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A new method for 3D radiative transfer with adaptive grids

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Abstract. We present a new method for 3D NLTE radiative transfer in moving media. We use short characteristics to set up a system of equations for each directed intensity. The entity of these systems is then re-formulated as one system of equations for the angle-integrated mean intensity. This system is solved with a fast, modern BiCGStab iterative solver. We recently have implemented an adaptive grid on a cell by cell basis. A major advantage of our approach is that convergence rates barely depend on the spatial discretization. In the rate equations, lines are treated by a 3D generalization of the Sobolev-approximation. The solutions of the transfer and the rate equations are iteratively coupled.

1. Introduction

The last decade has seen an enormous development of non-Monte-Carlo multi-dimensional radiative transfer, both with regard to techniques and range of applications (e.g. Auer & Paletou 1994; Vath 1994; Fabiani Bendicho, Trujillo Bueno, & Auer 1997; Folini 1998; Steinacker & Henning 1999; Busche & Hillier 2000; Dullemond & Turolla 2000; Richling et al. 2001; van Noort, Hubeny, & Lanz 2002).

We here present a brief discussion of new features, advantages, and limitations of our code TR3D. The technical basics of the code have been published before (Folini 1998; Folini & Walder 1999a). TR3D solves the optically thick NLTE radiative transfer problem for moving media in 3D. For a given 3D density, velocity, and temperature distribution, TR3D calculates the NLTE level populations as well as the mean intensity at each spatial grid point.

2. The approach

Our approach follows the idea of Turek (1994) and differs from other methods in several ways. In particular, we do not solve for each directed intensity separately and then iterate over all ordinate directions, but we solve for their combination in the form of the mean intensity. We start from the radiative transfer equation, which is the equivalent of the Boltzmann equation for photons, in the following form:

$$n\nabla_x I(x,n,\nu) + \chi(x,n,\nu)I(x,n,\nu) = \lambda(x,\nu)\int_\Omega I(x,n',\nu)d\omega' + f(x,n,\nu) \quad (1)$$

Here, χ, λ, and f are the coefficients for total losses (absorption plus scattering), scattering, and emission (atomic and external). I is the specific intensity, Ω the unit sphere. Neglecting frequency coupling, we can omit in the following the frequency index in the 1D discrete frequency space. Discretizing the 2D ordinate space we obtain for each discrete ordinate direction m ($m = 1, ..., M$):

$$n^m\nabla_x I^m(x) + \chi^m(x)I^m(x) = \lambda(x)\sum_{\tilde{m}=1}^{M} c^{\tilde{m}} I^{\tilde{m}}(x) + f^m(x). \quad (2)$$

$c^{\tilde{m}}$ are the quadrature weights for the integral over Ω. Discretizing 3D space, and using short characteristics to express $n^m\nabla_x I^m(x)$, one further gets:

$$T_h^m I_h^m = L_h \sum_{\tilde{m}=1}^{M} c^{\tilde{m}} I_h^{\tilde{m}} + f_h^m. \quad (3)$$

Here the vector I_h^m contains the specific intensity for direction m at each spatial grid point, L_h and f_h^m contain the scattering and emission coefficients. The matrix T_h^m describes the discretized transport term and the discretized loss coefficient χ^m. Note that for each given discrete direction m the spatial grid points can be numbered such that T_h^m is lower triangular. Next, we multiply the equation by the inverse of T_h^m (which can be done analytically as T_h^m is lower triangular), and apply a quadrature sum over all ordinate directions to the equation. With the discrete mean intensity $J_h = \sum_{m=1}^{M} c^m I_h^m$ we then obtain

$$\begin{aligned} J_h &= \sum_{m=1}^{M} c^m \left(T_h^m\right)^{-1} L_h J_h + \sum_{m=1}^{M} c^m \left(T_h^m\right)^{-1} f_h^m \\ &= T_h L_h J_h + F_h. \end{aligned}$$

Taking all J_h terms to the left one finally obtains, with $A_h = 1 - T_h L_h$,

$$A_h J_h = F_h. \quad (4)$$

This linear system of equations we solve with a BiCGStab algorithm. Of the matrix A_h the following can be said: A_h is definite (in a mathematical sense) for $\chi \geq \lambda \geq 0$; A_h is not symmetric; A_h is a full matrix; A_h is given only implicitly; based on the condition number of A_h convergence of the iterative solution should deteriorate as $\lambda \to \chi$ and $\chi h \to 1$, where h is the spatial cell size. Note that we cannot afford to build up the matrix A_h explicitly, as it has dimension n_{node}^2, where n_{node} is the number of spatial grid points. Instead, we construct on the fly the parts of A_h we need, apply them to a vector, and throw them away again.

