HYBRID MONTE-CARLO METHOD FOR ICF CALCULATIONS

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Abstract

We present a new numerical method for radiation transport equations well adapted to ICF calculations. It consists in a dynamic coupling, in space and frequency variables, between a full transport description and diffusion approximation of the radiative transfer equation. This method has been introduced in the 2D radiation hydrocode FCI2. Results are compared with full Monte-Carlo simulations of a simplified laser cavity.

Introduction

At the present time, scientific computing is the one of the main tools for an accurate design of Inertial Confinement Fusion (ICF) targets. In the indirect drive configuration, it requires the numerical simulation of radiation transport: laser energy is first converted to X-ray in a gold wall and then transferred to the fusion target through an hohlraum filled with gas. The emission region is moving in the gold wall which is rapidly expanding into the hohlraum so that the radiative transfer equations have to be coupled with hydrodynamic motion.

One of the difficulties is to compute the non-isotropic irradiation on the capsule and to control them by an appropriate balance between the energy of the different laser beams. Hence an approximate description of radiation transport is not relevant and a transport method has to be chosen. On the other hand, transport method are known to be more or less inefficient in optically thick regions: for instance in the gold wall before it is sufficiently heated and ablated to become optically thin. In these regions, diffusion approximation of the transfer equations is an accurate description of the physical phenomenon; moreover it is much more cheaper to solve numerically than the full transport equations. This is why we introduced an hybrid method for radiation transport where the lower part of the energy spectrum is treated in the diffusion approximation whereas the higher part is treated by a transport method.

This method has been introduced in a 2D ICF hydrocode FCI2 and its results have been compared with the standard method, i.e. full transport.

The paper is organized as follows: in next section, we shall briefly describe the FCI2 code and give the physical background. In third section, we will introduce the hybrid method. We will then give some numerical results on a simplified ICF calculation. Several issues are still to be addressed: at last, we shall briefly discuss these problems.

ICF calculations and ICF hydrocode

The goal of ICF is to use laser energy to bring a target in the conditions where fusion reaction occurs. More precisely, the ultimate goal is obtain to high gain targets, i.e. to get more fusion energy than the laser energy used to ignite the target.

In the indirect drive configuration, laser energy is not transferred directly into the target but first converted into X-ray: the target is a small Deuterium-Tritium sphere of 1 mm radius put in the center of a hohlraum filled with gas and the X-ray conversion take place in a cylindrical gold wall of 50 μm thickness. The whole cavity is a cylinder approximatively 1.2 cm long and 0.3 cm radius (see figure below) An accurate description of all physical phenomenons which occur in the cavity requires the use of numerical simulation. The FCI2 [3] hydrocode has been used for several years at the CEA for laser studies. It is a lagrangian code with Arbitrary Lagrangian Eulerian capabilities, flux-limited thermal (ionic and electronic) conduction and ray-tracing for laser description. It is coupled with non-equilibrium atomic physics package for opacities. Radiation transport is usually solved by a Monte-Carlo method either Implicit Monte-Carlo (IMC) [4] or Symbolic Implicit Monte-Carlo (SIMC) [6].

In an ICF calculation, the main part of CPU is used to solve the radiative transfer equations:

