The ANTARES code: recent developments and applications

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Abstract. ANTARES (A Numerical Tool for Astrophysical REsearch) is a multi-purpose numerical tool to solve different variants of the equations of hydrodynamics as they appear in problems of astrophysics, geophysics, and engineering sciences and which require the construction of detailed numerical simulation models. A presentation of the current feature set of the code with a focus on recent add-ons is given here in addition to a summary on several results from recent applications of ANTARES to solar physics, the physics of planets, and basic convection studies including the damping of pressure modes (solar oscillations) in numerical simulations of convection at the solar surface and the coupling of layers in numerical simulations of sheared and non-sheared double-diffusive convection.

1. Introduction

ANTARES (A Numerical Tool for Astrophysical REsearch) is a general purpose hydrodynamical simulation code which had been developed from both the perspectives of numerical mathematics and of astrophysics [1]. It has been applied to problems in stellar astrophysics (A-type stars [2]; turbulent solar convection [3] as well as solar granulation studies [4, 5] and studies of solar p-mode damping [6]; Cepheids [7, 8] and white dwarfs [9]), to the study of basic physical processes in stars, planets, and oceanography (double-diffusive convection [10, 11, 12]) and it motivated further development of advanced numerical methods (implicit-explicit Runge-Kutta methods for semi-implicit time integration of radiative and heat diffusion [13, 14, 15, 16]; semi-implicit integration of pressure gradient terms with an extension of Kwatra’s approach [17] for two-component fluids [18]) or their implementation and investigation in an astrophysical context (mapped grids [19]; effects of boundary conditions [20]; efficiency and convergence rates [21]). In the following we summarize recent progress that has been made in further developing ANTARES as a numerical simulation tool and we illustrate this with several successful applications.
2. Recent developments

During the last two years the ANTARES code has been subject to major improvements concerning its maintainability. These steps have now been completed. In particular, this has allowed merging several code branches which had developed during preceding years. The branches have now been unified into a single, self-consistent code base for which a private git repository has been set up and which is the basis for future code developments.

The input routines for starting models for the numerical simulations, which can process the output of various stellar structure and evolution codes as well as stellar atmosphere codes, have been simplified. Hydrodynamical simulations of stellar surface convection can now also be started from YREC stellar evolution models [22], which in turn can be patched on their top by ATLAS9 stellar model atmospheres [23] (for further details see also [24]). The pre-processing routines have been made capable to handle the new opacity distribution function format associated with the models of [23] and produce opacity binning tables which can be used by ANTARES. This allows the use of precomputed equation of state tables, Rosseland opacity tables, and tables of frequency integrated opacities (opacity binning tables) for more recent solar abundance distributions which are also used in current stellar evolution models.

For the numerical simulation of convective flows with a mean shear the vertical boundary conditions have recently been revised. Closed top and bottom vertical boundaries (no inflow from or outflow through vertical boundaries) can now optionally be subject to a constant, horizontally directed shear stress which is specified through a Richardson number $Ri$ [12] (squared ratio of shear and buoyancy). Applications of this feature include the study of numerical experiments of the influence of low Prandtl numbers and moderate shear on turbulent Rayleigh-Bénard convection at large aspect ratios and with periodic boundary conditions as a model to study the physics of large scale coupling through oscillatory motions [25] and the study of shear flows interacting with layer formation in double-diffusive convection [12].

Previously, improved methods of time integration have found a lot of attention when further developing ANTARES (see also [26]). This includes new implicit-explicit Runge-Kutta (IMEX-RK) methods which simultaneously have the following stability properties motivated by the classes of equations to be solved numerically: L-stability and positive definiteness of the implicit part, uniform convergence, non-trivial regions of absolute monotonicity, and more ([15]). The goal of this work had been to accelerate time integration while keeping dissipation at minimal values. Implicit time integration has become an additional option for hydrodynamical studies with linear viscous terms that constrain the time step due to stability requirements (see [16]).

Built-in error control has so far received little attention in hydrodynamical simulations of convective flows in astrophysics. For the purely explicit case ANTARES now offers an embedded Runge-Kutta method based on the standard TVD2 (SSP(2,2)) and TVD3 (SSP(3,3)) time integrator as an additional scheme with built-in error control.

