Cell Monte Carlo Radiative Transfer

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ABSTRACT

In this paper, we present a new radiative transfer technique we call cell Monte Carlo radiative transfer (CMC).

Subject headings: radiative transfer — methods: numerical — supernovae: general

1. INTRODUCTION

Monte Carlo radiative transfer (MC) is a method of doing radiative transfer by statistical sampling. One propagates photon packets through a model atmosphere and from counting their interactions in the atmosphere and the number of emergent packets, one can calculate the radiative transfer effects of interest. The individual packets represent aggregations of photons: for most radiative transfer situations, the number of actual photons far exceeds actual computational ability. (In this paper, we will almost always use the term photon packet for consistency even though much of the discussion applies equally well to real photons.)

The model atmosphere usually consists of cells that are isotropic and homogeneous in matter properties, but not in radiation field nor, if a moving atmosphere, in macroscopic velocity field in general. (For brevity, we use the neologism isohomogeneous??? meaning isotropic and homogeneous and related words when needed hereafter.) The discretization of the model atmosphere into cells is an adequate approximation as a long as the cells are sufficiently small. In general, one needs optically thin cells near the surface of an atmosphere where radiation and matter properties change relatively rapidly with optical depth and optically thick cells are adequate in the interior where those properties change relatively slowly with optical depth. The shape of the cells is usually chosen to exploit the geometry of the model. For plane-parallel atmospheres, one uses slab cells that are infinite in the parallel

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directions and finite in the perpendicular direction (which usually the radial direction of an atmosphere in astrophysics). For spherically-symmetric atmospheres, one uses shell slabs that are concentric about the center of symmetry. For 3-dimensional atmospheres, the simplest cell geometry is a cube.

MC has great advantages relative to other radiative transfer techniques:

1. Because it is a simulation of actual events, MC can usually treat systems with great physical realism in a relatively straightforward way and avoid approximations needed in other radiative transfer methods. The other methods are principally difference equations methods or analytic or semi-analytic methods. MC is also very general and flexible where other methods are often restricted to particular systems or approximations. Aspects of systems that MC treats relatively straightforwardly are complex photon-matter interactions, complex 3-dimensional geometry, and complex 3-dimensional velocity fields. MC is particularly useful for supernovae which are often significantly 3-dimensional in structure and are time dependent.
2. Often the main approximation of MC is its statistical nature. But the error due to this approximation ordinarily can reduced as much as desired simply by using sufficiently many photon packets in a MC run.
3. MC is embarrassingly parallelizable: it parallelizes approximately linearly in the number of processors. Each photon packet for a given radiative transfer calculation (which can be an iteration of a self-consistent atmosphere calculation) can be propagated on a single processor independently of what other packets are doing. Thus, one can propagate as many packets simultaneously as one has processors. One only has to sum the results from all the processors at the end of the propagation stage.
4. MC gives very stable, fast convergence in self-consistent atmosphere calculations for reasons we discuss below.
5. Monte Carlo codes are often relatively simple to develop.

But there are severe disadvantages:

1. The downside of advantage 2 is that error in MC can be dominated by statistical error because it can be computationally too expensive to reduce this error to a very low level by propagating sufficiently many photon packets. There is an explicit trade-off between computational speed and accuracy.

The nature of the statistical error in MC outputs is often as follows. Most outputs of interest in an MC calculation are proportional to counts in output bins and the mean values of each bin count are proportional to the total number of photon packets in the calculation. Say we do a calculation with N photons and have n counts in a bin with mean number of counts μ. The probability distribution for count-in-bin and no-count-in-bin is binomial: let p be the probability per photon packet of count-in-bin. Relative standard deviation for the count-in-bin is

$$\sigma_{\rm rel} = \sqrt{\frac{1-p}{\mu}} \propto \frac{1}{\sqrt{N}} \tag{1}$$

(e.g., Bevington 1969, p. 33). Often $p << 1$, and the probability for distribution for count-in-bin and no-count-in-bin is approximately Poissonian in which case

