion (cf Ed. Wright 1997, UCLA), and dynamical ejecta during mergers (Rosswog et al. 2014; Wu et al. 2022).

⁵The total opacity accounting for the effect of the Doppler-shifted of the individual photon frequencies at a give time during the expansion.

of NLTE on the population of main opacity sources, in this case Ce II, is demonstrated in Fig. 38, (c) Pognan et al. (2022a).

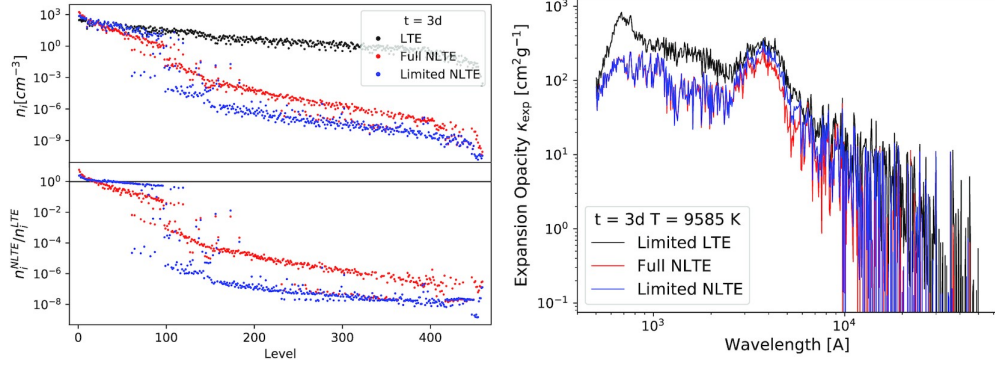


Fig. 38 NLTE effect on the population of singly-ionized cerium (Ce II). The effect on NLTE populations on total opacity of kilonova at 3 d after the merger event, computed for a low-density model with the ejecta mass of $0.01 M_{\text{Sun}}$ and expansion velocity of the ejected material of $0.2c$ (20% of the speed of light). Image reproduced with permission from Pognan et al. (2022a), copyright by ESO.

For He I and Sr II, due to their particular atomic structure, the NLTE effects may arise in strong IR lines at $1.08 \mu\text{m}$ (He I: $10830 \text{ \AA}$, and Sr II: $10037, 10327, 10914 \text{ \AA}$) due to the over-ionization (relative to Saha equilibrium) caused by non-thermal electrons produced in radioactive β -decays (Tarumi et al. 2023). These spectral lines are critical for the interpretation of the PCyg like feature around $700\text{--}900 \text{ nm}$ (Watson et al. 2019), which is thought to provide a strong evidence for r-process synthesis in NSM. We refer the reader to Pognan et al. (2023), who provide a parametric study of the evolution of thermodynamic structure and NLTE synthetic spectra of kilonovae.

From the available body of evidence, it can be concluded that a more comprehensive understanding of NLTE effects in light elements, like He, and in trans-Fe-group species, is critical for the interpretation and analysis of nucleosynthesis in compact binary mergers (Perego et al. 2022; Tarumi et al. 2023).

8.11 Red supergiants

RSGs are evolved core-He burning massive stars close (in the $T_{\text{eff}}\text{--}\log g$ space) to the Hyashi boundary (Maeder 1981; Levesque 2017), with convective envelopes occupying ~ 0.1 to 0.8 of their total mass (Stothers 1972). Thus, 3D radiation-hydrodynamics is imperative for understanding the outer structure of these systems (e.g. Chiavassa et al. 2009, 2011; Goldberg et al. 2022; Ahmad et al. 2023; Ma et al. 2024).

