Why Galaxies Care About AGB Stars:
A Continuing Challenge through Cosmic Time
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3D modelling of AGB stars with CO5BOLD

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Abstract. Local three-dimensional radiation-hydrodynamics simulations of patches of the surfaces of solar-type stars, that are governed by small-scale granular convection, have helped analyzing and interpreting observations for decades. These models contributed considerably to the understanding of the atmospheres and indirectly also of the interiors and the active layers above the surface of these stars. Of great help was of course the availability of a close-by prototype of these stars – the sun.

In the case of an asymptotic-giant-branch (AGB) star, the convective cells have sizes comparable to the radius of the giant. Therefore, the extensions of the solar-type-star simulations to AGB stars have to be global and cover the entire object, including a large part of the convection zone, the molecule-formation layers in the inner atmosphere, and the dust-formation region in the outer atmosphere. Three-dimensional radiation-hydrodynamics simulations with CO5BOLD show how the interplay of large and small convection cells, waves, pulsations, and shocks, but also molecular and dust opacities of AGB stars create conditions very different from those in the solar atmosphere.

Recent CO5BOLD models account for frequency-dependent radiation transport and the formation of two independent dust species for an oxygen-rich composition. The drop of the comparably smooth temperature distribution below a threshold determines to onset of dust formation, further in, at higher temperatures, for aluminium oxides (Al_2O_3) than for silicates (Mg_2SiO_4). An uneven dust distribution is mostly caused by inhomogeneities in the density of the shocked gas.

Keywords. convection, hydrodynamics, radiative transfer, shock waves, waves, methods: numerical, stars: AGB and post-AGB, stars: atmospheres, stars: oscillations (including pulsations), stars: winds, outflows

1. Introduction

Even classical (quasi-)stationary one-dimensional models of stellar interiors and atmospheres have to take into account the effects of convection on the transport of energy and the mixing of material and of stellar winds onto mass loss. As time- and space-resolving observations of the accessible surface layers demonstrate, these complex, truly dynamical processes are accompanied by time-dependent small- and large-scale fluctuations in brightness, density, and velocity (see, e.g., Nordlund *et al.* 2009).

Detailed radiation hydrodynamics (RHD) simulations can help to qualitatively understand these processes and are the only way to quantitatively model dynamical layers in and around stars. The first "local" simulations of small representative patches of the solar surface, comprising a few granules and the photosphere above, were performed decades ago (Dravins *et al.* 1981, Nordlund & Stein 2001, Stein & Nordlund 2001). They have since been improved on in terms of algorithms, numerical resolution, extension, boundary conditions and in particular concerning microphysics (opacities, etc.). Grids of local RHD models produced by different groups with various codes are available for the atmospheres of a wide range of different types of stars (CO5BOLD: Ludwig *et al.* 2009, Tremblay *et al.* 2015; Stagger code: Magic *et al.* 2013, Trampedach *et al.* 2013; MURaM: Beeck *et al.* 2013).

In the meantime, these atmosphere models have been extended into the chromosphere and corona (with the Bifrost code: see, e.g., Gudiksen *et al.* 2011), while interior models, that exclude the surface layers, can simulate flows in the solar interior (with the ASH code: see, e.g., Clune *et al.* 1999).

Global RHD models with CO5BOLD, using a fixed cubic Cartesian grid and a prescribed gravitational potential, were presented by Freytag *et al.* (2002) for a red supergiant (RSG), by Freytag & Höfner (2008) for an AGB star and by Freytag *et al.* (2017) for a small grid of AGB stars. Ohlmann *et al.* (2017) used AREPO to perform hydrodynamics simulations without radiation transport of an AGB star with a "moving-mesh" accounting for self gravity.

2. Challenges for 3D modelling of AGB stars

Global models of the sun and sun-like stars are currently out of reach, due to the disparity in spatial scales (a few grid points are needed per photospheric pressure scale height of about 150 km, for the entire surface of the sun with a diameter of about 1 400 000 km) and time scales (numerical time steps of around a second for at least several rotation periods of about a month and better several magnetic cycles, each spanning 22 years). See Freytag *et al.* (2012) for a discussion.