$$\sigma_{\rm rel} = \frac{1}{\sqrt{\mu}} \propto \frac{1}{\sqrt{N}} \tag{2}$$

(e.g., Bevington 1969, p. 40). In either case, μ can be approximated by n for a single calculation which is all that is often done. Actual errors in any calculation scale as the relative standard deviation. Thus from equations (1) and (2), we see that most outputs of interest will have relative errors that scale as $1/\sqrt{N}$. Consequently, we see that accuracy of outputs improves only very slowly with the number of photon packets N in the calculation. For example, to reduce the error of an output by a factor of 3, one must usually propagate about 10 times more packets. It can be computationally expensive to go from adequate accuracy to high accuracy.

2. Relative to other radiative transfer methods, MC is often particularly slow for optically thick atmospheres (e.g., supernovae in the interior in the photospheric phase). The origin of this slowness is simply that it takes a long computational time for photon packets to diffuse through optically thick atmospheres. The relative speed of other radiative transfer methods in regard to optically thick atmospheres is because they avoid tracking individual photon-matter interactions which MC is simulating. This is the downside of the high physical realism of MC.

To expand on the last-mentioned disadvantage, say, for example, one is injecting photon packets at the inner boundary of a pure-scattering, plane-parallel atmosphere of optical thickness τ in a Monte Carlo calculation. Figure 1 shows a cartoon a photon packet on a random walk through the atmosphere. The typical number of photon packet steps (or

flights) needed for an escaping packet to diffuse to the outer boundary is of order τ^2 from a random-walk argument (e.g., Jeffery 2009)???. From this result, one can see that in general the time of Monte Carlo calculation will increase like the square of a characteristic optical depth of the atmosphere. The slow diffusion of packets in optically thick atmospheres can make a Monte Carlo calculation prohibitively expensive for very optically thick atmospheres.

Can one do something about the slowness of MC in optically thick atmospheres? Yes. Various acceleration techniques have been developed that can give orders of magnitude speed-ups factors (e.g., Densmore et al. 2007). One of these is the random walk method of Fleck & Canfield (1984) in which ordinary photon packet steps are replaced by macrosteps: for simplicity, we call this method the macrostep random walk method (MRW). This procedure was independently rediscovered in part by Jeffery & Mazzali (2007) (and called giant steps) and perhaps by others. In astrophysical radiative transfer, the MRV method has recently been used by Min et al. (2009) and was used in an early giant-steps version by (Mazzali et al. 2001) without giving a discussion of the method. A method that give greater speed-up factors in many cases is the discrete diffusion Monte Carlo (DDMC) of Densmore et al. (2007).

In this paper, we offer a new accelerated MC method which we call cell Monte Carlo radiative transfer (CMC). The advantage of CMC over other accelerated MC methods is that it appears to have greater generality. Although we have done only limited calculations with CMC, we believe that it can be used in many radiative transfer cases (e.g., static, moving, time-independent, time-independent having complex 3-dimensional geometries, having complex velocity fields). It also seems to us that CMC should be relatively easy to implement in existing codes. Conceptually, CMC is simpler than either MRW or DDMC. Whether, it is competitive in speed-up factors with these or other accelerated Monte Carlo methods is left to future work.

The essence of CMC is to use standard MC to solve the radiative transfer in optically thick subcells (optically thick as measured by some characteristic optical depth), then use the subcell solutions to solve for the radiative in optically thick cells and then use the cell solutions and standard MC radiative in the optically thin cells to solve the radiative transfer for the whole atmosphere. The subcell and cell solutions involve calculating photon transmission probabilities and other quantities which are mostly needed for the thermal state solution. Because standard MC is used, CMC is a hybrid method like DDMC (Densmore et al. 2007). The complete self-consistent solution of radiative transfer and thermal state for all cells is obtained by a Lambda-iteration (e.g., Mihalas 1978, p. 147–150): radiative transfer and thermal state solutions are done in an alternating iteration in each depends on the other until both solutions converge to unchanging state.

