Fully threaded transport engine: new method for multi-scale radiative transfer

A. O. Razoumov1,2,3 and C. Y. Cardall1,2⋆

1Physics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6354, USA
2Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996-1200, USA
3Joint Institute for Heavy Ion Research, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6374, USA

Accepted 2005 July 6. Received 2005 July 5; in original form 2005 March 30

ABSTRACT

A new, very fast method for 3D radiative transfer on fully threaded grids with arbitrarily high angular resolution is presented. The method uses completely cell-based discretization, and is ideally suited for problems with diffuse background radiation, often encountered in cosmological and star formation models. We find that for accurate statistical study of intergalactic Ly α absorption lines, one needs of the order of a few hundred angular discretization elements even for models without radiative feedback from star-forming galaxies.

Key words: radiative transfer – methods: numerical – intergalactic medium.

1 INTRODUCTION

There are many astrophysical systems that require solution of the 3D radiative transfer equation. In the last decade, starting perhaps from the local optical depth approximation (Gnedin & Ostriker 1997), numerical transfer solvers started to appear in cosmological and galaxy formation simulations. A wide range of approximations have been used to deal with the multi-dimensional nature of the transfer equation. Among the most interesting original developments, one can mention an implicit variable Eddington tensor method (Norman, Paschos & Abel 1998), a massively parallel multiple wavefront implementation by the Tsukuba group (Umemura, Nakamoto & Susa 1999), long characteristics on a uniform grid (Razoumov & Scott 1999), Monte Carlo transport (Ciardi et al. 2001), optically thin variable Eddington tensor approach (Gnedin & Abel 2001), adaptive ray tracing around point sources (Abel & Wandelt 2002), nested trees of rays and sources (Razoumov et al. 2002) and the integral transfer method via fast Fourier transforms (Cen 2002). Depending on the problem, many of these methods effectively reduced the number of operations for single-frequency transport from $O(N^3 N_{\text{ang}})$, where $N$ is the number of data points in each spatial dimension and $N_{\text{ang}}$ is the number of sources, to scaling which is closer to but not the same as $O(N^2)$.

Recently, Juvela & Padoan (2005) proposed a new radiative transfer method for line emission on multi-resolution grids using a combination of long and short characteristics. In their implementation, the radiative transfer equation is solved on separate grids, and intensities are interpolated at the grid boundaries. On the other hand, Cardall et al. (2005) developed a method to solve the Boltzmann equation for neutrino transport on fully threaded grids. The fully threaded data model pioneered in astrophysical hydrodynamics by Khokhlov (1998) is very efficient in dealing with multi-resolution phenomena. In this paper, we extend the ray-tracing scheme of Juvela & Padoan (2005) to fully threaded structures moving from ray-based to cell-based discretization, and find that the resulting algorithm is extremely fast and does not require any significant additional memory allocation on top of a hydrodynamical solver.

We will show that in general, in order to recover the proper spatial distribution of the mean intensity in cosmological models, one cannot (and does not necessarily want to) achieve a scaling much better than $O(N^3 N_{\text{ang}})$.

We limit transport to plane-parallel fluxes, which enter the computational volume at arbitrary angles, assuming for now that there are no point sources of radiation in the volume. Extended sources, that is, those covering at least few dozen cells, can be accurately modelled with plane-parallel transport with a sufficient number of angles (current scheme), whereas an unresolved star-forming region would need a separate transfer scheme around point sources on refined meshes, which we have also developed and will present separately. Therefore, in this paper, we limit our tests to a cosmological model with no feedback.