However, due to the scaling of the pressure scale height H_p with the stellar radius R_* (ignoring the dependence on effective temperature, stellar mass, and composition),

$$H_\mathrm{p} \propto 1/g \propto R_*^2, \tag{2.1}$$

one derives

$$H_\mathrm{p}/R_* \propto R_*. \tag{2.2}$$

With the expectation that the typical horizontal size of surface granules is proportional to a local length scale – as, for example, the pressure scale height – Schwarzschild (1975) estimated that the surface of cool giants might be covered by a relatively small number of giant convection cells (already suggested by Stothers & Leung 1971). This picture is consistent with observations of surface inhomogeneities in red supergiants and AGB stars (e.g., Lim *et al.* 1998, Paladini *et al.* 2018). It brings "global" 3D RHD models covering the entire convective surface of cool giants into the realm of possibility, as several granules could already be resolved by early local RHD simulations.

The first global low-resolution model computed with CO5BOLD ("COnservative COde for the COmputation of COmpressible COnvection in a BOx of L Dimensions, $L = 2, 3$") was presented by Freytag *et al.* (2002). In spite of the similarities to the now commonplace local RHD simulations of the convective surface layers and the atmosphere of solar-type stars, global RHD models of cool (super-)giants face a number of additional difficulties, as outlined in the following.

The computational domain for local simulations can be extended to cover more granules or to reach deeper down into the interior or higher up into the upper atmosphere. Alternatively, the box can be shrunk to save grid points, i.e., CPU time and memory. Global simulations, in contrast, always have to include the entire star plus a bit of the environment, which, for a given number of grid points, limits the number of granules that can be resolved. It restricts current simulations therefore to the most "fluffy" stars with lowest surface gravity and/or low stellar mass (see Freytag *et al.* 2017). According to Eq. (2.2), stars with a smaller radius will require more grid points.

Local simulations not only cover most of the line-formation region in the optically thin atmosphere but also the optically thick top layers of the surface convection zone. Truly global simulations should ideally comprise these layers and include the stellar interior with the nuclear processes close to the core, the outer convective envelope with its violent dynamics due to convection and pulsations, the inner atmosphere with its network of small shocks, the outer atmosphere, where large-scale shock fronts create sufficient conditions for dust to form, and the wind-driving region further out. Current CO5BOLD models can neither resolve nor model the stellar core in detail, nor do they contain the wind-driving region or even the necessary physics to model radiative acceleration of matter.

A freshly started simulation should at least run long enough to cover the thermal relaxation phase (of typically a few years). For meaningful statistical results, averages have to be taken over several convective turnover times (of a few months for the small surface cells and several years for the global cells with downdrafts reaching deep into the interior) and pulsational periods (of about a year, see Table 1 in Freytag *et al.* 2017). This is still short compared to evolutionary time scales, but very long compared to the radiative time scales at the level of individual grid cells (of a few hundred seconds). It means that a typical global simulation requires several million radiation-transport sub steps, which is a much larger number than necessary for a local simulation of a sun-like star.

The steep sub-photospheric temperature step due to a peak in hydrogen opacity at low densities is accompanied by a drop in density. The resulting density inversion (dense above less dense material) contributes significantly to the driving of convective motions. However, the strong local gradients in temperature and density require a good numerical resolution – ideally more than in the current models – and pose high demands on the stability of the hydrodynamics and the radiation-transport solver. At higher densities, in local models, the problem is not quite as severe but still prevalent at higher effective temperatures (see, e.g., Mundprecht *et al.* 2013 and Vasilyev *et al.* 2017).

Due to the small ratio of radiation to gas pressure in local models of sun-like – and not too hot – stars, radiation pressure can usually be completely neglected. However, in AGB stars and in red supergiants, radiation pressure becomes significant in the interior and in the atmospheres. In the standard picture, radiative acceleration of dust grains is the driver for wind formation in AGB stars (see, e.g., Höfner & Olofsson 2018).

The formation of dust is a non-equilibrium process. This means that the properties of dust cannot just be inferred from temperature and pressure alone but require a detailed time-dependent treatment of formation, transport, and destruction of dust grains (see Gail & Sedlmayr 2013 for an overview and Freytag & Höfner 2008 about a way of treating dust in CO5BOLD). Most local solar-type models do not harbor conditions that allow dust to form, in contrast to models of brown dwarfs, that require a detailed treatment of dust (without radiative pressure onto grains but with gravitational settling of dust, see Freytag *et al.* 2010).