The speed-up factors achieved with CMC are because standard MC photon packets flights (which have mean distances of optical depth 1) are replaced by effective flights over subcells and cells. Each subcell and cell are many optical depth units thick. So far fewer effective flights need to be calculated. CMC could be extended to optically thin cells (i.e., those of optical depth of order 1 or less), but for these cells CMC would be tend to be slower than standard MC since CMC would require more flights rather than fewer compared to standard MC. Also certain approximations that we make for CMC are only appropriate for optically thick cells deep in the atmospheres.

We note that Lambda-iteration for optically thick atmospheres notoriously often fails to converge in any reasonable computational time in difference equation methods (e.g., Mihalas 1978, p. 147–150). However, with MC the Lambda-iteration has been shown to give fast convergence (in terms of number of iterations) for local-thermodynamic-equilibrium (LTE) atmospheres (Lucy 1999a; Kasen et al. 2006) and atmospheres with NLTE (Lucy 2003; Kromer & Sim 2009). The essential reason why the Lambda-iteration works well for MC seems to be that energy conservation is strictly enforced by using energy packets (which are often photon packets) that are indestructible (except for true energy sources and sinks) and indivisible (Lucy 1999a, 2005a). In difference equation methods, energy conservation is only necessarily satisfied in the limit of convergence. We see that MC can keep the atmosphere closer to physical reality during the Lambda-iteration than the difference equation Lambda-iteration. We also note that in the difference equation Lambda-iteration, information about changed thermal state conditions tends to be transported by about optical depth 1 in each radiative transfer calculation (e.g., Mihalas 1978, p. 149). In MC, the indestructible energy packets can transport information about changed thermal state conditions throughout the atmosphere in a single radiative transfer calculation. Thus, there is a global coupling of the atmosphere in each radiative transfer calculation beyond just energy conservation. The global coupling with MC probably greatly speeds up convergence to the atmosphere solution.

In developing CMC in this paper, we concentrate on plane-parallel and spherically symmetric atmospheres and only outline the generalization to 3-dimensional atmospheres. We also keep in mind the application of CMC to supernovae which are systems for the flexibility of MC is of great use (as mentioned above) and for which CMC was originally conceived. The use of MC for supernova analysis has flourished in recent years (e.g., Ambwani & Sutherland 1988; Mazzali & Lucy 1993; Lucy 1999b, 2003, 2005a,b; Kasen et al. 2006; Sim 2007; Sim & Mazzali 2008; Kromer & Sim 2009).

Section 2 describes the basics of CMC. In § 3 demonstration CMC results are presented for the plane-parallel grey atmosphere (e.g., Mihalas 1978, p. 53ff). The generalization of CMC for 3-dimensional atmospheres is outlined in § 4. Section 5 outlines ideas for a

relatively simple thermal state calculation with MC. Conclusions and discussion are given in § 6 Appendix B gives an introduction to standard MC.

2. BASICS OF CMC

Consider a plane-parallel or spherically-symmetric atmosphere divided into cells. The division into cells is the basic discretization approximation of MC. For the plane-parallel case, the cells are slabs, infinite in the planes of uniformity of the atmosphere (which we take to be x-y direction planes) and finite in the non-uniform direction (which we take to the radial direction). For the spherically-symmetric case, the cells are spherically symmetric shell concentric about the center of symmetry.

The matter thermal state of the cells is always homogeneous: e.g., uniform density, uniform electron density, occupation numbers, temperature, opacities, emissivities, line profiles, etc. This is not realistic, but the discretization is fine enough that it is an adequate approximation. The radiation field on the other hand is not usually homogeneous nor isotropic in reality and in the MC calculation.

The size of the cells must be appropriately determined for the atmosphere under consideration.

