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Radiation Hydrodynamics Simulations in 3D with COBOLD

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Abstract

Modelling a stellar atmosphere as a stationary 1D stratification is only valid if the expectations about the accuracy are not to high. As soon as observations become god enough, they reveal all kinds of time-dependent fluctuations as e.g. granulation, oscillations, shock waves, Sun/star spots and other magnetic phenomena, instationary winds, ...

To study at least some of these phenomena in cool star atmospheres and extend the previous two-dimensional models to three dimensions a new code ("COBOLD") has been written. It solves the coupled non-linear equations of compressible hydrodynamics in an external gravity field together with non-local frequency-dependent radiation transport.

The code can operate in two "modes" to simulate either a small piece of a stellar atmosphere with a constant gravity field ("solar mode") or to include the entire star with a central gravitational potential as appropriate for Betelgeuse ("supergiant mode").

In this poster some features of COBOLD as well as recent results from simulations of Betelgeuse are presented.

Introduction

Basic ingredients of a model of stellar surface convection are compressible hydrodynamics in the presence of a gravity field to describe the transport of energy by matter and non-local radiation transport to describe the cooling upper layers, where radiation is emitted into free space, and the horizontal energy exchange which reduces temperature fluctuations.

General features of granulation can be investigated with low-resolution models, grey opacities, and even in 2D. Detailed models need fully 3D geometry, some account for the frequency-dependence of the opacities, an refined grid and enlarged spatial extent of the model. Currently, no effort is undertaken to include Non-LTE effects, time-dependent ionization/chemistry or magnetic fields.

Development of COBOLD

To extend the previous two-dimensional Kiel models of stellar surface convection to three dimensions a new Fortran90 code (CO^5BOLD: "COnservative COde for the COmputation of COmpressible COnvection in a BOx of L Dimensions, L=2,3") based on a more modern algorithm has been written.

It solves the coupled non-linear equations of compressible hydrodynamics in an external gravity field together with non-local frequency-dependent radiation transport. Operator splitting is applied to solve the equations of hydrodynamics (including gravity), the radiative energy transfer (with a long-characteristics ray scheme), and possibly additional 3D (turbulent) diffusion in individual sub steps.

Some of the features of the code are described in the following.

Hydrodynamics

The hydrodynamics scheme of COBOLD uses a finite volume approach with a non-staggered Cartesian grid for the basic quantities. By means of operator (directional) splitting (Strang, G. 1968, SIAM J. Numer. Anal. 5(3), 506) the 2D or 3D problem is reduced to one dimension. To compute the fluxes across each cell boundary in every 1D column an approximate 1D Riemann solver of Roe-type is applied. Small amounts of extra smoothing can be added by activating a standard 2D/3D tensor viscosity.

Accuracy versus Stability

A hydrodynamics code should represent the true solution to an initial/boundary value problem as closely as possible on a given grid. This can be achieved by using high-order discretizations of all differential operators. A direct application leads to stability problems especially in regions where the true solution is not smooth. Therefore, an additional numerical viscosity can be applied, which has to be thoroughly tuned not to destroy the accuracy of the basic scheme, which can turn out to be a difficult task.

As an alternative, COBOLD separates the 3D hydrodynamic equations into three 1D sub step ("directional splitting"). To compute the fluxes across each cell boundary in every 1D column an approximate Riemann solver (Roe, P.L. 1986, Ann.Rev.Fluid Mech. 18, 337) is applied. The partial waves are advected with upwind-centered fluxes. A slope limiter or a reconstruction with monotonic parabolae is applied to decrease the order of the scheme to keep it stable in the neighborhood of discontinuities while preserving higher order accuracy in the case of smooth flow configurations.

While this hydrodynamics scheme is able to handle most 1D problems and many 2D/3D problems by its own build-in stabilization mechanism, there are certain multi-dimensional cases where instabilities occur near strong shocks that are nearly aligned with the grid (Quirk, J. 1994, Int. J. for Numerical Methods in Fluids 18, 555). To overcome such (possible) problems, an additional tensor viscosity sub step was included in the code that can add a dissipation in a way the Roe solver by its own is not able to produce.

Conservativity

Care was taken to write the discrete equations in conservative form to preserve some conservation properties of the original equations. This means that e.g. total mass or energy only change due to fluxes through the boundaries of the computational volume and are exactly preserved in case of closed boundaries.

