Monte Carlo discretization of general relativistic radiation transport

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An indirect, hybrid Monte Carlo discretization of general relativistic kinetic theory suitable for the development of numerical schemes for radiation transport is presented. The discretization is based on surface flux estimators obtained from a local decomposition of the distribution function, and can handle optically thick regions by means of formal solutions within each cell. Furthermore, the scheme is designed for parallel implementation, and it admits the use of adaptive techniques by virtue of leaving all probability density functions unspecified. Some considerations for numerical uses of the scheme are discussed.

PACS numbers: 05.20.Dd, 95.30.Jx, 05.10.Ln, 02.70.Uu, 47.70.-n

I. INTRODUCTION

Radiation transport is an important process in many astrophysical systems. In those models which involve compact objects, a notion which encompasses active galactic nuclei, supernovae, collapsars, X-ray binaries and microquasars, and compact binary mergers as models for short-hard gamma-ray bursts, either photons or neutrinos can have a role as a dynamical agent, influence the chemical and nuclear composition of the matter, and give rise to directly observable signals.

In recent years, numerical techniques for handling general relativistic models, in particular those involving black holes and relativistic magnetized fluids, have made substantial progress \cite{1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14}. Current numerical codes are able to evolve isolated, accreting and binary black holes and neutron stars for long times compared to the dynamical time scales of the compact objects.

Most models, however, do not account for radiation transport. In some cases this is a reasonable approximation, particularly when the radiation is trapped and only influences the system on diffusion timescales, but there are many interesting situations where the interaction of matter with radiation fields cannot be neglected. Radiation can remove or supply energy and momentum to the matter, and thus influence the local thermodynamical state and composition of the material. In turn, this affects the bulk dynamical properties of fluid elements in a numerical simulation.

A major difficulty with discretizing radiation transport is its high-dimensional nature. Each radiation field depends on three positional and three momentum variables, which makes even storing the full field state at a particular time, and with enough resolution, a challenging proposition. One popular strategy is to make the diffusion assumption \cite{15} with additional flux limiters to handle the regions near free-streaming \cite{16}. Another strategy reduces the problem by taking averages over the momenta and leaving the remaining dynamics of the radiation field hidden in a closure relation \cite{15}. In addition, systematical approximations are employed to reduce the computational cost, either by assuming symmetries and thus reducing the dimensionality, or by averaging quantities like the energy.

Practical implementations of transport in compact objects have been mostly limited to Newtonian gravity and flows \cite{17, 18, 19, 20, 21, 22, 23}. The motion of photons and neutrinos is a genuinely relativistic problem, so existing schemes for Newtonian fluid flow often approximate the coupling terms to order $O(v/c)$, an assumption which will be violated as soon as the matter moves relativistically itself: in particular, the important case of outflows in gamma-ray bursts is excluded in this manner. General relativistic spacetime curvature can also be a substantial effect when compact objects are involved.

Attempts to discretize the general relativistic transport problem were mostly focused on spherically symmetric spacetimes \cite{24, 25, 26, 27, 28, 29, 30, 31, 32, 33}, since the computational complexity of the problem simplifies considerably in this case and makes a direct finite differenting integration of the Lindquist equation \cite{34} a reasonable proposition.

Discretization schemes not restricted to spherically symmetric spacetimes have not been investigated by many authors. Schinder \cite{35} describes the problem in the particular case of polar-sliced spacetimes (which at that time had been successfully used to simulate the collapse of a polytrope to a black hole \cite{36}). Anile and Romano \cite{37} discuss covariant flux-limited diffusion in general spacetimes (see also \cite{38}). Cardall and Mezzacappa \cite{39} provide a conservative formulation of the transport equations, both in the general case and in restriction to spherical symmetry. Farris et al \cite{40} have recently added an effective treatment of the radiation field to their general relativistic magnetohydrodynamics code, which discretizes the radiation in the same way as the fluid, under the gray approximation and the assumption that the radiation energy-momentum tensor is nearly isotropic in the comoving frame.

The methods listed above are ultimately based on finite-differencing and finite-volume techniques, which apply polynomial approximants to reconstruct the radiation field or moments over it. These schemes have been very successful in numerical implementations for hy-
dynamics, magnetohydrodynamics, and Einstein’s field equations. There are at least two major differences compared to the radiation transport problem: the first is that both the fluid as well as the spacetime metric are only dependent on three spatial and one time variable, whereas the radiation field depends, at each spacetime point, on three momentum variables as well, as mentioned above. The second difference is that the radiation field can have strongly peaked distributions in momentum space which are not easy to approximate with polynomials.

This paper investigates a discretization of radiation transport based on Monte Carlo methods. Monte Carlo schemes are particularly well-suited for high-dimensional problems as outlined in section II B and provide a degree of flexibility which is difficult to achieve with polynomial techniques. The scheme is constructed to solve the full transport problem, in general spacetimes and including full angular and energy dependency, but it should be straightforward to restrict to particular spacetime symmetries, or to the $O(c^2/c)$ approximation needed for a coupling to Newtonian fluids. The scheme is indirect, i.e. it admits an arbitrary specification of all probability density functions, which is particularly useful to derive adaptive methods for application problems. It can also handle optically thick regions by virtue of its hybrid approach, that is by using cell-based surface flux estimators. Since the scheme is local, it admit parallelization with standard domain-decomposition methods.

