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# A full Monte-Carlo resolution scheme of a photon-phonon model for conducto-radiative heat transfer in heterogeneous media

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## Abstract

In this paper, we tackle the problem of solving the system of radiative heat transfer coupled with the diffusion equation for material temperature with a full Monte-Carlo (MC) scheme in heterogeneous media, i.e. possibly containing discontinuities of thermophysical material parameters. MC schemes based on Brownian paths for the diffusion equation in layered media are known to present some issues: corrections at the interface between media are usually mandatory or must be replaced with complex samplings. In this paper, based on the observations that transport models are easily solved by MC methods in layered media, and that state-of-the-art MC schemes capture the diffusion limit, we suggest to build a phonon like model and to solve it with an MC scheme. For capturing the diffusion limit, physical constraints are explicated and enforced within the MC resolution. These constraints can even help revisiting the Brownian paths for efficient corrections. Numerical results are provided in different regimes in order to highlight the relevance of the strategies suggested in this paper.

*Keywords:* Radiative transfer, Diffusion, Monte Carlo, Numerical scheme, layered media, stratified media

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## 1. Introduction

Heat transfer in heterogeneous and porous media mixing conduction and radiation has attracted much attention, due in particular to its applications in alternative energy development like concentrated solar power [1] and in thermal protection systems design [2].

Varieties of solvers have been proposed to address this problem [3, 4, 5, 6, 7]; here, we are mostly interested by Monte-Carlo/Random Walks schemes. This technique has long been one of the favorites for the solution of the radiative part of heat transfer, especially in case of complex geometries [8, 9]; here, the random walk algorithm is directly based on the physics of radiative heat transfer, simulating scattering, absorption and emission with Poissonian processes. On the other hand, in the diffusive limit – that is, for very small free path lengths –, it has been found handy

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to design algorithms based on the laws of Brownian motion, sometimes called “walk-on-sphere” methods [10, 11, 12].

When heat conduction and radiation are mixed in opaque/semitransparent heterogeneous media, it has been proposed to design “hybrid walks” whereby the walk rules are differing, depending on whether the walker lies in the opaque or the transparent medium, with specific rules for the transitions between both types of media. Successful implementations with Poissonian behavior in the semi-transparent subdomains and Brownian behavior in the opaque ones were reported by Vignoles [13] and Tregan *et al.* [14]. Another type of coupling has been proposed in the case of semi-transparent media in which both types of transport occur in the same regions of space [15, 16, 17]. Despite these successes, as will be shown in this paper, there exist some uncertainties linked to the solution of Brownian motion problems close to an opaque/semitransparent interface.

Here our goal is to design a fully “kinetic” (Poissonian) scheme in which the essence of the random walk algorithm is the same everywhere, but in which discontinuities of material thermophysical properties are handled properly, i.e. without introducing any bias in the results and recovering the correct diffusive limits when appropriate. We will see that analysing Poissonian paths will also help us have a better understanding of Brownian ones.

We are interested in the Monte-Carlo (MC) resolution of the time-dependent, nonlinear, radiative transfer equations coupled to heat diffusion in layered media. By layered media, we mean configurations in which several layers of media with very different characteristics (conductivity, density, heat capacity etc.) are superimposed. The model has general form (see [18, 19]):

$$\begin{cases} \frac{1}{c} \partial_t I + \omega \cdot \nabla I + \sigma_t I = \sigma_a B(T_m) + \sigma_s \int_{4\pi} I \frac{d\omega'}{4\pi}, \\ \partial_t E(T_m) - \nabla \cdot (\kappa(T_m) \nabla T_m) = \int_{4\pi} c \sigma_a \left( \frac{I}{4\pi} - B(T_m) \right) d\omega'. \end{cases} \quad (1)$$