Despite recent advances in resolving surface structures on AGB stars (see Paladini *et al.* 2018 and Paladini, this volume), there are no observations of stars available that are even remotely close to the level of detail achievable by observations of the solar surface. This means that there is no sun-equivalent to check simulations against. A further complication for the comparison of numerical models and observations is the fact that parameters of AGB stars are known with much less accuracy than the parameters of the sun.

3. 3D models with CO5BOLD: current status

The CO5BOLD code (Freytag *et al.* 2012) is able to perform radiation-(magneto)-hydrodynamics simulations of the optically thick top layers of a stellar surface convection zone and the optically thin atmosphere above. Its bread-and-butter job is to compute

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local "box-in-a-star" models covering small patches on the surface of the sun (see, e.g., Wedemeyer *et al.* 2004), other roughly sun-like stars (see, e.g., Ludwig *et al.* 2009) and even brown dwarfs (see Freytag *et al.* 2010). Gravity is assumed is to be constant, pointing downward. The lateral boundary conditions are periodic, while energy enters at the lower boundary by radiation or matter transport, and radiative energy leaves through the upper boundary (see Freytag 2017).

However, for the global "box-in-a-star" models of AGB stars presented in this paper, an external central gravitational potential for a given stellar mass is assumed. It is smoothed in the center, because the small-scale flows in the tine stellar core cannot be resolved with the current grid (see also Freytag & Höfner 2008, and Chiavassa *et al.* 2009). A central energy source corresponding to the stellar luminosity is driving the convective flows in the outer stellar layers. All the outer boundaries are very similar to the upper boundary in the local models. They allow radiation to escape and the free flow of matter. More details about boundary conditions are given in Freytag (2017). Already early simulations containing only the topmost layers of the solar convection zone demonstrated that granulation is a genuine surface phenomenon and not caused by hot bubbles produced deep inside the star. Therefore, one can expect that the simplified treatment of the stellar core in CO5BOLD only has a minor impact on the properties of the surface convection. And for stellar pulsations the extended outer layers with relatively low sound speed (i.e., long sound-travel times) are more important than the small core region with high sound speed. Still, some downdrafts reach from the surface down into the core region. Their inner overturning behavior and their interaction with pulsations in the core region via a modulation of the convective over the pulsation cycle is somewhat affected by the details of the treatment of the core region.

The computational box, that covers about 2 stellar radii, limits studies to stellar pulsations (see Freytag *et al.* 2017), surface features (see Chiavassa *et al.* 2018) or near-surface features such as shocks (see Liljegren *et al.* 2018) and the formation of dust (see Freytag & Höfner 2008 and Höfner & Freytag, in prep.). The large wind-formation region, spanning several stellar radii, is not included in current models. The outer boundaries are implemented by filling a few layers of ghost cells with extrapolated values for density, internal energy, and velocity (see Freytag 2017). While the efficient radiation transport adjusts the temperature of the gas inside the computational box rapidly to its local equilibrium value, the gas density in the outer layers during long phases of material infall to some degree depends on the detailed settings for the outer boundary. A future enlargement of the computational domain and the inclusion of radiation pressure will get rid of these shortcomings of the current setup. The omission of radiation-pressure terms might also be responsible for the inability of current models to properly reproduce the observed large extension of supergiant atmospheres (see Arroyo-Torres *et al.* 2015).

The CO5BOLD code numerically integrates the Euler equations of hydrodynamics (HD) or, alternatively, the ideal magneto-hydrodynamics (MHD) equations explicitly in time, accounting for a tabulated equation of state and an external gravity field (Freytag *et al.* 2012 and Freytag 2013). The hydrodynamics module employs a Roe solver (Roe 1986) and is used for the examples below. In both cases, the fully compressible equations are used, so that sound waves and shocks can be modelled. However, these solvers are bound to the Courant-Friedrichs-Lewy condition, which imposes a limit to the numerical time step. It is not severe for the high-Mach-number flows with efficient radiative energy exchange in AGB models but becomes important for the low-Mach-number flows in brown dwarfs (see Freytag *et al.* 2010). The MHD solver is – in principle – capable of dealing with magnetic reconnection. However, such an event will only lead to a local heating of the gas and not to the acceleration of a small number of charged particles to very high (super-thermal) velocities. This would require a different kind of solver for a more complex set of plasmaphysics equations, necessary to adequately model thin plasmas far away from the stellar surface.

