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Hydrodynamics and radiative transfer of 3D model atmospheres

current status, limitations, and how to make headway

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Abstract. 3D MHD models are important tools for advancing our understanding of stellar atmospheres. A major computational challenge is the treatment of radiative transfer; both to get a realistic treatment of the energy transfer in the 3D modelling and for the diagnostic problem of calculating the emergent spectrum in more detail from such models. The current status, limitations and future directions of 3D MHD atmospheric modelling and the treatment of radiative transfer are here discussed.

Key words. Methods: numerical – hydrodynamics – MHD – radiative transfer – Stars: atmospheres

1. Introduction

Most of our knowledge of stars comes from studying the electromagnetic radiation from them. We do not directly observe the physical conditions, like the temperature, the density, the velocity field and the magnetic field, but spectral features that carry information about the regions where they are formed, by definition called the stellar atmosphere. In addition, the radiation does not only play a diagnostic role but is often also the dominant means of energy transport in stellar atmospheres.

An important tool to disentangle this information is to calculate the emergent spectrum from synthetic 3D models and compare with observations. A major computational challenge is the treatment of radiative transfer; both to get a realistic treatment of the energy transfer in the 3D modelling and for the diagnostic problem of calculating the emergent spectrum in more detail from such models.

The layout of this contribution is as follows: in Section 2 we discuss the problems of calculating 3D models of stellar atmospheres, in Section 3 we discuss the diagnostic problem of calculating the emergent spectrum in detail from a given 3D atmosphere and we finish in Section 4 with conclusions. For a more detailed account of 3D radiative transfer in stellar atmospheres the reader is referred to Carlsson (2008).

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2. 3D model atmospheres

Radiation is the dominant energy transport mechanism in the outer part of most stellar atmospheres and it is therefore imperative to include a good description of radiative transfer when modelling stellar atmospheres. The computational difficulty arises from the many atomic processes that contribute to the opacity of a stellar atmosphere. The very large number of narrow spectral lines makes it necessary to solve the transfer equation at a very large number of frequencies to obtain an accurate description of the spectrum — To cover the spectrum from 50 nm to 10 μm with 10 points per width of 2 km/s means 8 million frequency points. Fortunately it is not necessary to have a good description of the detailed spectrum when modelling stellar atmospheres — it is the radiative flux divergence (which is a quantity integrated over frequency) that must be accurately described. Several methods have been devised to reduce the number of frequency points needed to accurately describe the flux divergence.

Opacity Distribution Function (ODF) methods split the spectrum into small wavelength bins (over which the Planck-function is approximately constant) and sort the opacities over the bin. The opacity distribution function can be described with much fewer points than the detailed run of opacity over wavelength. On the order of 1000 frequency points give a good description of the frequency integrated quantities like the flux divergence.

The ODF approach was taken further by Nordlund (1982) by introducing *Group mean opacities*. On the order of four opacity bins describe the radiative flux divergence in the solar photosphere remarkably well. This method is used in almost all codes used for realistic modelling of cool star atmospheres: Nordlund & Stein (e.g. Nordlund 1982; Stein & Nordlund 1998, 2000), the CO^{5}BOLD code (Freytag et al. 2002; Wedemeyer et al. 2004), the MuRAM code (Vögler et al. 2005) and the Oslo Stagger Code (Hansteen 2004, Hansteen, Carlsson & Gudiksen 2007). Computing power has increased by about a factor of two every 18 months ("Moore's law"). What used to be run on the very biggest machines can now be run on a workstation (like a simulation of solar convection in a box of 6 Mm horizontal extent). To take advantage of the large increase in computing power it is now necessary to have a code adapted to massive parallelism. The above codes can all be run in parallel on machines with global memory. The Oslo Stagger Code was recently completely rewritten using the MPI protocol to enable running on machines with distributed memory (all large computers today). The new code has been named Bifrost (Gudiksen et al., in preparation) and it joins MuRAM and the Copenhagen stagger code being MPI parallelized.

