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Notes

Integral formulation of null-collision Monte Carlo algorithms

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ABSTRACT

At the kinetic level, the meaning of null-collisions is straightforward: they correspond to pure-forward scattering events. We here discuss their technical significance in integral terms. We first consider a most standard null-collision Monte Carlo algorithm and show how it can be rigorously justified starting from a Fredholm equivalent to the radiative transfer equation. Doing so, we also prove that null-collision algorithms can be slightly modified so that they deal with unexpected occurrences of negative values of the null-collision coefficient (when the upper bound of the heterogeneous extinction coefficient is nonstrict). We then describe technically, in full details, the resulting algorithm, when applied to the evaluation of the local net-power density within a bounded, heterogeneous, multiple scattering and emitting/absorbing medium. The corresponding integral formulation is then explored theoretically in order to distinguish the statistical significance of introducing null-collisions from that of the integral-structure underlying modification.

1. Introduction

The introduction of null-collisions in the process of modelling photon transport consists in transforming the standard radiative transfer equation

$$\frac{\partial f}{\partial t} + c\boldsymbol{\omega}.\nabla f = -(k_a + k_s)cf + \mathcal{S} + \int_{4\pi} k_s c f' p(\boldsymbol{\omega}|\boldsymbol{\omega}')\, d\boldsymbol{\omega}' \qquad (1)$$

into

$$\frac{\partial f}{\partial t} + c\boldsymbol{\omega}.\nabla f = -(k_a + k_s + k_n)cf + \mathcal{S} + \int_{4\pi} k_s c f' p_S(\boldsymbol{\omega}|\boldsymbol{\omega}')\, d\boldsymbol{\omega}' + \int_{4\pi} k_n c f' \delta(\boldsymbol{\omega}-\boldsymbol{\omega}')\, d\boldsymbol{\omega}' \qquad (2)$$

where

- $f \equiv f(\mathbf{x}, \boldsymbol{\omega}, t)$ is the distribution function at location $\mathbf{x}$, propagation direction $\boldsymbol{\omega}$ and time t. The distribution function is used here, instead of the specific intensity $I = h\nu cf$, in order to help readers from other particle transport communities such as neutron transport, plasma physics and rarefied gas dynamics, that have made an intensive use of null-collision approaches [1–3] (see Appendix A for a brief description of the rather complex structure of the corresponding literature).
- c is the speed of light, $k_a(\mathbf{x}, t)$ the absorption coefficient, $k_s(\mathbf{x}, t)$ the scattering coefficient, $p_S(\boldsymbol{\omega}|\boldsymbol{\omega}') \equiv p_S(\boldsymbol{\omega}|\boldsymbol{\omega}', \mathbf{x})$ the single scattering phase function, that is to say the probability density that the scattering direction is $\boldsymbol{\omega}$ for a photon initially in the direction $\boldsymbol{\omega}'$. The

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notation f' in the scattering source integral stands for $f' \equiv f(\mathbf{x}, \boldsymbol{\omega}', t)$.

- $\mathcal{S} \equiv \mathcal{S}(\mathbf{x}, \boldsymbol{\omega}, t)$ is any source term. We will define $s \equiv s(\mathbf{x}, \boldsymbol{\omega}, t)$ such that $\mathcal{S} = k_a c s$, and therefore $s = f^{eq}(\mathbf{x}, t)$ in the particular case of thermal emission under the assumption of local thermodynamic equilibrium, where $f^{eq}(\mathbf{x}, t)$ is the distribution function at equilibrium at local temperature (related to the Planck specific intensity B according to $B = h\nu c f^{eq}$).
- k_n is the null-collision coefficient and δ is the Dirac distribution.

Additional collisions are introduced via the term $-k_n c f$ but these collisions are cancelled out, as they are scattering events in the pure forward direction (the phase function is $\delta(\boldsymbol{\omega}-\boldsymbol{\omega}')$ in the scattering source integral), and leave the f field unchanged, which is a direct consequence of the property $\int_{4\pi} k_n c f' \delta(\boldsymbol{\omega}-\boldsymbol{\omega}')\, d\boldsymbol{\omega}' = k_n c f$. To the best of our knowledge, outside the above mentioned transport physics literature, the only reported practical use of null-collision approaches for radiative transfer applications is in the fields of computer graphics and medical imaging [4,5].

