Improved Radiative Transfer in the ANTARES Code

D. Krüger∗,1,2,3, N. Kostogryz2, D. Fabbian1, F. Kupka1

1 Institut für Astrophysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen
2 Max-Planck-Institut für Sonnensystemforschung, Justus-von-Liebig-Weg 3, 37077 Göttingen
3 Fakultät für Mathematik, Universität Wien, Oskar-Morgenstern-Platz 1, 1090 Wien

*Contact e-mail: daniel.krueger@uni-goettingen.de

Abstract. One of the most difficult and time-consuming tasks in multi-dimensional stellar radiative-hydrodynamics simulations is the calculation of the radiation field. We present two major improvements we achieved for the ANTARES code in this context. The first one is the use of Bezier splines in combination with the short characteristic method, resulting in a radiative transfer solver which shows more realistic results (less artifacts) and an increased stability compared to the method used so far. The second improvement presented is a radiative transfer solver based on the Eddington approximation. It allows for fast calculation of the radiation field with only a minor loss of precision. Additionally, it shows good numerical properties. These methods for radiative transfer, as newly-implemented within ANTARES, allow improved numerical results in the case of the Bezier method and much faster calculations in the case of the Eddington approximation.

1. Introduction

The ANTARES code was developed to perform numerical simulations of stellar hydrodynamics with realistic microphysics and radiative transfer in 1D, 2D, and 3D [1]. One important focus of these simulations lies on the upper convection zone. A box covering the physical domain to be simulated is thus adopted accordingly and the compressible Navier-Stokes equations are then solved at subsequent time steps on the chosen grid points of the simulation box. Since the stellar plasma and the radiation field exchange energy, the Navier-Stokes equations are coupled with the radiative transfer equation (RTE). The calculation of the radiation field via solution of the RTE usually takes up to 70 – 80% of the whole calculation time in ANTARES.

We consider simulations of convection zones of solar-like stars and white dwarfs with a focus on applications to astero- and helioseismology. Thus, the physical domain simulated is the upper part of the convection zone including the lower part of the photosphere. Calculations covering many sound crossing times to follow a sufficient part of the temporal evolution are needed (e.g. to simulate solar-like p-mode oscillations [2]). Therefore, stable and/or fast computational methods for the radiative transfer are very useful. We present two methods, that are promising in those aspects.

2. Methods for Solving Radiative Transfer in ANTARES

The original radiative transfer scheme in ANTARES uses multiple methods for computation. These shall shortly be described in the following.
The radiation field is found by calculating the formal solution of the radiative transfer equation (RTE), which reads

\[ \vec{r} \cdot \nabla I_\nu = \rho \kappa_\nu (S_\nu - I_\nu) \]  

with \( I_\nu \) being the frequency-dependent intensity, \( \rho \) being the density, \( \vec{r} \) the direction of the ray, \( S_\nu \) the source function and \( \kappa_\nu \) the opacity. We note that dropping velocity- and time-dependent terms in the radiative transfer equation is an approximation which is made in all 3-D radiation hydrodynamics codes used to simulate stellar convection that we are aware of. This is justified by large spatial scales in such simulations where the flow speed is small compared to the speed of light. The validity of this approximation can be derived from the discussion presented in Chap. 6.5 and Chap. 7.2 (Sect. 93) of Mihalas & Mihalas (1984) [3].

We solve the RTE along several rays, thus the equation simplifies to the 1-D case for each ray,

\[ \partial_{\tau_\nu} I_\nu = S_\nu - I_\nu, \]  

where \( \tau_\nu \) is the optical depth. The dependence on frequency is treated by using the opacity binning method [4, 5]. Usually 4 or 12 bins are used in ANTARES for non-grey atmospheres and the Rosseland mean opacity is used for grey simulations. Additionally, we assume local thermodynamical equilibrium (LTE), i. e. \( S_\nu = B_\nu \), where \( B_\nu \) denotes the Planck function.

For the integration along the rays we use the short characteristic method [6], by fitting a parabola through the points \( (\tau_k, I_k) \) and \( (\tau_{k+1}, I_{k+1}) \), thus using the drawback that a parabola can overshoot between those two points. This can lead to non-physical results. For horizontal interpolation onto the grid points two equal stencils are used, thus using 4 points in 2-D and 16 points in 3-D [1].