A large number of studies of spectral line formation in 3D media has been performed using these codes. See Carlsson (2008) and other contributions in these proceedings for examples. Given the existence of numerical viscosity to stabilize the schemes and therefore Reynold's numbers many orders of magnitudes away from the solar case and a very approximate treatment of the detailed radiative transfer, a legitimate question to ask is: Are these realistic simulations really realistic? Can we trust the results?

The most obvious testing bed is our closest star, the Sun. Current simulations reproduce line profiles very accurately, including line bisectors that are very sensitive to the detailed correlations of flows and temperature. The long standing difference between calculated and observed granulation contrast seem to have been resolved (Wedemeyer-Böhm & Rouppe van der Voort 2009) and also the center-to-limb variation of the intensity is well reproduced in the latest models (Pereira et al. 2009a). For photospheric simulations we thus seem to be doing well but further tests should be done using the full information in the observations and simulations: comparisons using high spatial and temporal resolution (e.g. Pereira et al. 2009b).

A worry is still the crude approximation of the radiative flux divergence description using only on the order of four frequency bins. Most of the energy transport happens in the optical region of the spectrum where almost all the opacity ends up in the lowest opacity bin. We thus describe the dominant energy transport with only one opacity bin. An improvement is to do the opacity binning separately in different wavelength regions, thus approaching the original ODF approach. It is then possible to have more opacity bins in the optical region and still catch the high opacities in the UV in other bins. Another possibility explored by Trampedach is to use an opacity sampling method but choose the wavelengths not by random but using some criterion like accurate description of the radiative flux divergence in a test-model (e.g. a 1D horizontally averaged model) for the limited wavelength set when compared with a full opacity sampling set. Initial tests indicate that on the order of 100 wavelength points may be sufficient. This *Sparse Opacity Sampling* method will also catch the effect of Doppler-shifts of line absorption on the transfer.

It is almost 30 years since the ground-breaking simulations by Nordlund and that timespan corresponds to a factor of 10^6 following Moore's law. We should thus be able to use full opacity sampling with 10^5 frequency points for small computational domains. Such simulations should be carried out and serve as test beds for the further development of the approximate methods that are still needed in order to use the increase in computational capabilities to increase the domain size, increase the resolution or incorporate more physics (see below).

Going to layers of the atmosphere above the mid-photosphere the standard models described above are not sufficient. Scattering in the radiative transfer starts to become important, time-dependent out-of-equilibrium hydrogen ionization is very important to take into account to get the energetics and electron densities right in the lower chromosphere (Carlsson & Stein 2002) and the magnetic fields start to dominate the pressure and energetics. The radiative losses of the solar chromosphere are dominated by strong lines of calcium, magnesium and hydrogen where the approximation of Local Thermodynamic Equilibrium (LTE) is no longer valid.

Ideally one would thus want to solve the full MHD problem together with the NLTE rate equations for the dominant species with an implicit code (to handle time-dependent rates without having the timestep being set by the fastest rates which have timescales of less than 10^{-8}s). This was done in 1D by Carlsson & Stein (1992, 1994, 1995, 1997, 2002) but employing the same methods in 3D would be computationally prohibitive; instead of brute-force we need to start with approximate methods.

Skartlien (2000) generalized the group mean opacity method of Nordlund to also take into account coherent scattering in continua and lines. Although the method only works for coherent scattering, it is a first step to include the effect of scattering in the problem with a moderate cost (about a factor of 10 in a serial code and less than that in a domain-decomposed parallelization that needs iterations for consistency). Recently, Hayek (2008) implemented treatment of scattering in the Bifrost code using the Gauss-Seidel method of Trujillo Bueno & Fabiani Bendicho (1995) with promising results at a similar numerical cost.