For RSGs, 3D radiation transfer and spectrum synthesis has been so far primarily exploited in the context of the atmospheric dynamics and convective flows (see Chiavassa et al. 2024, for a review). These calculations make use of 3D LTE radiation transfer simulations in selected spectral lines to invert the asymmetric observed profiles of selected photospheric lines (Kravchenko et al. 2018). These are, for example, the TiO

band features that are sensitive to both temperature and velocity inhomogeneities due to large-scale convective motions (Kravchenko et al. 2019). The tomographic methods can be applied to different wavelength regimes, including the optical spectral lines, and they are also useful as diagnostics of relationships between photometric variability of red supergiants and sub-surface convection, as e.g., shown for Betelgeuse in the context of its Great Dimming event (Kravchenko et al. 2021). As Ma et al. (2024) show, 3D RT models are furthermore key to the interpretation of the widths of molecular lines, such as SiO and CO, that can be observed in the sub-mm with ALMA. These are relevant in the context of measurements of RSG rotation rates with ALMA (Kervella et al. 2018) and the tantalising possibility that rapidly-rotating RSG may represent a product of merger in a massive binary system (Chatzopoulos et al. 2020; Sullivan et al. 2020).

NLTE calculations for RSG stars have been carried out with 1D hydrostatic MARCS models (Bergemann et al. 2012b, 2013, 2015) owing to their comprehensive treatment of molecular line blanketing. Since RSGs are brightest in the infra-red, abundance diagnostics typically rely in spectral lines in the J, H, or K bands (e.g. Davies et al. 2017). The available evidence suggests that NLTE effects in the IR diagnostic features are typically driven by line scattering. Hence, for most diagnostic transitions, such as strong lines of Fe I (Bergemann et al. 2012b), Ti I (Bergemann 2011), Mg I (Bergemann et al. 2015), and Si I (Bergemann et al. 2013), NLTE radiation transfer predicts significantly stronger spectral lines compared to LTE. Consequently, the chemical abundances inferred via LTE IR spectroscopy of RSG stars may be significantly over-estimated, and detailed NLTE calculations are needed to retrieve robust chemical composition of RSGs (e.g. Patrick et al. 2016; Davies et al. 2017; Asa'd et al. 2020) and young super-star clusters (Gazak et al. 2014).

9 Summary written by AI

Given the increasing relevance and integration of AI tools in research workflows, we have included in this section a summary of this document generated with the assistance of ChatGPT. Each point in the summary has been thoroughly reviewed and, where deemed necessary, revised by the authors to ensure accuracy, clarity, and scientific precision. No other content in this document — apart from this section — was produced using ChatGPT.

In Fig. 39, we also summarize the theoretical estimates of 3D NLTE abundance corrections for different types of stars and metallicities.

Motivation & Scope

- Radiative transfer (RT) modeling is essential for deriving physical parameters from astronomical spectra.
- 3D Non-LTE (NLTE) models are computed from first principles using hydrodynamics, radiation transfer, atomic and molecular physics, and statistical physics.
- 3D Non-LTE (NLTE) overcome limitations of traditional 1D LTE models that are highly-parameterized; the synthetic observables (spectra,

Impact of 3D + NLTE on abundances

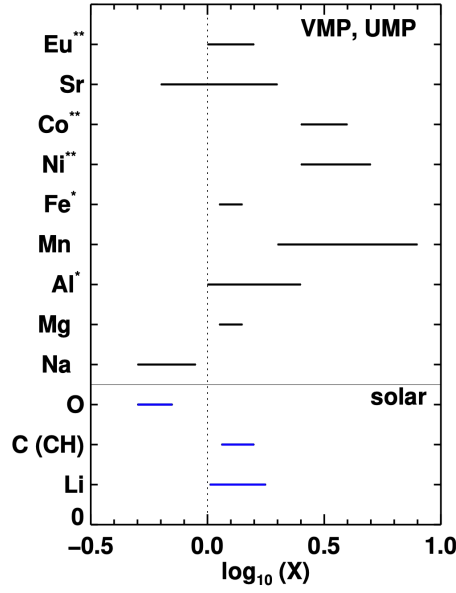


Fig. 39 3D and/or NLTE effects on chemical abundances of chemical elements in metal-poor (very metal-poor and ultra-metal-poor) and Sun-like stars. The figure only shows selected representative results and does not aim for completeness. The 3D NLTE and 1D NLTE abundance corrections are adopted from the sources described in Sect. 8.5. For Fe and Al, only 1D NLTE results are provided. For Co, Eu, and Ni, the data represent only turn-off and subgiant atmospheres. For all other elements, the bars represent the results for red giants and main-sequence stars.

