Chapter 1

Introduction

Contents

The information we have to study distant stars comes from the photons they have emitted. Radiation escaping the atmosphere provides the single diagnostic tool for the study of these stars. Of central importance in this context are stellar atmospheres, the transition regions which separate the optically thick stellar interiors where the electromagnetic radiation is generated from the optically thin outer layers from where the photons can leave the star. The atmosphere of a star is the region which is "visible" from the outside (i.e., where most of the observable radiation is emitted), and its complexity grows as we move towards the stellar surface.

In order to truly understand stellar atmosphere, it is crucial to incorporate all underlying physics into numerical simulations. Synthetic spectra are absolutely necessary for the interpretation of observations and the extraction of fundamental data such as chemical abundances, effective temperatures, radii, etc. They allow us to generate observables from theoretical models, thereby enabling us to validate models which are necessary for deriving fundamental stellar quantities. The computation of spectra requires knowledge of the thermal structure usually provided by a model (one-dimensional or three-dimensional models, Sect. 2.1). Then, assuming local thermal equilibrium (LTE) or Non-local thermal equilibrium (NLTE), the calculation of synthetic spectrum can be done using continuous as well as line opacities.

1.1 Red Supergiant Stars

Fig. 1.1 shows the evolutionary tracks for stars of different masses. By definition, massive stars have an initial mass of at least $\sim 10\mathrm{M}_\odot$ (i.e., the minimum mass for single star

to explode latter as supernova). In order to attain hydrostatic equilibrium, these stars must produce enormous amounts of energy to counter their large gravities; the hydrogen core is burned into helium within few million years. This is followed by helium burning (about one million years), carbon burning (a few hundred years) and finally silicon-to-iron burning which takes only a fraction of a year. When the star has built up a sufficiently large iron core, exceeding the Chandrasekhar mass of $1.4\mathrm{M}_{\odot}$, it collapses into a neutron star or a black hole (expelling the envelope through a supernova explosion). As for its structure, a massive star appears first as a blue (super)giant with a radiative envelope. When hydrogen shell burning starts together with the helium core burning, the envelope expands and the star becomes convective and red. This is the red supergiant (RSG) phase that is characterized by a strong mass loss ($\mathrm{M} \sim 10^{-6}\mathrm{M}_{\odot}\ \mathrm{yr}^{-1}$; Castor 1993) of unknown origin. Once the hydrogen envelope is lost, the star becomes a Wolf-Rayet (WR) star. The WR stars can expel products of central helium burning, turning into carbon rich WR stars or oxygen rich WR stars.
An outline of the RSG phase is shown in Fig. 1.2 as well as a photo of α Ori taken by the Hubble Space Telescope in the ultraviolet (which reveals its actual size).

RSG stars have an initial mass of $10 \leq \mathrm{M}_{\mathrm{initial}} \leq 40\mathrm{M}_{\odot}$ and they precede WR stars and/or type II supernovae. Thanks to their high-peak infrared luminosity, RSGs are potential tracers of galactic structure, efficiently probing regions of high interstellar extinction. They may also become extragalactic distance indicators, if their fundamental parameters are properly calibrated.

RSG stars are late-K and M-type stars with an effective temperature ranging from 3450 for M5 spectral type to 4100K for K1 spectral type (solar metallicity, Levesque et al. 2005). The effective temperature of RSG stars is cool enough for molecules to form. The effects of molecular lines on the atmosphere of RSGs are much more significant than those of atomic lines. The most important molecular opacity sources are CO and CN at near infrared wavelengths (1-2.5 μm), TiO at optical and near infrared wavelengths and H_2O in the near- and mid-infrared wavelengths.
It is important to notice that the numerous electronic bands of TiO are in the visual and in the infrared, and their integrated absorption coefficient per molecule is much higher than, for example, CO vibration-rotation bands located in the infrared. Therefore, the TiO bands block out a considerable fraction of the total flux. The action of CO is less significant in RSG stars (in spite of its much greater abundance) because the electronic transitions fall in the ultraviolet, where there is very little flux from RSGs, and the vibration-rotation bands, though quite strong, are concentrated in a few limited wavelength regions.
Fig. 1.3 shows an example of an observed spectrum of α Ori (Josselin & Plez 2007). The rich spectra of RSGs, in which the continuum may be very difficult to trace, consists of tens of thousands of spectral features that can be identified in high-resolution spectra. A large fraction of these features are blends of several spectral lines. As a consequence, the compilation of vast tables of spectral line data is crucial to understand and model the spectra and atmospheres of RSGs.