3. DEMONSTRATION CALCULATIONS WITH THE GREY ATMOSPHERE

4. GENERALIZATION OF CMC FOR 3-DIMENSIONAL ATMOSPHERES

5. THE THERMAL STATE CALCULATION

6. CONCLUSIONS AND DISCUSSION

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A. ERROR IN MONTE CARLO RADIATIVE TRANSFER CALCULATIONS

As stated in § 1 the error in all MC calculations for all statistically-determined quantities tends to scale as $1/\sqrt{N}$ where N is the number photon packets in the calculation. In this appendix, we review a special case derivation of this general result.

First note that the scaling tendency goes to an exact result in the limit that the relative standard deviations for statistical quantities grows small. To give an example where the scaling does not apply consider a quantity determined from a count of photon packet interactions that rarely occur. For sufficiently, small N the count may stay a constant zero as N is varied, and so the error in the quantity stays constant.

Now say we want to calculate statistically-determined quantity Q. For example, Q could be the mean specific intensity in a frequency bin, or the emergent flux in a frequency bin. Determining Q is done by finding the mean contribution to Q per photon packet. This process may be disguised in some cases, but it is the essence of the determination process for all statistically-determined quantities.

Let us say that there are N packets in the calculation, but only the fraction f of them can contribute to Q: $f \leq 1$, of course. For example, the calculation may be time-dependent and the count bin for Q may only exist for some time period in the calculation. Because the calculation is statistical f itself will have a mean value $\bar{f}$ and a standard deviation σ_f. The calculated Q value is

$$Q = \frac{C}{fN} \sum_{i=1}^{fN} \sum_{j=1}^{n_i} q_{ij} \ , \tag{A1}$$

where C is some scaling constant, fN is the number of packets that can cause a contribution to Q, n_i the number of interaction of the ith packet that contribute to Q, and q_{ij} is the contribution of the jth interaction of the ith packet to Q. For simplicity, we will assume that mean ($\bar{n}$) and standard deviation (σ_n) for the number of interactions per packet is the same for all packets and that these values are constant in time. Similarly for simplicity, we will assume that mean ($\bar{q}$) and standard deviation (σ_q) for the contribution per interaction is the same for all interactions and that these values are constant in time. We assume that there is no correlation between n_i and q_{ij}. Exception to this assumption are hard to think for actual MC calculations.

The mean value of Q obtained by infinite number of repeats of the calculation is

$$\bar{Q} = C\bar{n}\bar{q} \ , \tag{A2}$$

where

$$\bar{n} = \lim_{fN\to\infty} \frac{1}{fN} \sum_{i=1}^{fN} n_i \qquad \text{and} \qquad \bar{q} = \lim_{fN\to\infty} \frac{1}{fN} \sum_{i=1}^{fN} \sum_{j=1}^{n_i} q_{ij} = \lim_{fN\to\infty} \frac{1}{fN} \bar{n}\bar{q}_i = \bar{n} \lim_{fN\to\infty} \frac{1}{fN} \bar{q}_i \ , \tag{A3}$$

where $\bar{q}_i$ is the mean contribution from the ith packet.

To determine the standard deviation of Q, we assume that the standard deviations of the input variables (i.e., f, n_i, and q_{ij}) are small enough that we can drop all terms higher than 1st order in these quantities in a Taylor expansion of Q around $\bar{Q}$. This is just following the usual 1st order error propagation procedure (e.g., Bevington 1969, p. 56–60). Note

$$\left.\frac{\partial Q}{\partial f}\right|_{f=\bar{f}} = \left.\frac{\partial}{\partial f}\left[\bar{Q} + (f-\bar{f})\left.\frac{\partial Q}{\partial f}\right|_{f=\bar{f},nk=\bar{n},q_{k\ell}=\bar{q}} + \ldots\right]\right|_{f=\bar{f},nk=\bar{n},q_{k\ell}=\bar{q}} = 0 \ , \tag{A4}$$