Such applications are related to Monte Carlo simulations in which the heterogeneity of the absorption and scattering coefficients does not allow the implementation of simple free path sampling algorithms. When defining the location of the next collision event, the common practice is indeed to first sample an extinction optical thickness τ according to the probability density function $p_T(\tau) = \exp(-\tau)$, and then derive the corresponding path length λ by inverting the function relating τ to λ: $\tau(\lambda) = \int_0^\lambda k(\mathbf{x} + \sigma\boldsymbol{\omega}, \boldsymbol{\omega}, t + \sigma/c)\, d\sigma$, where $k = k_a + k_s$. However, if k_a and k_s are complex functions of space, this inversion is difficult to perform analytically. Most usually, k_a is then approximated with discretization approaches, but this implies a rigorous control of the corresponding approximation level. Introducing null-collisions is a way to avoid such approximations.

A null-collision k_n field can indeed be introduced so that the modified extinction coefficient $\hat{k} = k_a + k_s + k_n$ (corresponding to absorption plus true scattering plus null-collision) allows tractable $\tau(\lambda)$ inversions (e.g. $\hat{k}$ uniform). Practically,

- $\hat{k}$ is arbitrarily chosen as an upper bound of the true extinction field k ($\hat{k} > k$) and k_n is then defined as $k_n = \hat{k} - k$ (note that the choice is made on $\hat{k}$, not on k_n, so that $\hat{k}$ has the expected inversion properties);
- a collision location is sampled by first sampling $\hat{\tau}$ according to p_T and inverting $\hat{\tau}(\lambda) = \int_0^\lambda \hat{k}(\mathbf{x} + \sigma\boldsymbol{\omega}, \boldsymbol{\omega}, t + \sigma/c)\, d\sigma$;
- a random number r is sampled uniformly on the unit interval and the collision is considered as an absorption event if $0 < r < k_a/\hat{k}$, as a real scattering event if $k_a/\hat{k} < r < (k_a + k_s)/\hat{k}$, or as a pure forward scattering event if $(k_a + k_s)/\hat{k} < r < (k_a + k_s + k_n)/\hat{k} = 1$ (fortune wheel).

This technique is well suited to the recent Monte Carlo developments toward flexible validation tools for accuracy control of fast radiation solvers (interacting with chemistry and fluid mechanics). In such contexts, field representation is bound to the specificity of each solver in an intricate manner and null-collision algorithms make it possible to design transversal meshless[1] Monte Carlo codes that are immediately applicable whatever the retained solver numerics be.

The present technical note addresses the question of using integral formulation techniques for refining Monte Carlo algorithms involving null-collisions. For didactic reasons, we first consider the academic question of evaluating the distribution function (at a given point in a given direction) in an heterogeneous emitting/absorbing infinite medium using a backward algorithm (Section 2). The corresponding integral formulation is constructed step by step as a translation of the above described null-collision algorithm. This formulation is then modified so that the constraint $\hat{k} > k$ is relieved: negative values of the null-collision coefficient are accepted. This is practically very significant because $\hat{k}$ must be chosen to match k as closely as possible (otherwise too many useless collisions are sampled), which is a delicate task when the constraint $\hat{k} > k$ is strict. This first technical proposition is detailed in Section 3, with the complete description of a Monte Carlo algorithm evaluating the local net-power density within a bounded, heterogeneous, multiple scattering and emitting/absorbing medium. A second technical proposition is made in Section 4: an integral formulation is constructed that helps clarify the significance of introducing null-collisions, in particular as far as convergence is concerned. This formulation indicates that the problem of sampling free paths in heterogeneous fields could be bypassed without introducing any null-collision concept, but sign alternations would appear that would be the sources of statistical variance. It is then shown that further benefit of introducing null-collisions is to break this sign alternation. We therefore suggest to preserve the idea of introducing a $\hat{k}$ field, but without imposing that free paths to be sampled according to $\hat{k}$, or that the type of collision (absorption, true scattering or forward continuation) be sampled according to the respective proportions of k_a, k_s and $k_n = \hat{k} - k_a - k_s$. A wider class of Monte Carlo algorithms is therefore identified that could be explored for convergence enhancement.

2. Theoretical justification and extension to negative values of the null-collision coefficient

In the particular case of stationary radiation[2] in a non-scattering infinite medium, the distribution function at location $\mathbf{x}$ in the direction $\boldsymbol{\omega}$ takes the following integral

[1] "Meshless" is here used to indicate that the Monte Carlo algorithm requires no volume discretization. Therefore, if the input fields of temperature and extinction coefficients are analytical (as in benchmarking exercises) no mesh is used at all. However, if the input fields are provided using a volume discretization and an interpolation procedure, the grid is rigorously respected. The idea is that the input fields can take any form and that the Monte Carlo algorithm introduces no mesh by itself.

[2] Transient radiation would induce no specific theoretical difficulty, but it would make the integral formulation much heavier. The extinction coefficients would indeed be functions of time and time would itself depend on path-length.