The continuous absorption of RSGs is dominated by H^{-} bound-free and free-free ab-

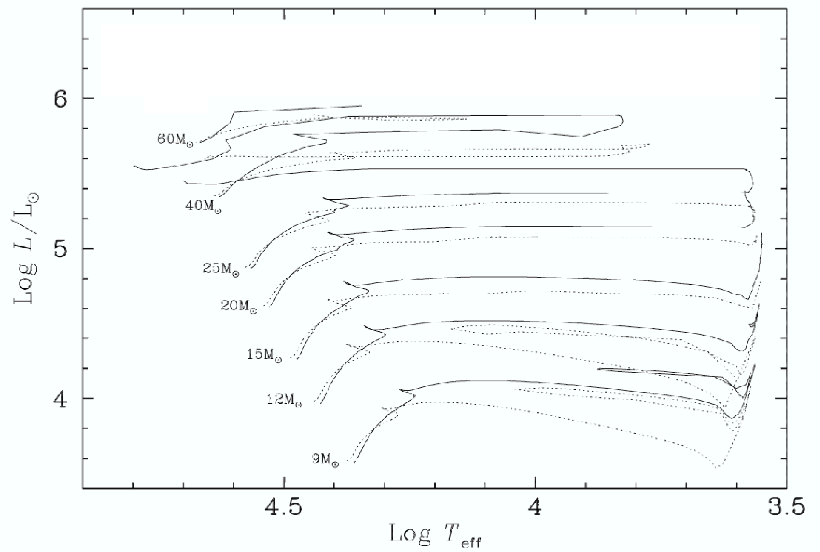

Figure 1.1: Evolutionary track from Meynet & Maeder (2003). Full line tracks represent non-rotating models and dashed line tracks correspond to models with an initial rotational velocity of 300 km/s.

sorption throughout the spectrum (except for the ultraviolet and violet spectral range).The stellar flux maximum is shifted out into the infrared, so the 1.6 μm H^- absorption minimum is clearly visible in the spectrum as a peak. Another source of continuous opacity is the free-free absorption by H_2^-, for which an electron passing a hydrogen molecule temporarily induces a dipole momentum in the molecule that interacts with the radiation field. The H_2^- absorption fills in the H^- minimum especially in the cool outer layers. In the deepest atmospheric layers, HI absorptions, excited by the higher temperatures, dominate the H^- absorption.

Rayleigh scattering by H atoms and H_2 molecules is also significant compared to the H^- absorption coefficient. Because it varies with λ^{-4}, scattering is more important at shorter wavelengths.