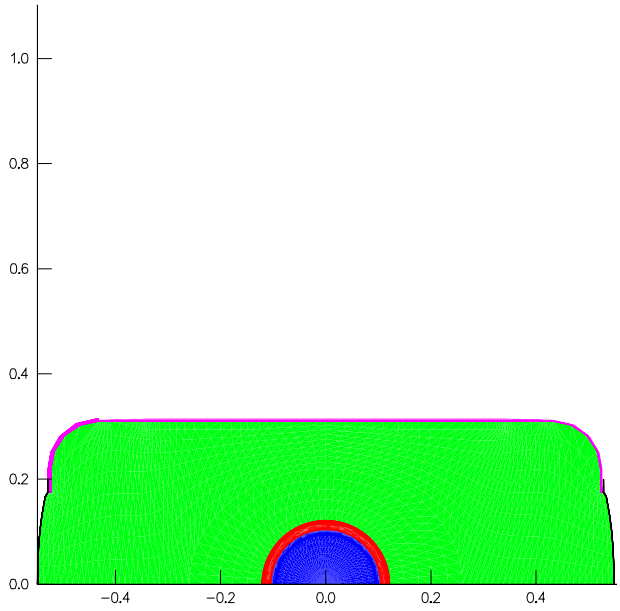

Figure 1: ICF cavity: DT fuel (blue), Helium gas (green), Ablator (red) and Gold wall (pink)

it consists in an integro-differential equation in phase space coupled with energy-balance equation which writes as (neglecting hydrodynamic motion)

$$\begin{cases} \partial_t I_\nu + c\vec{\Omega}.\nabla I_\nu + c\sigma_\nu(I_\nu - \dfrac{B_\nu(T)}{4\pi}) = 0 \\ \partial_t E(T) + c\displaystyle\int\int \sigma_\nu(\frac{B_\nu(T)}{4\pi} - I_\nu)d\nu d\vec{\Omega} = 0, \end{cases} \tag{1}$$

where radiative intensity I_ν depends on frequency ν, direction $\vec{\Omega}$, space position x and time t. c is the speed of light, σ_ν the emission-absorption opacity, T the matter temperature, $E(T)$ the internal energy and the Planck function $B_\nu(T)$ is given by

$$B_\nu(T) = \frac{2h\nu^3}{c^2}\frac{1}{\exp(\dfrac{h\nu}{kT}) - 1}.$$

Despite the rapid progress of deterministic algorithms (see [1] for a recent contribution), Monte-Carlo methods are still very popular for solving radiative transfer equations. This is especially the case for 2D and 3D problems because the number of unknowns becomes rapidly prohibitive.

When σ_ν is large, we have

$$I_\nu \sim \frac{B_\nu(T)}{4\pi} + \frac{1}{4\pi\sigma_\nu}\vec{\Omega}.\nabla B_\nu(T) \tag{2}$$

and radiative energy $E_r = \dfrac{1}{c}\displaystyle\int I_\nu d\nu d\vec{\Omega}$ is solution of the diffusion equation

$$\partial_t(E(T) + E_r) = \mathrm{div}(\frac{c}{3\sigma^R}\nabla E_r) \tag{3}$$

with $E_r = aT^4$ and σ^R is the Rosseland mean of σ_ν (see [5] for details). Because equation (3) is much cheaper to solve than equation (1) it is highly desirable to solve the diffusion equation as soon as the approximation is justified: this is the purpose of hybrid methods.

Hybrid Method

The principle of hybrid method is to solve equation (1) in one part of the domain and equation (3) in another part. For stationary problems, when photon mean-free path is somewhat constant, it is possible to decide which equation is relevant in any given part of the simulation. This is no longer the case in ICF problems.

In particular, the gold wall is initially cold and hence optically thick. When laser beams hit the wall, a heat conduction wave travels toward the exterior and the gold becomes progressively transparent: a fixed boundary between diffusion approximation and transport description is not appropriate.

Another important issue is the variation of σ_ν with respect to the spectral variable ν. In a fully ionized plasma σ_ν behaves as ν^{-3}; in gold, the variation is much more complicated but σ_ν is, at first approximation, decreasing with respect to ν (except for some specific frequencies). It means that approximation (2) may be justified only at low frequencies.

In [2], we have introduced a new hybrid method based on the notion of spectral cut-off. We will only give the main features of the method and refer to [2] for more details. After spectral discretization, the continuous variable ν takes its value in some discrete set $\cap K = (k_0, k_1, \ldots, k_N)$. The spectral cut-off, is a function $k(x,t)$ with values in $\cap K$ such that:

- For $k \leq k(x,t)$, we approximate I_k with the help of (2) with the Planck function at some temperature T_t which may differ from the matter temperature T.
- For $k > k(x,t)$, we do not make any approximation and solve the transport equation.