$$\left.\frac{\partial Q}{\partial n_k}\right|_{n_k=\bar{n},nk=\bar{n},q_{k\ell}=\bar{q}} = \left.\frac{\partial}{\partial n_k}\frac{C}{fN}\sum_{i=1}^{fN} n_i(\bar{q}+\ldots)\right|_{n_k=\bar{n},nk=\bar{n},q_{k\ell}=\bar{q}} = \frac{C\bar{q}}{\bar{f}N} \tag{A5}$$

$$\left.\frac{\partial Q}{\partial q_{k\ell}}\right|_{n_k=\bar{n},nk=\bar{n},q_{k\ell}=\bar{q}} = \left.\frac{C}{fN}\sum_{i=1}^{fN}(\bar{n}_i+\ldots)q_{ij}\right|_{n_k=\bar{n},nk=\bar{n},q_{k\ell}=\bar{q}} = C\bar{n} \tag{A6}$$

$$\tag{A7}$$

where we have made using of limiting values for $f \to \bar{f}$, $n_k \to \bar{n}$, and $q_{k\ell} \to \bar{q}$. Now Taylor expanding Q to 1st order in small quantities, we find

$$Q = \bar{Q} + \frac{C\bar{q}}{fN}\sum_{i=1}^{fN}(n_i-\bar{n}) + \frac{C\bar{n}}{fN}\sum_{i=1}^{fN}\sum_{j=1}^{\bar{n}}(q_{ij}-\bar{q}) \tag{A8}$$

$$= \bar{Q} + \frac{C}{fN}\sum_{i=1}^{fN}(n_i-\bar{n})\bar{q} + \frac{C}{fN}\sum_{i=1}^{fN}\sum_{j=1}^{\bar{n}}(q_{ij}-\bar{q}) \ , \tag{A9}$$

where we note that the partial derivative with respect to f is actually zero to 1st order in small quantities.

We now subtract $\bar{Q}$ from both sides of equation (A9), square the equation, and average over all quantities to obtain the variance in Q

$$\sigma_Q^2 = \left(\frac{C}{fN}\right)^2 \left[\sum_{i=1}^{fN}\sum_{k=1}^{fN}\langle(n_i-\bar{n})(n_k-\bar{n})\rangle\bar{q}\right. \tag{A10}$$

$$\left. + \sum_{i=1}^{fN}\sum_{j=1}^{\bar{n}}\sum_{k=1}^{fN}\sum_{\ell=1}^{\bar{n}}\langle(q_{ij}-\bar{q})(q_{k\ell}-\bar{q})\rangle\right] \tag{A11}$$

$$+\sum_{i=1}^{fN}\sum_{k=1}^{fN}\sum_{\ell=1}^{\bar{n}}\langle(n_i-\bar{n})(q_{k\ell}-\bar{q})\rangle\Bigg] \tag{A12}$$

$$= \left(\frac{C}{fN}\right)^2\left(\sum_{i=1}^{fN}\sigma_n\bar{q}+\sum_{i=1}^{fN}\sum_{j=1}^{\bar{n}}\sigma_q+\sum_{i=1}^{fN}\sum_{\ell=1}^{\bar{n}}\sigma_{nq}\right) \tag{A13}$$

$$= \left(\frac{C^2}{fN}\right)(\bar{q}\sigma_n+\bar{n}\sigma_q+\bar{n}\sigma_{nq}) \tag{A14}$$

The relative standard deviation for Q is

$$\sigma_{Q\,\mathrm{rel}} = \frac{\sigma_Q}{\bar{Q}} = \sqrt{\frac{(\sigma_n/\bar{n})+(\sigma_q/\bar{q})+[\sigma_{nq}/(\bar{q}\bar{n})]}{fN}}\ . \tag{A15}$$

B. INTRODUCTION TO STANDARD MONTE CARLO RADIATIVE TRANSFER

REFERENCES

Ambwani, K., & Sutherland, P. G. 1988, ApJ, 325, 820

Bevington, P. R. 1969, Data Reduction and Error Analysis for the Physical Sciences (New York: McGraw-Hill Book Company)

Chandrasekhar, S. 1960, Radiative Transfer (New York: Dover Publications, Inc.)