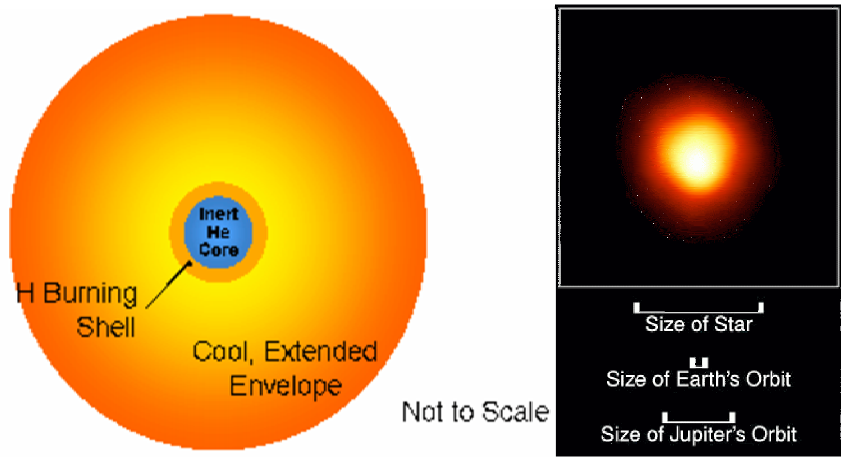

Figure 1.2: *Left panel :* outline of the red supergiant phase. The helium core contracts and heats up, and the hydrogen burns in a shell around the helium core. The envelope is huge and as big as the size of the orbit of Jupiter. *Right panel :* image of RSG α Ori (Betelgeuse) in the ultraviolet (courtesy of the NASA/STScI).

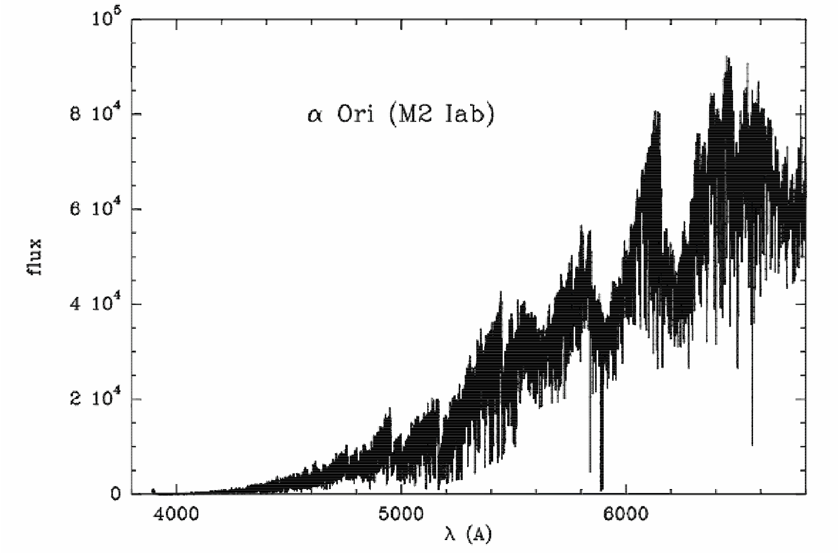

Figure 1.3: Observed optical spectrum of α Ori by Josselin & Plez (2007). The spectrum is dominated by strong molecular bands.

1.2 Principal questions about RSG

With its granules and spots, the dynamical nature of the solar surface layers has been known for a long time. A granulation pattern is also expected also on RSG star surfaces because their atmospheres are convectively unstable. For the RSG α Ori, there is a backlog of visual observations of its brightness which covers almost a hundred years. The irregular fluctuations of its light curve are clearly aperiodic and rather resemble a series of outbursts. Already more than 30 years ago, inspired by Stothers & Leung (1971), Schwarzschild (1975) claimed that very few large-scale convective cells exist at

any one time over the entire surface of RSG stars. He supposed that the pressure scale height[1] determines the characteristic scale of the convection (in agreement with the Mixing Length Theory, MLT) and adopted a constant ratio (diameter of the granule)/(depth of the granule)$\simeq$3. Extrapolating solar values, he found that the whole surface of a red supergiant should be occupied by at most a dozen cells. The fluctuations in the light curve would be the result of their combined stochastic brightness changes. Schwarzschild argued that the surface brightness varies from the hot portions of a convective element to its cool portions by a very large factor, owing to temperature fluctuations of the order of 1000 K.
The relevant scale of convection on the surface of RSGs is still uncertain.

