A 3D radiative transfer framework

III. Periodic boundary conditions

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ABSTRACT

Aims. We present a general method to solve radiative transfer problems including scattering in the continuum as well as in lines in 3D configurations with periodic boundary conditions.

Methods. The scattering problem for line transfer is solved via means of an operator splitting (OS) technique. The formal solution is based on a full characteristics method. The approximate A operator is constructed considering nearest neighbors exactly. The code is parallelized over both wavelength and solid angle using the MPI library.

Results. We present the results of several test cases with different values of the thermalization parameter and two choices for the temperature structure. The results are directly compared to 1D plane parallel tests. The 3D results agree very well with the well-tested 1D calculations.

Conclusions. Advances in modern computers will make realistic 3D radiative transfer calculations possible in the near future. Our current code scales to very large numbers of processors, but requires larger memory per processor at high spatial resolution.

Key words. radiative transfer – scattering

1. Introduction

Interest in 3-D radiative transfer in stellar atmospheres has grown with the calculations of Asplund and collaborators (Asplund et al. 1999, 2000; Asplund 2000; Asplund et al. 2005; Grevesse et al. 2007). This work has indicated that the solar oxygen abundance needs to be revised downward. However, the revised abundances are difficult to reconcile with helioseismological results (see Basu & Antia 2008, and references therein). The work of Asplund et al. is based on comparisons of synthetic spectra produced by formal solutions of hydrodynamical models of solar convection. We present a framework for solving the full scattering problem that is applicable to hydrodynamical calculations of stellar atmospheres. Hauschildt & Baron (2006, hereafter Paper I) and Baron & Hauschildt (2007, hereafter Paper II) described a framework for the solution of the radiative transfer equation for scattering continua and lines in 3D (when we say 3D we mean three spatial dimensions, plus three momentum dimensions) for the time independent, static atmospheres. Hauschildt & Baron (2006) and continuing of the characteristic until it leaves the other boundary. The direction of a bundle of full characteristics is determined by a set of solid angles (θ,ϕ) which correspond to a normalized momentum space vector (p_x,p_y,p_z). The periodic boundary conditions are simply implemented as a wrap-around (e.g., passing x_{max} for p_x > 0 wraps around to x_{min}) and continuing of the characteristic until it leaves at the z boundary. Characteristics with very small |p_z| would require a large number of wrap-arounds (and eventually would lead to infinitely long characteristics), therefore, we limit the number of wrap-arounds per voxel to a prescribed value, typically around 16

2. Method

In the following discussion we use notation of Papers I and II. The basic framework and the methods used for the formal solution and the solution of the scattering problem via operator splitting are discussed in detail in Papers I and II and will thus not be repeated here.

In the following we assume (without restriction) that we have periodic boundary conditions in the x and y coordinates, and for the z coordinate that the “bottom” (large optical depth) is at z = z_{min} and the “top” (interface to empty space) is at z = z_{max}. The implementation of the periodic boundary conditions within our framework is simple: we use a “full characteristics” approach that completely tracks a set of characteristics of the radiative transfer equation from the outer boundary through the computational domain to their exit voxel and takes care that each voxel is hit by at least one characteristic per solid angle. One characteristic is started on each boundary voxel (in this case these are the planes z = z_{min} and z = z_{max}) and then tracked until it leaves the other boundary. The direction of a bundle of full characteristics is determined by a set of solid angles (θ,ϕ) which correspond to a normalized momentum space vector (p_x,p_y,p_z). The periodic boundary conditions are simply implemented as a wrap-around (e.g., passing x_{max} for p_x > 0 wraps around to x_{min}) and continuing of the characteristic until it leaves at the z boundary. Characteristics with very small |p_z| would require a large number of wrap-arounds (and eventually would lead to infinitely long characteristics), therefore, we limit the number of wrap-arounds per voxel to a prescribed value, typically around 16
configurations, this is a typical situation one encounters in a full
We did not require the line to thermalize at the center of the test
file, including wavelengths outside the line for the continuum.

\[ \tau \]

law in the continuum optical depth \( \tau \)
\[ \epsilon \]
to simulate a strong line, with varying
\[ z \]
axis. The grey continuum opacity is parameterized by a power
conditions (PBCs) are realized in a plane parallel slab. We use
setup is similar to that discussed in Paper II. Periodic boundary
for the line transfer problems discussed in this paper. Our basic
We use the framework discussed in Papers I and II as the baseline
(tests have shown that larger values do not affect the results, val-
ues as small as 4 are usable in plane-parallel tests). The code is
parallelized as described in Paper II.