3. Advantages of the approach

A main advantage of our approach is that the convergence rate of the solution of the transfer equation depends only on χ, λ, and χ/λ, but essentially not on the size of the spatial grid cells. This behaviour is in essence due to the fact that the matrix A_h contains only the inverse of the derivative operator T_h^m and not the operator itself. This property is particularly attractive with regard to the use of adaptive grids in space. If T_h^m were used directly, convergence properties would be dominated by the smallest cells. In this case, convergence can again be improved by, for example, the use of multi-grid techniques (e.g. Steiner 1991; Fabiani Bendicho, Trujillo Bueno, & Auer 1997). However, implementing an efficient, non-linear multi-grid is rather demanding.

The comparatively moderate storage requirements we consider another advantage. Currently, we store the n_ν frequency dependent mean intensity as well as the n_{lev} NLTE level populations and the n_{lev} LTE level populations at all n_{node} grid points. The LTE populations could be constructed on the fly, but storing them allows for an efficient construction of χ, λ, and f. The working memory needed on top of these three large portions makes up only a few more percent. In essence, our approach thus requires storing $(n_\nu + n_{lev}) \cdot n_{node}$ variables.

As mentioned before, in our approach we have to solve only one linear system of equations which contains the contributions from all discrete ordinate directions. We do not know so far whether this results in an overall reduction of the computational costs, compared to methods where one solves the transfer equation for one individual ordinate after the other and iterates over the total of ordinates. On the one hand, we have to solve only one linear system, instead of solving one linear system per ordinate direction per global iteration step. On the other hand, our linear system consists of a full matrix and is, therefore, expensive to solve, whereas the linear system for a single ordinate direction is sparse and can be solved rather cheaply.

Finally, although we currently use first order finite differences in our scheme this is not mandatory. At least in principle, any other choice which fulfills upwinding is possible.

4. Limitations of the approach

A restriction is the fact that our approach depends on the ability to make the matrix T_h^m lower triangular for a given direction m. First of all, this means that only such discrete formulations of the transfer equation are allowed which fulfill upwinding. Only points lying in the direction m where the specific intensity is coming from can be considered. Second, the upwind discretization must be such that the corresponding numbering of the grid points, which is what finally ensures T_h^m to be lower triangular, can be done in an efficient way. For example, a different numbering for each direction m would be too costly either with regard to memory (store all these numberings) or CPU (construct them whenever needed). In practice, this means that the grid must fulfill certain regularity conditions. For an equidistant Cartesian grid, as an example, six different numberings of the grid are sufficient.

Another limitation with regard to discretization is that with each ordinate in direction (ϕ, θ) its counterpart in direction (-ϕ, -θ) should also be used. Otherwise, convergence can deteriorate. For the applications we so far have primarily envisaged, namely wind-wind collision in binary star systems (Folini & Walder 1999b), this is no severe restriction. In situations where photons primarily propagate into a small solid angle segment this probably changes.

5. Conclusions

While TR3D also has its limitations, it has some definite advantages: near independence of the convergence rate on the grid spacing, moderate storage requirements, no need to iterate over ordinate directions. With regard to future development, parallelization is a must, in view of both CPU and memory. 100^3 grid points, 100 atomic levels, and 100 frequency points result already in roughly 2 GB of memory. A generalization to non-isotropic scattering is desirable for many applications. While formally this should not be a problem with the current approach, the practical realization may not be easy (Steinacker, private communication). Concerning adaptivity, TR3D already has some adaptivity (spatial grid, some crude ordinate adaptivity). Yet more adaptivity is a must to save memory and computer time. Desirable are, in a first step, different grids for different frequencies, but in the long run also some kind of 'physical adaptivity': for a particular spatial and frequency range, solve only that part of the total set of physical equations which is really relevant.

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