2 METHOD

2.1 2D algorithm

We start with a 2D example to demonstrate the basic ideas of fully threaded transport, and extend the scheme to 3D in the next subsection. Consider a 2D Cartesian grid of size $N_x \times N_y$, each element of which can be refined recursively by a factor of 2 in each dimension, resulting in four subcells within a refined element (Fig. 1). We tag individual cells with a variable-length label according to their positions in the tree hierarchy.
Assume that a plane-parallel wavefront enters the grid in some direction $\theta$, which we restrict to $\pi/2 < \theta < \pi$. Let us discretize the wavefront with $N_x$ long characteristics (thick lines in Fig. 1) separated in $x$ by the base grid resolution $\Delta x$, so that each characteristic starts in its own base grid cell at the bottom of the computational grid (cell 1, parent cell of 21–24, and parent cell of 31–34 in our example), and crosses the entire grid. Let us now divide each long characteristic into segments falling into individual cells, and consider these ray segments to be elements of their parent cells. Each ray segment can be described by several attributes such as the geometric length and the optical depth, the orientation of the side it starts on (lower horizontal or left vertical, for $\pi/2 < \theta < \pi$), and the position of its origin on that side. Using a terminology that will be particularly useful in 3D, the ray segments starting on the lower horizontal side of a cell, we call the $x$-rays, and the ones starting on the left vertical side, we call the $y$-rays. In Fig. 1, the cell 1 has only one $x$-ray, whereas cell 21 has both an $x$- and a $y$-ray. Note that for our choice of angle $\pi/2 < \theta < \pi$, every cell on any level of refinement will have exactly one $x$-ray, and zero or one $y$-ray. Depending on geometry, these segments might be very short, for example, the $x$-ray in the cell 4, but this ray count rule applies to all cells at all levels, and is central to our scheme. One can easily note that any cell will have only the $x$-ray and no $y$-ray if the $x$-ray ends at the upper horizontal side of this cell, and an additional $y$-ray if the $x$-ray ends at the right vertical side.

We discretize the rays entirely on the grid storing all information in computer memory in the form cell : rayType : rayAttribute, and each cell is in turn an element in the grid tree hierarchy. Inside each cell, we measure all lengths and coordinates in units of that cell’s size, independently of its level of refinement.

We now note the second important property of such ray construction. Since all rays are parallel and separated in $x$ by the local grid resolution $\Delta x$ (which varies from region to region), the ray geometry inside each cell — number of segments, their lengths and orientations — is the same for all cells of a given refinement level within each horizontal layer. For example, in Fig. 1, cells 21, 22, 31 and 32 have the same ray geometry, and so do the cells 511, 512, 521 and 522. Similarly, the cells 513, 514, 523 and 524 have their own geometry. It immediately follows that the ray geometry has to be computed only once per level, per layer.

We start calculation by computing the ray geometry of cell 1 and recording it in pattern $P_1$. Next, we subdivide this pattern into two elements $P_{11}$ and $P_{12}$, the first one containing the ray geometry of cells 21, 22, 31 and 32, and the second one — ray geometry of cells 23, 24, 33 and 34. In the second base grid layer, we have one additional level of refinement, and store the patterns $P_2, P_{211}, P_{212}$ and $P_{22}$. In each cell, we record a pointer to its pattern, although this association can also be recovered from the position of that cell in the tree, with a few extra integer operations. In addition, we compute the optical depth along each ray element.

Before actual transport, we introduce the concept of $x$- and $y$-neighbours of each cell into which the $x$- and $y$-ray ‘back-trace’. Neighbours can be of the higher, lower, or same level of refinement as the current cell. Cell 1 in Fig. 1 does not have any neighbour since its only $x$-ray starts on the grid boundary. Cell 21 has cell 1 as its $y$-neighbour, since its $y$-ray starts on the interface with cell 1, but it has no $x$-neighbour. Cell 511 has one $x$-neighbour (23) and one $y$-neighbour (4). Cell 53 has one $x$-neighbour (514) and one $y$-neighbour (4), and so on. For each cell, we store its $x$- and $y$-neighbours as pointers $C : X$ and $C : Y$.

Next we perform transport, starting from cell 1, continuing in cells 21, 22, 23, 24, 31, 32, 33, 34, 4, 511, 512, and so on until we cover the entire grid. In each cell, we start by computing transfer of the intensity along the $x$-ray. The input intensity $C : xray : I_{in}$ is either the cosmic background intensity (cells 1, 21, 22, 31, 32, i.e. those along the lower edge of the grid), or the outgoing intensity of the respective $x$-neighbour, either $C : X : xray$ or $C : X : yray$, depending on which ray segment hits the horizontal interface between $C$ and $X$. Note that by construction only one ray segment in $C : X$ reaches this interface, so there is no ambiguity in the choice of the incoming intensity $C : xray : I_{in}$. When we continue a ray from a lower-resolution into a higher-resolution cell, that is, when $C : level > C : X : level$, we do not interoperate across the wavefront and instead just propagate the ‘unrefined intensity’ $C : X : xray : I_{out}$. We found that, in practice, the error associated with this approximation is negligible, since it is in the refined region that radiation starts to show a non-zero gradient across the wavefront on scales smaller than the size of $C : X$.