3. Plane-parallel tests

3.1. Testing environment

We use the framework discussed in Papers I and II as the baseline
for the line transfer problems discussed in this paper. Our basic
setup is similar to that discussed in Paper II. Periodic boundary
conditions (PBCs) are realized in a plane parallel slab. We use
PBCs on the \( x \) and \( y \) axes, \( z_{\text{max}} \) is at the outside boundary, \( z_{\text{min}} \)
the inside boundary. The slab has a finite optical depth in the
\( z \) axis. The grey continuum opacity is parameterized by a power
law in the continuum optical depth \( \tau_{\text{rad}} \) in the \( z \) axis. The basic
model parameters are

1. thickness of the slab, \( z_{\text{max}} - z_{\text{min}} \approx 10^3 \) cm;
2. minimum optical depth in the continuum, \( \tau_{\text{rad}}^{\text{min}} \approx 10^{-8} \) and
maximum optical depth in the continuum, \( \tau_{\text{rad}}^{\text{max}} = 10 \);
3. constant temperatures (in all axes), \( T = 10^4 \) K;
4. outer boundary condition, \( \tau_{\text{rad}} = 0 \) and diffusion inner bound-
ary condition for all wavelengths;
5. parameterized coherent & isotropic continuum scattering by

\[ \chi_c = \epsilon_c \kappa_c + (1 - \epsilon_c)\sigma_c \]

with \( 0 \leq \epsilon_c \leq 1 \). \( \kappa_c \) and \( \sigma_c \) are the continuum absorption and
scattering coefficients.

The line of the simple 2-level model atom is parameterized by
the ratio of the profile averaged line opacity \( \chi_l \) to the continuum
opacity \( \chi_c \) and the line thermalization parameter \( \epsilon_l \). For the test
cases presented below, we have used \( \epsilon_l = 1 \) and a constant tem-
perature and thus a constant thermal part of the source function
for simplicity (and to save computing time) and set \( \chi_l/\chi_c = 10^6 \)
to simulate a strong line, with varying \( \epsilon_l \) (see below). With this
setup, the optical depths as seen in the line range from \( 10^{-2} \) to
10^6. We use 32 wavelength points to model the full line pro-
file, including wavelengths outside the line for the continuum.
We did not require the line to thermalize at the center of the test
configurations, this is a typical situation one encounters in a full
3D configurations as the location (or even existence) of the ther-
alization depths becomes more ambiguous than in the 1D case.
The slab is mapped onto a Cartesian grid. For the test cal-
culations we use voxel grids with the same number of spatial
points in each direction (see below). The solid angle space was
discretized in \( (\theta, \phi) \) with \( n_{\theta} = n_{\phi} \) if not stated otherwise. In the
following we discuss the results of various tests. In all tests we
use the full characteristic method for the 3D RT solution as
described above. Unless otherwise stated, the tests were run on
parallel computers using 128 CPUs. For the 3D solver we use
\( n_x = n_y = n_z = 2 \times 32 + 1 = 65 \) points along each axis. The solid
angle space discretization uses \( n_{\theta} = n_{\phi} = 64 \) points.

3.2. Results

We test the accuracy of the 3D PBC solution by comparing it
to the results of the 1D code for several line scattering para-
eters. The 1D solver uses 64 depth points, distributed logarithmi-
cally in optical depth. Figures 1–4 show the mean intensities \( J \) at
\( \tau_{\text{rad}} = 0 \) and the \( z \) component of the emergent flux \( F \) as function
of wavelength for both the 1D (+ symbols) and the 3D solver.
The mean intensity $J$ and the $z$ component of the radiation flux $F$ at $\tau_{std} = 0$ as function of wavelength. The + symbols are the comparison results with the 1D solver, the full lines the results from the 3D PBC solution. The results are for $\epsilon_l = 10^{-8}$ and constant temperatures.