When introducing $k(x,t)$ into (1) we arrive at:

$$\left\{\begin{array}{l} \partial_t I_k + c\vec{\Omega}.\nabla I_k + c\sigma_k(I_k - \dfrac{B_k(T)}{4\pi}) = 0,\ k > k(x,t) \\ \partial_t \left(\displaystyle\sum_{k\leq k(x,t)} B_k(T_t)\right) + c \displaystyle\sum_{k\leq k(x,t)} \sigma_k(B_k(T_t) - B_k(T)) = \mathrm{div}\left(\displaystyle\sum_{k\leq k(x,t)} \frac{c}{3\sigma_k}\nabla B_k(T_t)\right) \\ \partial_t E(T) + c\displaystyle\int \sum_{k>k(x,t)} \sigma_k(\frac{B_k(T)}{4\pi} - I_k)d\vec{\Omega} + c \sum_{k\leq k(x,t)} \sigma_k(B_k(T) - B_k(T_t)) = 0, \end{array}\right. \tag{4}$$

With this formulation, transport and diffusion formulation occur at the same space location. A generalized Marshak condition appears a discontinuity of the function $x \mapsto k(x,t)$. (see figure (2).

So far, we have not yet specified the numerical algorithms which will be used to solve the transport and the diffusion equation. We could have the choice between deterministic or stochastic method for transport equation (diffusion equation is solved using a finite volume approximation). In coupling diffusion approximation and transport description, the difficult

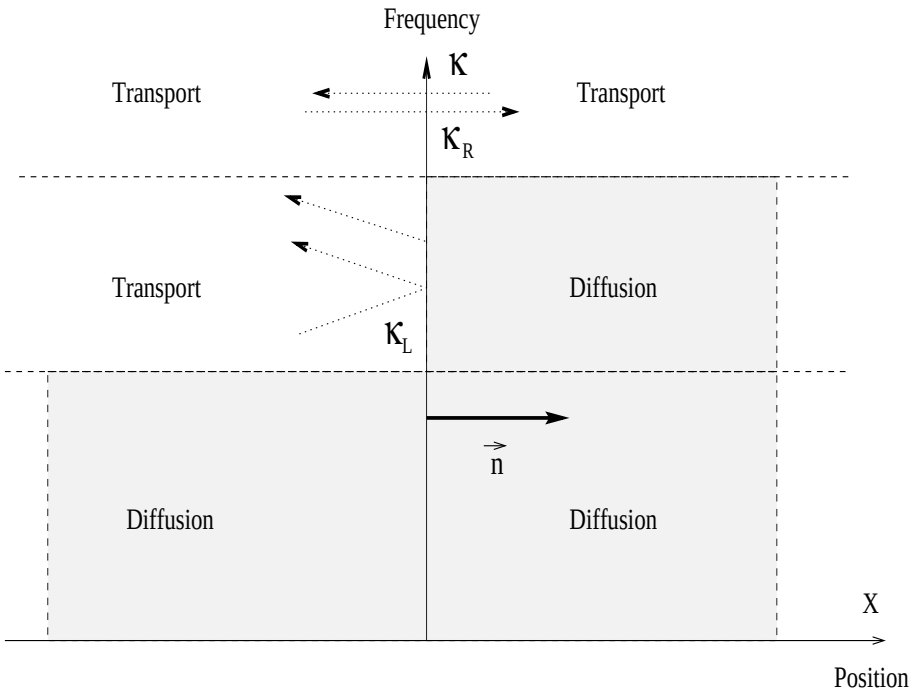

Figure 2: Transport-diffusion interface

part comes from the need for an implicit time discretization of the emission-absorption term. It appears that Symbolic Monte-Carlo method is a good candidate for system (4). It consists in computing the linear operator (i.e. the matrix) $\mathcal{M}$ and the vector $\mathcal{S}$ such that

$$c \int \sum_{k>k(x,t)} \sigma_k I_k d\vec{\Omega} = \mathcal{M} \begin{bmatrix} T_t^4 \\ T^4 \end{bmatrix} + \mathcal{S}.$$

matrix $\mathcal{M}$ is called the Monte-Carlo matrix and is obtained by solving the transport equations of (4) by a Monte-Carlo method (see [6]). Putting this expression in the third equation we arrive at a non-linear diffusion-like equation which is solved by Newton's method.