Going back to our example, to get the input $x$-ray intensity in both the cells 511 and 512, we use the outgoing $x$-ray intensity from their $x$-neighbour, cell 23. In cell 53, the incoming $x$-ray intensity is the outgoing $y$-ray intensity from cell 514 (the thick line in Fig. 1). After an $x$-ray update in each cell, we proceed to a $y$-ray update in that cell if a $y$-ray segment is present. The incoming $y$-ray intensity is again either the cosmic intensity for border cells (cell 4), or the outgoing $x$-ray (only!) intensity of the corresponding $y$-neighbour. Note that by construction, a $y$-ray in any cell never reaches the cell’s right vertical side, always ending at the upper horizontal side. The only special case for a $y$-update, which does not arise in $x$-updates, is when $C : Y : yray$ ends on the upper horizontal side of $C : Y$, instead of the right vertical side. This in fact happens in cell 21 for which its $y$-neighbour’s $x$-ray (cell 1) does not end on the right vertical side.

In this case, we use $C : yray : I_{in} = cell : Y : xray : I_{out}$.

2.2 3D unigrid implementation

Now consider a 3D uniform Cartesian grid of size $N_x \times N_y \times N_z$, and a plane-parallel wavefront entering the volume in some direction $\phi, \theta$. As in the 2D case, we limit the angles $\phi, \theta$ in such a way that a ray entering a cubic cell through its lower left front corner ($x = y = z = 0$ in Fig. 2) would leave this cell through its upper $xy$-face without hitting the side faces first. Such restriction on the angles means that for new $\phi, \theta$ can cover only a solid angle of $\pi/6$. We
discretize the wavefront with $N_x \times N_y$ long characteristics, each one of which starts in its own base grid cell at the bottom ($z = 0$) of the computational volume and crosses the entire grid until it leaves the volume. In analogy with the 2D scheme, each long characteristic is divided into cell segments, but now each segment can start on a $xy$-plane, $xz$-plane, or $yz$-plane (Fig. 2). We continue the notation from the previous section and call these segments the $xy$-, $xz$- and $yz$-rays, respectively, and consider them to be elements of their parent cells. As before, $C_{i,j,k} : xyray : x_0$ stands for the $x$-coordinate of the starting point of the $xy$-ray inside cell $C_{i,j,k}$, and we assume that inside each cell all lengths are measured in units of that cell’s size, so that the starting position of each long characteristic is described by the same pair of numbers $C_{i,j,k} : xyray : x_0, y_0$, which do not depend on indices $j, k$, and we wrote $i = 1$ since all long characteristics start in the bottom layer cells.

As long as $\phi, \theta$ stay inside the solid angle we chose above, each base grid cell in the volume will have exactly one $xy$-ray in it, zero or one $xz$-ray and zero or one $yz$-ray. Since the grid is Cartesian, and we have fixed the angles, all base grid cells in each layer have exactly the same set of ray segments, which can be conveniently stored in a pattern $P_i$, to which each cell in that layer has a pointer $C_{i,j,k} : P \rightarrow P_i$. We have to compute and store this pattern only once per layer. The starting points $P_{i+1} : xyray : x_0, y_0$ for each subsequent layer can be computed entirely from $P_i$.

Without refinement, one can compute radiative transfer one layer at a time, starting from the very bottom layer $i = 1$. In each layer, except for $i = 1$, the first step would be to compute a pair of starting points $P_i : xyray : x_0, y_0$ from $P_{i-1}$, and then calculate the entire pattern $P_i$ starting from the length of the $xy$-ray and the type of the plane it finishes on ($xy, xz$ or $yz$). If the $xy$-ray ends on the $xy$-plane, then it is the only ray segment in this pattern. However, if it finishes on the $xz$-plane, there will be an $xz$-ray inside this pattern (Fig. 2). If the $xz$-ray is present, it will end on either the $xy$- or $yz$-plane, but not on the $xz$-plane, due to the restriction in angles we chose above. In the latter case, we will have one $yz$-ray in this pattern, and so on. For each additional ray segment, we need to compute its starting point, either $P_i : xyray : x_0, y_0$ or $P_i : xyray : y_0, z_0$ and the length of that ray segment. We also record, for quick reference, the type of the ray that hits each of the planes ($xy, xz, yz$) in that cell.