This guarantees that in a scheme, which is stable and where the discrete equations are consistent with the original ones, shocks move with the right speed and have correct jump conditions. The time-and-space-averaged total energy flux through a convection model must be constant with height. This was not exactly fulfilled for the former code which was hardly any problem for the relatively moderate flow velocities of solar granulation. But it becomes a problem for the more violent convection in early main-sequence F-type stars and is crucial for simulations of a red supergiant with its enormous velocities. Exact conservation of mass and energy is particularly useful in low-resolution calculations.

Equation of State

Ionization effects are treated by taking the pressure and its derivatives as function of density and internal energy from a table

The differences in the code compared to the case of an ideal gas with constant γ manifest themselves in modifications of the formulae for the Roe averages (e.q. the dimensionless quantity Γ_1 has to be averaged) and an additional term for the advection of "ionization energy". Instead of accounting for the transport of the "ionization energy" with a term proportional to the mass flux, a "sixth partial wave" was introduced exclusively for it. It is always zero in the case of a simple gas (without gravitation).

Source Terms due to Gravity

Gravitational source terms destroy the hyperbolic character of the hydrodynamical equations and inhibit the direct application of an (approximate) Riemann solver to it.

On the other hand, the separation via operator splitting is not a good idea in this case because in stratified atmospheres the terms describing pressure gradient and gravity tend to cancel each other (nearly). Their application in sequence – and not together in a single step – would cause spurious unwanted accelerations back and forth. And the naive combination of the Roe solver and the source terms due to gravity into a single operator just by adding them leads to problems, because the Roe solver interprets the strong pressure gradients in a stratified atmosphere as indication of shock waves, which are then treated as such. The result might turn out to be quite unexpected.

Luckily, there is some freedom in the choice of the exact run of the reconstructed quantities inside the cells (Mellema, G., Eulderink, F., Icke, V. 1991, A&A 252, 718). This freedom is used to amalgamate the hydrodynamics and the gravity operator by compensating the pressure jump across a boundary by the pressure gradient of an hydrostatic stratification. The latter is subtracted from the actual pressure inside the cells during the computation of the amplitudes of the partial waves.

The idea is, that only pressure deviations from a hydrostatic equilibrium – and not already pressure gradients – should give rise to fluxes of the partial waves. In the exactly hydrostatic case the Roe solver should "sense" no sound waves.

Grid and Geometries

The grid has to be Cartesian. But it is allowed to be non-equidistant. The code can handle 1D, 2D, and 3D models.

Speed

During each directional sub step the individual columns are independent from each other and can be collected into chunks and processed efficiently by different CPUs. The parallelization is done with OpenMP directives, which restricts the application to shared memory architectures, so far. The size of the chunks can be chosen to make them fit into the L2 cache each at a time. The numerical operators are grouped together to optimize the reuse of quantities in the L1 cache. But the number of quantities and the complexity of the operators turned out to be to large to get an opimal reuse of the (few) CPU registers available. Therefore, the impressive performance values of some linear algebra packages could not be reached.

However, the radiation transport routines consume most of the CPU time and are prime candidates for further optimization.

Simplicity

Ideally, a code should stay simple and maintainable, while being accurate and fast. The operator splitting in COBOLD separates hydrodynamics and radiation transport very well and allows independent development and testing of the respective modules.

However, the original Roe solver itself has lost part of its simplicity and elegance during the transformation to a "real world" code. Especially the inclusion of gravitational source terms and also of a general equation of state resulted in several additional equations, temporary quantities, and numerical steps, and turned out to be far from straightforward (at least for me).

Radiation Transport

Is is separated from the hydrodynamics steps via operator splitting. This is exact in the case of a stratification in hydrostatic and radiative equilibrium, when the individual operators cause no change at all and therefore the entire operator gives no change.

The radiation sub step uses a long characteristics method, in which the equation of radiation transport is solved along a representative number of rays with various inclinations. First, some quantities (e.g. temperature and density) are interpolated from the hydrodynamics grid onto a ray. Here, the equation of radiative energy transfer is solved with a Feautrier method. The source function is computed in strict LTE. Non-LTE effects and scattering are ignored. The resulting radiative fluxes and the energy changes per volume on the ray have to be distributed back onto the hydrodynamics grid, where the energy is updated in a conservative way. The opacity table are grey or account for frequency-dependence by some binning technique.