The paper is organized as follows: In section II general relativistic kinetic theory as needed for purposes of the Monte Carlo discretization is reviewed, and the basic idea of (indirect or deterministic) Monte Carlo techniques is presented. Section III contains the derivation of the Monte Carlo estimators for all terms in the collision integral, and also estimators for the energy-momentum contained in the radiation field. Section IV gives an outline of how such a scheme may be realized and coupled to existing evolution codes for general relativistic magnetohydrodynamics, and discusses some particular features of the Monte Carlo approach. Finally, section V concludes the paper with a summary and short discussion of future work.

II. BACKGROUND

A. General relativistic kinetic theory

Any attempt to represent a gas of photons, neutrinos, or other particles invites the application of kinetic theory. The original formalism for general relativistic kinetic theory is described in the seminal paper by Lindquist. This section will review some essential aspects of this theory needed for the discrete representation, following closely Ehlers and also Cardall and Mezzacappa.

In classical physics, the state of an ensemble of $n$ particles can be described by a point in the product phase space $M = M_1 \times \ldots \times M_n$, where each phase space $M_i$ is spanned by the configuration variables $x_i = (x_{i,1}, y_{i,1}, z_{i,1})$ and the momenta $p_i = (p_{i,1}^1, p_{i,1}^2, p_{i,1}^3)$. However, if one is rather interested in average properties of the ensemble, it is useful to introduce, for each type of particles, a distribution function defined on a one-particle phase space:

$$f(x, p, t) = \frac{dN}{d^3x d^3p}.$$  

Here, $N$ denotes the particle number in a particular phase space volume element, i.e. the object $f$ is the phase space density of particles of that type.

A similar object can also be introduced in general relativity. Let $(M, g)$ be the space-time manifold with metric $g$. Given the collection $T_x(M)$, $x \in M$ of tangent spaces associated with events in $M$, a new object, the eight-dimensional tangent bundle $T(M)$, can be constructed with the metric $g \otimes g$ and volume form $-\det(g_{ab}) dx^0 \wedge \ldots \wedge dx^3 \wedge dp^0 \wedge \ldots \wedge dp^3$.

Since particles of mass $m$ and momentum $p \in T_x(M)$ satisfy the mass-shell constraint $g(p, p) = -m^2$, the (one-particle) phase space of that particle type is given by $M_m = \{ x \in M, p \in T_x(M), g(p, p) = -m^2 \}$. If the mass shell is parametrized by the three-components of the momentum, a volume form on the shell is given by

$$\pi_m \equiv \sqrt{-\frac{3}{|p_0|}} dp^1 \wedge dp^2 \wedge dp^3.$$  

where $p_0$ is now a function given by the mass-shell constraint.

It will later be useful to employ proper frame coordinates on the mass shell, which we will denote by a wedge, i.e. $\hat{p} = (p^1, p^2, p^3)$ [39]. In this frame the element $\pi_m$ assumes the form

$$\pi_m = \frac{1}{E(\hat{p})} dp^1 \wedge dp^2 \wedge dp^3$$  

where $E(\hat{p}) = \sqrt{\hat{p}^2 - m^2}$.

A volume form on the one-particle phase space $M_m$ can then be constructed canonically, given the configuration space four-volume form $\eta = \sqrt{-g} dx^0 \wedge \ldots \wedge dx^3$.

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1 For Monte Carlo schemes as applied to Newtonian background flows, see [42, 43, 44, 45, 46, 47, 48, 49] and references therein.

2 This space is sometimes also called the sphere bundle in analogy to Riemannian geometry.
by the exterior product
\[ \Omega \equiv \eta \wedge \pi_m \]
\[ = \frac{-\hat{\Sigma}}{|p_0|} \, dx^0 \wedge \ldots \wedge dx^3 \wedge dp^1 \wedge dp^2 \wedge dp^3 \]
\[ = \frac{\sqrt{-\hat{\Sigma}}}{E(\hat{p})} \, dx^0 \wedge \ldots \wedge dx^3 \wedge dp^1 \wedge dp^2 \wedge dp^3 , \]
where the second equality is obtained from the specific form \( \mathbf{3} \).

Particle flow in phase space can be approximated by separating two different physical regimes: The first are long-range interactions with large-scale fields, most notably the interaction of charged particles with an electromagnetic field, and the second are short-range interactions, which we will approximate as point interactions for the present purpose, in particular containing direct interactions with matter (emission, absorption, scattering). The former can be represented as a four-force, while the latter are modifications to the distribution function in any domain containing the interaction event.

The particle flow itself is represented by orbits of the Liouville operator, which, in the absence of long-range forces, is given by the geodesics of the particles and their associated momenta. In explicit form, given a connection with coordinate coefficients \( \Gamma^{ab}_{bc} \), the Liouville operator is the vector field
\[ L \equiv p^a \frac{\partial}{\partial x^a} - \Gamma^a_{bc} p^b p^c \frac{\partial}{\partial p^a} . \]  

We will often need to integrate over hypersurfaces in the manifold \( M_m \) when considering the particle flow through a particular surface. Consider a hypersurface \( \Sigma \subset M_m \). On \( \Sigma \), we can introduce the 6-form \( \mathbf{50} \)
\[ \omega = p^a \sigma_a \wedge \pi_m , \]
where \( \sigma_a \) is the vectorial 3-surface element of configuration space, i.e. \( \sigma_a = \frac{1}{3!} \eta_{abcd} dx^b \wedge dx^c \wedge dx^d \), and \( \pi_m \) as given above.