Time-dependent out-of-equilibrium hydrogen ionization was studied in detail in 1D by Carlsson & Stein (2002) and approximate methods for including such effects in 3D without solving the non-local radiative transfer problem were developed by Sollum (1999). These methods were implemented in the CO^{5}BOLD code by Leenaarts & Wedemeyer-Böhm (2006) and they showed that, indeed, hydrogen ionization is much higher in cool pockets in the chromosphere than instantaneous equilibrium would indicate. The back-coupling on the energy equation was not taken into account in the hydrodynamic simulations. This was done in a 2D simulation in the context of the Oslo Stagger Code by Leenaarts et al. (2007) but the effect of the increased electron density on the opacities and heating in the H^- continuum still is not included self-consistently. Furthermore, the approximate methods have only been shown to work well in the 1D case and further testing (and possibly modifications) have to be made in 3D. The computational cost of these approximate methods is considerable since eight linear equations need to be solved at every grid-point of the simulation in an implicit scheme needing several iterations for convergence. Furthermore, the strong temperature dependence of ionization introduces very strong gradients in the population densities of hydrogen which need care in the numerical scheme.

Magnetic fields are straightforward to include and the standard codes mentioned previously can all treat full MHD. The cost paid is three extra equations to solve and much more complicated boundary conditions to allow all different waves through without reflection. The Courant-Friedrich condition is also quickly dominated by the fast magneto-acoustic waves (especially for simulations extending into the corona) cutting down the allowed timestep size by several orders of magnitude.

Incorporating full NLTE into the MHD simulations is not possible at the moment and smart recipes have to be designed based on the computationally tractable 1D problem. This has been done in the Bifrost code where the radiative losses in the chromosphere in strong lines from calcium and hydrogen are described using temperature dependent, local, collisional excitation rates from atomic physics and escape probabilities based on the vertical optical depth and calibration using 1D simulations.

Simulating the full region from the convection zone to the corona with realistic descriptions of the physics is the ambition of the Oslo Stagger Code (Hansteen 2004, Hansteen, Carlsson & Gudiksen 2007) and the rewritten MPI-code Bifrost. One experiment typically covers 16x16x16 Mm (2 Mm below the photosphere, 14 Mm above) with open boundaries, detailed radiative transfer along 48 rays with group mean opacities in 4 bins with scattering, added NLTE radiative losses in the chromosphere from Ca II and hydrogen lines and continua, optically thin losses in the corona and conduction along magnetic field-lines. The convection moves the magnetic field around and provides a pointing-flux that is large enough to heat up the corona to 0.5 to 2 million K (depending on the initial magnetic field configuration). The simulations also show the existence of Alfvénic waves that are very similar to waves observed with the Hinode satellite (De Pontieu et al. 2007) and carry an energy flux that is similar to what is needed to accelerate the solar wind. Simulations of magnetic flux emergence into the chromosphere and corona have also been carried out (Martínez-Sykora et al. 2008, 2009a) and spicule-like structures are seen to be excited in the simulations (Martínez-Sykora et al. 2009b).

3. 3D NLTE

Once 3D models have been calculated with an approximate description of the radiation, it is time to calculate the emergent spectrum with much more detail in order to compare with observations. In LTE this reduces to a 1D problem - calculating the radiative transfer along a ray (or rather, very many rays) through the known 3D model. The rays are independent from each other and the problem is what is called trivially parallelizable.

The computing demand is rather modest; a 253x253x160 solution involving 3000 frequency points using MULTI (Carlsson 1986) takes 5s per column on a MacBook laptop computer resulting in 90 hours for the complete simulation box. Parallelization results in a linear speedup giving a total of one hour on 90 CPUs. Other codes for the LTE solution from a 3D atmosphere are Linfor3D developed in Potsdam and Meudon [1] and ASSϵT (Koesterke et al. in preparation, see also Koesterke et al. 2008).

In NLTE it is necessary to solve the statistical equilibrium equations simultaneously with the transfer equations. Many 1D methods can easily be generalized to 3D with most of the complication being the formal solution (solving the transfer equation with known source function) in 3D.

One example of such a code is the generalization of the 1D code MULTI (Carlsson 1986) to 3D (Botnen 1997). This code, MULTI3D, employs linearization of the statistical equilibrium equations following Scharmer & Carlsson (1985), the approximate operator of

[1] `http://www.aip.de/~mst/Linfor3D/linfor_3D_manual.pdf`

Rybicki & Hummer (1991) and a short characteristics formulation of the formal solution. A rewritten form of MULTI3D uses domain decomposition and MPI parallelization (Leenaarts et al. 2009).