In the high-Reynolds-number flows in stellar atmospheres, kinetic energy is supposed to be generated on large granular scales, transferred via a turbulent cascade to smaller and smaller scales and finally dissipated on scales given by the mean-free-path length of particles. All these scales are impossible to resolve by current or foreseeable computers. However, the assumption, that the numerical viscosity inherent in all hydrodynamics schemes has a similar net effect, explains the success of RHD simulations of stellar surface convection with their relatively coarse grids (see Nordlund *et al.* 1997). Tests with – slightly – different numerical resolutions (see, e.g., Asplund *et al.* 1999, Freytag *et al.* 2017 or Collet *et al.* 2018) don't give reasons for major concerns. However, limitations due to the finite numerical resolution should also be kept in mind, for instance, when it comes to (radiative) shocks or small-scale magnetic phenomena.

The non-local transfer of radiative energy in optically thin or thick layers is based on detailed opacity tables merged, for example, from Phoenix (Hauschildt *et al.* 1997) and OPAL (Iglesias *et al.* 1992) data. The employed short-characteristics method is designed to be able to handle large variations of opacity and source function, among others by using a piecewise linear interpolation of the source function (see Freytag *et al.* 2012). Most previous global CO5BOLD models have used grey opacities only, adequate for the study of pulsations or (near-) surface features (see, e.g., Freytag *et al.* 2017, Chiavassa *et al.* 2018, Liljegren *et al.* 2018). However, for applications that require a more realistic photospheric temperature stratification, like spectrum synthesis (see Chiavassa *et al.* 2011) or dust formation (see the example below), the frequency dependence of the opacities is treated in an approximate way by an opacity-binning technique based on a method laid out by Nordlund (1982) and further refined later on (see Freytag *et al.* 2012 and references therein). For the sample model below, going from grey (single bin) to non-grey (simple 3-bin) opacities, increases the computational effort per time step by a factor 3 and reduces the time step by a factor 2. The increase of the total computational cost per simulation by a factor 6 makes it clear why grey models are still utilized in some cases. Currently used opacity tables treat scattering as true absorption and ignore dust completely. Radiation pressure is ignored. In other words, the microphysical processes necessary to drive a stellar wind are not completely implemented, yet.

The frequency resolution of the radiation-transport step in CO5BOLD is only designed to model the exchange of heat and is not fine enough to give a meaningful stellar spectrum. Instead, a detailed spectrum synthesis is performed in a post-processing step with OPTIM3D based on stored snapshots from CO5BOLD simulations (see Chiavassa *et al.* 2009).

One pillar of the concept of (magneto)hydrodynamics is the assumption that matter is locally in thermal equilibrium and that the local material properties can therefore be completely described by two state quantities, for example pressure and temperature or, typically in numerical simulations, gas density and internal energy. Further quantities (heat capacities, sound speed, etc.) can be derived from the equation of state, i.e., by interpolation in a table. It accounts for hydrogen and helium ionization, the formation of H_2 molecules, and a representative neutral metal. Other atoms or molecules contribute only relatively little to, e.g., the partial pressure and heat capacity and are therefore ignored in the equation of state, while they are accounted for in great detail in the opacity tables. Models of time-dependent non-equilibrium processes, for example, for carbon monoxide in the solar atmosphere (see Wedemeyer-Böhm *et al.* 2005), amorphous carbon dust around AGB stars (see Freytag & Höfner 2008) or forsterite dust clouds in the atmospheres of brown dwarfs (see Freytag *et al.* 2010) assume that the contributing species do not affect the equation of state but – possibly – the opacities.