The general relativistic distribution function \( f \) is then related to the number \( N[\Sigma] \) of particles crossing the surface \( \Sigma \) by the integral
\[ N[\Sigma] = \int_\Sigma f \, \omega . \]  

In the specific case where \( \Sigma \) is a small element of the phase space containing an observer at \( x \in M \), it can be written as \( \Sigma = G \times K \), where \( G \) is a spacelike hypersurface containing \( x \), and \( K \) is its associated set of mass shells. In the proper frame of this observer, the expression \( \mathbf{7} \) then limits (for vanishing spatial volume) in the differential \( f \, d^3 x \, d^3 p \). Therefore, the function \( f \) as defined above corresponds to the classical distribution function defined in \( \mathbf{1} \).

From the surface integral \( \mathbf{7} \), one can get a statement of particle conservation by considering a domain \( D \) of the sphere bundle. Application of the surface integral to the boundary \( \partial D \) of that domain, and using Stoke’s theorem, one obtains \( \mathbf{50} \)
\[ \Delta N[\partial D] = \int_{\partial D} f \, \omega = \int_D L[f] \Omega , \]
which relates the number of collisions in \( D \) to the Liouville flow \( L[f] \). The differential form of this equation is the relativistic Boltzmann or Lindquist equation \( \mathbf{54} \):
\[ L[f] = p^a \frac{\partial f}{\partial x^a} - \Gamma^a_{bc} p^b p^c \frac{\partial f}{\partial p^a} = C[f] , \]
and here \( C[f] \) stands for a source term which is the limit of \( \Delta N[\partial D] \) for a differential domain size \( D \).

A concept closely related to the distribution function is the invariant intensity \( \mathbf{13} \). Starting from the traditional definition of the radiation intensity \( I_\nu \), which is the energy emitted per time interval, surface area, angle and frequency interval, one can construct the Lorentz invariant
\[ \mathcal{J} \equiv \frac{I_\nu}{\nu^3} , \]
also called the invariant intensity. This object is related to the distribution function by only a numerical factor in the Planck constant \( h \) and the speed of light \( c \):
\[ f = \frac{c^2}{h^4} \mathcal{J} . \]  

The source term \( C[f] \) of the Lindquist equation is commonly splitted into the invariant emissivity \( e \) and the invariant opacity \( a \), which in general are functionals of \( f \) and may contain contributions from spontaneous emission, absorption, and scattering:
\[ C[f] = e[f] - a[f] f . \]  

**B. Monte Carlo techniques**

The simplest application of Monte Carlo techniques\(^3\) is to calculate properties of statistical systems by generating numbers with a particular random distribution, and thus constructing a sample of the ensemble space. This approach is called a direct simulation of a probabilistic problem, where the probability density functions (PDFs) are fixed by the problem to solve.

Monte Carlo methods can also be applied to deterministic problems, however. In this case, an estimator is defined, which is a map from the set of samples to a real number designed to approximate the value to solve for.

\(^3\) A general introduction to Monte Carlo methods is given in Hammersley and Handscomb \([\mathbf{13}]\).
A simple example is given by the integration problem: Consider the definite integral of a function \( f \) over the real interval \([a, b]\):

\[
I = \int_a^b f \, dx
\]  

(13)

A standard numerical technique is to use polynomial approximants, e.g., the trapezoidal rule, to obtain a sequence of approximate values which converge to \( I \) provided \( f \) satisfies certain conditions.

An indirect Monte Carlo method solves this problem in a different way: First, random samples \( x_i \in [a, b] \), \( i = 1, \ldots , N \) are generated according to an arbitrary PDF \( p \), also defined on \([a, b]\). Then, the estimator

\[
\{I\} = \frac{1}{N} \sum_{i=1}^{N} f(x_i) p(x_i)
\]  

(14)

is computed from the samples. For increasing number of samples, this estimator approximates the integral \( I \), limiting in the correct value for \( N \to \infty \), which is also expressed by saying that the estimator is unbiased. The asymptotic error behaves like \( 1/\sqrt{N} \).

A direct comparison to a polynomial technique of order \( k \) (\( k = 2 \) in the case of the trapezoidal rule) seems, at first sight, rather unfavorable for the Monte Carlo approach: the error of the polynomial scheme goes like \( 1/N^k \) and is therefore asymptotically superior to the Monte Carlo estimator. However, an interesting observation concerns multi-dimensional integrals: the Monte Carlo estimator retains the error \( 1/\sqrt{N} \), whereas a polynomial approximation by dimension has an error \( 1/N^{k/d} \), where \( d \) is the number of dimensions. For \( d = 4 \), the Monte Carlo scheme and the trapezoidal rule have the same accuracy, whereas for \( d > 4 \) Monte Carlo is asymptotically superior. Therefore, Monte Carlo techniques are considered particularly useful for high-dimensional problems.

This fact is of some interest for radiation transport: a second-order polynomial scheme should be asymptotically superior to a Monte Carlo scheme only for four dimensions or less. The full radiation transport problem, however, is six-dimensional, suggesting that using a Monte Carlo scheme may be preferable in that case. These estimates are only based on the asymptotic error, of course.

The actual magnitude of the local error can be reduced, sometimes by orders of magnitude, with variance-reduction techniques \[41\] like control variates, importance sampling and stratified sampling. Importance sampling, which makes use of the fact that the PDF can be chosen arbitrarily in indirect Monte Carlo schemes, could be particularly useful for radiation transport problems (see discussion in section\[IV\]).