SEDs, photometry) generated by 1D LTE models depend on input ad-hoc free parameters and hence any diagnostic based on 1D LTE is user-dependent.

- Applications span stellar types (OBA to FGKM), exoplanet atmospheres, and kilonovae.

Conceptual Foundations

- LTE assumes local equilibrium; NLTE solves statistical equilibrium (or rate) equations for greater realism.
- 3D RT accounts for spatial inhomogeneities and dynamics (e.g., convection, pulsations, magnetic fields), if multi-D RHD models are used as inputs.

Model Inputs

- Utilizes 3D radiation-hydrodynamics models (e.g., STAGGER, MURaM, CO⁵BOLD, M3DIS) and atomic/molecular databases (e.g., NIST, VALD).
- Requires comprehensive equations of state (EoS) and partition functions and opacities for complex media.

- Full time-dependent 3D RHD model atmospheres available for FGKM-type stars of different metallicities $[\text{Fe}/\text{H}]$ at <https://nlte.mpia.de/> (196 full 3D and average 3D stellar models) and at <https://staggergrid.wordpress.com/> (204 average 3D stellar models)

Spectral Features & Observational Phenomena

- *Convective Line Asymmetries*: Captures line bisectors and Doppler shifts from stellar surface granulation.
- *Centre-to-Limb Variation (CLV)*: 3D NLTE models describe the center-to-limb variation of solar intensities.
- *Limb Darkening*: Magnetic field effects accounted for in 3D SSD and 3D MHD simulations; near-UV discrepancies remain.
- *Rossiter–McLaughlin Effect*: 1D NLTE and 3D NLTE models outperform 3D LTE in simulating planet transits across stellar surfaces.

Applications

- **Cool Stars**: Accurate fundamental stellar parameters and chemical abundances;
- **Cool Stars**: 3D RT essential for spectral lines with strong asymmetries, e.g., due to isotopic structure, hyperfine splitting, or shifts due to variation of fundamental physical constants.
- **Exoplanets**: NLTE RT aids in atmospheric characterization; NLTE-driven strong heating in the outer atmospheres of exoplanets.
- **Kilonovae**: Adaptation of RT methods from supernovae for evolving spectra; transition from LTE early to a fully NLTE-dominated regime in late phases (several days) after the merger; fluorescence as a key NLTE effect.
- **Red Supergiants**: 3D models explain observed surface granulation and variability (e.g., Betelgeuse), as revealed by interferometric data (VLT, ALMA).

Computational Techniques

- *1.5D RT*: Approximation using independent vertical columns.
- *Lambda Iteration & Accelerated Methods*: Solve coupled RT and statistical equilibrium equations.
- *Opacity Binning & Mesh Refinement*: Optimize resolution vs. cost.

Challenges & Future Work

- High computational demands limit broad application; grids of 3D atmosphere models and synthetic spectra are needed to enable physical analysis of data from next-generation astronomical surveys, such as 4MOST, WEAVE, and SDSS-V.
- Need improved observational validation, especially for metal-poor stars (line shifts and asymmetries), exoplanet atmospheres (molecular lines), and kilonovae (opacities due to neutron-capture elements).

- Magnetic field treatment is needed; small-scale dynamo and magnetic fields to be explored over the entire parameter space of FGKM-type stars.
- Required for diagnostics of stellar physics with facilities, such as the ESO’s Extremely Large Telescope (ELT), permits studies of time- and spatially-dependent phenomena (oscillations, variability) from first principles.
- Methods from stellar atmospheric conditions can be adapted to studies of kilonova and exoplanet atmospheres; A notable success in physical domain transfer is the `Cloudy` code, which has been widely adopted in astrophysical modeling.