For the two different geometries (box contains only a small fraction of a stellar surface with periodic side boundaries, "solar case", or box contains an entire star with all six boundaries open, "supergiant case") there exist two different modules relying on the same microphysics (opacities, equation of state).

"Solar" Module

It has been developed mainly by Matthias Steffen and is a 3D extension of the routines used in the old 2D Kiel code (see Ludwig, H.-G. 1992, PhD thesis (German), University of Kiel; Ludwig, H.-G., Jordan, S., Steffen, M. 1994, A&A 284, 105). Periodic lateral boundary conditions are appropriate for the solar surface layers. Special care is taken to model the flux in the preferred vertical direction precisely by choosing fixed optimized θ angles, whereas there are e.g. no nearly horizontal rays, because they would cause problems in connection with the periodic boundaries. All rays in a given direction have the same length.

“Supergiant” Module

It has been newly developed for the “Star-in-a-box” case. All side boundaries are open, which implies that the individual rays might have different lengths. On the other hand, all directions are equivalent and have to be treated with the same accuracy. Each radiative time-step uses only a small number of rays (e.g. 3 orthogonal rays). Their orientation is varied randomly between sub time steps to cover all directions equally.

Radiative Time-Scales

In the surface layers of hot stars and also of red supergiants like Betelgeuse the ratio of radiative to hydrodynamic time-scales is smaller than in the Sun. This poses severe restrictions on the numerical time step, if the radiation transport is treated explicitely.

As a consequence, in COBOLD the numerical solution can be advanced alternatingly by several small radiative sub time step and a larger hydrodynamics step.

A more clever alternative is to treat the radiation transport implicitely. Unfortunately, this means that even in the case of strict LTE the source functions is not independent of the radiation field anymore: the temperature changes due to radiative energy exchange within a time step have to be taken into account. This can be done by an ALI scheme, which has been successfully implemented and used in the old Kiel code. Its application in COBOLD is not yet satisfying, because the gain in the size of the time step is not larger than the number of iterations needed, so far. Clearly, some more work is needed here.

Some Facts about Betelgeuse

Parameters

- α Orionis, HD39801, HIP27989
- M2 Iab Supergiant
- Star with largest apparent diameter (after the Sun)
- Distance $d_{\rm Hipparcos}$=131±30 pc
- Apparent radius R=22.1 mas ⇒ R=620 $R_\odot$
- M=6 $M_\odot$, $T_{\rm eff}$=3600 K, $\log g$=-0.5,
  (or M=15 $M_\odot$, $T_{\rm eff}$=3500 K, $\log g$=0.0)
- Solar atmospheric composition

Observations

Observations reveal temporal brightness fluctuations, an extended hot atmosphere, and an irregular temporally variable surface structure.

By now, there are photometric data available covering a time span of almost 100 years. They come from various short-term photometric campaigns and from collected observations of amateur astronomers (Leo Goldberg 1984, PASP 96, 366). The overall brightness of Betelgeuse varies on time-scales of weeks, months, and years.

Observations with optical interferometers started 12 years ago. They still have an extremely low resolution but definitely show deviations of the image from circular symmetry. The measurements can be fitted by a model comprising a circular disc plus 0 to 3 bright spot(s) (Buscher et al., 1990, MNRAS 245, 7p; Wilson et al., 1992, MNRAS 257, 369; Tuthill et al., 1997, MNRAS 285, 529; Wilson et al., 1997, MNRAS 291, 819; Klueckers et al., 1997, MNRAS 284, 711; Burns et al., 1997, MNRAS 290, L11; Young et al., 2000, MNRAS 315, 635).

In the last paper, the possibility of a fit with a circular disk and a single *dark* spot is discussed.

Ronald L. Gilliland and Andrea K. Dupree took a direct UV image with HST (1996, ApJ 463, L29) with obvious deviations from circular symmetry. The VLA radio-observations by Jeremy Lim, Chris L. Carilli, Stephen M. White, Anthony J. Beasley, Ralph G. Marson (1998, Nature 392, 575) cannot resolve the very surface of the star, but reveal an asymmetric extended outer atmosphere.

Spectra (even some spatial resolution is possible) indicate large atmospheric and chromospheric velocities. But in general, spectroscopic observations of Betelgeuse are difficult to interpret due to the lack of a reliable (3D) model atmosphere (see David F. Gray 2000, ApJ 532, 487 for an attempt).