### III. MONTE CARLO APPROXIMANTS FOR RELATIVISTIC KINETIC THEORY

#### A. Cell discretization, and decomposition of the collision integral

Assume \( D \subset M_{\text{int}} \) to be a domain of the phase space associated with particles of mass \( m \). From \[8\] we see that the number of interactions in \( D \) is given by the boundary integral

\[
\Delta N[\partial D] = \int_{\partial D} f \, \omega.
\]  

(15)

Consider configuration space to be parametrized by coordinates \((t, a, b, c)\), and a spacetime cell given by a region \( G = [t', t' + \Delta t'] \times \ldots \times [c'_j, c'_j + \Delta c'_j] \), where \( i, j \) are integers obtained from the discretization. We would like to characterize the emission of particles newly created in this spacetime interval by means of the source functions, the invariant emissivity \( \epsilon \) and the invariant opacity \( \kappa \).

For this purpose, first decompose the integral \[15\] into terms for each surface in configuration space and its entire associated future-directed mass shells:

\[
\Delta N[\partial D] = \int_{T^-} f \, \omega + \int_{T^+} f \, \omega + \ldots
\]  

(16)

where we label the cell surface \( t = t' = \text{const} \) by \( T^- \), the surface \( t = t' + \Delta t' = \text{const} \) by \( T^+ \), and all remaining six surfaces likewise. Next, further decompose each surface into an ingoing and outgoing component with respect to the space-time cell, and label the resulting surfaces \( A_{-in} \), \( A_{-out} \) and so on\[4\].

\[
\Delta N[\partial D] = \int_{T^-} f \, \omega + \int_{T^+} f \, \omega + \ldots
\]  

(17)

Every point on an outflow boundary surface can be backpropagated by the Liouville operator to a point on an ingoing boundary surface, and the evolution of the distribution function is given by the Lindquist equation

\[
\frac{\hbar^4}{c^2} L[f] = \frac{\hbar^4}{c^2} \frac{df}{d\lambda} = \frac{d}{d\lambda} = e - a \, \mathcal{J},
\]  

(18)

where \( \lambda \) is an affine parameter, and the last relation is the usual form involving the invariant emissivity and opacity. In general, both \( e \) and \( a \) are not only functions of the local fluid variables (and further macroscopic fields), but also functionals of the full distribution function on the past light cone at that point, making the relation \[18\] an integrodifferential equation.

The numerical scheme presented here separates between particles newly emitted in a volume element and

\[4\] Since all mass shells are future directed, this decomposition is trivial for the surfaces \( T^- \) and \( T^+ \).
those injected and absorbed subsequently. To formalize this separation, define, for a particular orbit of the Liouville operator, the function \( \tilde{f} \) to be a solution of the pure absorption component with initial condition \( \tilde{f}(\lambda_0) = f(\lambda_0) \) at the ingoing boundary point \( \lambda_0 \):

\[
\frac{d\tilde{f}}{d\lambda} = -a[\tilde{J}] \tilde{f}
\]  

(19)

This function represents the absorption of injected particles. Next, define another function \( \hat{f} \) as the solution of the full Boltzmann equation, but for vanishing inflow, i.e. \( f(\lambda_0) = 0 \). This represents particles newly created (and possibly immediately reabsorbed) inside the cell:

\[
\frac{d\hat{f}}{d\lambda} = e[\hat{J}] - a[\hat{J}] \hat{f}.
\]  

(20)

Now construct the sum \( \hat{f} \equiv \tilde{f} + \hat{f} \), which has the same inflow condition as \( \tilde{f} \), and insert this into the Lindquist equation:

\[
\frac{d\hat{f}}{d\lambda} = e[\hat{J}] - a[\hat{J}] \hat{f} - a[\tilde{J}] \hat{f}
\]  

(21)

In the particular case where \( e \) and \( a \) are independent of the changes in the distribution function while propagating inside the cell, the function \( \hat{f} \) is a solution to the Lindquist equation.\(^5\)

With an expression of the collision integral and the separation of \( f \) into \( \tilde{f} \) and \( \hat{f} \), we define \( \tilde{J}, \hat{J} \), and \( J \) by multiplying the corresponding invariant intensities by \( \frac{e^2}{h^4} \), and decompose (17) into contributions from \( \tilde{f} \) and \( \hat{f} \), yielding

\[
\Delta N[\vartheta D] = \Delta N_{em}[\vartheta D] + \Delta N_{abs}[\vartheta D]
\]  

(22)

\[
\Delta N_{em}[\vartheta D] = \int_{T^+} \tilde{f} \omega + \int_{T^+} \tilde{J} \vartheta \omega + \ldots
\]

\[
\Delta N_{abs}[\vartheta D] = \int_{T^+} \hat{f} \omega + \int_{T^+} \hat{J} \vartheta \omega + \ldots
\]

Physically, these represent the changes in the particle numbers due to emission of new particles as measured on the outflow surface, or absorption of particles injected at the inflow surface. In the next section, we will employ a Monte Carlo scheme to solve for the terms involving \( \hat{f} \). The remaining terms are treated in section III C.

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\(^5\) Note that both the emissivity and the opacity are still allowed to depend on the boundary values of \( f \) and on the affine parameter \( \lambda \), which in particular admits to model scattering processes. To treat the general case in some approximation, it is also conceivable to either neglect or approximate the non-linear coupling between the partial distributions, and treat each one independently as a nonlinear ODE.
where the components of $x$ depend on the surface as above, and each direction is sampled according to

$$Q_i(x') = \frac{1}{x_{i,\text{high}} - x_{i,\text{low}}}, \quad (27)$$

with $x_{i,\text{high}}$ and $x_{i,\text{low}}$ denoting the boundaries of integration.