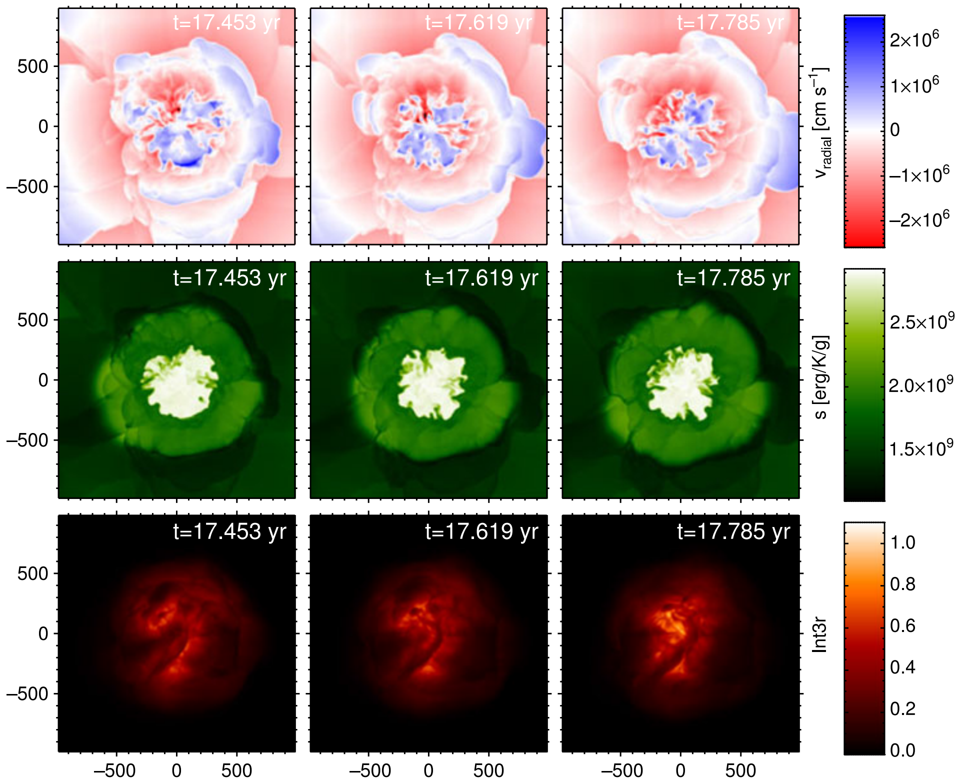

Figure 1. Time sequences of radial velocity and entropy for slices through the center of the model (st28gm06n038, rows 1–2), and the variation of relative surface intensity (bottom row). The snapshots are about 2 months apart (see the counter in the top of the panels).

4. Dust formation in 3D models

The latest 3D CO5BOLD model (st28gm06n038) of an AGB star, with $1\,M_\odot$, $7000\,L_\odot$ and solar composition, has a box size of $1970\,R_\odot$ with 401^3 grid points and uses a non-grey opacity table (see Figs. 1 and 2). It incorporates terms to describe the formation, transport, and destruction of aluminium-oxide (Al_2O_3) and silicate (Mg_2SiO_4) dust. For further details see Höfner & Freytag (in prep.).

The new extended high-resolution model confirms previous results about the dynamics in the convective envelopes and inner atmospheres of AGB stars (see Freytag & Höfner 2008, Freytag *et al.* 2017, Liljegren *et al.* 2018). Downdrafts reach from the surface of the convection zone into the core region of the model and outline a few global convection cells with lifetimes of several years. Surface cells on the other hand, driven by the narrow layer with strong superadiabaticity, flow on top of the global cells (cf. Fig. 1). Usually, they do not extend far below the surface. They have lifetimes of months. Particularly during merging events of small or large downdrafts, non-stationary convection excites acoustic waves. In the current models, only the fundamental radial mode shows up as distinct peak in a power spectrum (see Freytag *et al.* 2017). Waves with shorter wavelengths and periods do exist but are affected too much by changes in velocity field and sound speed of the background flow to achieve a lifetime that would cause a local peak in a power spectrum. When waves travel into the thin atmosphere with low sound speeds,