Some Theory

Based on simple scaling arguments, Martin Schwarzschild suggested in 1975 (ApJ 195, 137) that a few giant granules on the surface of Betelgeuse are the cause for the observed temporal brightness variations: if the typical horizontal extent of a granule is a fixed multiple of some characteristic vertical scale length (e.g. the pressure scale height), granules on a supergiant will be much larger than on the Sun, not only in absolute but also in relative size.

In the meantime pulsations, shocks, rotation, and magnetic fields have been invoked besides convection to be responsible for some of the observed phenomena (see e.g. Gilliland & Dupree 1996).

Setup for first “realistic” Betelgeuse Model

To put the star in the box, a spherical potential for given stellar mass M_*=6 $M_\odot$, inner smoothing radius $r0_{\rm grav}$=166 $R_\odot$, and outer smoothing radius $r1_{\rm grav}$=1175 $R_\odot$ is prescribed by

$$\phi(r) = \frac{-G_{\rm grav} M_*}{\sqrt[4]{r0_{\rm grav}^4 + r^4 \sqrt{\frac{1}{1+\left(\frac{r^2}{r1_{\rm grav}^2}\right)^4}}}} \tag{1}$$

with r as the distance to the center of the star. The computational volume is a cube with an edge length of $2{\times}988 R_\odot$ and 127^3 grid points.

Within a sphere of radius $r0_{\rm grav}$ the internal energy is adjusted to keep the entropy close to a prescribed value ($3.25\,10^9$ erg/K/g). This mimics the energy production by nuclear fusion in the real stellar core.

The outer boundaries are open, i.e. transmitting for waves.

The opacity tables rely on realistic data but are simple grey Rosseland means. They are a merger of the PHOENIX opacities (Hauschildt, P.H., Baron, E., Allard, F. 1997, ApJ 483, 390) and OPAL tables (Iglesias, C.A., Rogers, F.J., Wilson, B.G. 1992, ApJ 397, 717), kindly provided by Hans-Günter Ludwig.

The model is characterized by the parameters $T_{\rm eff}{\sim}3200$ K, $\log g{\sim}$-0.5, $L_*{\sim}50000\,L_\odot$.

The model turns out to be slightly to cool for Betelgeuse and is lies at the lower end of the allowed surface gravity range but should be sufficient to draw some first conclusions and to demonstrate what the simulations can provide (and what they are not yet able to do).

The simulations were performed on a SGI at TAC in Copenhagen and a Cray at the computer center at the CAU in Kiel.

Results

The initial model for the simulation is a sphere in hydrostatic equilibrium. Due to convective instability, a pattern of convective cells forms, which is highly symmetric because of the initial conditions. After some time the symmetry is destroyed due to the influence of small non-isotropic numerical terms.

A sequence of surface intensity images from a later stage with completely irregular surface structures is given in Fig. 1. A sequence of entropy slices is presented in Fig. 2 which nicely shows the deep-reaching downdrafts. The temperature slices in Fig. 3 demonstrate the formation of shock waves in the atmosphere.

Although envelope convection in a red supergiant is still driven by a network of surface cells, they significantly differ in properties and appearance from solar granulation. Convection in a red supergiant is characterized by

- smaller ratio of radiative to hydrodynamic time-scales
- larger convective cells (measured in atmospheric pressure scale heights)
- larger convective velocities (with particularly strong tangential flows)
- larger pulsations, stronger interactions with convection
- larger surface intensity fluctuations, less obvious "granular" pattern

While in the solar case small granules or the rims of some granules are the brightest structures, the surface images of the red supergiant (Fig. 1) shows its brightest features over intergranular lanes. This is due the temperature dependence of the opacities and sensitively depends on the surface temperature of the star.

Temporal variations of the surface intensities up to a factor 2 are due to irregular pulsations with a period of around 1.5 years plus some phenomena of convective origin on shorter time-scales.

