Pulsation – convection interaction

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Abstract. A lot of effort has been devoted to the hydrodynamical modelling of Cepheids in one dimension. While the recovery of the most basic properties such as the pulsational instability itself has been achieved already a long time ago, properties such as the observed double-mode pulsation of some objects and the red-edge of the classical instability strip and their dependence on metallicity have remained a delicate issue. The uncertainty introduced by adjustable parameters and further physical approximations introduced in one-dimensional model equations motivate an investigation based on numerical simulations which use the full hydrodynamical equations. In this talk, results from such two-dimensional numerical simulations of a short period Cepheid are presented. The importance of a carefully designed numerical setup, in particular of sufficient resolution and domain extent, is discussed. The problematic issue of how to reliably choose fixed parameters for the one-dimensional model is illustrated. Results from an analysis of the interaction of pulsation with convection are shown concerning the large-scale structure of the He II ionization zone. We also address the influence of convection on the atmospheric structure. Considering the potential of hydrodynamical simulations and the wealth of ever improving observational data an outlook on possible future work in this field of research is given.

Keywords. convection, stars: oscillations, stars: variables: Cepheids, stars: variables: RR Lyrae

1. Motivation

Astrophysics has enormously benefitted from the advent of large scale surveys and from ever improving high precision measurements. The data on Cepheids observed in the OGLE-III field of the LMC (Soszyński *et al.* 2008), for instance, comprises a unified sample of the observed distribution of various types of Cepheid pulsators. This set of data is capable of challenging theoretical models well beyond what had been possible when discrepancies between first generation models and observational data on the famous pulsational mass problem had become evident (Stobie 1969). Likewise, the identification of non-radial modes in the classical pulsator V445 Lyr, an RR Lyr type star (Guggenberger *et al.* 2012), widens future possibilities to constrain the models of such types of stars.

Although these developments are intriguing from the viewpoint of hydrodynamics and stellar physics, the non-specialist might be tempted to ask: how is it possible that classical pulsators such as Cepheids, after all those years of research, are still of interest to astrophysics in general? The most straightforward answer is that Cepheids are one of the most crucial parts of the cosmic distance ladder (cf. de Grijs 2011). Their precise quantitative description holds the key to them becoming an instrument of simultaneous precision measurement of distance and chemical composition in galaxies beyond the Local Group.

Well-known problems of research on Cepheids that keep reappearing include the already introduced discrepancies found when comparing masses from stellar evolution with those resulting from stellar pulsation modelling (Keller 2008, Pietrzyński *et al.* 2010, Cassisi & Salaris 2011) and explanations to the location of double-mode (and even triplemode) pulsators (cf. the data discussed in Soszyński *et al.* 2008). 1D models that have previously been claimed to have resolved this question (Kolláth *et al.* (1998) and Feuchtinger (1998) for RR Lyr stars; cf. the critical discussion in Buchler (2009)) eventually turned out only to have done so by chance, lacking a solid physical justification for their success (see the general discussion in Smolec & Moskalik (2008a) and the work on double-mode Cepheids in Smolec & Moskalik (2008b) as well as the discussion of beat Cepheids in Smolec & Moskalik (2010)). This is unfortunate also since the period ratios of such objects are sensitive to metallicity Z (cf. Buchler & Szabó 2007) which would allow their use for simultaneous metallicity and distance determinations in more distant galaxies. This is even more so since similar investigations exist now, e.g., for short-period classical Cepheids (Klagyvik *et al.* 2013). It thus appears natural to question whether we can trust one dimensional (1D, averaged over spherical shells) models to interpret the relations of period P, luminosity L, colour, and metallicity Z when convection is important.

The main challenges to previous modelling of 1D hydrodynamical pulsation and stellar evolution originate from their dependence on variants of non-local mixing-length theory (MLT) which entails up to 8 free parameters (Buchler & Kolláth 2000, Smolec & Moska-lik 2008b) that are either calibrated or guessed while their values determine the model predictions themselves such as the location of red edge of the instability strip of Cepheids. The latter, given here as an example, depends on turbulent pressure and thus its modelling which requires the specification of closure parameters. Likewise, the parameter determination with spectroscopy relies mostly on the assumption of static, homogeneous atmospheres (e.g. Luck *et al.* 2013, Takeda *et al.* 2013). One might wonder whether that at least approximately holds and whether any systematic differences might be introduced this way.