Having fixed $Q(x)$, we need to specify $R(p)$ as well. The use of proper frame coordinates in the momentum space volume form $\pi$ is motivated by the often simpler form of emission and absorption coefficients in a frame comoving with a fluid. This suggest to use a factorized PDF $R(p) = N(\nu) M(\Omega)$, where $\nu$ is the frequency and $\Omega = (\Theta, \Phi)$ denotes directional variables in momentum space. Sampling frequency and direction separately is often useful on physical grounds, and a simple form of the directional component of the PDF can be obtained from a uniform distribution over the variables $(\cos(\Theta), \Phi)$.

There is a complication with selecting suitable samples with the form of $R(p)$ given above: Since the integrals only contain outgoing points in the phase space with respect to that surface, not all samples provide valid surface points. It is possible to represent the boundary by a transformation from coordinate space to a rest frame and adjust the PDF accordingly. However, another (simpler) way exists: sample the full directional PDF without regard to the boundary surface, but, after a transformation of the constructed momentum vector to the coordinate frame, reject those samples which are ingoing.\(^6\)

Finally, we need a value for $\tilde{f}$ at each sample point. This is obtained from the solution of the Lindquist equation as in \(20\), under the inflow boundary condition $\tilde{f}(\lambda_0) = 0$. In those cases where $e$ and $a$ are approximately constants within the cell, we can construct the formal solution of the Lindquist equation \(15\)

$$\tilde{f}(\lambda) = \frac{e}{a} + C \exp(-a\lambda) \quad (28)$$

where $C$ is a constant of integration. W.l.o.g. assume $\lambda_0 = 0$ and $\lambda = \Delta \lambda$ at the outgoing point. The condition $\tilde{f}(0) = 0$ leads to $C = -\frac{e}{a}$ and the solution at the outgoing point:

$$\tilde{f}(\Delta \lambda) = \frac{e}{a} (1 - \exp(-a\Delta \lambda)) \quad (29)$$

This is the well-known result that emission in optically thick sources $(a\Delta \lambda \gg 1)$ rapidly approaches the source function $\tilde{f}$. If $e$ or $a$ are varying substantially with $\lambda$ inside the cell, equation (28) can be numerically treated with an appropriate ODE integrator.

Given the estimators \(25\), we can consider each summand a bundle contributing a particular number of particles to the total estimate:

$$\{ \int_{\Sigma} \tilde{f} \, \omega \} = \frac{1}{N(\Sigma)} \sum_{i=1}^{N(\Sigma)} \tilde{f}(x_i, p_i) \, \omega(x_i, p_i) / P(x_i, y_i) \quad (30)$$

\(^6\) This technique, rejection sampling, is generally useful to sample under constraints, although it can also increase the variance in adverse conditions.
$$\frac{N(\Sigma)}{\partial^D} = \sum_{i=1}^{N(\Sigma)} \{N_i\}$$

These bundles provide a Monte Carlo discretization of the distribution function. The estimate \{N_i\} associated with a bundle will be called its weight. Physically, we may imagine a set of directed bundles of \{N_i\} photons to be emitted from the cell.

In contrast to a sampling of the emissivity following a particular fluid world line, which gives a direct Monte Carlo scheme and is a grid-less technique as far as the radiation field is concerned, the estimator (24) is grid-based and indirect, i.e. the PDFs are not fixed and can be chosen arbitrarily. We will discuss some particular uses of this level of freedom in section IV.

It is sometimes useful to obtain a representation for \(f\) itself from the bundles. This can be obtained by assuming a distributional form

$$\{\tilde{f}\} = \sum_{i=1}^{N(\Sigma)} \{N_i\} \alpha_i \delta(x - x_i) \delta(\hat{\nu} - \hat{\nu}_i)$$

where \(x\) is the tupel of coordinates spanning the particular surface, and \(\alpha_i\) is yet unspecified. We perform the integral over the surface \(\Sigma\):

$$\int_\Sigma \tilde{f} \omega = \int_\Sigma \sum_{i=1}^{N(\Sigma)} \{N_i\} \alpha_i \delta(x - x_i) \delta(\hat{\nu} - \hat{\nu}_i)$$

where \(\omega\) has the particular form appropriate for that surface as above. This allows us to fix the coefficients \(\alpha_i\) by comparison with (31) to

$$\alpha_i = \frac{1}{\omega(x_i, \hat{\nu}_i)}$$

and we therefore obtain

$$\{\tilde{f}\} = \sum_{i=1}^{N(\Sigma)} \frac{\{N_i\}}{\omega(x_i, \hat{\nu}_i)} \delta(x - x_i) \delta(\hat{\nu} - \hat{\nu}_i).$$

### C. Monte Carlo estimators for absorption

Return to the expression (25) for the emission estimators:

$$\int_\Sigma \tilde{f} \omega = \frac{1}{N(\Sigma)} \sum_{i=1}^{N(\Sigma)} \frac{\tilde{f}(x_i, \hat{\nu}_i) \omega(x_i, \hat{\nu}_i)}{P(x_i, y_i)}.$$

The particular surface \(\Sigma\) considered here also appears as boundary surface of an adjacent cell \(\Sigma’\), but with a reversed normal vector and thus an inverse association with ingoing and outgoing mass shell components. Consider \(\Sigma\) to be the complement of \(\Sigma\) in the union of ingoing and outgoing hypersurfaces associated with a specific configuration space surface: then both are also subsets of \(\partial \Sigma’\) and in particular \(\Sigma\) is ingoing and \(\Sigma\) is outgoing with respect to \(\partial \Sigma’\).

It follows that the estimator (25) also serves as an estimator for the integral over the function \(\tilde{f}\) as defined in the previous section, effectively giving inflow boundary condition in form of a Monte Carlo estimator. A distributional representation of the function \(\tilde{f}\) on \(\Sigma \subset \partial \Sigma’\) can be reconstructed as in equation (34).

