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A Boundary-Based Net Exchange Monte-Carlo Method for absorbing and scattering thick media

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Abstract

A boundary-based net-exchange Monte Carlo method was introduced in [1] that allows to bypass the difficulties encountered by standard Monte Carlo algorithms in the limit of optically thick absorption (and/or for quasi-isothermal configurations). With the present paper, this method is extended to scattering media. Developments are fully 3D, but illustrations are presented for plane parallel configuration. Compared to standard Monte Carlo algorithms, convergence qualities have been improved over a wide range of absorption and scattering optical thicknesses. The proposed algorithm still encounters a convergence difficulty in the case of optically thick, highly scattering media.

Key words: Monte Carlo, net-exchange formulation, scattering, numerical optimization, convergence

1 Introduction

The Monte-Carlo Method (MCM) has been widely used in the field of transport phenomena simulation, and more specifically in the field of radiative transfer computing [2–4]. In this particular case, the method mainly consists in simulating numerically the physical statistical model of photons transport, from their emission to their absorption in a potentially scattering medium. A well known advantage of this method is that the corresponding computing

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code is easy to set up and to modify. Another main advantage is that it is a reference method : as the MCM is a statistical method, a standard deviation may be computed in addition to each result, that may be interpreted as a numerical uncertainty. Also, it has recently been shown that the MCM allows the computation of parametric sensitivities with no extra significant computing [5]. This can be helpful for design needs, or when radiative transfer is coupled with other physical processes. Finally, the MCM is known to be well adapted to the treatment of configurations with a high level of complexity (complex geometries, complex spectral properties, ...). However, in spite of these advantages over other methods and in spite of the regular increase of available computational powers, the computational effort requirement of MCM often remains a significant drawback.

Different works in the last fifteen years tried to preserve the main advantages of the method, in particular its strict analogy with physical processes, and the ability to solve complex problems, while trying to improve convergence qualities. There are mainly two ways MCM convergence can be enhanced : formulation changes and adaptation of sampling laws [2]. As far as formulation is concerned, most attention has been devoted to reverse Monte Carlo algorithms [6], that make use of reciprocal transport formulations (application of the reciprocity principle to the integral form of the radiative transfer equation), and to net-exchange Monte Carlo algorithms [7–10], that make use of net exchange transport formulations (combination of forward and reciprocal formulations, photons being followed both ways along each optical path). Net-exchange Monte Carlo algorithms allowed in particular to bypass the problem of standard Monte Carlo algorithms for quasi-isothermal configurations. As far as sampling laws optimization is concerned, numerous works have successfully used the biasing of sampled directions toward the parts of the system that most contribute to the addressed radiative quantity [11], or the biasing of sampled frequencies as function of temperature field and spectral properties [7,12].

Recently, the combination of formulation efforts and sampling laws adaptations permitted to solve the well known convergence problem of traditional Monte-Carlo algorithms in the case of strong optical thickness configurations [1]. If a gas volume is optically very thick, most emitted photons are absorbed very close to their emission position, and thus do not take part to the exchange of the gas volume with the rest of the system. Consequently, very large numbers of statistical realizations are required to reach satisfactory convergences. This problem could be solved in the case of purely absorbing systems thanks to a net-exchange formulation in which emission positions are sampled, starting from the volume boundary, along an inward oriented sampled direction (a formulation that will be named here a "boundary-based net-exchange formulation"). All sampling laws (frequency, boundary position, direction and emission position) were also finely optimized in order to insure that the al-

gorithm automatically adapts to system optical thickness in the whole range from the optically thin to the optically thick limits.

The present paper is one of a series that seek to improve the MCM through such methodological developments. It proposes techniques to take into account scattering in the above mentioned boundary-based net-exchange algorithm. The formulation used in [1] has been generalized and clarified in order to take into account the scattering phenomena. Developments are fully 3D, but convergence illustrations are presented for plane parallel configurations that are specifically meaningful in the atmospheric science community.

Sec. 2 of this article puts the emphasis on the multiple integral theoretical developments on which our Monte-Carlo algorithm is based. Sec. 3 presents gas volume emission results in a simple test case, thus revealing the algorithm convergence qualities together with its limits of applicability. Finally, Sec. 4 completes this convergence illustration in terms of radiative flux divergence profiles.

2 Theoretical developments

The three next paragraphs deal with improvements that were brought to the standard bundle transport MCM during the last few years, through a number of different methodological developments.

2.1 Exchange Formulation

Let us consider that, for the purpose of a 3D radiative transfer computation, the considered system is divided into volume and surface elements. Until further mention, this geometric division is only motivated by the required level of analysis and it therefore implies no physical assumption : the volume and surface elements have any geometrical shapes and are inhomogeneous.

The energy rate $E_{i,j}$ emitted by an arbitrary gas volume i and absorbed by an arbitrary gas volume j may be expressed as :

$$E_{ij} = \int_{V_i} dV_i(P) \int_{4\pi} d\omega(\mathbf{u}_0) \int_{\Gamma(P, \mathbf{u}_0)} p(\gamma; P, \mathbf{u}_0) d\gamma k_a(P) \sum_{n=1}^{\infty} T_{\gamma,n} \int_{l_{\gamma,n}^-}^{l_{\gamma,n}^+} d\sigma_n(P'_n) k_a(P'_n) B(P) \exp\left(-\int_{l_{\gamma,n}^-}^{\sigma_n} d\sigma' k_a(\sigma')\right) \quad (1)$$