In the above equations,  $I = I(t, x, \omega, \nu)$  and  $T_m(t, x)$  are the unknowns of the system and stand respectively for the density of radiation energy and the material temperature. Variables  $t \geq 0$ ,  $x \in \Omega \subset \mathbb{R}^3$ ,  $\omega \in \mathbb{S}^2$  and  $\nu \in \mathbb{R}^+$  are respectively the time, space, solid angle and frequency variables. The opacities  $\sigma_t = \sigma_t(x, t, \nu)$ ,  $\sigma_a = \sigma_a(x, t, \nu)$  and  $\sigma_s = \sigma_s(x, t, \nu)$  are given functions standing for the total, absorption and scattering opacities. In particular, we have  $\sigma_t = \sigma_a + \sigma_s$ . The density of internal energy  $E$  depends on  $T_m$  *via* an equation of state (EoS)  $dE = \rho c_v(T_m) dT_m$  with  $\rho$  the mass density and  $c_v$  the heat capacity (constant for a perfect gas). Quantity  $B(x, t, \nu)$  is the Planckian distribution and is such that  $B(x, t) = B(T_m(x, t)) = \int B(x, t, \nu) d\nu = a T_m^4(x, t) / 4\pi$  is the frequency-integrated Planck function with  $a$  the radiative constant. Here,  $c$  denotes the speed of light. The conductivity of the medium is denoted by  $\kappa$ . In this paper, emphasis is set onto the case of spatially discontinuous  $\rho c_v$  and/or  $\kappa$  in order to model layered media. In other words, let  $(\Omega_i)_{i \in \{1, \dots, M\}}$  denote  $M$  different media (or “phases”) involved in our configuration of interest, i.e. such that  $\cup_{i=1}^M \Omega_i = \Omega$ , then for  $\alpha \in \{\rho c_v, \kappa\}$ , we have  $\alpha(\mathbf{x}) = \sum_{i=1}^M \alpha_i \mathbf{1}_{\Omega_i}(\mathbf{x})$  where  $\mathbf{1}_{\Omega_i}(\mathbf{x})$  equals 1 if  $\mathbf{x} \in \Omega_i$ , 0 otherwise. Note that the discontinuities may also come from the temperature dependence of  $\kappa$ : suppose there is only one material but the discretisation is such that  $T_m$  is piecewise constant in each of the  $N$  cells, i.e.  $T_m(x) = \sum_{i=1}^N T_m^i \mathbf{1}_{\Omega_i}(x)$ : this naturally leads to a piecewise constant conductivity given by  $\kappa(x) = \sum_{i=1}^N \kappa(T_m^i) \mathbf{1}_{\Omega_i}(x) = \sum_{i=1}^N \kappa^i \mathbf{1}_{\Omega_i}(x)$ . The two different cases shall be treated the same way in this paper, without lack of generality. Initial and boundary conditions must be supplemented to system (1):

$$I(0, x, \omega) = I^0(x, \omega), \quad T_m(0, x) = T_m^0(x), \quad x \in \Omega, \quad \omega \in \mathbb{S}^2, \quad (2)$$

$$I(t, x, \omega) = I_b(t, \omega), \quad t \geq 0, \quad x \in \partial\Omega, \quad \omega \cdot n_s < 0, \quad (3)$$

where  $n_s$  is the outward normal to  $\Omega$  at  $x$ . System (1) together with initial and boundary conditions (2) + (3) define the well-posed [20] mathematical problem we want to solve.

System (1) is nonlinear. Its resolution consequently needs some linearisation hypothesis. System (1) is often solved by performing some operator splitting on a time step [21] before choosing numerical schemes for the different splitting steps. The choice of the splitting is not unique but a classical and convenient one is the following:

- A radiative transfer phase

$$\begin{cases} \frac{1}{c} \partial_t I + \omega \cdot \nabla I + \sigma_t I = \sigma_a B(T_m) + \sigma_s \int_{4\pi} I \frac{d\omega'}{4\pi}, \\ \partial_t E(T_m) = \int_{4\pi} c \sigma_a \left( \frac{I}{4\pi} - B(T_m) \right) d\omega', \end{cases} \quad (4)$$

- followed by a heat conduction one

$$\begin{cases} \partial_t I = 0, \\ \partial_t E(T_m) - \nabla \cdot (\kappa(T_m) \nabla T_m) = 0, \end{cases} \quad (5)$$

during which  $I$  remains constant.

This splitting is especially convenient when one only needs to focus on radiative transfer for example (i.e. when  $\Omega = \cup_{i=1}^M \Omega_i$  has many non conducting phases for which  $\kappa_i \ll 1$ ):

Once a splitting chosen, it remains to choose the resolution scheme for both steps