Once the layer pattern is computed, we can use it for every cell in that layer. In each cell $C_{i,j,k}$, we start by doing transfer along the $xy$-ray. The starting intensity is either the cosmic background intensity ($i = 1$), or the outgoing intensity of the ray segment ($xy$, $xz$, or $yz$) in $C_{i-1,j,k}$ that hits the upper $xy$-plane in that cell. An angle-dependent source function discretized on this ray segment can also be added to the transport step. Next, if the segment $C_{i,j,k} : xzray$ is active, we perform corresponding transfer of the incoming intensity, which is taken to be either the cosmic background ($j = 1$), or the outgoing intensity of the ray segment in $C_{i,j-1,k}$ that ends on the $xz$-plane of that cell. A similar update is done for the segment $C_{i,j,k} : yzray$ if it exists in this cell.

### 2.3 3D implementation with refinement

Let us finally consider a fully threaded 3D data structure in which each cell $C_{i,j,k}$ can be refined, in which case it contains eight sub-cells $C_{i,j,k} : C_{i',j',k'}$ of size $1/2$ of the parent, and assume that this refinement can proceed to any arbitrary level. Then the ray pattern $P_i$ for each layer will also be recursively refined to form structures of the type $P_i : P_j$, up to the deepest level of cell refinement in that layer. Unlike in the unrefined case, each ray segment is not necessarily a simple continuation of the corresponding ray segment in a neighbouring cell. If we just entered a refined region, new ray segments are created, and there are several strategies one can use to refine intensities across the wavefront. In complete analogy with the 2D construction above, we choose not to interpolate the intensities, but just to use the outgoing intensity of the cell into which the refined ray ‘back-traces’. However, we need an extra step to find out which cells the $xy$, $xz$- and $yz$-rays ‘back-trace’ into, or what we call the $xy$, $xz$- and $yz$-neighbours of the current cell. For each ray segment present, we store the pointers to their respective neighbours, which can be of the same, higher or lower level of refinement. Note that every cell containing, for example, an $xz$-ray must have an $xz$-neighbour, unless it starts on the boundary of the computational volume.

As in the unrefined scheme, before we perform transfer in a particular layer, we need to compute the base grid ray pattern for that layer. We then proceed to perform transfer in all base grid cells, following $xy$-rays and, if present, $xz$-rays and $yz$-rays, from their respective neighbours. When we hit a refined cell, we need to compute the corresponding refined ray pattern to which this cell has a pointer, if that pattern has not been computed before, and do that for each cell and refinement level in the layer. Each pattern at each level of refinement needs to be computed only once per layer.

The radiative transfer calculation itself is very fast, since all we need to do is follow the interconnected data structures of cells and ray segments we have already created for a particular choice of angles $\phi, \theta$. We always compute radiative transfer on the deepest level of refinement available, thus eliminating the need to store intensities at the boundary between regions of different refinement levels. The only floating point operations we need are the pattern calculation ($O(N_i)$), the calculation of the optical depth $\tau$ in each cell ($O(N_i \times N_x \times N_y)$), and the optical depth attenuation $e^{-\tau}(O(N_i \times N_x \times N_y))$. If we include emission, we also need to compute the source function ($O(N_i \times N_x \times N_y)$). There are one, two or three ray segments in each cell, the average number falling between one and two and depending on the grid size and hierarchy complexity. The total number of operations per iteration or time-step is then $O(N_i \times N_x \times N_y \times N_{\text{angles}})$, plus some overhead for refinement.
To generalize this scheme for any direction \( \phi, \theta \), we just need to rotate the indices used to access the grid elements, both on the base grid and in the refined cells, to cover all 24 angular zones of \( \pi/6 \), three (\( xy \), \( xz \), or \( yz \)) for each of the eight octants in a cube.

For discretization in angles, we use the HEALPix algorithm (Górski et al. 2002), dividing the entire sphere into \( 12 \times 4^{n-1} \) equal area pixels, where \( n = 1, 2, \ldots \), so that in computing the mean, angle-averaged intensity (which then goes into the ionizational balance module), all quadrature terms have the same weight. The angle-dependent intensity in each cell is obtained by averaging over all ray segments in a given direction present in that cell. We do not correct for the fact that the centre of the ray segment does not coincide with the centre of the cell, since in our discretization, the intensity is viewed more as a cell-averaged quantity. In addition, we find that averaging over few (one, two or three) ray segments cancels the errors faster than interpolation to the cell centre.