The implicit time integration of radiative transfer, thermal diffusion, viscous processes, and sound waves required by stability driven time step restrictions in various application has motivated the creation of an extensive suite of elliptic solvers contained within ANTARES. Recent additions to this part of the code include a 3D linear elliptic solver, fully parallelized, based on a geometric multigrid approach and its extension for the non-linear case ([16]), suitable for periodic, (non-) homogeneous Dirichlet and Neumann boundary conditions (with Dirichlet and Neumann conditions restricted to the vertical direction and currently without mixing them on opposite boundaries). More recently, this solver package was extended to be also applicable to spatial subdomains. Since the implicit time integration of stiff radiative transfer terms coupled to the energy equation of the hydrodynamical equations leads to a system of elliptic equation instead of a single, scalar equation, algebraic multigrid methods are going to become part of future versions of this package.

Finally, improvements to the treatment of radiative transfer in ANTARES for the case of
implicit time integration have been implemented. The quadratic Bézier spline method suggested in [27] for the integration of the source function and of optical depth has been implemented alongside a careful treatment of cell boundaries [24]. This has contributed to the removal of artifacts in the numerical solution of the radiative transfer (RT) equation introduced by various ad hoc limiters. The method is more accurate than that one originally implemented into the code [1] also on the relatively coarse spatial grids typically used in numerical simulations of solar and stellar surface convection. Simultaneously, the implementation of a solver for the (non-grey) 3D Eddington approximation [28] to radiative transfer has been completed. The solver is currently tuned for speed and is available for explicit time integration. (Semi-) Implicit time integration of radiative transfer will become feasible as soon as the algebraic multigrid solver package is available (this is all work currently in progress). The goal of this project is to accelerate solutions of the RT equation also on computer systems with more moderate resources (few dozen to at most few thousand CPU cores) for applications where very accurate angular integration is not crucial while stiff terms limit the integration time steps of the numerical solution for reasons of stability rather than accuracy. This occurs in classical variables such as Cepheids and in A-type stars, for example, (see [2, 7, 14]).

In addition to improvements inspired by astrophysical applications, extensions of ANTARES to be applicable to new problems posed in the engineering sciences are in development as well. These will be reported elsewhere.

3. Numerical simulations of the convective surface of the Sun

3.1. Statistical properties of granulation

Radiation hydrodynamical (RHD) simulations allow the study of properties of granulation. The latter appears on the top of stellar convection zones that continue from the envelope of a star into its photosphere. This is well known to occur also for our Sun which permits a direct comparison of numerical simulations with (solar) observations. A large scale simulation of the solar surface with sufficient resolution featuring more than 100 granules during each point in time was performed and discussed in detail by [4]. This simulation, internally called wide4, represents the time evolution of the solar surface within a box with Cartesian geometry that is 18 Mm wide in both horizontal directions and has a vertical extent of 4.45 Mm. Its limited vertical extent allows the assumption of a constant and vertical rather than radial surface gravity. Due to its width the simulation box contains about a dozen granules along each horizontal direction which reduces the influence of assuming lateral periodicity. Vertically, open in- and outflow of fluid is permitted (see also [20], conditions BC3b in their Table 1). The simulation volume is sliced into 510 cells in each of the horizontal directions while vertically the domain consists of 405 cells (without grid cells used to implement the simulation boundary conditions). This results in a horizontal resolution of 35.3 km and a vertical one of 11.1 km. In spite of minimized numerical diffusion (cf. [1]) the simulations are only moderately turbulent ($Re_{eff} \sim 123$ following the estimate suggested in [29, 30] for $H_{gran} \sim 1300$ km and bearing in mind that downdrafts between the granules are only 5 to 10 grid cells wide).

As demonstrated by [4] in a detailed analysis of general statistical properties of wide4 and in [5] through a detailed analysis of the average diameters and lifetimes of granules the simulation matches observed data from the Sunrise IMaX experiment [31] quite well apart from differences which are due to the lower time resolution of the observations and the magnetic fields which are present in the Sun also in otherwise “quiet” areas of low (magnetic) activity.