Surface Intensity

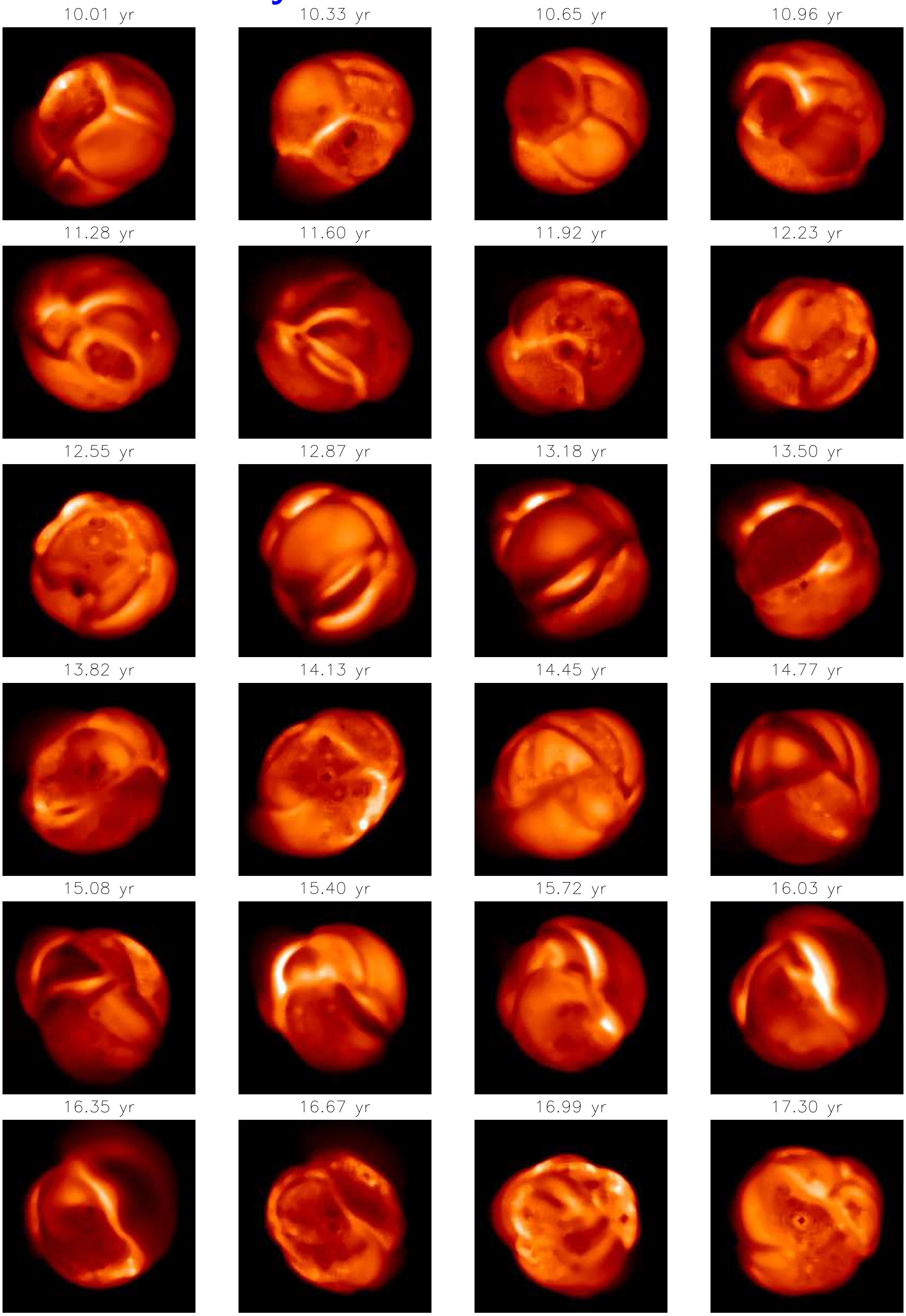

Figure 1: Sequence of surface intensity snapshots ($T_{\rm eff}$=3200 K, $\log g$=-0.5, 127^3 grid points). At the top the simulated stellar time is indicated in years. The surface cells are similar to solar granulation at 10.65 yrs. But occasionally, there are small bright features near the disk center (16.03 yrs) or the at the rim (15.40 yrs) above downdrafts.