At each step of Newton's algorithm, the Monte-Carlo matrix is added to usual diffusion matrices for radiative (and thermal) conductions: we finally arrive at a non-symmetric linear system to invert. It can be proven that this problem is well posed but one issue is the sparsity of the matrix (see next section).

Simplified ICF calculation

To test and validate our method, we used a simplified Laser cavity. Main differences between a full simulation are:

- The target (ablator and fuel) is replaced by a vacuum and we impose the law of displacement of the boundary.
- We do not take into account the plastic window which usually close the cavity, preventing the helium gas to leave the hohlraum.

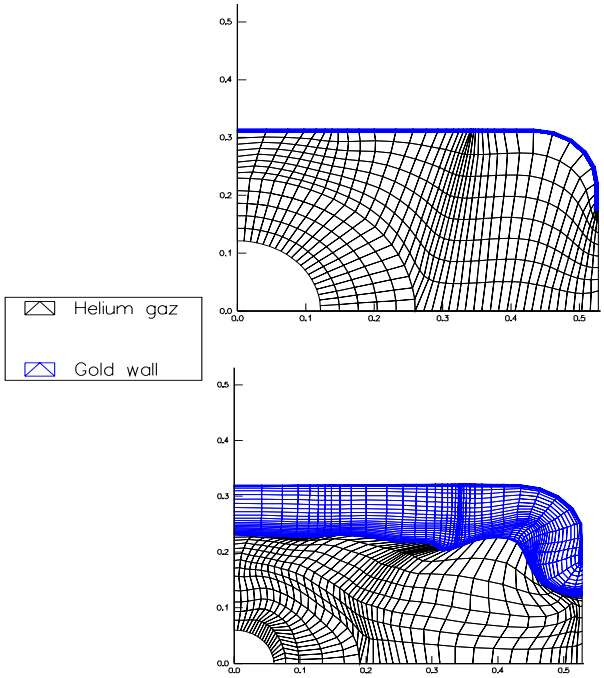

Figure 3: Geometry at t=0 ns (top) and t=20 ns (bottom)

- We use only equilibrium values for Equation of state and opacity.

So we only concentrate on the behavior of the radiative intensity as the wave enters the gold wall. One important quantity is the so-called temperature cavity, i.e. the mean radiative temperature in the gas, because it accounts for the incoming radiative energy emitted by gold and power losses through gold wall and laser entry holes.

Full Monte-Carlo Simulation

Figure (3) shows the evolution of the cavity and the radiative temperature from 0 to 20 ns (i.e. the duration of laser pulse). We observe the large mesh distortion due to the expansion of the gold plasma into the gas.

The mesh size is very small in gold at the interface (first cell is $4.10^{-8}\,cm$ thick at the beginning of the simulation and $10^{-2}\,cm$ thick at the end). Temperature is very high and density very low hence cells are optically thin and the Monte-Carlo treatment is always accurate at the boundary between gas and gold. However, in the interior of the wall, the mesh size is much higher, the temperature lower and the density higher: Monte-Carlo treatment is questionable. At exterior interface temperature remains low so that opacity remains large and cells remain optically thick: Monte-Carlo treatment is no longer correct but as it does not affect the temperature inside the cavity it is not important. Figure (4) represents the evolution of the optical depth of three distinct gold cells (at the interior boundary, in the middle and at the exterior boundary).