3.2. Powerspectra and p-modes

Another way to probe RHD simulations of convective stellar surfaces is to analyze their results with respect to the properties of global stellar oscillations which occur in many types of such stars. If we average a time series of numerical simulation snapshots horizontally, we can expect
to retrieve p-modes excited in the simulation box vertically as standing waves alongside a signal background caused by stellar granulation. This can be seen from published power spectra such as those presented in [6]. Their simulation run cosc13, performed with ANTARES, was done for the same boundary conditions, equation of state, non-grey opacities, and resolution as wide4 but was based on a smaller simulation box (with 6 Mm horizontal and 3.88 Mm vertical extent requiring only 170 cells in horizontal direction and 350 in the vertical one). The second importance difference is the run time available for statistical averages which is 40012 sec for cosc13 as opposed to 12420 sec for wide4 and an even higher output frequency for the latter (1/8.54 Hz in wide4 compared to 1/15.84 Hz available for cosc13).

In Fig. 1 a comparison is shown for the spectral power of the vertical velocity evaluated at the solar surface defined as the vertical layer for which the time average of the horizontal average of temperature equals about the solar effective temperature (since at a vertical resolution of 11.1 km the temperature difference between adjacent layers is more than 100 K a more precise definition does not matter here). The acoustic cut-off for p-modes in the Sun is around 5 mHz. Since in the numerical simulations we actually observe vertical standing waves defined by the box size, the frequencies of the modes depend on that size. On the other hand, modes with $\nu > 5$ mHz are subject to the damping processes operating in the solar photosphere. Thus, only modes with no, one, and two internal nodes can appear at the chosen box sizes (fundamental,
Figure 2. Spectral power of the vertical component of radiative flux evaluated at the layer for which the time average of the horizontal average $\bar{T} = T_{\text{eff}}$. An additional scaling factor has been applied. For this quantity data is only available for the cosc13 run. Only the two lower order vertical $p$-modes are visible. The power spectrum contribution of the granulation background behaves similarly as that one for vertical velocity.

First and second overtone) and this is just what is observed in Fig. 1. The shift of the modes in wide4 towards lower frequencies than in cosc13 is due to its larger vertical extent, particularly below the solar surface. The longer run time of cosc13, however, allows a higher resolution in frequency space and indeed the damping processes are much better resolved. This explains the much smaller line width for the modes in cosc13 (modes around 3.5 mHz require a simulation time of just the length of cosc13 to be resolved, see [6]). Studies of $p$-modes clearly need a long enough run time (of several solar days) to resolve damping processes and indeed wide4 had instead been designed to study granulation statistics.

The effects of the different domain with on the granulation background are quite remarkable though. Model wide4 has clearly more power in the range beyond about 20 mHz while in the range from 6 mHz to about 12 mHz it appears to be lower. Since both simulations have the same resolution, the same microphysics, the same non-grey radiative transfer (in LTE with 4 opacity bins), almost the same height above the solar surface, and are deep enough as well, the remaining differences have to be caused by the averaging time, the sampling rate, or the box width. The data are shown just to about half of the Nyquist frequency of each set and taking into account that the difference is also observed in the frequency domain well resolved by cosc13, the most likely explanation for it appears to be the influence of the domain width. This has to be checked carefully before performing more systematic studies of the granulation background based on numerical hydrodynamical simulations for applications in exoplanet and
asteroseismology missions such as TESS or PLATO.

Similar analyses can be done for other observables such as the radiative flux as shown in Fig. 2 for the case of cosc13. Note that here only two p-modes can be clearly identified (from the fundamental and the first overtone). Provided the RHD simulation is sufficiently long, the physical processes behind mode damping can be studied in detail with such simulations (see, for instance, [32] for the underlying principles and [6, 33] for recent results). Dedicated numerical simulations of the granulation background can be expected to permit the same type of analysis also for the convective flow itself in addition to the study of the p-modes generated by it.