Densmore, J. D, Urbatscha, T, J., Evans, T. M., & Buksas, M. W. 2007, Journal of Computational Physics, 222, 485

Firestone, R. B., & Ekström, L. P. 2004, LBNL Isotopes Project-Lunds Universitet: WWW Table of Radioactive Isotopes (Berkeley, California: Lawrence Berkeley National Laboratory), http://ie.lbl.gov/toi/

Fleck, Jr., J. A., & Canfield, E. H. 1984, Journal of Computational Physics, 54, 508

Hauschildt, P. H., & Baron, E. 1999, J. Comp. Applied Math., 109, 41

Hauschildt, P. H., & Baron, E. 2005, Mitteilungen der Mathematischen Gesellschaft in Hamburg, 24, 63

Jeffery, D. J. 1990, ApJ, 352, 267

Jeffery, D. J. 2009, in preparation[1]

Jeffery, D. J., & Mazzali, P. A. 2007, in The Multicoloured Landscape of Compact Objects and their Explosive Origins, AIP Conf. Pro. 924, Vol. 1 Cefalù, Sicily, 2006 June 11—24, ed. L. A. Antonelli et al. (Melville, New York: American Institute of Physics), 401

Kasen, D., Thomas, R.C., & Nugent, P. 2006, ApJ, 651, 366

Kromer, M., & Sim, S. A. 2009, MNRAS, submitted

Lucy, L. B. 1999a, A&A, 344, 282

Lucy, L. B. 1999b, A&A, 345, 211

Lucy, L. B. 2002, A&A, 384, 725

Lucy, L. B. 2003, A&A, 403, 261

Lucy, L. B. 2005a, A&A, 429, 19

Lucy, L. B. 2005b, A&A, 429, 31

Mazzali, P. A., & Lucy, L. B. 1993, A&A, 279, 447

Mazzali, P. A., Nomoto, K., Cappellaro, E., Nakamura, T., Umeda, H., & Iwamoto, K. 2001, ApJ, 547, 988, arXiv:astro-ph/0009490v1

Metcalf, M., Reid, J., & Cohen, M. 2004, Fortran 95/2003 Explained (Oxford: Oxford University Press)

Mihalas, D. 1978, Stellar Atmospheres, (San Francisco: W. H. Freeman and Company)

Min, M., Dullemond, C. P., Dominik, C., de Koter, A., & Hovenier, J. W. 2009, A&A, 497, 155

Placzek, G. 1947, Phys. Rev., 72, 556

Press, W. H., Teukolsky, S. A., Vetterling, W. T., & Flannery, B. P. 1992, Numerical Recipes in Fortran (Cambridge: Cambridge University Press), http://library.lanl.gov/numerical/index.html

[1]See http://www.nhn.ou.edu/~jeffery/astro/sne/spectra/spectra.html for a draft version of *A Study of Energy Deposition Estimators for Monte Carlo Radiative Transfer* under the heading *Papers of Current Interest*.