If this convection picture is true for RSG stars, the velocity field would strongly affect their spectra. The Doppler broadening of photospheric spectral lines is a direct manifestation of the velocity field in the layers were lines form. In standard spectroscopic analyses with one-dimensional models, microturbulent and macroturbulent[2] parameters are used in order to reproduce the line broadening. A typical value of macroturbulence is 15 km/s, found by Josselin & Plez (2004) with a non-gaussian convolution.
The signature of convection is asymmetries and shifts in spectral lines (see Dravins 1982 and Dravins 1987) with a resulting bisector[3] which is typically "C"-shaped (e.g. for the Sun, Asplund et al. 2000b).
Gray (2008) found velocity and temperature variations in α Ori which were interpreted as systematic and chaotic rise and fall of photospheric material with a typical time-scale of 400 days. The bisectors measured in his work show a predominant shape resembling a reversed "C" with shifts much larger than the shape variations. In another work, Josselin & Plez (2007) measured velocity gradients in the atmosphere of RSGs and suggested the presence of both ascending and descending gas in the outermost layers of RSGs atmospheres. They argued that these movements may have a convective origin. Josselin & Plez also found time-variable Doppler shifts, line depressions, and asymmetries. They argued that they are a natural and necessary consequence of giant convective cells.
Since RSGs are so big and sometimes relatively nearby, they have also been observed with interferometers and there is a series of observations that support the convection hypothesis; observations from WHT and COAST (Buscher et al. 1990; Wilson et al. 1997; Burns et al. 1997; Tuthill et al. 1997; Young et al. 2000) revealed an irregular shape of the image of Betelgeuse, which is the signature of the giant convective pattern. The existence of hot spots has been questioned by Young et al. (2000), who achieved an equally good fit

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[1] The pressure scale height is defined as $\mathrm{H_p} = \frac{\mathrm{P}}{\mathrm{g}\rho}$

[2] In dealing with stellar spectra, it is useful to make two asymptotic approximations: (i) the *microturbulence* limit is valid when the size of the turbulent elements is small compared to the unit optical depth; (ii) the *macroturbulence* limit when the size of the turbulent elements is large compared to the unit optical depth. In practice, the microturbulence can be brought into the radiation transfer by increasing the thermal velocity in the atomic absorption coefficient, while the macrotubulence bypasses the radiation transfer altogether and it is convolved with the resulting one-dimensional spectra. Both cases incorporate only kinematic effects, the velocities and their associated Doppler shifts, and neglect the dynamics such as changes in temperature and pressure caused by motions.

[3] It is the locus of the midpoints of the line. A symmetric profile has a straight vertical bisector, while the "C"-shaped line bisector reveals asymmetries.

to the interferometric data with a model of a disk and a cool spot. A large spot was also detected on Betelgeuse with the Hubble Space Telescope (Gilliland & Dupree 1996). The evidence of small scale structure was also found by di Benedetto & Bonneau (1990) on the giant β Andromedae.

With the increasing spatial resolution of interferometers like ESO's VLTI, resolved images of RSGs will be obtained in the near future. Observations of this type are of great significance for giving information on convective inhomogeneities and on other dynamic modes and surface structures. Moreover, the investigation of the signature of the convection on the visibility curves and phases is of great interest and their interpretation must go beyond the simple circular-symmetric parametric models. For this purpose, more complex models are needed for a qualitative and quantitative analyses.

In order to be able to interpret observed spectra in terms of abundances and fundamental parameters (such as luminosity, radius and mass) it is crucial to fully characterize the convection in RSGs. This includes a proper understanding of the size of the convective cells, their evolutionary time-scales as well as their velocity fields.

Unfortunately, the radius of these stars is difficult to define because of the extended atmosphere of RSGs. Consequently, the effective temperature and the surface gravity remain ambiguous.

Fundamental parameters can be estimated with spectrophotometry observations (e.g., Lançon et al. 2007 or Levesque et al. 2005) where the continuum flux spectra can be compared with the synthetic spectra obtained from stellar models. As an example, Levesque et al. (2005) used the new generation of MARCS models which include a much improved treatment of molecular opacity (Gustafsson et al. 1975, Plez et al. 1992 and Gustafsson et al. 2008). Using absolute spectrophotometry (both continuum fluxes and the strengths of the G bands for K stars and the TiO bands for M stars), they determined the effective temperature, luminosity, mass and reddening of a large sample of RSGs and they found a good agreement with evolutionary tracks.

The determination of elemental abundances is very sensitive to the value of fundamental parameters. Such determinations offer insight on the role played by these stars on the nucleosynthesis in galaxies. RSGs are among the brightest stars and are apt for determining the general abundance characteristics of galaxies.

