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Null-collision meshless Monte-Carlo—Application to the validation of fast radiative transfer solvers embedded in combustion simulators

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ABSTRACT

The Monte-Carlo method is often presented as a reference method for radiative transfer simulation when dealing with participating, inhomogeneous media. The reason is that numerical uncertainties are only of a statistical nature and are accurately evaluated by measuring the standard deviation of the Monte Carlo weight. But classical Monte-Carlo algorithms first sample optical thicknesses and then determine absorption or scattering locations by inverting the formal integral definition of optical thickness as an increasing function of path length. This function is only seldom analytically invertible and numerical inversion procedures are required. Most commonly, a volumic grid is introduced and optical properties within each cell are replaced by approximate homogeneous or linear fields. Simulation results are then sensitive to the grid and can no longer be considered as references. We propose a new algorithmic formulation based on the use of null-collisions that eliminate the need for numerical inversion: no volumic grid is required. Benchmark configurations are first considered in order to evaluate the effect of two free parameters: the amount of null-collisions, and the criterion used to decide at which stage a Russian Roulette is used to exit the path tracking process. Then the corresponding algorithm is implemented using a development environment allowing to deal with complex geometries (thanks to computer graphics techniques), leading to a Monte Carlo code that can be easily used for validation of fast radiative transfer solvers embedded in combustion simulators. "Easily" means here that the way the Monte Carlo algorithm deals with both the geometry and the temperature/pressure/concentration fields is independent of the choices made inside the combustion solver: there is no need for the design of a new path-tracking procedure adapted to each new CFD grid. The Monte Carlo simulator is ready for use as soon as combustion specialists provide a localization/interpolation tool defining what they consider as the continuous input fields best suiting their numerical assumptions. The radiation validation tool introduces no grid in itself.

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1. Introduction

Industrial applications, such as combustion processes, require radiative transfer modeling, often coupled with other energy transfer mechanisms. Numerical radiative transfer solvers used in such applications need to reach the best compromise between numerical accuracy and

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computation cost. These tools also need validation, and therefore reference numerical methods have to be used. The Monte-Carlo method (MCM) is known to be one of these reference methods. Like all other methods, MCM evaluates numerically the solution of the radiative transfer equation (RTE) and its "reference" status is only due to the existence of a rigorous measure of its uncertainty: from its statistical nature, MCM allows the systematic calculation of a standard deviation associated to each numerical result, and this standard deviation is translated into a numerical uncertainty thanks to the central limit theorem. However, designing Monte-Carlo algorithms to be used in complex geometries has long been a quite challenging task, mainly because of prohibitive computational costs. Using MCM to produce references and validate the radiative parts of heat-transfer or combustion solvers was therefore hardly feasible outside academic configurations. Recent developments, such as the work reported by Zhang et al. [1,2], show that this is now practically feasible whatever the complexity of industrial geometries. We here propose to further develop such tools using a meshless Monte-Carlo algorithm based on the null-collision technique introduced in [3].

Monte-Carlo algorithms dealing with participating media [4–10] are commonly formulated so that they sample the optical thickness. One major feature of such algorithms is that a correspondence must be established between any value of the optical thickness, along any optical path, and the physical position associated to this optical thickness within the heterogeneous participating medium. As optical thickness is an increasing function of path-length, this inversion is always possible, without approximation, using standard numerical inversion techniques, but these techniques rapidly require prohibitive computation powers. A possibility to speed-up the inversion procedure is the use of a volumic grid [37] together with simple enough approximate profiles for optical properties within each cell, allowing an analytic inversion of position from optical thickness. However, introducing such a volumic grid involves an unwanted consequence: simulation results depend on the retained particular grid (as with any deterministic approach), and MCM looses its "reference" status.

Concerning volume discretization, let us clarify some vocabulary to be used throughout the text. The question that we address is the production of reference solutions of the RTE for temperature, pressure and concentration fields provided by combustion specialists wishing to validate their radiation solvers. These *input fields* may have any form. They may be analytic when academic benchmarks are considered, they may be based on local measurements at structured or unstructured grid points in experimental contexts, or based on the structured or unstructured outputs of fluid-mechanics/chemistry codes in pure numerical contexts. In all cases the input fields will be *complete*, meaning that temperature, pressure and concentrations are defined at all locations. In experimental and numerical contexts, this requires that combustion specialists provide not only the grid point data, but also a meaningful *interpolation model* to complete the fields throughout the volume (meaningful with regard to fluid mechanics and chemistry). *Reference RTE solutions* will be produced without discussing this interpolation model, and the corresponding algorithm will be called a *meshless algorithm* if it is fully independent of the input-field type, and if it introduces no discretization procedure in itself.

Recent methodological developments [3,11,12] indicate that it is possible to use so-called null-collision Monte-Carlo algorithms in the field of radiative transfer simulation. One major characteristic of null-collision algorithms (NCA) is that they do not require any volumic grid. They are no longer formulated using optical thicknesses. Path-length (and thus position) is directly sampled according to a probability density function of the form $p_\Lambda(\lambda) = \exp(-\int_0^l \hat{k}(\sigma)\, d\sigma)$, that is to say according to a Beer–Lambert extinction law in which the true extinction coefficient k is replaced by an overestimate $\hat{k}$, chosen in such a way that sampling p_Λ is mathematically straightforward. In neutron and plasma physics, where the method was first introduced, the $\hat{k}$ field was most commonly chosen uniform (or uniform by parts) and λ was sampled as $\lambda = (1/\hat{k})\log(r)$, with r a uniformly sampled value in the unit interval. Of course, sampling λ using an overestimate of the true extinction field introduces a bias, but this bias is compensated by the use of a rejection test: when rejection occurs the path is continued straightforward as if no collision occurred.

These algorithms can be interpreted (and rigorously justified) using simple physical pictures. Let us note $k_n = \hat{k} - k$. This additional extinction coefficient, k_n, can be interpreted as due to null-collisions, i.e. collisions that lead to a pure forward scattering event. Obviously such additional collisions change nothing to the radiative transfer problem. However, k_n can be chosen in such a way that the new total extinction coefficient $\hat{k} = k + k_n$ has a simple shape (for instance uniform) and allows easy path-length sampling procedures. But then, when a collision occurs, it can either be a true collision, with probability $P = k/\hat{k}$, or a null collision, with probability $1-P$, and this is how the rejection method is justified: if a null-collision occurs, the path is continued straightforward as if no collision occurred.

The only reported practical difficulty is the choice of the $\hat{k}$ field (or of k_n as they are directly related). Indeed $\hat{k}$ must be greater than k at all locations, but it must also be as close to k as possible in order to avoid that too many rejections occur, which would lead to computationally expensive sequences of path-length sampling and forward continuations until a true collision occurs. This compromise can be hard to reach, even in the most standard combustion configurations because of the flame heterogeneities as well as the non-linear dependence of gaseous absorption with temperature, pressure and concentrations. But most of this difficulty vanishes thanks to the theoretical developments of [3] that allow to handle rigorously the occurrence of negative null-collisions: the authors show indeed that the best choice is still that $\hat{k}$ be as close an overestimate of k as possible, but such a close adjustment can now be achieved without strictly excluding that $\hat{k} < k$ in some parts of the field.

We present hereafter an implementation of a slightly modified version of the null-collision algorithm (that of [3]).

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