Sim, S. A. 2007, MNRAS, 375, 154

Sim, S. A., & Mazzali, P. A. 2008, MNRAS, 385, 1681

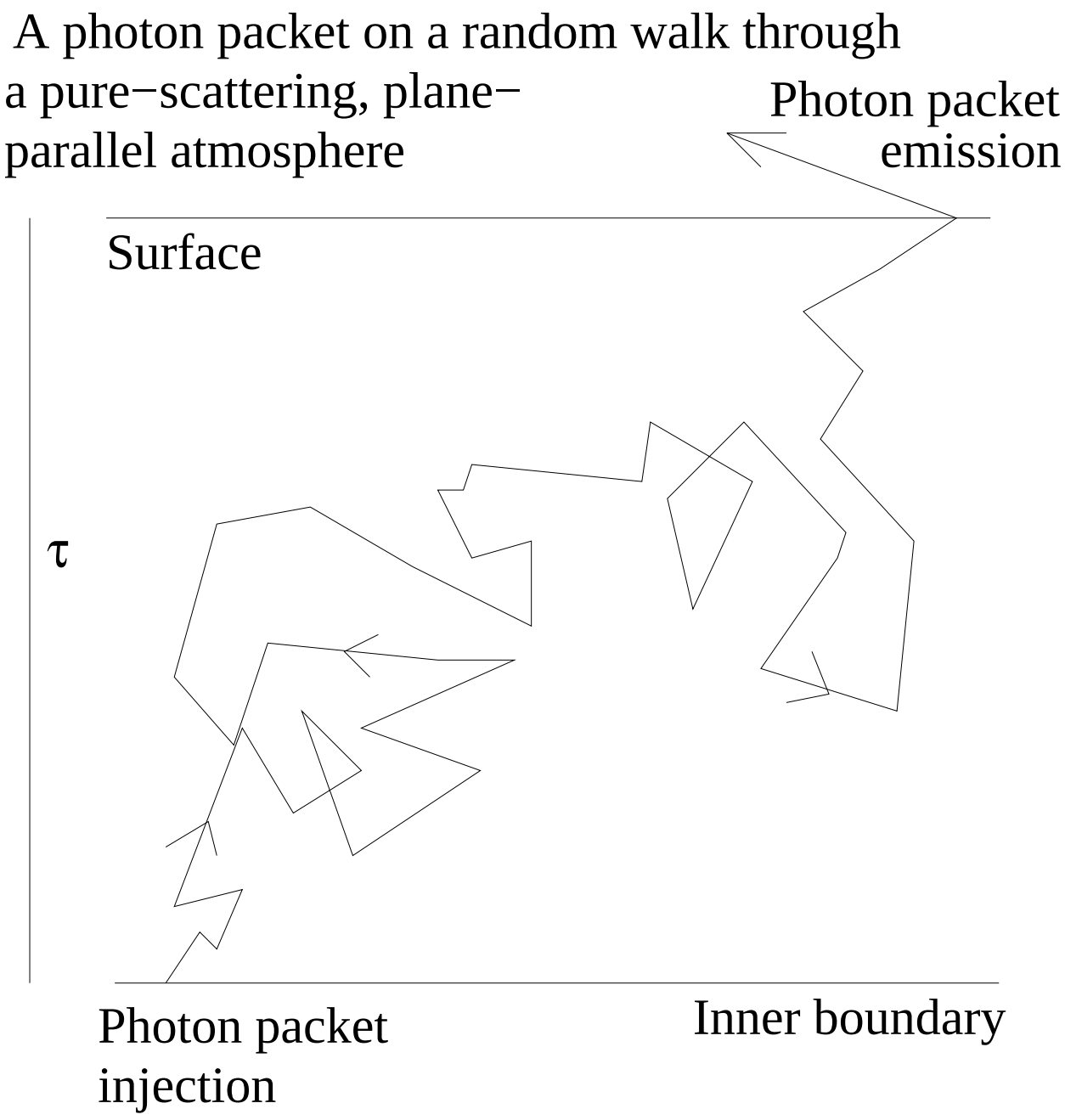

Fig. 1.— A cartoon of a photon packet on a random walk through a pure-scattering, plane-parallel atmosphere.