Another code for the solution of the 3D NLTE statistical equilibrium equations, called MUGA (from MUltilevel GAuss-Seidel), has been developed by Fabiani Bendicho, Trujillo Bueno, Auer and co-workers (Auer et al. 1994; Trujillo Bueno & Fabiani Bendicho 1995; Fabiani Bendicho et al. 1997). The code uses the preconditioning approach of Rybicki and Hummer, employs a short characteristic formal solver, a Gauss-Seidel iteration scheme and a multi-grid scheme. See also Fabiani Bendicho & Trujillo Bueno (1999) and Asensio Ramos & Trujillo Bueno (2006) for details on horizontal periodic boundary conditions and spherical geometry.

Uitenbroek has developed a general NLTE code for 1D, 2D and 3D problems in complete or partial redistribution. The code, called RH, uses preconditioning, short characteristics and the approximate operator of Rybicki & Hummer (1991).

In a series of papers Hauschildt and Baron and coworkers develop a 3D framework resulting in a 3D version of the atmospheric code Phoenix. A general method to calculate the radiative transfer including scattering in the continuum as well as in lines in 3D static atmospheres is presented (Hauschildt & Baron 2006, 2008) and (Baron & Hauschildt 2007). The scattering problem for line transfer is solved with an operator splitting technique. The formal solution is based on a long-characteristic method and the approximate Λ operator is constructed considering nearest neighbors exactly. The code is parallelized over both wavelength and solid angle using the MPI library and scales to very large numbers of processors. The framework is expanded in later papers in the series to spherical and cylindrical coordinate systems (Hauschildt & Baron 2009) and homologous flows (Baron et al. 2009).

MULTI3D has been used to study the 3D NLTE effects on abundance determinations of lithium (Asplund, Carlsson & Botnen 2003) employing a 21-level model atom and oxygen (Asplund et al. 2004) employing a 23-level model atom and a 50x50x100 3D model atmosphere. The MPI version of MULTI3D has been used to solve the NLTE problem of calcium in a 3D cube from the Oslo Stagger Code (Leenaarts et al. 2009).

Cayrel et al. (2007) used a 3D NLTE code developed by Steffen & Cayrel to study the line shift, line asymmetry and the ^{6}Li/^{7}Li isotopic ratio in the halo star HD 74000 employing an 8-level model atom. They find that the convective asymmetry generates an excess absorption in the red wing of the ^{7}Li absorption feature that mimics the presence of ^{6}Li at a level comparable to earlier published value.

The MUGA code is of great potential; one example of a NLTE 3D calculation is the computation of the level populations of Sr I from a 3D convection model snapshot utilizing a 5-level model atom (Trujillo Bueno & Shchukina 2007). The population densities were then used to predict the linear polarization signals we would see in the Sr I λ4607 line if we could observe it at the diffraction limit resolution of a 1m telescope. Trujillo Bueno & Shchukina (2009) also formulated and solved the 3D radiative transfer problem of the linear polarization of the solar continuous radiation. Their 3D modelling of the polarization of the Sun's continuous spectrum using a standard 3D hydrodynamical model of the solar photosphere shows very good agreement with the semi-empirical determination, significantly better than that obtained via the use of one-dimensional atmospheric models. Also the calculated center-to-limb variation of the continuum intensity is very close to the observed one.

Trujillo Bueno et al. (2004) performed 3D radiative transfer modelling of scattering polarization in atomic and molecular lines indicating the presence of hidden, mixed-polarity fields on subresolution scales. Combined with observational data these calculations indicate a tangled magnetic field with an average strength of about 130 G giving a magnetic energy density in the quiet solar photosphere at least two orders of magnitude greater than that derived from simplistic one-dimensional modelling. This conclusion was reinforced by an analysis of the Hanle effect in MgH lines (Asensio Ramos & Trujillo Bueno 2005).