10 Summary and conclusions

Over the past decade, the community has faced extraordinary advances in the area of radiation transfer in different astrophysical environments. The two primary developments are systems in non-local thermodynamic equilibrium (NLTE) and inhomogeneous three-dimensional (3D) thermo-dynamical systems, which include convection and turbulence arising from first principles. The latter can be computed in the plane-parallel Cartesian geometry or in the full spherically symmetric geometry with depth-dependent gravitational potential. These advances have been mainly motivated by the development of instrumental facilities and, so the availability of new types of observational data for different kinds of astronomical objects, including stars, exoplanets, and compact binary mergers. The typical questions that can be asked in the framework of 3D NLTE calculations are as follows

1. How wrong are the astrophysical parameters of stars, planets, etc, obtained using simplified (1D LTE) models?
2. Which qualitative advance [over 1D LTE] do 3D and/or NLTE models bring about, which cannot be learned from 1D LTE models?
3. How wrong are the 3D NLTE models and what are their observationally testable predictions?
4. What is the effect of magnetic fields?

Technically, 3D NLTE calculations are very similar in their technical skeleton, but differ in the level of detail, micro-physics, and implementation of all sub-grid effects, such as interpolations, extrapolations, smoothing. At the NLTE level, various approaches are used, ranging from full comprehensive (and highly, many orders of magnitude, more time-consuming) solution of rate equations for all known energy states of a specie to various approximations and simplifications, such as the two-level atom coronal approach or even a double-temperature approximation in the Boltzmann equation for a mixed plasma in LTE. Regarding geometry or dynamics, or both, the approaches range from standard 1D system in hydrostatic equilibrium and analytical recipes to represent depth-dependent convective fluxes, through more sophisticated 1D hydrodynamics (e.g., “Parker wind” profiles used for stars and exoplanets, [Linssen et al. 2022](#); [Kubyshkina et al. 2024](#)), to finally full 3D RHD hydrodynamics calculations

(Nordlund et al. 2009; Kupka and Muthsam 2017; Chiavassa et al. 2024). The latter, for the sake of maintaining the balance between relaxation and computational expense, have to assume LTE opacities or ignore them entirely adopting grey RT, or ignoring RT all together, as, e.g., in kilonovae for the early stages before the 1D homologous expansion can be assumed or in early phases of 3D RHD calculations of sub-surface stellar convection where Newton cooling is used (Eitner et al. 2024).

On the observational side, the most direct information comes from solar telescopes, which provide spatially-resolved high-resolution optical spectra for the solar surface. Such information is only barely accessible for other stars. However, first attempts have been made to reconstruct centre-to-limb intensity variation of a few nearby stars using exoplanet transit data (Dravins et al. 2017a,b, 2021). More extensive and convincing observational arguments for 3D convective models come from imaging of stellar surfaces, such as, e.g., possible with interferometers. Although limited to large stars, the observed data reveal asymmetries and inhomogeneities on stellar surfaces. This sub-structure, driven by gigantic sub-photospheric convective cells, exhibits correlations between velocity and temperature. As a result, it gives rise not only to surface granulation, but also to hot spots, mass loss, stellar winds, and circumstellar shells. Finally, evidence for more complex 3D models of stellar atmospheres — beyond the classical 1D LTE models — is rooted in the failure of these models to describe key diagnostic features in observed spectra. This can be particularly well demonstrated for the spatially-resolved spectroscopy of the Sun. These do not require any larger or more powerful instruments, but are sufficiently well-known already from data acquired with small medium-resolution facilities.