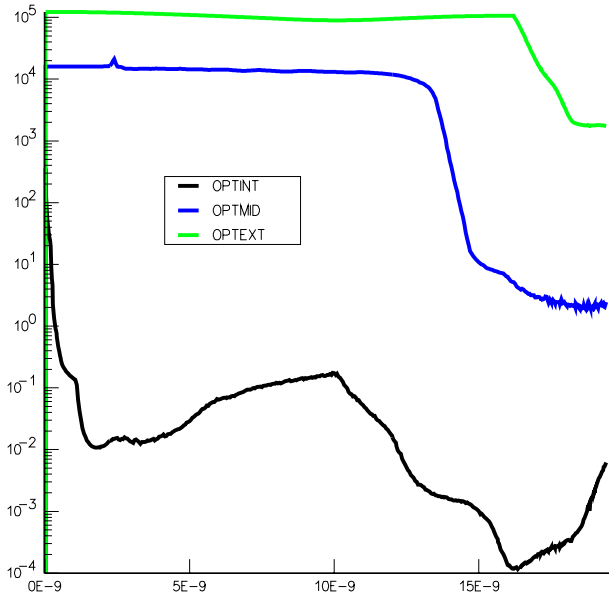

Figure 4: Evolution of optical depth of cells in gold

Hybrid Monte-Carlo simulation

The basic ingredient for using the Hybrid Monte-Carlo method is a criterion for the choice of the spectral cut-off. This criterion should be based on the comparison of one typical length scale and one typical mean-free path. The simplest criterion is the following:

$$k(x,t) = \min\{k,\ \forall k' > k,\ \sigma_{k'}(x,t)L(x,t) < C\} \tag{5}$$

where $L(x,t)$ is the cell size and C some given number. If $C = 0$ then $k(x,t) = N$ and the diffusion approximation is applied everywhere and everytime. If $C = +\infty$ then $k = 0$ and we recover full transport description. It is important that the results remain stable even for a large variation of C because this constant is quite arbitrary. In the following simulations, C takes the values $C = 1$, $C = 3$ and $C = 10$. We represent at time $t = 15\ ns$ the fraction of radiative energy which is represented by Monte-Carlo particles in gold (see figure (5)) and its evolution with respect to time.

S We observe that this value increases when C increases: a larger part of the gold is treated by the transport method. The extension of the region where diffusion is applied for low frequencies and transport for high frequencies remains small. We observe also that the boundary between transport and diffusion treatment is regular (there is no small "transport" region embedded in a larger "diffusion" region).

When looking at the cavity temperature, the differences between full Monte-Carlo and hybrid Monte-Carlo with three different values of the criterion C are small (see figure (6)).

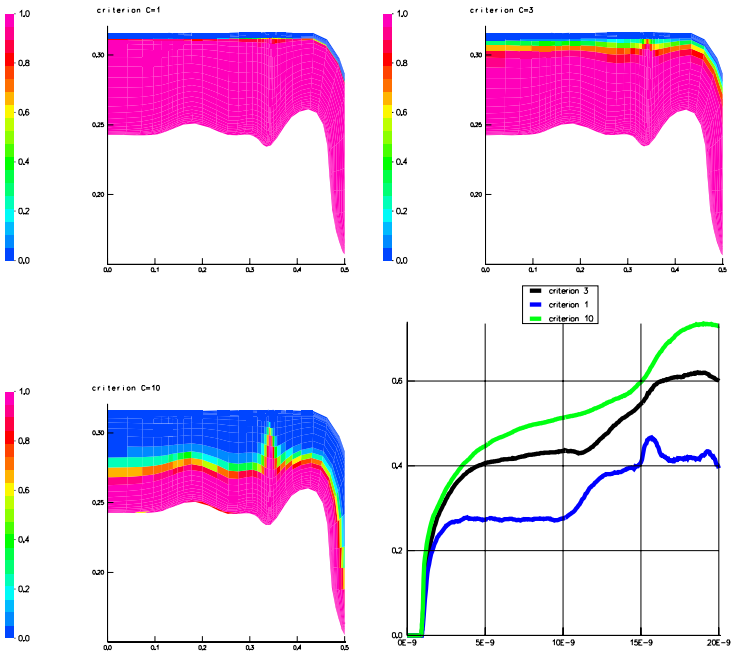

Figure 5: fraction of radiative energy represented by Monte-Carlo particles and its evolution with respect to time for three values of the criterion