4. Semiconvection

Semiconvection or diffusive convection (as it is called in oceanography) is distinguished from simple thermal convection by the competition of the gradients of two active scalars, the temperature field on the one hand and the mean molecular weight on the other, as well as by the role of the ratio of the molecular (or radiation based) diffusivities of the fluid for these two fields for the stability of a given stratification. A review on this topic has recently been published by [34]. In principle, a layer of fluid which is unstable to convection due to the steepness of its (mean) vertical temperature gradient (Schwarzschild criterion, predicting a convective instability for sufficiently cooler fluid located on top of hotter fluid) may be stabilized by an at least equally steep gradient of mean molecular weight (Ledoux criterion, predicting stability for this scenario if the fluid on top has sufficiently lower mean molecular weight than the fluid at the bottom). If the ratio of the two gradients is given by \( R_\rho = \frac{\kappa_T}{\kappa_S} < 1 \), then stability in the sense of the Ledoux criterion is found if \( R_\rho > 1 \). However, an additional, oscillatory type of instability can occur easily if heat diffuses faster than the species concentration that causes the mean molecular weight gradient: \( \kappa_T > \kappa_S \) or \( \text{Le} := \frac{\kappa_S}{\kappa_T} < 1 \) (in the literature this Lewis number is also defined as the inverse ratio \( \kappa_T/\kappa_S \)). As linear stability analysis demonstrates the region of such an instability depends also on the Prandtl number \( \text{Pr} = \frac{\nu}{\kappa_T} \), the ratio of kinematic viscosity and thermal (or radiative) heat diffusivity. The region for the ODDC (oscillatory double-diffusive convective) instability is given by \( 1 < R_\rho < \frac{(\text{Pr} + 1)}{(\text{Pr} + \text{Le})} \approx 1 + \frac{1}{\text{Pr}} \) for \( \text{Le} \ll \text{Pr} = R_{\rho,\max} \) which holds for stars, giant planets, and the ocean despite those three systems have drastically different Prandtl numbers.

These theoretical results can be investigated for linear stratifications of temperature \( T \) and solute \( S \) (or mean molecular weight which mathematically leads to the same equations) with 3D hydrodynamical simulations (for example, [35, 36]) and effective diffusivities can be derived for them. Such results are of particular interest for the regime of layer formation which is found for values of \( R_\rho \) below a certain upper limit \( R_{\rho,\text{crit}} \) as indicated by the inequality chain \( 1 < R_\rho < R_{\rho,\text{crit}} < R_{\rho,\text{max}} \). Interestingly, this is also found for other types of boundary conditions ([10, 11]). However, it is also known from experimental evidence that this criterion for layer formation is far too restrictive: in both lakes and in the ocean such layers are found for values \( R_\rho > R_{\rho,\text{crit}} \) and even \( R_\rho > R_{\rho,\text{max}} \). In [37] it was demonstrated that for Prandtl numbers representative for salt water a shear flow can enlarge the range of the ODDC region, i.e., increase \( R_{\rho,\text{max}} \) and also \( R_{\rho,\text{crit}} \) which was proposed as an explanation for the formation of *staircases*, layers of different \( T \) and \( S \) piled on top of each other as found in the oceans. On the other hand, [38] demonstrated that a more general (than just plain linear) stability analysis is required to understand the behaviour of interfaces between such layers which feature steep gradients at their boundaries and the results of their work agree well with observations.

In [12] this scenario was investigated in more detail for the case of both a larger value of \( \text{Pr} = 7 \), typical for oceanographic problems, and for a low value which is representative for the interior of giant planets, \( \text{Pr} = 0.1 \). In addition, the influence of different rates of plain Couette-like shear on this system was investigated, as parameterized by the Richardson number (with \( -\infty \) representing no shear, a value of \( -1 \) representing shear and buoyancy rates to be the same
Figure 3. Layer formation in a stratified fluid for the case $Pr = 0.1$, $Le = 0.01$, $R_\rho = 4$, $Ri = -10$, and $Ra = 5.0 \times 10^8$. Light material is located on top of heavy one. On top of the third layer several smaller layers form due to the ODDC instability. Note that the narrow plumes inside the convective layers are strongly tilted due to the shear flow interacting with convection.

Figure 4. Local stability parameter $R_{\rho,loc}$ as a function of depth, with and without shear (see main text for details).

Figure 5. Average temperature and solute concentration as a function of depth, with and without shear (see main text for details).

and the sign distinguishing a convectively unstable stratification, $Ri < 0$, from a stable one with $Ri > 0$). These simulations demonstrate that the first seed layer, triggered by the initial condition of a jump in $T$ at the bottom and a linear stratification in $S$, after 5% to 10% of the thermal time scale as defined through the ratio of the squared box height to the heat diffusivity $\kappa_T$, causes the formation of further layers. If the conditions become favourable for the ODDC
instability as well, additional small layers can form on top of the stack due to this mechanism. However, this process only occurs at the top of the entire stack of layers. The formation of new, non-ODDC layers is directly linked to the stability of the first interface layer which instead of breaking up triggers the formation of more layers on top of the stack. This can be concluded from a detailed study of its dynamics [12]. Shear on the other hand just slows down the formation of the first layer and then mainly dilutes the layer interfaces. No enhancement of the ODDC instability could be found for the case Pr = 7 and the range of values of Ri studied (−0.1, −1, −10). Thus, for understanding the dynamics of layer formation in double-diffusive convection, it is essential to also have an accurate model of the initial conditions of the stratification, since these determine the time evolution of the system at least over a full thermal time scale.