Entropy Slices

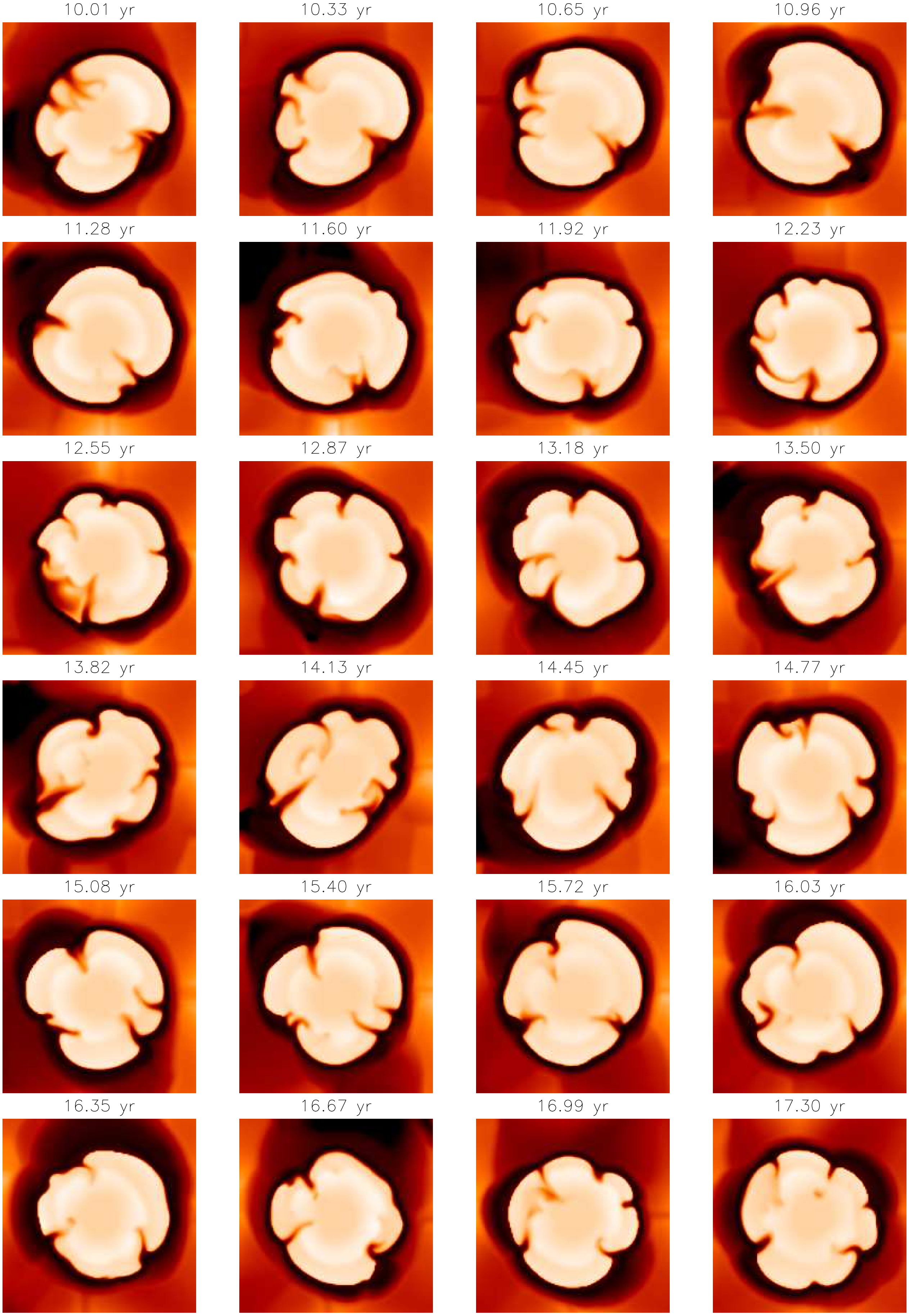

Figure 2: Sequence of entropy slices ($T_{\rm eff}$=3200 K, $\log g$=-0.5, 127^3 grid points). The star is not really spherically symmetric anymore. In a slice there are 3 to 6 downdrafts, some of them reaching deep into the star.