The agreement is excellent for all values of $\epsilon_l$ from unity to $10^{-8}$, indicating that the 3D code produces an accurate solution even for extreme cases of line scattering. In the case with $\epsilon_l = 10^{-8}$ the continuum processes lead to earlier thermalization than the classical approximation $J \propto \epsilon^{1/2}$ as the line strength is limited compared to the continuum. The convergence rate of the line source function (here used together with Ng acceleration) is the same as discussed in Paper II, in the case of $\epsilon_l = 10^{-8}$ the 3D code needed 29 iterations with the nearest-neighbor $\Lambda^*$ to reach a relative accuracy of $10^{-8}$ using the simple starting guess $S = B$. The nearest-neighbor $\Lambda^*$ does allow stopping the iterations earlier than a diagonal (local) $\Lambda^*$ due to the improved convergence rate (see Paper I). This can easily cut the number of iterations by factors of two or more, even greater savings are possible if the accuracy limit is relaxed.

In addition to the mean intensities, we checked that the flux vectors $F$ have vanishing components in the $x$ and $y$ directions, typically $\max(|F_x|, |F_y|)/|F_z| \leq 10^{-13}$ in all voxels. We stress that this result is the result of the calculations and is not forced by the numerical scheme.

4. Tests with 3D structures

For a test with a computed 3D structure, we obtained an example snapshot structure from Ludwig (Caffau et al. 2007; Wedemeyer et al. 2004) of a radiation-hydrodynamical simulation of convection in the solar atmosphere. The radiation transport calculations were performed with a total of $141 \times 141 \times 151$ grid points in $x$, $y$, and $z$, respectively, for a total of 3 002 031 voxels, the periodic boundary conditions were set in the (horizontal) $x, y$ plane. The transport equation is solved for $n_\theta = 16$ and $n_\phi = 32$ solid angle points, so that a total of about $1.5 \times 10^9$ intensities are calculated for each iteration and wavelength point. For the tests described here, we are only using the temperature-density structure of the hydro model and ignore the velocity field for the simple tests presented here. We set the continuum opacity proportional to the density $\rho$ by choosing a rough temperature independent estimate for the Rosseland mean opacity per unit mass of 0.1 cm$^2$/g and parameterizing the line in the same form as discussed above.
4.1. Results

We ran a number of line transfer tests with $\epsilon_l = 1, 10^{-2}$ and $10^{-4}$. The convergence rates for the two scattering cases are shown in Fig. 5 together with the convergence rates for a small plane parallel test model and the results of the $\Lambda$ iteration for continuum transfer (for computer time reasons) for a continuum $\epsilon_c = 10^{-2}$. The convergence rate for the plane-parallel tests and the hydro model are remarkably similar, the $\Lambda^*$ operator delivers very reasonable and practically usable convergence rates.

4.1.1. Images

Figures 6 and 7 show visualizations of the results for individual wavelength (continuum, line wing and line center) and a composite image. The images are significantly different for these wavelengths. The line scattering produces a similar “fog effect” as the scattering in the continuum transfer model, however, the images appear not that different. While one might expect that the line images would look vastly different from the continuum visualization, part of the similarity is due to the fact that they were scaled individually in order to highlight the differences in structure between the wavelengths rather than comparing them on an absolute scale. The composite image (best viewed in color available in the online version of this paper) shows the differences in the visible structures between the different wavelengths.

4.1.2. Limb darkening and contrast

In Fig. 8 we show the limb darkening and contrast for a continuum test case with different values of $\epsilon$. To compute the
limb darkening, we calculate the intensity average $\langle I \rangle$ over the visible surface for different values of $\cos(\theta)$ where $\theta$ is the angle between the observer and the normal to the surface. We similarly calculate the contrast as $\sqrt{\langle (I - \langle I \rangle)^2 \rangle} / \langle I \rangle$ over the visible surface for different $\theta$. The absolute values of the limb darkening and the contrast depend strongly on $\epsilon$, scattering dramatically reduces the contrast and “flattens” the limb darkening law. Overall, the limb darkening is nearly linear in $\cos(\theta)$, as would be expected from a plane parallel atmosphere with grey temperature structure.

5. Conclusions

Using rather difficult plane parallel test problems, we have shown that our 3D full-characteristics method gives very good results when compared to our well-tested 1D code. The periodic boundary conditions method discussed here is particularly well-suited to 3-D hydrodynamical simulations of convection in stellar atmospheres and in future work we will compare our results to observations as well as to previous calculations. The results for the computed 3D structure show that $\Lambda^*$ leads also to good convergence for a true 3D structure, with convergence rates that are comparable to the simple test cases (see also Papers I and II).

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