All these problems motivate the attempt to perform numerical hydrodynamical simulations of classical pulsators (see also the work of Gastine & Dintrans 2011a and Gastine & Dintrans 2011b on such simulations for idealized microphysics and the work of Geroux & Deupree 2011 and Geroux & Deupree 2013 on simulations of RR Lyrae stars in this context). Initially, such work may be restricted to two spatial dimensions (2D), while in the long-term three dimensional (3D) simulations probably will prevail.

2. The ANTARES code

A recently developed tool to perform such simulations is ANTARES (A Numerical Tool for Astrophysical RESearch), a general purpose Fortran95 code for hydrodynamical simulations (for details see Muthsam *et al.* 2010). Its development has been initiated by H.J. Muthsam and has mostly been done at the Faculty of Mathematics at Univ. of Vienna, Austria and during earlier stages also at the Max-Planck-Institute for Astrophysics in Garching, Germany. More recently, development work has also occurred at the BTU Cottbus, Germany, and at the Lab. d'Astrophys. Toulouse, France. Presently, the code is available to developers and direct collaborators and consists of about 150,000 lines of code in active modules. It is a modular, fully MPI parallelized program (with optional OpenMP parallelization for load balance) and has been demonstrated to scale up to more than 1 000 CPU cores (see Happenhofer *et al.* 2013). Post-processing of simulation results is mostly done with the Paraview system, available at http://www.paraview.org/, but also with separate statistics programs operating on the output data.

3. Numerical challenges

The numerical challenges ensuing from any attempt to pursue a 2D or 3D hydrodynamical simulation of a classical pulsator are best illustrated by an example. To this end we

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model a Cepheid with the following basic stellar (and simulation) parameters. We assume a $T_{\rm eff} = 5125$ K, a mass of $M = 5 M_{\odot}$ as well as a radius of $R \sim 38.5 R_{\odot}$. This results in a luminosity of $L \sim 913 L_{\odot}$ and a surface gravity of $\log(g) \sim 1.97$. For the chemical composition we assume X = 0.7, Y = 0.29, Z = 0.01 and the GN93 mixture (Grevesse & Noels 1993). In the simulations the LLNL equation of state (Rogers *et al.* 1996, Rogers & Nayfonov 2002) is used in combination with OPAL opacities (Iglesias & Rogers 1996) to compute a model with ANTARES for realistic microphysical conditions. Since the surface layers, for which a radiative transfer solver is used, extend to a temperature range below the limits of the OPAL tables, the latter are supplemented by opacity data from Ferguson *et al.* (2005).

For a Cepheid with these parameters pulsations in the fundamental mode with a period of P = 3.85 d are eventually found in the model simulations discussed in the following. In these simulations only the outer 42% of the radius is modelled with a typical vertical grid spacing of 0.47 Mm near the surface and 124 Mm in the interior (modelling of only the outer 42% implies that P is somewhat too short in comparison with 1D models that extend into the stellar core region). For these conditions, a 1D stellar structure model has kindly been provided to us by G. Houdek which can be used to start the simulations.

The computational concept underlying the following work is based on the idea to simulate the flow in a wedge with a fixed opening angle. Azimuthally this wedge is open for inand outflow and periodic boundary conditions are assumed in that direction. An integer multiple of such wedges constitutes a closed ring located at the stellar equator (thus, there is no flow in polar direction, but the geometry assumed for the radiative transfer is that of a fully three dimensional configuration (cf. Mundprecht 2011, Mundprecht *et al.* 2013 for further details). Vertically (i.e. along the radial direction) the boundaries are considered to be closed (a very recent development is an open boundary at the top though this is not used for the simulations discussed in the following). Due to self-gravity of the star there is an extreme stratification with respect to density (and pressure) along the radial direction. This is particularly pronounced in the stellar atmosphere layers. To handle this problem it has hence been necessary to introduce a radially stretched grid which is co-moving with the mean radial, pulsational velocity (Mundprecht 2011, Mundprecht *et al.* 2013).