Hence, although the Monte-Carlo treatment of the whole gold wall could appear unjustified when looking at optical depths, it seems that it does not affect the radiative energy which is emitted in the cavity.

Performances

In this section, we will compare the benefits and the drawbacks of hybrid Monte-Carlo compared to full Monte-Carlo with respect to computational issues. We will concentrate on the criterion $C = 1$. This discussion only applies to full Monte-Carlo with Symbolic Monte-Carlo method: in the IMC method of [4] extra collision events appear that may become the dominant part of the tracking in the cold part of gold so the method is less efficient than SIMC for this kind of problem.

First, we emphasize the fact that, for a given number of Monte-Carlo particles to track, Hybrid Monte-Carlo requires more arithmetic operations due to collisions at transport-diffusion interfaces. Moreover, there is some extra computational time spent for the calculation of the frequency cut-off at each time-step and in every-cell and an extra diffusion matrix to assemble. On the other hand, a significant part of the domain is treated only in the diffusion approximation so the number of particles tracked is lower in the hybrid case. Finally the inversion of the linear system and Newton's algorithm for the non-linear diffusion equation requires a different number of iterations (it appears that this number is usually higher for the Hybrid method). Finally, we find that the total CPU[1] cost are approximatively equal for the two methods (see figure (7):

[1] The results were obtained on one single alpha processor.

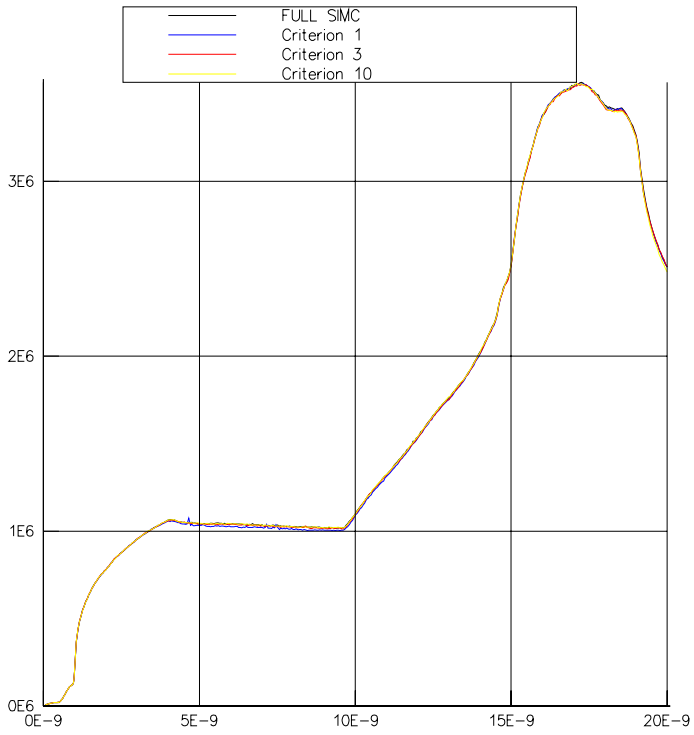

Figure 6: Radiative temperature in the cavity for full Monte-Carlo and hybrid Monte-Carlo with three different values of the criterion

this is of course strongly problem-dependent.