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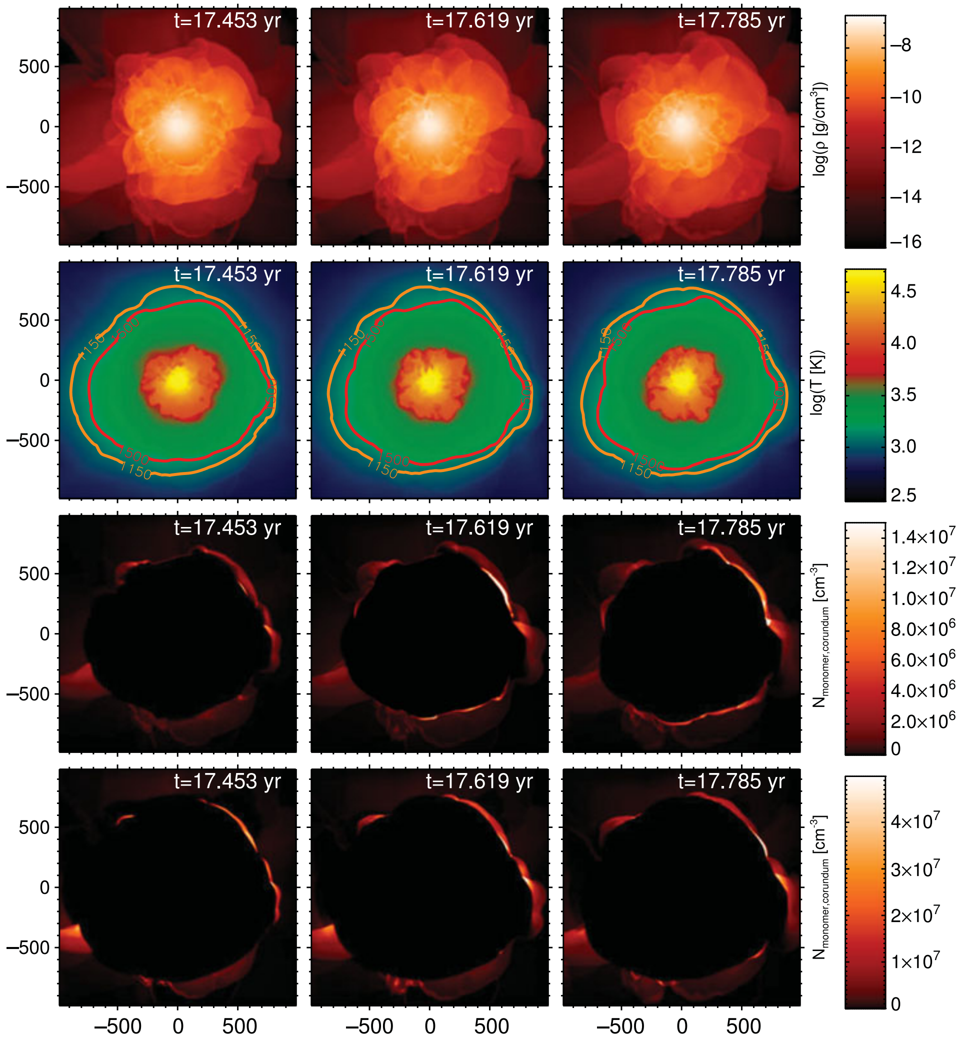

Figure 2. Time sequences of density, temperature, aluminium-oxide density and silicate density for slices through the center of the model (st28gm06n038). The snapshots are about 2 months apart (see the counter in the top of the panels).

they turn into shocks (see the velocity plots in Fig. 1 and the density plots in Fig. 2). Shorter-wavelength waves cause a complex small-scale network of shocks in the innermost atmosphere, while the fundamental pulsation mode causes a more or less spherical shock front, that is able to travel far out (see Liljegren *et al.* this volume).

New features in the current model generation are the source and sink terms for aluminium-oxide and silicate dust, based on a kinetic description of grain growth and thermal evaporation as discussed in Höfner *et al.* (2016). Once the temperatures are low enough, dust forms rather rapidly due to the high gas densities in the wake of shock fronts or at the bottom of a region with infalling material. While magnesium silicates can reach higher densities than aluminium oxides due to the higher amount of available magnesium compared to aluminium, the aluminium-oxides form further in, at higher temperatures, than silicates (compare the dust-density and the temperature plots in Fig. 2). The large

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density fluctuations of the shocked gas are reflected in the densities of the dust species (compare the dust-density and the gas density plots in Fig. 2).