RSGs are undergoing a particular nucleosynthesis[4] and dredge-up which modify their surface composition. This dredge-up is not yet well understood, but we know that convection plays a crucial role. **The effect of granulation on abundance determinations is of capital importance for the study of galactic chemical evolution.**

In the literature, studies of abundance determinations for RSGs are scarce (see, e.g., Carr et al. 2000 and Cunha et al. 2007). This is due to many factors. (i) RSGs are so crowded with lines from atoms and molecules that there is little hope to see the continuum. Therefore, it is difficult to measure reliable equivalent widths in the optical wavelength range. (ii) More reliable molecular data is needed for the model atmosphere. (iii) The derivation

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[4] RSGs are expected to be a source of elements beyond the iron peak, the so-called weak s-elements. For example, Lundqvist & Wahlgren (2005) reported the presence of weak s-elements on α Ori.

of the fundamental parameters is far from trivial. (iv) The velocity field must be know in order to characterize the line broadening.
Once the dynamical structure of the red supergiants will be known and correctly represented by theoretical models, abundance analyses will inevitably progress.

Another point of concern is the mass-loss of RSGs. The mass-loss rates are particularly significant ($M \sim 10^{-6}$ $M_\odot$ yr^{-1}; Castor 1993). **The exact mechanism driving the mass loss in RSG stars is still unknown**. A precise derivation of the mass loss rate, the associated wind's expansion velocity and its geometry are difficult because RSGs show, at best, very weak circumstellar molecular emission (Josselin et al. 1998).
A stellar wind requires a source of momentum, i.e., an outward-directed force that can overcome gravity. Stellar winds can be: (i) *thermal winds* driven by the gradient of the gas pressure, which requires a high pressure in the wind-formation zone, and may be created by, e.g., dissipation of sound waves or by radiative heating of the gas; (ii) *radiation-driven winds* (mostly in hot stars) driven by the gaz and/or the dust absorbing the outward-directed stellar radiation and reemitting photons in all directions, this creates a radiation pressure directed away from the star; (iii) *wave-driven winds* driven by sound waves, shocks and magneto-hydrodynamics waves. Even if these waves are not sufficiently efficient for directly driving a wind by momentum input, they should considerably help in generating thermal winds (by heating, increasing the gas pressure) or radiation-driven outflows (by enhancing the density of the outer atmospheric layers so that relevant absorbing species like molecules, or dust can form more efficiently and the radiative pressure can act on molecular lines).
One possible mass-loss scenario for RSGs could be from large-scale motions of the outer layers, resulting in waves that propagate through the density gradient of the atmosphere thus developing strong radiating shocks. As the shock front passes, the gas is compressed, heated, and pushed outwards. Eventually, the temperature in the shocked gas drops by radiative cooling, resulting in a relatively cool, dense and outward-moving wind.
In the asymptotic giant branch stars (AGBs), the favorable conditions (high density and sufficiently cool temperatures) give rise to dust grains formation. A combination of stellar pulsation (shock waves) and radiative driving (dust) can produce realistic mass-loss rates (see the review by Gustafsson & Höfner 2003). The result is a source of momentum for the wind. In RSGs the situation is different. Josselin et al. (2000) analysed infrared photometric and millimeter spectroscopic observations of a sample of RSGs. They showed that the molecular gas-to-dust ratio (the gas mass-loss rate is estimated from CO emission following Olofsson et al. 1993) shows a very large scatter and is generally higher than what is observed for AGB stars. RSGs are generally low amplitude and irregular variables, indicating that they cannot be pulsators of the same type as most AGBs. In addition, significant amounts of dust are found at larger radii (∼20 stellar radii, Danchi et al. 1994) so the radiation pressure on dust cannot occur in the wind acceleration zone. Hence, models of mass loss for AGB stars, based on pulsations and radiation pressure on dust grains, are not applicable to RSGs.