- due to the high dimensionality of the problem (with  $(x, t, \omega, \nu) \in \mathbb{R}^7$  in (1) and  $(x, t, \omega, \nu, v) \in \mathbb{R}^8$  later on for the photon-phonon model (10)) we aim at tackling, we focus on MC based numerical solvers for the radiative transfer phase. MC schemes are known to be costly but insensitive to the dimension of the problem and to the regularity of the solution [22]. In order to solve (4), we rely on the ISMC scheme described in [23] based on both the seminal works of [24, 25]: the MC scheme is implicit and teleportation error free. For the spectral dependance, we rely on the material of [26] (even if in this paper, without lack of generality with respect to the numerical difficulties we aim at tackling, the grey approximation is enough). The ISMC scheme discretises both  $I$  and  $E$  with MC particles which are transported (at velocity  $c$  for photons  $I$ ) or not (for matter at rest  $E$ ). The nature of the MC particles eventually changes at a collision at which a photon can become *sensible heat* or *a phonon* and sensible heat becomes photons, see [23, 26]. At the end of the time step,  $I$  and  $E$  are approximated in each cell by tallying the contributions of, respectively, the photon MC particles and the sensible heat MC particles. The temperature  $T_m$  is deduced from  $E$  by inversion of the EoS.
- The second step (5) of the splitting, in lower dimension (with  $T_m$  only depending on  $(x, t) \in \mathbb{R}^3 \times \mathbb{R}^+$ ), is usually solved thanks to deterministic solvers. From the temperature computed during the previous phase and the application of a diffusion scheme, the energy and the temperature are updated.

This solution strategy is efficient in practice but one must realise that in order to end the time iteration, the weights of all the sensible heat MC particles must be updated in accordance with the

new values of  $E$  determined by the diffusion step, before starting the radiative transfer phase of the next time step. This step is sequential (i.e. hard to parallelise [27]) and can lead to unbalanced weights. On the other hand, equation (5) can also be solved with an MC scheme: in practice, this is based on the application of Itô's lemma [28, 29, 30, 19, 31, 32, 33, 34, 35, 36]. In a homogeneous media, the application is quite simple as it only consists in solving

$$\begin{cases} \partial_t T - D\Delta T = 0, \\ T(t=0, x) = T_0(x), \end{cases} \quad (6)$$

on the time step where we defined  $D = \frac{\kappa}{\rho c_v}$  (for a homogeneous isotropic material). Itô's lemma then states that in order to solve (6), the position of the MC particles  $X_t$  must be updated by solving the stochastic ordinary equation

$$\begin{cases} dX_t = \sqrt{2D} dW_t, \\ X_0 = x, \end{cases} \quad (7)$$

where  $W_t$  denotes a Brownian motion (or a Wiener process). Then  $T(x, t) = \mathbb{E}[T_0(X_t)]$  is solution of (6). In practice, (7) is often solved thanks to an explicit Euler scheme.

Let us now consider a simple test-case for (6) and illustrate the difficulty we aim at tackling in this paper: it is a one dimensional test-case  $x \in \Omega = [0, 1] \subset \mathbb{R}$ , with initial condition

$$T_0(x) = 2 \times \mathbf{1}_{[0.45, 0.55]}(x),$$

where  $\mathbf{1}_{[a,b]}$  is the Heaviside function for interval  $[a, b]$ . The initial condition in terms of temperature is displayed in the left plots of figure 1. Quantities  $x \rightarrow \kappa(x)$  and  $x \rightarrow \rho(x)c_v(x)$  are also displayed (left vertical axis) together with the reference solution of the test-case. The boundary conditions are Neumann ones but the final time  $t = 10^{-2}$  is such that the solution does not have enough time to significantly interact with the edges of the domain. Now, the domain is composed of two layers of material in  $\Omega_1 = [0, \frac{1}{2}]$  and  $\Omega_2 = [\frac{1}{2}, 1]$  such that  $\Omega_1 \cup \Omega_2 = \Omega$  and with diffusivities  $D_1$  and  $D_2$ . If<sup>1</sup>  $D_1 = D_2$ , then the previously described MC resolution strategy is efficient: on picture top right of figure 1, the reference solution obtained with a deterministic code and the MC ones are in very good agreement (the number of cells is  $N_x = 100$ ), especially as  $\Delta t \leq 10^{-6}$ . On the other hand if<sup>2</sup>  $D_1 \neq D_2$  ( $D_1 = 10$  and  $D_2 = 1.0$  in the bottom picture of figure 1), the MC results (Brownian paths) do not converge toward the same temperature profile as the one obtained by the deterministic solver (reference). It is well-known that such an MC resolution scheme is not efficient for layered media and that the physical solution for this problem is the one obtained with the deterministic solver [28, 29]. In this case, increasing the number of particles, the number of cells or decreasing the time step does not ensure obtaining more physical results [28, 29, 32]. In this paper, we want to suggest a new way to deal with this phenomenon, i.e. jumps in  $x \rightarrow \rho(x)c_v(x)$  and/or  $x \rightarrow \kappa(x)$ .