To obtain the propagation and absorption estimator, we turn to the second half of the terms in the collision integral (17), namely those associated with \(\tilde{f}\):

$$\Delta N_{\text{abs}}[\partial \Sigma’] = \int_{T} \tilde{f} \omega + \int_{T} \tilde{f} \omega + \int_{A_{\text{in}}} \tilde{f} \omega + \ldots$$

Here, all integrals will contribute in the general case.

Using the distributional representation of \(\tilde{f}\) (31) on each ingoing surface \(\Sigma_{\text{in}}\), we can represent those integrals by a sum of integrals over non-intersecting, arbitrarily small control regions containing each discretization point (see also figure 2):

$$\int_{\Sigma_{\text{in}}} \tilde{f} \omega = \int_{\Sigma_{\text{in}}} \sum_{i=1}^{N(\Sigma_{\text{in}})} \frac{\{N_i\}}{\omega(x_i, \hat{\nu}_i)} \delta(x - x_i) \delta(\hat{\nu} - \hat{\nu}_i)$$

The particular surface \(\Sigma\) considered here also appears as boundary surface of an adjacent cell \(\Sigma’\), but with a reversed normal vector and thus an inverse association with ingoing and outgoing mass shell components. Consider \(\Sigma\) to be the complement of \(\Sigma\) in the union of ingoing and outgoing hypersurfaces associated with a specific configuration space surface: then both are also subsets of \(\partial \Sigma’\) and in particular \(\Sigma\) is ingoing and \(\Sigma\) is outgoing with respect to \(\partial \Sigma’\).

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Here, all integrals will contribute in the general case.

Using the distributional representation of \(\tilde{f}\) (31) on each ingoing surface \(\Sigma_{\text{in}}\), we can represent those integrals by a sum of integrals over non-intersecting, arbitrarily small control regions containing each discretization point (see also figure 2):

$$\int_{\Sigma_{\text{in}}} \tilde{f} \omega = \int_{\Sigma_{\text{in}}} \sum_{i=1}^{N(\Sigma_{\text{in}})} \frac{\{N_i\}}{\omega(x_i, \hat{\nu}_i)} \delta(x - x_i) \delta(\hat{\nu} - \hat{\nu}_i)$$

where the surfaces \(\Sigma_i\) satisfy \(\Sigma_i \subset \Sigma_{\text{in}}\), \(\Sigma_i \cap \Sigma_j = \emptyset\) for \(i \neq j\) and \((x_i, \hat{\nu}_i) \in \Sigma_i\).

Now define flux tubes \(D_i\) from the orbits of the Liouville operator intersecting \(\Sigma_i\). These tubes intersect the cell at a surface \(\Sigma_i\) contained in the union of its ingoing surfaces. Since the tube has been constructed from the Liouville flow, the general relation (8) holds for the tube:

$$\mid \Delta N[\partial D_i] \mid = \int_{\partial D_i} f \omega = \int_{D_i} L[f] \Omega.$$

Since the tube boundaries are parallel to the Liouville orbits, they have zero volume with respect to \(\omega = L \cdot \Omega\) and do not contribute to the surface integral. Therefore an estimator for the difference in particle number between \(\Sigma’\) and \(\Sigma_i\) is given by

$$\Delta N_{\text{in}} = \left\{ \int_{\Sigma_{\text{in}}} f \omega \right\} - \left\{ \int_{\Sigma_{\text{in}}} f \omega \right\}$$

$$\left\{ \int_{D_i} L[f] \Omega \right\}$$

Introduce a 6+1 decomposition of the tube with the generating function given by an affine parameter \(\lambda\). Then we can employ the same distributional representation as in (31) for each slice. The integral over the slices defines a function \(N_i(\lambda)\) which takes the role of \(f(\lambda)\) as
averaged over the slice, and thus follows the same equation as \( \dot{f} \) in equation (19):

\[
\frac{dN_i(\lambda)}{d\lambda} = -a N_i(\lambda),
\]

with initial condition given by \([N_i]\). If \( a \) is approximately constant inside the cell, we can easily construct a formal solution providing the difference estimate:

\[
[N'_i] = [N_i] \exp(-a\Delta\lambda)
\]

Here \( \Delta\lambda \) is the affine distance between the sample \((x_i, \hat{p}_i)\) and its Liouville development at \(\Sigma'_i\). This relation reflects the expected result that the particle number in a bundle stays constant without source, and decreases exponentially with the effective optical depth. In those cases where \( a \) varies substantially with \( \lambda \), a numerical solution for the ODE can be obtained.

Having obtained an estimate for the number of particles on all \(\Sigma'_i\), we can define the remaining part of the estimator for \( \dot{f} \) by using equation (31) for all outgoing surfaces of \( D \):

\[
\{ \int_{\Sigma_{out}} \dot{f} \omega \} = \int_{\Sigma_{out}} \sum_{i=1}^{N(\Sigma_{out})} \frac{[N'_i]}{\omega(x_i, \hat{p}_i)} \delta(x - x^i) \delta(\hat{p} - \hat{p}^i) \omega
\]

The sample locations are the Liouville developments of the samples on the ingoing surfaces, or solutions of the geodesic equation in the absence of long-range forces. This completes the definition of estimators for all terms in the decomposition of the collision integral.

D. Estimators for energy-momentum

To couple a radiation transport scheme to Einstein’s field equations or general relativistic magnetohydrodynamics, we need an estimate of the energy-momentum tensor \( R \) of the radiation field. Since the Monte Carlo scheme defines the kinetic function \( f \) only in a distributional sense, the energy-momentum tensor can be estimated in an integral form, which also translates well into finite-volume schemes usually applied to obtain a correct weak solution for fluids [51, 52].