An important issue is the sparsity of the Monte-Carlo matrix. For a given column j, the number of non-zero terms in the matrix is equal to the number of cells visited by particles issued from cell j this is bounded by $\frac{c\Delta t}{\Delta x}$ where Δt is the time step and Δx the typical mesh around cell j. The time step is usually constrained by a CFL condition which writes as $c_s \frac{\Delta t}{\Delta x} \leq 1$ where c_s is the speed of sound waves. So we see that the number of non-zero terms is only bounded by $\frac{c}{c_s}$ which is very large. However, we notice that, when opacity is large, particles are absorbed very close to their originating cell so that the number of cells is small and, when opacity is small, particles can travel very far without being absorbed so that the number of cells may becomes large but on the other hand the whole matrix becomes strongly diagonally dominant so there is no problem with the inversion of the linear system (problems arise rather from memory storage). We represent in figure (8) the evolution of the density of the Monte-Carlo matrices for full and hybrid method (the density is defined as $\frac{\text{number of non-zero terms}}{(\text{mesh size})^2}$): we observe that no storage problem occurs, the density decreases toward the end of the simulation because of decreasing time step.

Because a non-negligible part of gold is treated in the diffusion approximation when and where it is a correct approximation, Monte-Carlo oscillations are lower in the hybrid simulation than in full Monte-Carlo (see figure (9). As the CPU time is similar in both cases, we can conclude that, for this kind of simulation, the figure of merit is better with the hybrid method

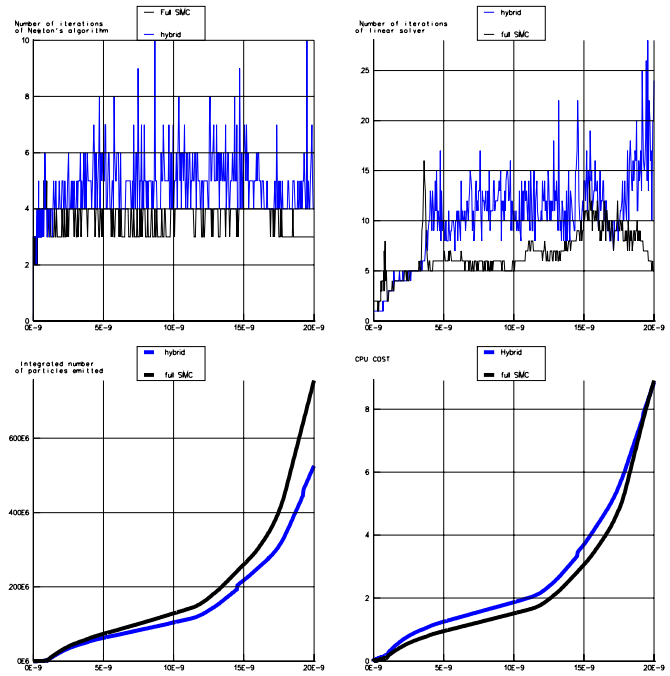

Figure 7: Numbers of iteration for conjugated gradient and inversion of linear system, integrated number of particles tracked and total CPU time (in hours) as a function of time