Finally, the directional intensity along each ray segment is computed as the average over that segment:

\[
(I)_{\text{seg}} = \frac{I_{\text{in}}}{L} \int_0^L e^{-\kappa l} dl = \frac{I_{\text{in}}}{\kappa L} (1 - e^{-\kappa L}) = \frac{I_{\text{in}} - I_{\text{out}}}{\ln(I_{\text{in}}/I_{\text{out}})},
\]

(1)

where \( L \) is the geometrical length and \( I_{\text{in}} \) and \( I_{\text{out}} \) are the incoming and attenuated intensities at the ends of that segment. Using this form instead of the simple average \((I_{\text{in}} + I_{\text{out}})/2\) ensures that we get a correct answer in cells that have large absorption but are, nevertheless, exposed to a strong radiation background.

### 3 APPLICATION

We ran a number of standard tests of the type described in Razoumov & Scott (1999) to make sure that we recover the proper mean intensity on uniform grids. To test the method with cell refinement, we took an output from a cosmological simulation computed with ENZO, an Eulerian adaptive mesh refinement structure formation code (Bryan & Norman 1999), in the 8-Mpc (comoving) volume at \( z = 3 \) at \( 128^3 \) base grid resolution, assigned some constant cross-section \( \sigma \) which is typical – within a factor of 2 – for photons above the Lyman limit propagating in the intergalactic medium, and ran a simple optical attenuation calculation with the variable number of angles \( 12 \times 4^{n-1} = 12, 48, 192 \) and 768. The entire data set included 501 nested grids with up to five levels of refinement, which for the purpose of our transfer, we projected on to a fully threaded data structure. Full calculation – computing ray geometry, finding neighbours and doing actual transport – takes about 3 s in one direction on the full tree hierarchy on a 2-GHz Pentium 4 processor.

In Fig. 3, we plot the angle-averaged intensity in a cross-section through one of the dense haloes, in units of the mean cosmic background. At lower angular resolution, the radiation field is extremely clumpy forming long shadows behind shielded and semishielded regions. Visually, the quality of the solution improves drastically when we switch from 48 to 192 angles, and the latter seems to be an almost converged solution as there is very little difference in radiation fields computed at 192 and 768 angles. We conclude that for a volume of several megaparsecs on a side at \( z = 3 \), one needs at least

---

Figure 3. Grey-scale map of the mean intensity in a slice through the 8-Mpc (comoving) volume, in units of the mean background intensity, at \( z = 3 \), for a \( 128^3 \) run with five levels of refinement by a factor of 2. The upper left-hand panel shows the calculation with 12 angles, the upper right-hand panel with 48 angles, and the bottom panels are with 192 and 768 angles, respectively (see text for details). Only three levels of refinement are plotted for simplicity. The grey-scale map is chosen to peak at intensities that differ the most from panel to panel.
a hundred angular resolution elements to compute the diffuse component. In general, this number depends on the size of the volume, the redshift and the photon frequency.

Fig. 4 shows the mean intensity as a function of the local density using data from all cells on all levels of refinement, for a high angular resolution model. The vertical error bars demonstrate a large rms mean intensity dispersion for all cells of the given density, indicating that radiative transfer effects are not negligible in modelling the thermal state of the intergalactic medium.

4 DISCUSSION

In our implementation, since transfer is done layer by layer, there is no need to store any transfer-related variable in more than two base grid layers at any given time: the current layer and the one below. Of course, one would prefer to keep grid variables such as density, temperature and ionization state of the entire volume in memory at once, otherwise these variables would need to be read from the disk at every new time-step or iteration. Overall, if all cells are kept in memory, our implementation does not require any more storage than a hydrodynamical part. For parallel implementation, if the entire cell hierarchy can fit on one processor, parallelization via angle decomposition is preferable to volume decomposition.

In a hydrodynamical structure formation code, radiative transfer is followed by the calculation of ionizational balance and gas temperature. We find that for large hydrodynamical time-steps, 10–20 iterations are normally required to compute an equilibrium position of H I, He I and He II ionization fronts. Interestingly enough, fewer iterations are needed to obtain a solution in higher spatial resolution models in which cosmological filaments and sheets are better resolved and tend to leave more open space for radiation to reach the higher-density regions.

ACKNOWLEDGMENTS

AOR would like to thank Åke Nordlund for organizing the radiative transfer and MHD workshop in Copenhagen in 2004 December, which inspired this work, and Mika Juvela and Eric Lentz for stimulating discussions. This work was supported by Scientific Discovery Through Advanced Computing (SciDAC), a programme of the Office of Science of the US Department of Energy (DoE), and by Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the DoE under contract DE-AC05-00OR22725.

REFERENCES

Gnedin N. Y., Abel T., 2001, New Astron., 6, 437

This paper has been typeset from a TeX/LaTeX file prepared by the author.