Several grid and geometry configurations have been considered more closely: a model with an opening angle of 1° and 800 × 300 points (radially and azimuthally, respectively, here and in the following). This model is suitable to resolve the zone of hydrogen ionization and thus also the photospheric layers. Secondly, a model with an opening angle of 10° and 510×800 points has been constructed to study the dynamical behaviour of the He II ionization zone. For a satisfactory simulation of both regions simultaneously a model with 3° opening angle and grid refinement has been constructed as well (further details on these models are given in Mundprecht *et al.* 2013).

We summarise first some results of this work on the numerical requirements. One important realization has been that the number of grid points cannot be scaled from solar simulations. For the similar case of A-type stars this has already been discussed in Kupka *et al.* (2009). Instead, a much higher resolution is required to resolve the divergence of the radiative flux, $Q_{\rm rad}$, and thus the radiative cooling in the H I ionization zone. This was concluded from 1D models of various resolutions in which case an 8 to 16 times finer grid spacing is needed. Even if the smoothing effect of a convective rather than radiative structure is considered, the resolution has to be at the very least four times higher which consequently places more restrictive conditions on the permitted time step. An increased number of grid points is inevitably required in both the radial and the azimuthal direction to avoid artificial numerical viscosity along the azimuthal direction and to resolve layers temporarily inclined with respect to the radial direction which altogether increases the computational costs. To illustrate the practical implications of a poorly resolved calculation Mundprecht *et al.* (2013) show how light curves computed from an insufficient default resolution and from a four times higher resolution differ in the case of a 1D radiative Cepheid model (no non-local MLT used to model the convective flux and turbulent pressure). Indeed, artifacts (a high frequency noise and a shift of the intensity level) are introduced in the lightcurve computation from this simulation. They are caused by the insufficient resolution and cannot be removed by simply averaging the predicted lightcurve in time.

As can be illustrated with a model with a 3×4 increased resolution obtained through a grid refinement zone (triple resolution radially and quadruple resolution azimuthally), which ranges from the top region of the model to optical depths slightly above 100, the photosphere becomes much more dynamical. The maximum convective flux in the H I ionization zone increases by factors of five to eight. The price to pay in this case is a much smaller radiative time scale where the most stringent restrictions are due to layers just underneath the H I ionization zone. The grid refinement zone thus has to be placed such that it ends closely to the bottom of this zone to reduce the computational costs.

4. Pulsation–convection interaction

The models with different opening angles and thus different resolution can be used for a variety of investigations. High resolution models such as the 1° model by Mundprecht *et al.* (2013) are suited for studying the temporal development of the H I ionization zone and the dynamics of the photosphere. Models with large opening angle such as the 10° model by the same authors can be used to investigate the development of convection in the He II ionization zone, in particular with respect to phase shifts and the interaction between convection and pulsation. Moreover, they can be used to probe models for the computation of $F_{\rm conv}$ and determine, for instance, one of the model parameters of the Kuhfuß and Stellingwerf models. The simulations are also useful to directly compute work integrals and study their behaviour as a function of phase and location within and outside the convection zone.

In the following subsection we will discuss global properties of the He II convection zone by considering a whole annulus instead of a sector of some relatively small opening angle. Subsequently, we will provide some results regarding the structure of the atmosphere of our model Cepheid.

4.1. The ring model

One might wonder whether a full ring instead of a wedge with finite opening angle is an affordable simulation domain for models of Cepheids. Indeed, this turns out to be feasible. Reducing the radial solution somewhat, a grid of 277×13000 points (rather than just 510×800) can be set up such that the domain azimuthally covers a full 360° angle. With physical parameters otherwise identical to the 10° case and with 500,000CPU-core hours available, it has been possible to conduct such a simulation for no less than 14 pulsation cycles.

The aim in setting up this model has been to perform a study of the natural azimuthal width of the flow structures. Figure 1 provides an insight to some of the properties. At some instance of time, the convective vortices are visualized by displaying the convective flux $F_{\rm conv}$. It turns out that during the evolution of the model the vortices had some tendency to group together so that in effect the distribution of vortices is quite irregular.