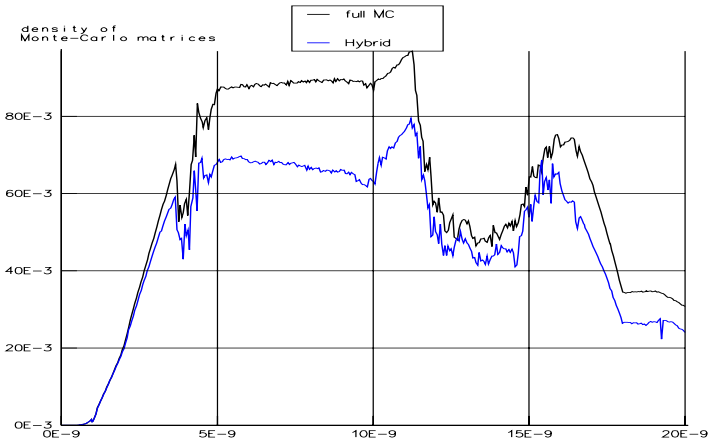

Figure 8: density of Monte-Carlo matrices as a function of time

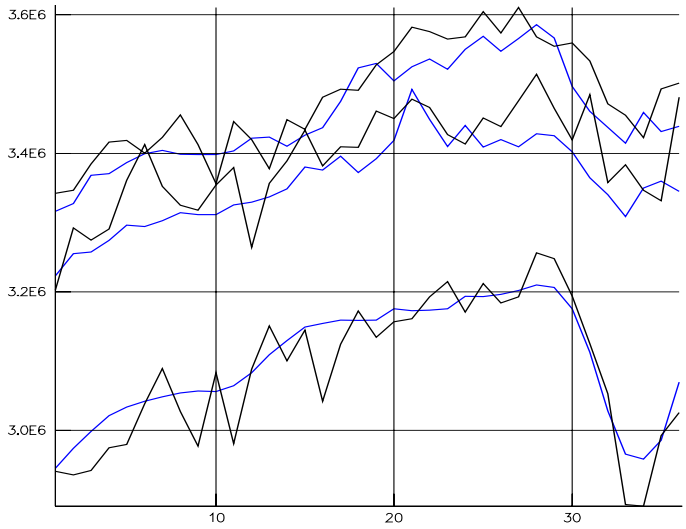

Figure 9: temperature along a gold section at $t = 18\,ns$ at gold/gas interface, in the middle of gold and in the wave front (blue: hybrid, black: full MC)

than with full Monte-Carlo.

Miscellaneous

We want now to list some issues that will have to be addressed in the future.

Choice of the criterion.
An important issue for the robustness of the method is to find a criterion that really detects when diffusion approximation is valid. For this study, we took the simplest possible (5) but we could consider many other choices. For example, the characteristic length scale could be related to the gradient length

$$L(x,t) \sim \frac{T}{|\nabla T|}.$$

Some specific algorithm can also be considered to take into account opacity lines. Finally, if the choice of the spectral cut-off only depends on a local criterion, it may make the number of transport-diffusion coupling interfaces large because of Monte-Carlo oscillations (a small difference in temperature between two cells could create an artificial coupling interface between the cells): it may be efficient to introduce a local smoothing of the spectral cut-off to prevent this.

Coupling with remapping.
When remapping the lagrangian mesh (which happens when using Arbitrary Lagrangian Eulerian method), it is necessary to reconstruct the cut-off function from the new local variables. Some Monte-Carlo particles may become located in a diffusion region and some Monte-Carlo regions may contain no Monte-Carlo particle. In this case, particles must be killed or created under the constraint of conservation of radiative energy. The drawback

is that important information about the anisotropy of the distribution may be lost. A solution could be to adapt the remeshing algorithm so that it does not affect the boundary between two cells whose spectral cut-off are too different.

Parallelization.
Monte-Carlo methods are relatively easy to parallelize on shared memory processors. When using domain decomposition and distributed memory, it is necessary to deal with particles escaping from one domain to another one. Because the number of Monte-Carlo events in each domain is evolving with time, load balancing is a difficult task. The situation is still more complicated with hybrid method since the domain on which Monte-Carlo events occur is evolving with time.

Conclusion

In this paper, we have presented a first realistic application of a new Hybrid Monte-Carlo method for the numerical simulation of radiative transfer equations. A simplified laser cavity was used as a test problem to compare the Hybrid method with full Monte-Carlo simulation. It appears that, for a given computational cost, results are slightly better (in term of smaller Monte-Carlo oscillations) for the hybrid method. More important, the use of Hybrid method remove some doubts about the use of a Full Monte-Carlo method in regions where Monte-Carlo behaves poorly. These results have to be confirmed for other configurations.

Some important work remains to be done either from a numerical point of view (choice of spectral cut-off criterion, coupling with A.L.E.) as well as for computational issues (parallelization). At last examination of the density of the Monte-Carlo matrix makes us confident in the extension of the method to three-dimensional configurations.

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