## 2. An overview of the strategies of the literature

As explained in the introduction, the flaw illustrated in figure 1 for the Brownian path in layered media is well-known, see [37] for example. Many authors have suggested ways to circumvent it. The suggested solutions can be decomposed in two different families of methods:

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<sup>1</sup> $x \rightarrow \kappa(x) = 1$  and  $x \rightarrow \rho(x)c_v(x) = 1$  are displayed on the right vertical axis.

<sup>2</sup> $x \rightarrow \kappa(x) = 10^{-1}\mathbf{1}_{[0, \frac{1}{2}]}(x) + \mathbf{1}_{[\frac{1}{2}, 1]}(x)$  and  $x \rightarrow \rho(x)c_v(x) = 1$  are displayed on the right vertical axis.

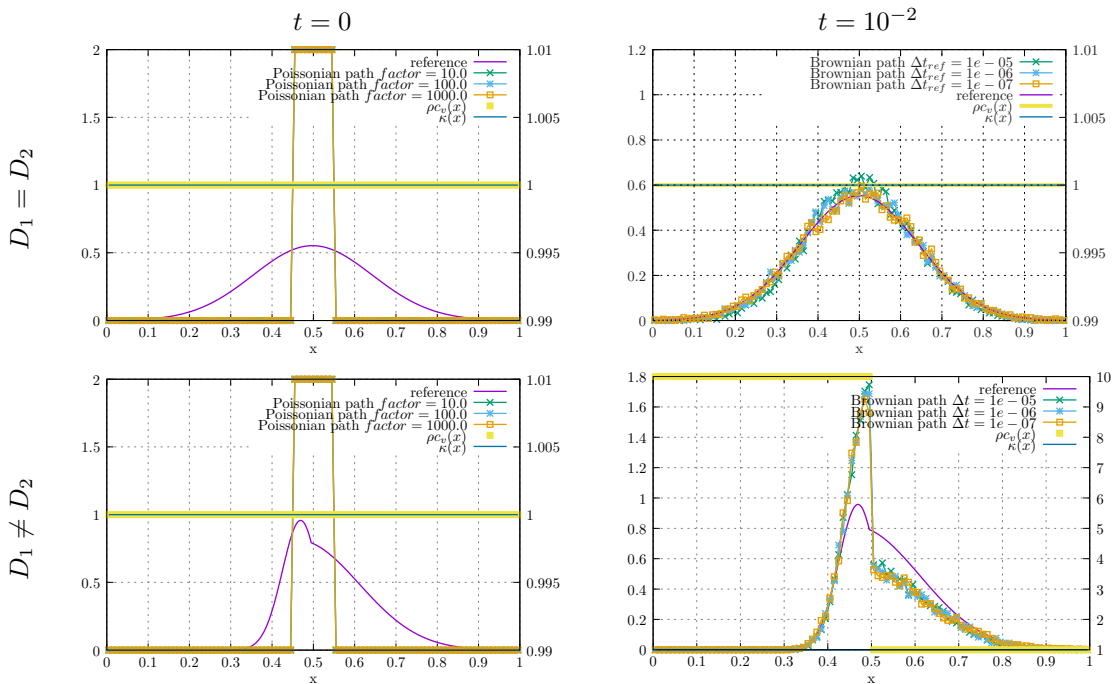


Figure 1: Left: initial conditions. Right: numerical solutions. For the top pictures, the diffusivities are the same ( $D_1 = D_2$ ) in domains  $\Omega_1$  and  $\Omega_2$ . The plot presents the simulated temperatures at time  $t = 10^{-2}$  obtained with a reference deterministic code and an MC one with  $10^5$  and  $10^6$  particles. Bottom: the diffusivities are different ( $D_1 = 0.1 \neq D_2 = 1.0$ ) in domains  $\Omega_1$  and  $\Omega_2$ . The plot presents the simulated temperatures at time  $t = 10^{-2}$  obtained with a reference deterministic code and an MC one with  $10^5$  and  $10^6$  particles.

- the ones working on adapting the time steps,
- the ones having a fixed time step but with interface corrections.