5. Conclusions and outlook

The first global radiation hydrodynamics simulations with CO5BOLD of RSG stars (Freytag *et al.* 2002) and AGB stars (Freytag & Höfner 2008) were performed several years ago, but are much more demanding than local RHD models of sun-like stars or M-type main-sequence stars of the same effective temperature. That causes restrictions in numerical resolution, model extension, microphysics (e.g., opacity treatment) and number of models available. However, 3D effects can partly be incorporated in 1D atmosphere and wind models, e.g., by extracting a description of the surface velocity field from the 3D models and using this as an inner boundary condition for 1D models (see Freytag & Höfner 2008, Liljegren *et al.* 2018, and Liljegren, this volume). Grids of 1D models can easily cover large ranges of stellar parameters (see Bladh *et al.* 2015, Bladh, this volume and Eriksson, this volume).

The existing 3D models give interesting insights about the dynamics of the near-surface layers of cool giant and supergiant stars. For example, they confirmed previous ideas (e.g., of Stothers & Leung 1971 and Schwarzschild 1975) about the presence of giant convection cells but also showed that the contrast of surface features is much higher than on the sun. In addition, convective motions are much more violent, producing sound waves (as on the sun but with larger amplitudes), that turn into shocks as soon as they reach the thin atmosphere (and not higher up in the chromosphere as on the sun, see, e.g., Wedemeyer *et al.* 2004). The latest AGB model presented above demonstrates that the largest-scale shocks are able to lift high-density material into layers sufficiently cool for dust to form. The distance to the star is dictated by the temperature (i.e., the radiation field) with an inhomogeneous distribution caused by density fluctuations of the shocked gas. Aluminium oxides (Al_2O_3) form further in than silicates (Mg_2SiO_4) indicating that the combination of both plays a role for the generation of a stellar wind (see also Höfner *et al.* 2016 and references therein).

Future development will, on the one hand, focus on improving the treatment of the stellar interior to better model deep reaching convection and pulsations. This will be achieved by including terms for radiation pressure and by hierarchically refining the grid in the core region. On the other hand is the (more) refined treatment of dust (including detailed opacities and radiation pressure) crucial for the modelling of the stellar atmosphere and the wind-driving mechanism and for the computation of synthetic emergent spectra (the latter computed as a post-processing step). The inclusion of the wind-driving zone will require an enlargement of the computational box. Furthermore, first attempts are under way to include magnetic fields or stellar rotation.

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Discussion

QUESTION: How do you define the radius of the star in your simulations?

FREYTAG: In contrast to, for example the stellar mass or the luminosity, the stellar radius and with it effective temperature and surface gravity are not well-defined quantities. A radius definition consistent with observations would require the generation of synthetic images in appropriate filter bands, the degradation of the images with the instrumental profile, and the application of a similar radius-measurement algorithm as used for observed images. To circumvent this, the radius is defined as the point where the luminosity (computed with $4\pi r^2 \sigma T^4$) from the averages of the temperature over spherical shells and time matches the stellar luminosity.

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Decin: What is the physical reason for shock temperatures to be around 2000 K in the 3D models and not reach values around 10 000 K?

Freytag: The peak temperatures, that shocks can reach, decreases with distance from the star. In the layers of the atmosphere that are relevant for dust formation, efficient non-grey radiative energy transfer smoothes small-scale temperature fluctuations on very short time scale of a few hundred seconds. With the current numerical mesh, the travel time of a shock front across a grid cell is so long, that the shock is essentially not adiabatic but isothermal. Simple grey radiation transport causes longer relaxation time scales, so that shocks are accompanied by a noticeable rise in temperature. However, they never reach 10000 K, even remotely. A proper modelling of radiative shocks would require very high numerical resolution and a non-LTE treatment of gas chemistry and radiation transport – completely out of reach for our 3D simulations.

Decin: How is the dust formed, and in particular, the first seeds in your models?

Freytag: The multi-dimensional simulations can only afford a relatively simple dust model. Seeds are assumed to be always present, in a prescribed concentration. The amount of available monomers is computed from the gas and the dust density in a grid cell. The rate of grain growth or evaporation is computed via a number of of temperature- and density-dependent reaction rates.

Question: How do you manage to resolve the surface structures of an AGB star with your current numerical grid? Do you have enough grid points to resolve, for example, a pressure scale height?

Freytag: With currently feasible grids of 400^3 points or so, we can only model stars with lowest surface gravities, i.e., largest pressure scale heights and largest granules relative to the star, at the tip of the asymptotic giant branch. Going down the AGB will require a significant refinement of the grid.

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