ANTARES uses different methods of angular integration like Gauss-Radau 3 [7](GR3) or Carlson A4 [8], which means that we typically solve Eq. 2 for 10 rays in 2-D and 18 rays in 3-D (in the case of GR3). The direction of each ray differs depending on the method used.

Using the calculated ray-dependent intensities, the mean intensity can easily be derived by summing up over all rays,

\[ J_\nu = \frac{1}{4\pi} \int I_\nu d\omega \approx \sum_i w_i I_\nu(\vec{r}_i), \]  

where \( w_i \) denotes the corresponding angular weights and \( \vec{r}_i \) the ray direction.

The calculation of \( J_\nu \) gives us an alternative option to calculate the radiative heating \( Q_{\text{rad}} \). We can either calculate it as the gradient of the radiative flux,

\[ Q_{\text{rad}} = -\nabla \cdot F_{\text{rad}}, \]  

or as the difference between \( J_\nu \) and \( B_\nu \),

\[ Q_{\text{rad}} = 4\pi \kappa_\nu (J_\nu - B_\nu). \]  

In the following section we will drop the index \( \nu \) but still keeping in mind that the corresponding variables depend on the frequency.
3. Bezier Solver of the Radiative Transfer Equation

The method described above has at least one major problem which is the interpolation of rays. Depending on the method of interpolation, the corresponding function can overshoot leading to a larger error for the interpolated values. This overshooting can especially cause the positive definite source function to turn negative leading to unphysical results.

The Bezier method [9] offers a new way to compute the formal solution of Eq. 1, namely controlling the overshooting of the source function. This increases the stability of the calculation of radiative transfer.

To approximate the source function with quadratic Bezier interpolation, the numerical solution of Eq. 3 is written as:

\[ I_k = I_{k-1}e^{-\delta_k} + \alpha S_k + \beta S_{k-1} + \gamma C_k, \]  

where the coefficients \( \alpha, \beta, \) and \( \gamma \) are calculated by using the expressions from [9] and depend only on optical depth. Note that the coefficients are defined in a different way from the coefficients in Eq. 4. \( C_k \) is the Bezier control point that can be expressed using the derivative at the grid points intersecting layer \( k \) and \( k-1 \):

\[ C^0_k = y_k + \frac{x_{k-1} - x_k}{2} \frac{dy_k}{dx}, \]

\[ C^1_{k-1} = y_{k-1} - \frac{x_{k-1} - x_k}{2} \frac{dy_{k-1}}{dx}. \]

\[ C_k = \frac{C^0_k + C^1_{k-1}}{2}. \]  

For the application to Eq. 8, \( y \) corresponds to \( S \) and \( x \) corresponds to \( \tau \). As \( \tau_{k-1} - \tau_k < 0 \), both \( C^0_k \) and \( C^1_{k-1} \) lie between \( U \) and \( P \) and thus \( C_k \in [U, P] \).

In order to prevent the parabola from overshooting (thus staying between \( y_k \) and \( y_{k+1} \) with known function values), the harmonic derivatives are calculated at the intersection with the \( k-1 \) layer and the intersection with the \( k \)-th layer.

\[ \frac{dy_k}{dx} = \frac{d_{\text{front}} \cdot d_{\text{back}}}{\alpha \cdot d_{\text{back}} + (1 - \alpha)d_{\text{front}}} \]
where

\[ d_{\text{back}} = \frac{y_{k-1} - y_k}{x_{k-1} - x_k}, \]  

(11)

\[ d_{\text{front}} = \frac{y_k - y_{k+1}}{x_k - x_{k+1}}, \]  

(12)

Overshooting is avoided when the condition \( d_{\text{back}} \cdot d_{\text{front}} > 0 \) is satisfied. When that is not the case, the derivative \( \frac{dy}{dx} \) is set to zero.

As is seen from the definition of the harmonic derivative, the function’s values have to be determined at three consecutive intersection points. Due to the usage of the short characteristic method and its specific implementation into ANTARES and given that the RTE is solved locally, we only know the values at three points for every step. These values allow us to define the harmonic derivative for a central point \( P \) but not for the previous point \( U \). Therefore, the derivative at \( U \) is provided by the slope defined by Eq. 11.