In Fig. 3 we illustrate a case simulated in [12] with simulation parameters Pr = 0.1, Le = 0.01, $R_p = 4$, $R_i = -10$, and $R_a = 5.0 \times 10^8$. This corresponds to a case with moderate shear (convection dominates since the buoyancy rate is smaller than the shear rate, as follows from $R_i = -10$). The state shown is the result of an evolution from the initial conditions after 0.5 thermal time scales. Shear introduces some qualitative differences when directly comparing to the non-sheared case as it leads to sharper, more inclined plumes (cf. Fig. 11a in [12] which is depicted there for a somewhat earlier state after 0.39 thermal time scales). To gain further insight Fig. 4 compares $R_{\rho,\text{loc}}$, which is $R_\rho$ scaled by the local ratio of solute jump $\delta S$ to temperature jump $\delta T$ between adjacent vertical grid points, averaged horizontally and over the last 0.02 thermal time scales before the state shown in the snapshot Fig. 3, for the case with no shear and with moderate shear. In Fig. 5 the same is done for the horizontal average of mean temperature and solute concentration, again averaged over the same time interval. In both figures each quantity is given as a function of depth for both the case of shear and no shear. The most evident influence of the moderate amount of shear implied by $R_i = -10$ is visible at the boundary of the top layer to the adjacent, diffusive region: local stability increases more quickly with height for the case of a moderate shear (Fig. 4).

5. Discussion and conclusions
We have provided a summary of recent, advanced numerical techniques implemented into the ANTARES hydrodynamical simulation code. A lot of attention has been devoted to radiative transfer methods, suitable for both explicit and implicit time integration, and scalability of the code, particularly also with respect to fast elliptic solvers which are essential in applications where processes operating on short time scales appear that contribute but little to the development of the solution but crucially influence numerical stability. Methods implemented into the code are designed to deal with such cases without sacrificing conservation properties and the self-consistency of equations of state characterizing the problems to be investigated.

Additionally, we have selected two recent applications of ANTARES to problems from astrophysics and geophysics as examples of its capabilities. Indeed, modern radiation hydrodynamical simulations provide an excellent tool to investigate the physics of stellar surfaces with methods which complement observations. Considering the contributions to damping processes of solar p-modes as an example, the numerical simulations allow a direct computation of the individual contributions which limit the lifetime of oscillation modes that in turn are continuously driven by the convective flow. With their numerical simulations based on ANTARES [6] demonstrated that in the solar photosphere the large, opposing contributions of radiative and convective flux nearly cancel each other while turbulent pressure and the dissipation of (turbulent) kinetic provide a moderate, net damping effect in this region. Such delicate balances are very difficult to model analytically [39] and their computation on the basis of observational data is equally challenging, along with the resulting (p-mode) line width which in turn is a benchmark for the numerical simulations (see also [33] for related work on p-mode amplitudes by means of numerical simulations). The same type of numerical simulations can also
be used to support observational studies of the so-called granulation background against which the p-modes are measured. This background carries a lot of information on its own, among them surface gravity and the presence or absence of magnetic activity (cf. [40]) and its detailed characterization is of major interest to exoplanet search and asteroseismology space missions.

An equally challenging task is the quantification of the energy and species concentration transport capabilities of convection in a medium with an additional gradient in chemical composition. Initially mainly a problem concerning the evolution of the core regions of massive stars and certain regions in the oceans of Earth, a much wider field of applications now demands for more accurate physical models of such transport processes (cf. [41, 42], for example). With now more than 4000 planets discovered outside the solar system exoplanet research can pose new constraints on our physical models of the interior of gaseous giant planets for which convection is considered to occur in the context of competing gradients of temperature and composition. Complementing work on oscillatory double-diffusive convection as reviewed in [34], recent numerical simulations with ANTARES for the case of convection with an imposed initial step in temperature rather than a plain linear stratification and, optionally, an imposed shear stress, revealed [12] that the whole stack of layers has to be considered to understand its local dynamics. This further advances earlier work by [38] who provided a detailed analysis of the stability of layer interfaces in the case of water without an imposed shear.

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