The starting point for obtaining conservative schemes is the general conservation law derived from \( \partial \sigma = 0 \) [53], given a spacetime region \( \Omega \):

\[
\int_{\Omega} d^4R = \int_{\partial\Omega} \sigma R = 0.
\]

Given a tangent space basis \([e_a]\) and the surface form \( \sigma_a \), the surface integral can be expressed in components as

\[
\int_{\partial\Omega} \sigma R = \int_{\partial\Omega} e_a R^{ab} \sigma_b.
\]

The surface \( \partial\Omega \) can be decomposed into parts \( G_i \cup G_i = \partial\Omega \) as needed for the spacetime discretization.

The energy-momentum tensor associated with a distribution function \( f \) is given by [50]

\[
R^{ab} = \int_{\Sigma_i} p^a p^b f \pi,
\]

where the integration covers the mass shell at the configuration space point under consideration.

Inserting this form into equation (14), and using the distributional representation of \( f \) in equation (34), yields the desired estimator for a configuration space surface \( G_i \subset \partial\Omega \):

\[
\{ \int_{G_i} \sigma R \} = \int_{\Sigma_i} e_a p^a p^b \{ f \} \sigma_b \land \pi
\]
\[ = \int_{\Sigma_i} e_a p^a \{ f \} \omega \]
\[ = \int_{\Sigma_i} e_a p^a \sum_{i=1}^{N(\Sigma_i)} \omega(x_i, \hat{p}_i) \delta(x - x_i) \cdot \delta(\hat{p} - \hat{p}_i) \omega \]
\[ = \sum_{i=1}^{N(\Sigma_i)} \{N_i\} e_a(x_i) p_i^a\]

where we have used \( \omega = p^a \sigma_a \wedge \pi \), and where \( \Sigma_i \) is the union of \( G_i \) with all its future-directed mass shells as in section III B.

IV. SOME CONSIDERATIONS FOR NUMERICAL IMPLEMENTATIONS OF THE SCHEME

This section contains a brief discussion of how to realize the Monte Carlo estimators discussed in section III in a practical application, and also contains some remarks on potential uses of the arbitrary probability density functions in astrophysical models.

Numerical codes which solve the (magneto-) hydrodynamics equations coupled to Einstein’s field equations\(^7\) regularly employ a finite-volume discretization of the fluid\([51, 52]\) and either the BSSN\([54, 55, 56]\) or generalized harmonic\([57]\) form of Einstein’s field equations, discretized with finite differences.

If a radiation transport module is to be coupled to such a system, the amount of energy-momentum in the radiation field \( R \) needs to be accounted for in the BSSN or generalized harmonic system, and since conservation is satisfied by the total energy-momentum tensor (fluid, magnetic field, and all radiation species), all emission, absorption and scattering processes extract or supply energy and momentum to the fluid.

A simple approach is to perform the coupling in an operator-split manner, in which the radiation field estimators are updated separately. The spacetime projection of the cell \( S \) employed in section III can be identical to the cells employed in the finite-volume method, but that is not a requirement, and different grid resolutions can be prescribed as needed. The spacetime metric updated by the BSSN/harmonic code enters in the volume forms and the geodesic equations, whereas the fluid variables provide the rest frame and thermodynamic state of the matter, possibly including chemical and nuclear composition variables, from which emission, absorption and scattering coefficients can be derived. In turn, the estimators\([47]\) yield approximations to the amount of energy-momentum in the radiation field and act as sources and sinks for both the spacetime and the fluid.

The radiation transport step itself may be performed in this order:

- **Choose a set of probability density functions.** For each cell surface \( \Sigma \), construct a PDF \( P_{\Sigma}(x, p) \), on the spacetime surface and all associated mass shells. This function can be chosen arbitrarily, and it can be different between all cells.

- **Create random samples.** For each cell surface \( \Sigma \), sample the PDF chosen above with an arbitrary number of samples \( N(\Sigma) \). The sample locations \( (x_i, p_i) \) on the surface can be obtained by generation of pseudorandom numbers in the unit interval \([0, 1]\), e.g. with the popular Mersenne twister algorithm\([58]\). For a one-dimensional PDF, the sample location is then formally the inverse of the cumulative distribution function applied to the value on the unit interval obtained above\([41]\). Factorizations like those suggested in section III B can greatly simplify the multidimensional case. In general, tabulated values can be employed for complicated PDFs.

- **Create new bundles.** The samples admit to defining surface emission estimators as given by equation \(25\). The necessary values of the surface element can be obtained from the spacetime metric and equations \(26\). The value of \( f \) in general calculated by integrating an ODE, but for constant emissivity and opacity a formal solution as discussed in section III B can be used. The effective emissivity and opacity are, in the simplest case, a function of the material thermodynamic state alone, but may also depend on the radiation field estimate at inflow when scattering is dominant.

  The affine length \( \Delta \lambda \) needed in this expression is a function of the intersection of the particle geodesic curve with the cell boundaries, which can be approximated by a Taylor expansion.

- **Propagate existing bundles.** The set of existing (and newly created) bundles is propagated up to each surface \( T^+ \). The bundle weight is adjusted according to equation \(40\), which needs to be treated as an ODE in general. In the case of constant opacity, the affine length can again be approximated by a Taylor expansion.

- **Estimate radiation energy-momentum.** For newly emitted particles, the estimators for the energy-momentum in the radiation field, equation \(47\), approximate the amount of energy and momentum removed from the fluid. In turn,

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\(^7\) See e.g. [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14] and references therein.