To implement the full Bezier technique an intersection point of the ray with the layer \( k - 2 \) is needed. As this results in a fourth-order method (compared to a second-order method when using only three intersection points), it will lead to a further improvement in the accuracy and precision of the computed models. However, compared to our implementation of the Bezier method (which we call the one-sided Bezier method in the following) this change would decrease the speed of calculations because an additional interpolation at the fourth intersection point is necessary. In comparison to the short characteristic method the one-sided Bezier method usually takes the same amount of calculation time (while being more accurate). The larger number of calculations that need to be done for the one-sided Bezier method are compensated by the higher number of if-statements which only need to be evaluated for the original short characteristic method. These statements take care that variables like the intensity \( I \) do not become negative at the boundaries which could happen due to the way of interpolation in the original short characteristic method.

The above integration scheme is described for downward integration, i.e. for a ray from \( U \) to \( P \) (see Fig. 1). In ANTARES, for each ray the downward and upward integration are performed. For the latter, the points \( U \) and \( D \) are flipped so we integrate again from \( U \) to \( P \) and the above formulae do not change.

The Bezier method is also used to calculate the optical depth (with \( y = \kappa_\nu \) and \( x \) as the height). To solve the RTE, the optical depth at three consecutive intersection points \( U \), \( P \), and \( D \) has to be known.

As shown by the results of a comparison for a solar 1-D atmosphere (see Fig. 2), the difference between the methods becomes especially important for the optical depth if the density is very low. This is the case for the photosphere, which is covered by the upper \( \sim 20\% \) of our simulated box. The difference found in optical depth results fulfills our expectations since our implementation of the Bezier scheme is a second-order method compared to the trapezoidal rule being a (globally) first-order method. This difference thus becomes especially important in those parts of the atmosphere where the optical depth is strongly nonlinear as a function of opacity.

Fig. 3 shows two snapshots for the radiative flux \( F_{\text{rad}} \) of a 2-D solar simulation, performed respectively using the Bezier method and the short characteristic method. Weighted parabolas were used for interpolation. We ran the simulation on a \( 223 \times 171 \) (vertical \( \times \) horizontal) grid with a resolution of 35.08 km in the horizontal direction and 16.5 km in the vertical direction. As time integration method we used a strong-stability-preserving (SSP) method. As boundary conditions we assumed an open top and bottom [10]. We used an adaptive stepwidth ensuring a maximum courant number of \( C_{\text{max}} = 0.4 \) and thus making sure that the Courant-Friedrichs-Lewy condition

\[ C_{\text{max}} = \frac{u \times \Delta t}{\Delta x} \]  

(13)
Figure 2. Comparison of values for the optical depth calculated with the Bezier method and the trapezoidal rule for integration. The residual shows that the methods differ mostly towards outer layers (large positive height values), where the density is low. A height value of 0 denotes the solar surface, negative x-values point inside the Sun.

Figure 3. Radiative flux $F_{rad}$ in 2-D ANTARES simulations of the solar atmosphere with the original short characteristic method (upper image) and the Bezier method (lower image) used for integration. In both cases weighted parabolas were used for interpolation.

holds. Here $u$ is the velocity, $\Delta t$ the width of the timestep and $\Delta x$ the resolution of the grid. As one can see from Fig. 3, visible differences between the two simulations lie in the upper part of the box. A comparison of the two images shows that the artifacts along the rays near the areas of orange-yellow $F_{rad}$-values, generate a cone-like structure which does not represent the real physics. Those artifacts can also partially be seen in the case of the Bezier method but
they are weaker. The difference can more easily be seen in a difference plot (Fig. 4) showing $F_{\text{rad,SC}} - F_{\text{rad,Bezier}}$ normalized by the largest value of $|F_{\text{rad,SC}} - F_{\text{rad,Bezier}}|$. As the differences between the two simulations lie in the upper part of the box, the difference plot is cut off and only shows the upper 100 vertical gridpoints. The main differences appear around the superadiabatic peak, which is the same area where the mentioned areas denoted by yellow-orange colours in the plot of $F_{\text{rad}}$ show up (see Fig. 3). One can see that the differences are larger along the rays forming a valley-like structure in the difference plot, even though the differences are smaller than in the area around the superadiabatic peak.