Overall, 3D RT modelling in the context of stars has been driven mainly by an interest in convection (Stein and Nordlund 1998; Vögler et al. 2004; Freytag et al. 2012), atmospheric structure (Gudiksen and Nordlund 2002; Carlsson et al. 2016; Rempel 2017), and activity (Vögler and Schüssler 2007; Rempel and Cheung 2014; Chen et al. 2017), the results of which could be compared to high precision observations. Atmospheric models of other stars were also developed for a handful of individual stars (Caffau et al. 2011; Nordlander and Lind 2017; Lagae et al. 2023) and grids of effective temperature and surface gravity were computed by Ludwig et al. (2009b) and Magic et al. (2013a) and more recently by Rodríguez Díaz et al. (2024) and Eitner et al. (2024).

For stars, the necessity for NLTE has been argued primarily from the theoretical standpoint. Recent calculations of cross-sections for reactions of collisional type suggest that classical formulations have to be used with caution, as these sometimes overestimate the cross-sections by orders of magnitude (Barklem and Collet 2016). However, in general we conclude that the NLTE effects obtained by different authors (Amarsi et al. 2015; Osorio and Barklem 2016; Bergemann et al. 2017; Mashonkina and Belyaev 2019; Gallagher et al. 2020; Mashonkina et al. 2022; Storm et al. 2024) are consistent, despite the differences in the atomic models, atmospheric physics, and numerical approaches in NLTE RT. Recent calculations for stellar conditions (Fig. 28, 29 in this review) confirm significant NLTE effects on lines in the UV, optical, and near-IR bands for most chemical elements in the periodic table, including the lightest (H, He, Li) through Fe-peak (Mn, Co, Ni) to heavy neutron-capture elements (e.g.,

Ba, Y, Sr, Eu). NLTE abundances strongly depend on stellar parameters (T_{eff} , $\log g$, $[\text{Fe}/\text{H}]$) and the effects cannot be calibrated out, thus requiring NLTE modelling of stellar spectra from first principles. These effects can be included either directly (via spectrum synthesis) or indirectly, by correcting the inferred 1D LTE abundances for effects of 3D NLTE.

Coupled calculations of NLTE RT in 3D hydrodynamical atmospheric models of stars are still rare. However, the available evidence (for lighter species like H and Li, but also heavier like Na, Al, Mn) suggests that 3D NLTE modelling is crucial and may have a profound impact on the analysis of stellar chemical composition, especially so for low metallicity and/or low gravity stars (e.g. [Amarsi et al. 2019b](#); [Bergemann et al. 2019](#); [Nordlander et al. 2019](#)). A comprehensive analysis of 3D NLTE abundance corrections and their relevance in studies of Galactic Chemical Evolution was recently presented by [Storm et al. \(2025\)](#) and [Koutsouridou et al. \(2025\)](#). Given major computational overheads associated with 3D RT, it is essential that the next step in observational stellar physics involves 3D NLTE spectroscopic grids, and ideally includes magnetism, for instance by employing 3D SSD (or MHD) model atmospheres ([Bhatia et al. 2022](#); [Ludwig et al. 2023](#); [Witzke et al. 2023](#); [Kostogryz et al. 2024](#)) in spectroscopic RT calculations.

The prime advantage of 3D NLTE atmospheric and spectroscopic models is that they do not include ad-hoc free parameters (micro- or macroturbulence, mixing length), and thereby allow for analyses of fundamental stellar parameters, chemical abundances, but also studies of spatially- and time-dependent phenomena, from first principles.

Beyond chemical composition, model stellar spectra from 3D time-dependent RHD and MHD models for stars are relevant in the context of other applications. These include: diagnostics of stellar oscillations from multi-epoch spectra and light-curves for asteroseismology, variability and surface structure of stars in the context of studies of exoplanets, as well as studies of stellar multiplicity and pulsations. These models are also particularly important for science questions for which tiny effects on spectral line shifts or asymmetries may have drastic implications for conclusions. One interesting example is constraining the variability of the fundamental fine structure constant (e.g. [Murphy et al. 2022](#)).