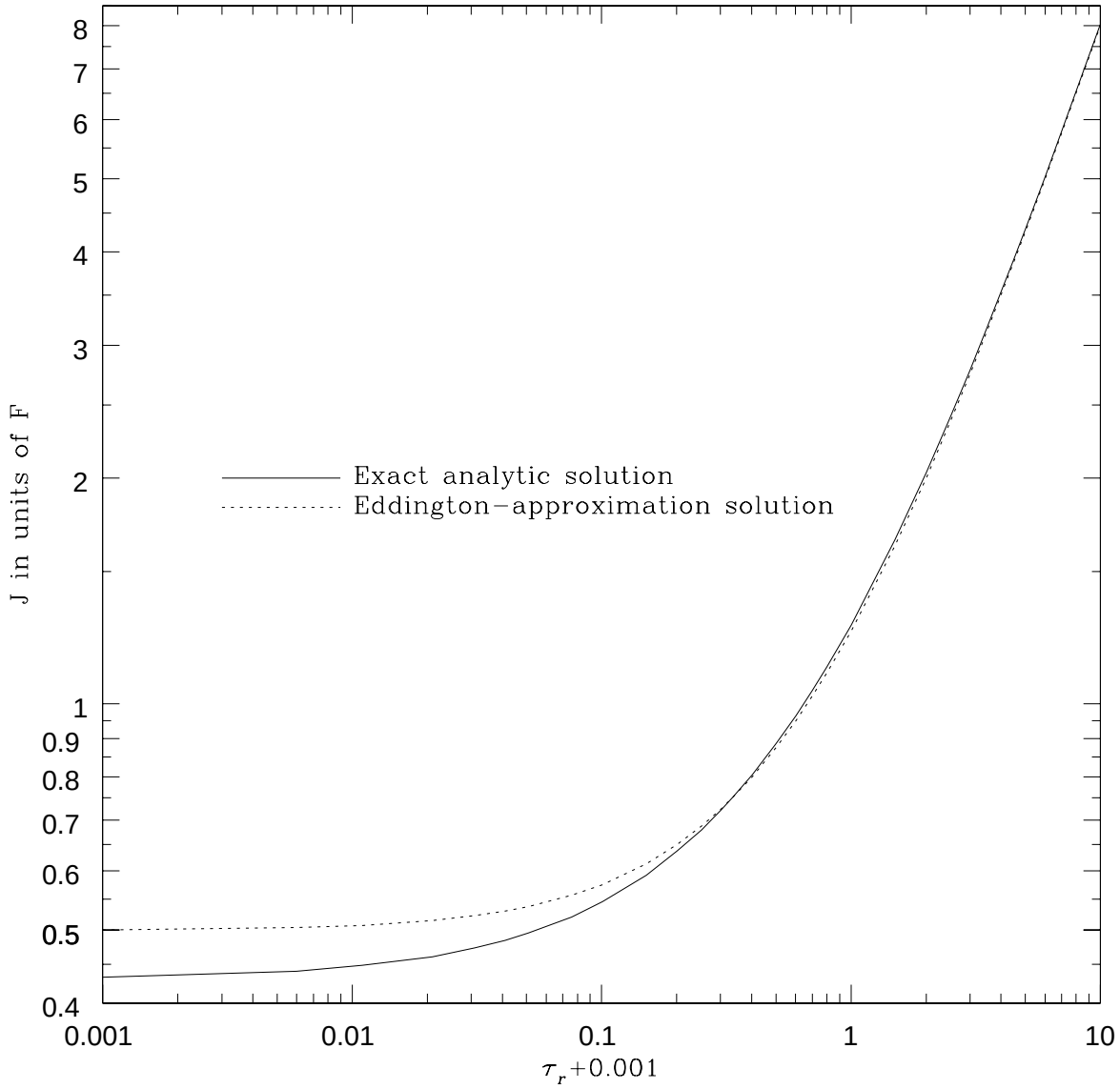

Fig. 2.— The exact analytic, time-independent, isotropically-scattering, semi-infinite, plane-parallel grey atmosphere solution and the Eddington approximation to it. To plot the solutions on a logarithmic plot, we plot the solutions versus $\tau_r + 0.001$. Thus, 0.001 on the plot is physical optical depth zero. The solution extends to infinite optical depth in a nearly linear extrapolation of the solution near optical depth 10.