Figure 1. Convective flux in the ring model (in erg s⁻¹ cm⁻²). This model serves to investigate the He II ionization zone. In order to better represent its flux carrying vortices, the colour scale for the has been limited to approximately the central ten percent of the total range of the convective flux. For discussion see text.

This is in contrast to what does, or even can, happen when working with a sector just 10° wide.

Naturally, such findings provoke thoughts whether or not such mechanisms may ultimately lead to the excitation of nonradial pulsations. While the present 360° simulation is not suitable yet to study the excitation of nonradial modes, this is certainly an exciting perspective of future simulations of this kind.

4.2. The atmosphere

As already mentioned, interpretation of spectroscopic observations overwhelmingly relies on the use of one-dimensional, static atmospheres. As a matter of fact, however, one has to deal with pulsation and convection and to consider, in addition, the interaction of these two phenomena which posess characteristic times which are, moreover, not too dissimilar. There are observations which cast doubt on the simple static picture usually assumed in analysis. Even setting aside standard spectroscopic investigations showing, for example, a varying degree of microturbulence as a function of phase, other hints to complications have popped up. Analyzing an eclipsing binary, one component of which is actually a Cepheid, it has been noticed in Pilecki *et al.* (2013) that the limb darkening is in strong disagreement with theoretical predictions from static model atmospheres. Obviously, this indicates a wrong temperature structure of the static atmospheric models.

Let us provide a short discussion of atmospheric properties based on our 1° model. Figure 2 shows the temperature structure at an instance of time. The steep rise of temperature in the hydrogen ionization front is easily visible. (The top of the star is to the left side of the figure.) As is clearly seen in the temperature, an outgoing ray hits several shock fronts in the atmosphere. Details can be discerned more closely when moving to Fig. 3. Here, the course of several quantities extracted along the line visible in Fig. 2 is displayed, namely, the density of gas, the temperature (labelled by t) and the vertical velocity vx. All those quantities are normalized so as to range from 0 to 1 along the probing line. The shock visible in the middle has a density contrast of about 3.9 and a temperature jump of about 270 K, the temperature there being about 5800 K. The difference in Mach numbers across the shock is 1.6. In contrast to the case of solar granulation, where shocks appear only rather high in the atmosphere, our model also exhibits shocks throughout all atmospheric depth ranges. Often, they dissolve from the hydrogen ionization zone and move upwards. We have observed shocks of up to Mach 4 strength.



Figure 2. Temperature (labelled t and in units of K) in regions near and above the hydrogen ionization zone. The top of the atmosphere is to the left in the figure. Data are probed along the line inserted and displayed in the next figure.



Figure 3. Various physical quantities (all normalized to be located in the range from 0 to 1) extracted along the probing line visible in the preceding figure). dg: density of gas; t: temperature; vx: vertical velocity.

In addition, when looking into the properties of the atmospheric convection at various phases a rather strong phase dependency is obvious.

5. Recent work and outlook

Since simulations of Cepheids and related stars are so demanding numerically, we have ongoing work regarding numerical methodology. Significant progress has recently also been made on the subject of upper open boundary conditions, which are required for stable long-term runs of high resolution models. Such conditions, similar to what has recently been discussed by Grimm-Strele *et al.* (2013), have been ported to the scenario of a polar, co-moving grid and are currently being tested.

Implicit time integration to further ease the restrictions imposed by radiative diffusion are not only necessary for a more efficient model computation, but are even a prerequisite for the simulation of long time series. A new, strong stability-preserving, implicit-explicit Runge-Kutta (SSP IMEX RK) method has been developed for this purpose (Higueras *et al.* 2012). The method is already operational and working for 1D simulations with ANTARES. It has now been implemented and is currently being tested for the 2D case. A parallelized, non-linear multigrid solver has been developed to perform such simulations on suitable hardware (see Happenhofer 2013 for these developments). The simulation of wedges at moderate opening angle but very high resolution and the computation of full 360° models will become much more accessible by these improvements.

Of course, the long-term goal remains to be 3D simulations for the same scenarios and with similar resolution and model accuracy. However, in the near future, the astrophysical interpretation of existing results and their detailed comparisons with observational data will have highest priority.

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