Temperature Slices

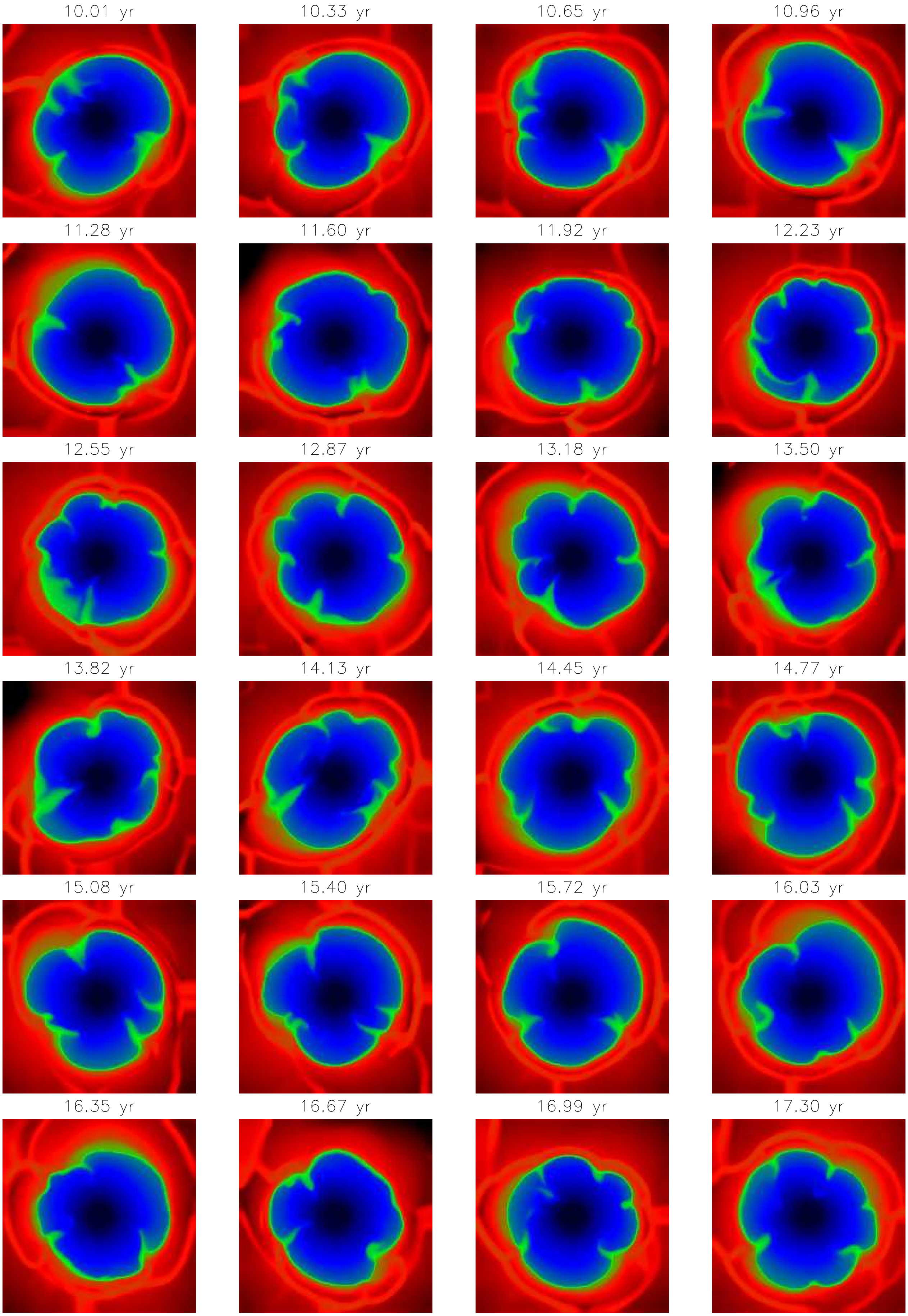

Figure 3: Sequence of temperature (ranging from 1500 K to 150 000 K) slices ($T_{\rm eff}$=3200 K, $\log g$=-0.5, 127^3 grid points). Shock waves run into the outer atmosphere, moving mainly radially.

Conclusions

- Simplified but realistic simulations of a red supergiant "star-in-a-box" including non-local radiative transfer are now becoming feasible. While the current model is slightly to cool to be appropriate for Betelgeuse, it nevertheless shows interesting results:
- The surface of a red supergiant is covered by giant convection cells.
- The deviations from spherical symmetry are significant.
- Atmospheric velocities are large (with peak values of 20 – 30 km/s). Shock waves are ubiquitous.
- The granulation appears not to be solar-like. The surface pattern is not simply composed of "bright granules and dark intergranular lanes". The intensity contrast exceeds the solar value.
- Occasionally, there are bright features (hot spots?) over downdrafts.
- Pulsations and their interaction with convection play an important role.

Main Problems

- The short radiative time-scales make the computation of the radiation field very time-consuming.
- A high number of grid points is needed to resolve all features, particularly the steep temperature jump just below the photosphere.

Future Development

- An adjustment of the basic parameters is necessary to find values most appropriate for Betelgeuse.
- A faster version of the code is needed to allow an increase of the number of grid points, frequency-bins,. . .
- Improved input physics (frequency-dependent opacities, radiation pressure, self-consistent gravity, dust, . . .) will lead to more realistic models.