In order to improve the results for some non homogeneous diffusivity coefficients  $x \rightarrow D(x)$ , some authors relied on linearisations of  $x \rightarrow D(x) = D(x) + \Delta x \nabla_x D(x) + \mathcal{O}(\Delta x^2)$ . In [31], the authors empirically demonstrate the improvements made by correcting the time step of the resolution when  $x \rightarrow D(x)$  is not constant and  $\nabla_x D(x)$  is available. The numerical scheme does improve the results on the benchmarks of the paper but  $x \rightarrow D(x)$  is quite smooth ( $\mathcal{C}^2$ ), which is clearly not the case in layered media.

In [29], the idea is to accept the lack of regularity of  $x \rightarrow D(x)$  and consider discontinuous diffusivities. The stochastic process that governs the positions of the particles is fully characterised. Two algorithms are suggested. They rely on fixed time steps and the construction of an *interface layer*, a numerical vicinity of the interface, within which skew Brownian motions (SBM) are simulated. Several schemes are proposed in the literature in order to treat the samplings within this layer, see [29, 38, 39]. The SBM one [38, 39, 40] seems to outperform the others. But the scheme is quite complex to implement and its efficiency on multi-layered media is not obvious nor, to our knowledge, has been numerically demonstrated [36]. The question of what happens to the numerical interface layer when the mesh is refined remains: remember we aim at solving (1) and

the additional equation may require finer meshes for accuracy.

In [34], the samplings needed at the interface between two media are studied: it is explained that introducing reflections at the boundary aims at maintaining some no-flux boundary conditions for the random walk. Some treatments fail to solve the specified problem while it is explained that the methods of [41, 42] succeed. One can show that these methods relate to an analytical solution to the problem of one-dimensional diffusion at an interface. But the use of the analytical solution for the samplings at the interface [43, 35, 42] is quite complex, does not guarantee convergence properties as the number of layers grows and often needs the introduction of some artificial interface layers [41, 42]: in other words, it introduces some additional (in plus of  $\Delta t$ ) numerical parameter which must be tuned (and for which, to our knowledge, convergence is not guaranteed).

In [30, 19, 44], the authors suggest introducing some kind of albedo at the interface between the two domains: the particles have a certain probability of bouncing back into the domain they come from instead of crossing it. Note that some authors, in combination to the use of rebound probabilities, introduce the need for having negative weights for their particles [44]. This strategy can be efficient in practice [44] or even [45, 46] for some applications of negative weights for neutronics applications but they need to be combined with fine algorithm for population control (or the number of negative weight particles and the variance may increase [44, 45]).

To sum up, many numerical methods aiming at dealing with discontinuous material properties for the diffusion equation with random walkers are suggested in the literature. But they either

- rely on smoothness assumptions which do not hold for our applications,
- or seem to be efficient but complex to implement,
- or rely on numerical parameters which may need to be tuned without convergence guarantees.

For all these reason, we suggest a new numerical strategy to tackle the same kind of problems. It is based on what we consider simple modifications of the model (1) we aim at solving.

### 3. The photon-phonon coupled system for conducto-radiative transfer

From the previous simple example (see figure 1 and the comments), we can see that the resolution of the diffusion equation with Brownian paths is very efficient in almost homogeneous media but remains complex to treat layered ones. The main idea of this paper comes from two observations:

- the MC resolution of the transport equation (Poissonian paths rather than Brownian ones) does not suffer from the previous problem: layered media can easily and reliably be simulated.
- The diffusion equation is the limit of the transport one for both fast particles and opaque media and the SMC and ISMC schemes capture this limit [23]. By the way, the material of this paper can easily be applied with other (teleportation error free) MC solvers such as the ones in [47, 48, 49].

Hence the idea to solve a transport model, the one for phonons described in [50], in the equilibrium diffusion limit in order to simulate heat conduction. For this, we suggest solving

$$\begin{cases} \partial_t I + c\omega \cdot \nabla I + c\sigma_t I = c\sigma_a B(T_m) + c\sigma_s \int_{4\pi} \frac{I}{4\pi} d\omega', \\ \partial_t e + c_m\omega \cdot \nabla e + c_m\sigma_m e = c_m\sigma_m \int \int_{4\pi} P_m e \frac{d\omega'}{4\pi} dc'_m + \int_{4\pi} c\sigma_a \left( \frac{I}{4\pi} - B(T_m) \right) d\omega', \\ \text{with } E(T_m(x, t)) = \iiint e(x, t, \omega, c_m) d\omega dc_m. \end{cases} \quad (8)$$