Figure 4. Normalized differences $\frac{F_{\text{rad,SC}} - F_{\text{rad,Bezier}}}{\max(|F_{\text{rad,SC}} - F_{\text{rad,Bezier}}|)}$ between the radiative flux in the original short characteristic method $F_{\text{rad,SC}}$ and the radiative flux calculated with the Bezier method $F_{\text{rad,Bezier}}$ from diagonal viewpoint (upper image) and frontal viewpoint (lower image).

Thus, we expect that implementing the full Bezier method in the future will further improve the simulation results thanks to it being of higher order than our current implementation. In addition to the different order of the methods, the improvement with respect to artifacts is also
understandable in terms of the Bezier method being strongly monotone and positive, similarly to the physical problem being treated (see Eq. 1). These results agree with the (semi-)analytical investigations [11, 12, 13, 9] done by other groups.

4. The Eddington Approximation

Often calculation speed is more important than having highly-precise results for radiative transfer, since the additional error due to the faster method is of the order of only a few percent. For this reason, it is of significant interest to use a method that, while not increasing the error too much, is much faster than the standard methods based on ray integration.

Such a method has already been proposed more than fifty years ago [14]. By forming moments, one gets for the radiative transfer equation

$$\nabla \cdot \left( \frac{1}{3 \kappa_\nu \rho} \nabla J_\nu \right) - \kappa_\nu \rho J_\nu + \kappa_\nu \rho B_\nu = 0,$$

and the net radiative heating can be expressed as

$$Q_{\text{rad}} = \nabla \cdot \left( \frac{4\pi}{3 \kappa_\nu \rho} \nabla J_\nu \right).$$

This has already been used in the treatment of a grey atmosphere by [15], but it can easily be shown that it also holds for non-grey atmospheres as shall be demonstrated in the following. Keeping in mind that LTE holds and using the Eddington approximation we get

$$\int_0^\infty \kappa_\nu J_\nu d\nu = \int_0^\infty \kappa_\nu B_\nu d\nu.$$

With the opacity binning method we get the necessary condition

$$\sum_i \kappa_{\nu,i} J_{\nu,i} = \sum_i \kappa_{\nu,i} B_{\nu,i}$$

with the more restrictive condition $J_{\nu,i} = B_{\nu,i}$ holding in the special case of a grey atmosphere. This is a major improvement compared to the Eddington approximation used so far as this allows the inclusion of frequency dependence. Of course, this approximation cannot be used for all kinds of applications. It was shown [15] that the error of this approximation is largest for the part of the atmosphere above the superadiabatic peak. Thus, at the moment we do not recommend the use of this approximation for calculations like element abundance determination from spectral synthesis or limb darkening calculations.

As can easily be seen, Eq. 14 has the form of a generalized Poisson equation and thus can be solved by using a scalar multigrid solver. Such a solver has been implemented into ANTARES and has shown good numerical properties, e.g. weak scaling, meaning that the solution time scales with the number of used processors while keeping the problem size per processor fixed. Therefore, in the non-grey case Eq. 14 is solved for each bin and $\bar{J}$ is then retrieved by summing up over all bins, as opposed to the grey case considered in [15, 14] where $\bar{J}$ can be computed from a single solution of Eq. 14 per time stage (or time step).

The reason for the speed up expected from this approach is the much better scaling of parallelized multigrid solvers when compared to parallelized short characteristic solvers. It has already been shown ([15] for the grey case) that in the non-parallelized case the use of a multigrid solver based on the Eddington approximation is faster than using the most simple ray-integration based solver (10 rays in 3-D). Thus, we expect an even larger speed-up for the parallelized case.
due to the better scaling properties of the multigrid solver. Additionally, we expect the speed-up to be even higher in the non-grey case, as the speed-up holds for each individual bin.

A drawback of this method is that certain quantities like the intensity $I_\nu$ are not calculated and thus the method is not usable for all types of simulations and analysis. Another drawback is that the Eddington approximation has a higher relative error than the usual angular integration methods for depths around the superadiabatic gradient, as it is only exact in the limits of very high or very low optical depth [15].

5. Summary

Two new methods for the calculation of radiative transfer were implemented into ANTARES. The Bezier method shows improved results for the calculation of intensity along each ray by significantly reducing visible artifacts. The Eddington method achieves much faster calculations for grey atmospheres and we expect the same for non-grey atmospheres. The two methods now allow us to perform simulations providing physically more realistic results or to drastically reduce the computation time, respectively.

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