\(^8\) The implementations of the C standard library function \( \text{rand} \), or its Fortran equivalent, are often not sufficiently accurate for Monte Carlo applications.
when absorption is estimated, they determine the amount returned to the fluid. Scattering is formally treated in the same way, since the end result of scattering is always a particular surface state of the radiation field, and an associated flux coupled to the fluid flux.

A scheme constructed along these lines covers the simulation domain with a large set of bundles and separately integrates each bundle. The quality of the fluid-radiation coupling, and therefore also the coupling between curves in the Liouville flow, is determined by the cell size and the number of samples per cell.

Since the probability density functions are not related to the emissivity and opacity, a number of schemes can be employed to reduce the discretization error of the scheme. Importance sampling [41] is a basic technique in which approximately known properties of the solution are used to define probability density functions which reduce overall variance. In practice, a frequency sampling roughly based on the local emissivity and opacity should give better results than a linear or logarithmic distribution function.

More importantly, the directional distribution of bundles can be varied freely. This can be used to reduce variance in the radiation field in directions which are considered more important for a particular problem. One example would be the polar heating by neutrino-antineutrino annihilation in collapsar disks: If a geometrical region of interest is identified, the angular PDF can be selected such that the field has increased resolution in those Liouville orbits which intersect that region. In essence, the free choice of PDF gives rise to flexible adaptive techniques, which can be combined with actual adaptive mesh refinement in the cell-based discretization if required.

All these advantages can be used in the context of Newtonian approximations to the simulations of compact objects as well: In this case, a suitable background metric needs to be derived from the Newtonian gravitational potential, and the coordinate transformations to the rest frame are performed to $O(v/c)$ as in other approaches [15,23,59]. The geometric curvature introduced by non-Cartesian (spherical, cylindrical) grids is already contained in the covariant form of the expressions. Therefore the scheme is not restricted to general relativistic applications.

The discretization presented here is also conservative, which is a desirable property for radiation transport (see also [39]). All energy and momentum removed from a cell via the flux estimators is accounted for in the expression for the energy-momentum tensor, and only absorption and out-scattering can reduce the particle number, energy and momentum associated with each bundle.

A final but important remark concerns the parallelization of the scheme. Any full six-dimensional discretization of radiation transport will likely dominate the computational requirements of a simulation. In recent years, one of the traditional approaches to increasing computational performance, by raising the clock frequency of the processing core, has failed due to heat dissipation issues [60]. Therefore, future architectures will tend to employ massive parallelization in the order of $10^5 \ldots 10^6$ computing cores or more per machine, and numerical algorithms need to be designed to effectively use such resources. The hybrid Monte Carlo method is particle/cell-based and local, and therefore admits the use of standard domain decomposition techniques for load distribution. It should be possible to design implementations which are scalable to large parallel high performance architectures in the future.

V. CONCLUSION AND OUTLOOK

This paper contains an indirect Monte Carlo discretization of general relativistic radiation transport. Starting from the general expression for the collision integral applied to a cell decomposition of the configuration and phase space, Monte Carlo functions are introduced which provide unbiased estimates of phase space surface integrals over the relativistic distribution function. This approach is indirect, that is it leaves all probability density functions used to select samples in phase space unspecified.

The relativistic distribution function is split into two components with different inflow boundary conditions per cell. In the linear approximation, where the collision terms do not depend on the distribution, this decomposition is exact. For practical implementations, it provides an approximation which improves with diminishing finite volume of the cell. The split allows to treat two parts of the collision integral separately: one for the construction of new bundles, and one for the propagation of existing ones. In addition to collision estimators, a similar estimator for the energy-momentum in the radiation field is constructed, and can be used for coupling the radiation to general relativistic magnetohydrodynamics and Einstein’s field equations.

Finally, an outline of a numerical implementation of this transport scheme is given, with some additional remarks on expectations concerning the adaptiveness, parallel efficiency and conservative nature of the scheme.

The scheme exhibits a number of promising features compared to other approaches: the local nature of the operators which is expected to help parallelizing the scheme, the free choice of probability density functions which makes the use of adaptive techniques easier, and its fully covariant formulation which should make coupling to both general relativistic and Newtonian codes, possibly with non-Cartesian coordinates, straightforward. Besides these properties, an actual implementation and the associated tests are expected to be a major effort, particularly when a full coupling to general relativistic magnetohydrodynamics is considered.

Some advanced methods may also be worthy of in-
vestigation in the future: there exist a number of so-called variance-reduction methods, which are ultimately designed to reduce the discretization error of Monte Carlo estimators. Importance sampling has already been mentioned. Quasi-Monte Carlo is the name of a set of techniques where sequences are constructed with methods from number theory such that they minimize a particular distributional measure. Although these sequences are not random, they provide unbiased estimators with substantially lower variance than random sampling. Stratified sampling is another technique which cuts the sampling domain into intervals and therefore into separate estimators. And control variates split analytically tractable control functions from the estimator, thus reducing the average discretization error based on the approximation made by the variate. More advanced techniques are known in the literature, e.g. antithetic variables which reportedly reduce variances up to $10^{-6}$ in certain cases, according to Hammersley and Handscomb [41].

In the future, Monte Carlo techniques should deserve further attention, particularly when full six-dimensional radiation transport is to be calculated on upcoming large-scale parallel machines. With good parallel scaling and sufficiently large machine allocations, the simulation of $10^{11} \ldots 10^{12}$ bundles should be within the range of possibilities during the next five years, which may give enough resolution for an interesting class of problems.

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