A last point concerns the existence of molecular layers around RSGs. The first to put forward the idea of such a "MOLsphere" was Tsuji (1988). The MOLsphere is a stationary, warm envelope situated above the photosphere but within the cool, expanding circumstellar shell. The space between the layer and the photosphere is considered empty. The MOLsphere has been used in several cases for the interpretation of interferometric data to explain the near-infrared structure of α Ori by Perrin et al. (2004a) who described it with two main components, the photosphere and a surrounding shell possibly containing CO, H_2O and SiO; Perrin et al. (2005) found a surrounding shell also around μ Cep; Ohnaka (2004) has shown that the apparent near- and mid-infrared angular sizes of the two supergiants α Ori and α Her can be understood in terms of a star with an envelope of warm H_2O; Tsuji (2000) and Verhoelst et al. (2003) assumed that the signature of water vapor in spectra of α Ori originates from a layer around the star.

In this context, water is one of the most abundant molecules in RSGs and it is a dominant source of opacity in the infrared. Ryde et al. (2006) analyzed high-resolution spectroscopic data of water vapor at lines around 12 μm from α Ori. They argued that an inhomogeneous outer atmosphere could explain the observations. However, Ryde et al. show that neither published MOLsphere models, nor a synthetic spectrum calculated on the basis of a classical model photosphere match their spectra.

The existence or not of the MOLsphere around RSGs is still uncertain.

1.3 Radiation Hydrodynamic simulations

In this thesis, I use the three-dimensional radiation hydrodynamics (RHD) simulations calculated with CO^{5}BOLD (*COnservative COde for the COmputation of COmpressible COnvection in a BOx of L Dimensions with l=2,3"*) code (Freytag, Steffen, & Dorch 2002, F2002 therein). The key point of such simulations is the coupling of radiation field (treated using grey opacity tables) and hydrodynamics, which dominates the physics of the transition layers, where the gas becomes optically thin. These models are time dependent and they account for the convective motions and the horizontal inhomogeneities.

With this tool at hand, I will thoroughly explore the principal characteristics of the RHD simulations, establishing their advantages and limitations.
I will investigate the surface structure of RSGs and the impact of convection on stellar parameter determinations through spectroscopy and interferometry predictions.
I will also explore the impact of the granulation on visibility curves, phases, and will discuss the detection and characterization of granulation (contrast, size) on RSGs. In addition I will provide appropriate average limb-darkening coefficients.
I will investigated the presence of the so-called MOLsphere in terms of spatial distribution (interferometry in the near infrared).

Finally I will be able to answer or to propose a solution to some important questions:

- *Are the three-dimensional models consistent enough for the interpretation of observations?*
- *What does the surface of a RSG look like? How can the convection pattern be detected and characterized?*
- *How does the convection affect the spectral lines? Are the three-dimensional models better than the one-dimensional ones?*
- *What are the velocity fields in RSGs and what is the origin of their mass-loss?*

1.4 Thesis content

In this thesis, I study the atmospheric dynamics of red supergiant stars using RHD simulations and combining spectroscopy and interferometry to validate the models.
In Chapter 2, I introduce the three-dimensional hydrodynamical simulations of red supergiant stars based on the CO^{5}BOLD numerical code.
Chapter 3 reports the description of the 3D radiative transfer code (OPTIM3D) that I have developed and that is employed to solve in detail the radiation transfer problem and to create spectroscopic and interferometric observables.
In Chapter 4, I show the principal characteristics of the hydrodynamical simulations of red supergiant stars.
Thereafter, Chapter 5 and 6 introduce the results obtained with spectroscopic analyses.

Comparisons with observations in the optical and infrared are presented together with the determination of characteristic velocities in the atmosphere. Chapter 7 and 8 are centered on interferometric results: after a short introduction and the presentation of the code I have developed for computing visibility curves and phases from synthetic images, I detail the prospects for the detection and characterization of granulation (contrast, size) on RSGs and I conclude with the first interpretations of interferometric data in the infrared. In Chapter 9, I explore the effect of the non-grey treatment of opacity on three-dimensional hydrodynamical simulations.
The final Chapter contains the conclusion and perspectives.