Olshevsky & Shchukina (2007) studied the formation of the Ba II λ4554 line in solar hydrodynamic models. They find that NLTE and 3D effects have to be taken into account for reliable diagnostics of the solar atmosphere using this line.

Most applications of Uitenbroek's RH code have been in 2D; the one 3D example is Uitenbroek (2006) where the line bisector of the chromospheric line λ8542 from singly ionized calcium was investigated. This line, as well as other chromospheric lines, shows an inverse C-shaped bisector. The 3D computations, based on a solar convective snapshot, did not reproduce the observed shape but this could be because the convection model does not reach chromospheric heights. Similar 3D NLTE computations need to be carried out based on the new generation of chromospheric simulations.

There are thus several 3D NLTE codes around and up to 23-level atoms have been treated. With current computing resources more levels could be treated or larger computational boxes or higher spatial resolution. The computational effort is much larger than that required for one timestep in the MHD calculation; for smaller model atoms the computing time is dominated by the formal solution step in the operator perturbation methods. The increase in computational effort compared with the radiation-MHD timestep is thus approximately proportional to the increased number of frequencies multiplied by the number of iterations needed for convergence (often on the order of 50).

Since the computing time is dominated by the formal solution and the number of iterations, these are the areas where algorithmic improvements could make an impact. Strong jumps in velocity, density or temperature often lead to large jumps in optical depth. In 1D it is normally possible to solve these problems by adding grid-points in the troublesome regions. This is difficult to do in 3D simulations employing a global mesh without getting a very fine grid also in regions where it is not needed. The penalty of a fine grid is often slow convergence since large scale errors take many iterations to propagate over the fine grid. Ways out are multi-grid methods or possibly adaptive mesh refinement (refinement of the grid only locally where it is needed). More work is needed to explore these avenues. We also need a better understanding of when and why we get slow convergence or even divergence.

Another area of concern is memory demands. Storing frequency dependent quantities like opacities and profile functions (even worse: redistribution matrices) leads to very large memory demands and efficient strategies for storing on disk are needed.

Even with efficient codes available we have the problem that the quality of the output is never higher than the quality of the input. Of specific concern is the large amount of atomic data needed. Especially collisional rates are often poorly known and inconsistent sets of input data may give erroneous results. One example from the 1D world is Lemke & Holweger (1987) who had the right explanation for why the magnesium 12 μm lines are in emission but failed to get emission in their NLTE calculations because of systematically too high collisional rates in some transitions; see Carlsson et al. (1992) for a detailed account. Cross-sections for collisions with neutral hydrogen are even less known but important for the NLTE balance in many lines of importance for abundance analysis. This is known in 1D and of course also true in 3D.

4. Conclusions

3D Radiation Hydrodynamical models of solar type stars can now be routinely made with modest computational effort. These models reproduce remarkably well a wealth of observational constraints even though they are constructed with very few free parameters. Previous discrepancies with solar observations (center-to-limb variation and granulation contrast) have been resolved and for photospheric applications the "realistic" models do seem realistic and mature. Details can still be improved, especially the treatment of radiation going to wavelength split group mean opacities and opacity sampling methods. Detailed comparisons of simulations with high resolution solar observations will help improving these methods.

For the upper photosphere and chromosphere models are more experimental. More and more of the important physics is being implemented in the models: scattering, magnetic fields, conduction, non-equilibrium ionization and NLTE effects. Since the tractable computational domains are too small to include the *generation* of large scale magnetic features (like active regions) the field geometry is an imposed quantity and the simulations are not as parameter-free as the hydrodynamic, photospheric, simulations. However, much progress has been made in recent years and we may expect many exciting results in the near future.

Methods to calculate the emergent spectrum in detail from 3D models are mature. It is possible to solve the full NLTE diagnostic problem with realistic model atoms (10-100 atomic levels or more). For the upper atmosphere there are often convergence problems due to large jumps in optical depth and these difficulties need to be solved before we can routinely solve 3D NLTE for chromospheric lines. As in 1D there is a strong need for atomic data, especially collisional cross-sections.

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