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Radiative transfer and spectroscopic databases: A line-sampling Monte Carlo approach

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ABSTRACT

Dealing with molecular-state transitions for radiative transfer purposes involves two successive steps that both reach the complexity level at which physicists start thinking about statistical approaches: (1) constructing line-shaped absorption spectra as the result of very numerous state-transitions, (2) integrating over optical-path domains. For the first time, we show here how these steps can be addressed simultaneously using the null-collision concept. This opens the door to the design of Monte Carlo codes directly estimating radiative transfer observables from spectroscopic databases. The intermediate step of producing accurate high-resolution absorption spectra is no longer required. A Monte Carlo algorithm is proposed and applied to six one-dimensional test cases. It allows the computation of spectrally integrated intensities (over 25 cm^{-1} bands or the full IR range) in a few seconds, regardless of the retained database and line model. But free parameters need to be selected and they impact the convergence. A first possible selection is provided in full detail. We observe that this selection is highly satisfactory for quite distinct atmospheric and combustion configurations, but a more systematic exploration is still in progress.

1. Introduction

Recent advances in Monte Carlo methods [1,2] indicate that null-collision algorithms can be used to simulate radiative transfer in semi-transparent media in such a way that grids are no longer required. Even for highly non-homogeneous configurations the volume does not need to be discretized and this is achieved while still preserving all the statistical properties of standard Monte Carlo algorithms: convergence toward the exact solution is rigorous (no bias) and for a finite number M of samples, the estimate is associated with a faithful statistical uncertainty ($\frac{1}{\sqrt{M}}$ times the standard deviation of the Monte Carlo weights). The initial idea of null-collisions came from the plasma physics and neutron transport communities. It consists in adding a third type of collisional event to the absorption and scattering

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Nomenclature[1]

A_i	Bernoulli random variable
B_ν	blackbody intensity
d	distance
E	statistical expectation
$h_{a,\nu,j}$	contribution of transition j to the absorption coefficient
$\hat{h}_{\nu,j}$	contribution of transition j to the extinction coefficient
i	index of collision
i_b	narrowband index
I_ν	monochromatic specific intensity
j	index of molecular transition
$k_{a,\nu}$	absorption coefficient
$k_{n,\nu}$	null-collision coefficient
$k_{s,\nu}$	scattering coefficient
$\hat{k}_\nu$	extinction coefficient resulting from null-collision introduction
$\tilde{k}_\nu$	approximate absorption coefficient
m	index of independent realization
M	number of independent realizations
N_b	number of narrowbands
N_t	number of molecular transitions
P_a	probability of absorption
$P_{a,J}(j)$	probability of absorption for a given transition j
$P_b(i_b)$	probability of narrowband i_b
$P_J(j)$	probability of transition j
P_n	probability of null collision
$p_X(x)$	probability density function for absorption/emission location
$\hat{p}_X(x)$	probability density function for absorption/emission location considering null-collision events
$p_N(\nu)$	probability density function for wavenumber
$p_s(\boldsymbol{\omega}\|\boldsymbol{\omega}')$	single scattering phase function
$Q_J(j)$	second component of the proposed transition probability expression
r	random number sampled uniformly over the unit interval
S_k	moments of order k
t	time
T	temperature
$t_{1\%}$	computation time require to get a 1% standard deviation
$T_U(u)$	first component of the proposed transition probability expression
u	index of spectral bands
VOV	variance of variance
w	Monte Carlo weight
x	location (scalar)
x_0	observation location
$\mathbf{x}$	location (vector)
y	absorption/emission location at the end of a path involving null-collisions
α	multiplicative factor
γ_Q	half-width of an arbitrary Lorentz profile
δ	delta-Dirac distribution
δ_π	partial derivative with respect to parameter π
$\delta\nu$	spectral interval
ζ	extinction threshold
ν	wavenumber
π	generic parameter
τ	transmissivity
$\boldsymbol{\omega}$	direction (vector)

events. These new collisions change nothing with regard to the propagation of radiation. They are pure-forward scattering events: after the collision, the photon continues its trajectory as if no collision had occurred (the collision is "null" or "virtual"). The amount of such collisions can therefore be tuned to any value without modifying the resulting transfer. This tuning can then be such that the total density of the colliders is uniform: more null-collisions are added where true extinction is weak, fewer where it is strong, so that the total extinction coefficient is uniform (as in a homogeneous semi-transparent medium). The consequence is that collision locations can be sampled within a simple exponential-distribution, according to the Beer extinction law. It is thus only at the sampled location that the question is raised of evaluating the respective amounts of absorbers, true-scatterers and null-colliders, in order to sample one type of events out of the three possible ones (according to their respective probabilities). The photon-transport Monte Carlo algorithm is therefore decoupled from the spatial description of radiative properties. It is not required to "know" the true radiative properties when transporting photons until their next collision location.

In preceding null-collision algorithms, the radiative properties were indeed known and the only benefit was a simplification of the procedure for accessing the data (getting rid of the volume-discretization requirement). Here we assume that the monochromatic absorption coefficient $k_{a,\nu}$ is unknown and that the only available data are those of the molecular spectroscopic databases [3–6]. We still have $k_{a,\nu}=\sum_{j=1}^{N_t} h_{a,\nu,j}$, where N_t is the number of molecular transitions and $h_{a,\nu,j}$ is the known contribution of the j-th transition to the absorption coefficient at wavenumber ν, but this sum is not precomputed. Null-collisions allow us to initiate the Monte Carlo algorithm without computing $k_{a,\nu}$ and we then observe that the algorithm can be continued without ever making this computation: $\sum_{j=1}^{N_t} h_{a,\nu,j}$ is diluted into the photon-transport algorithm via successive samplings of the transition index.

Why this is possible is quite simple. Let us take only two transitions: $k_{a,\nu}=h_{a,\nu,1}+h_{a,\nu,2}$ and write $k_{a,\nu}=P_1\frac{h_{a,\nu,1}}{P_1}+P_2\frac{h_{a,\nu,2}}{P_2}$ with P_1 and P_2 in $]0,1[$ and $P_1+P_2=1$. This justifies a Monte

[1] We retain here the following standard statistical formalism: random variables are written in upper-case (*e.g.* X), free and bound variables in lower-case (*e.g.* x) and samples of random variables are subscripted (*e.g.* x_m).