In the domain of observational studies of exoplanets, neither strong evidence for NLTE effects nor sub-surface convection or mass motions exists yet. It is difficult to probe these effects observationally in the transmission spectra, even despite theoretical models forecasting NLTE effects of up to a factor of 2 to 5 in the line depths, or in the mean atmospheric structure, such as severe (up to several ~ 1000 K) NLTE-driven heating in the outer atmospheric layers of gas planets, such as hot Jupiters. Standard externally irradiated 1D LTE spectral models ([Mollière et al. 2019](#)) provide the first-order estimates of the atmospheric structure of exoplanets, and hence of abundance ratios of important molecular tracers, such as water, CO, CH₄, and CO₂. However, first attempts to compute models with NLTE radiative transfer highlight the substantial effects on atomic opacities and, hence, on the detectability of features in absorption or emission (e.g. [Young et al. 2020](#); [Fossati et al. 2021](#); [Wright et al. 2022](#)). Interest in 3D convective planet atmosphere models is rapidly growing. These models include

global atmospheric circulation, and thus yield fascinating observational predictions in the presence of stellar irradiation on the day-night side of tidally locked planets.

Methods of RT in the context of kilonova research (Jerkstrand 2011; Kerzendorf and Sim 2014; Pognan et al. 2023; Shingles et al. 2023) have mostly been inspired by NLTE simulations for SN Ia (Noebauer and Sim 2019) and numerical methods have been mostly taken over. However, adapting the micro-physics, such as the chemical composition and the equation of state to the chemical mixtures prevalent in the outcomes of compact binary mergers of NS and NS-BH mergers. Here, shift to progressively heavy species, actinides and lanthanides produced in r-process during the merger, has imposed a need for calculations of radiative data for NLTE modelling of opacities and SEDs of kilonovae. Detailed calculations confirmed strong pumping of critical transitions (e.g., He I and Sr II) by the radiation field emerging due to non-thermal NLTE effects (Tarumi et al. 2023). Also the NLTE effects on kilonovae opacities can be tremendous, leading to up to a factor of 1000 lower radiative opacities at late epochs compared to LTE conditions (Pognan et al. 2022b). More detailed and extensive calculations for different chemical species, but also coupled 3D NLTE modelling (van Baal et al. 2023) are imperative to consolidate the diagnostic of these enigmatic astrophysical systems.

In summary, the past decade has seen tremendous progress in the numerical aspects of atmospheric radiation transfer — moving towards multi-D geometry, convection, expansion, and non-local thermodynamic equilibrium — for vast classes of astronomical objects, ranging from exoplanets, to stars, and their post-explosion or post-merger remnants. These efforts, although tedious, technically (numerically and physically) complex, and barely accessible to the broader community of observers and phenomenologists, are exceptionally valuable and fundamental to progress in astrophysics. This is primarily because they are our primary (or even the only!) source of evidence that astrophysical inference, and hence all kinds of discoveries in astronomy, is reliable and trustworthy. To give an example, the importance of NLTE abundances and 3D stellar atmosphere grids was acknowledged quickly and unanimously in the studies of first stars (Beers and Christlieb 2005; Bonifacio et al. 2025), nucleosynthesis and nuclear physics (Käppeler et al. 2011; Sbordone et al. 2010), origins of elements and Galactic chemical evolution (Nomoto et al. 2006; Frebel and Norris 2015), formation and evolution of massive stars (Woosley and Heger 2007), as well as in asteroseismology (Aerts et al. 2010), and exoplanet science (Rauer et al. 2014). However, even today, a decade later, those fields are still heavily reliant on rapid synthesis of LTE 1D spectra (Sharma et al. 2018; Nelson et al. 2019; Gilmore et al. 2022). Therefore, we consider it essential to develop NLTE and 3D spectrum synthesis codes that surpass established 1D LTE codes in their capability of employing 3D radiation-hydrodynamical inputs.

We anticipate that the progress towards 3D NLTE will accelerate as RT codes become public, and this will enable a fundamentally new quality of observational astrophysics: the ability to understand, predict, and explain astronomical objects in space and in time. Unfortunately, is not possible to do this from first principles with any current 1D parameterized quasi-equilibrium (LTE) models.

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