In the above system,  $c_m$  may be understood as a kind of speed of sound in sensible heat and  $\sigma_m(x, t) = \sigma_m(x, T_m(x, t))$  is a kind of opacity for phonons of density  $e(x, t, \omega, c_m)$ . But the truth is their relevance will only be numerical (and not physical) in the following sections. We could better call them "Poissonian sensible heat energy carriers" than "phonons". The quantity  $P_m$  describes how the phonons' velocities and angles are scattered at a collision, i.e. it is a scattering kernel. For the moment, the only property we suppose it satisfies is

$$\int P_m(x \in \Omega_i, c'_m, v) dc'_m = \delta_{c_m, i}(v), \forall x \in \Omega, \forall v \in \mathbb{R}^3.$$

In the above expression,  $\delta_c(v)$  is the Dirac delta function such that  $\int f(v)\delta_c(v)dv = f(c)$  for all continuous compactly supported function  $f$ . Of course, in order to solve a heat conduction equation for sensible heat,  $c_m$ ,  $\sigma_m$  and  $P_m$  must be *astutely spatially* chosen. Their tuning will be the purpose of section 4. In this section, we focus on model (8), on its properties and on the resolution strategy we suggest in this paper.

First, system (8) is still conservative: indeed, integrating both equations (8) with respect to  $\omega$  and summing them up leads to

$$\partial_t \left( \int I + E(T_m) \right) + \int c\omega \cdot \nabla I + \int c_m\omega \cdot \nabla e = 0, \quad (9)$$

so that in a closed system (i.e. such that the fluxes cancel), the sum of the photons and phonons' energies are constant  $\int I + E(T_m) = \int I^0 + E(T_m^0)$ .

Now, system (8) is nonlinear and must be linearised in order to be solved with an MC scheme. For this, we rely either on the SMC discretisation [25] or the ISMC one [23] (in the stiff case or when stationary computations are needed) which we need to modify in order to take the streaming ( $c_m$ ) and the collision ( $\sigma_m$ ) terms of the phonons into account. Let us rewrite (8) as

$$\begin{cases} \partial_t I + c\omega \cdot \nabla I &= -c\sigma_t I + c\sigma_a \eta(E) \int_{4\pi} \frac{e}{4\pi} d\omega' + c\sigma_s \int_{4\pi} \frac{I}{4\pi} d\omega', \\ \partial_t e + c_m\omega \cdot \nabla e &= -c_m\sigma_m e - c\sigma_a \eta(E)e + \int_{4\pi} c\sigma_a \frac{I}{4\pi} d\omega' + c_m\sigma_m \int \int_{4\pi} P_m \frac{e}{4\pi} d\omega' dc'_m, \end{cases} \quad (10)$$

in which we introduced  $B(E) = \eta(E)E$ . This system is still nonlinear (due to the dependence of  $\eta$  with respect to  $E$ ). From now on, let us assume that  $\eta(E(x, t)) = \bar{\eta}(x, t)$  for  $t \in [t^n, t^n + \Delta t]$ . With the previous hypothesis, (10) becomes

$$\begin{cases} \partial_t I + c\omega \cdot \nabla I &= -c\sigma_t I + c\sigma_a \bar{\eta} \int_{4\pi} \frac{e}{4\pi} d\omega' + c\sigma_s \int_{4\pi} \frac{I}{4\pi} d\omega', \\ \partial_t e + c_m\omega \cdot \nabla e &= -c_m\sigma_m e - c\sigma_a \bar{\eta} e + \int_{4\pi} c\sigma_a \frac{I}{4\pi} d\omega' + c_m\sigma_m \int \int_{4\pi} P_m \frac{e}{4\pi} d\omega' dc'_m. \end{cases} \quad (11)$$



Independently of the choice of  $\bar{\eta}$ , system (11) is linear ( $\bar{\eta}$  is a function of  $x, t$  but not anymore of  $E$ ). An MC scheme can then be applied to solve it on time step  $[t^n, t^n + \Delta t]$ . Of course, in practice, a choice must be made for  $\bar{\eta}$  (explicit as in [25], implicit as in [23]): let us postpone this choice and rather go through a few properties of the above linearization (which remains independent of the choice of  $\bar{\eta}$ ).

**Remark 1.** *At this stage of the discussion it is important noting that if one has already access to an MC solver in order to solve the radiative transfer equation (4), a simple modification of the solver can be made in order to solve system (11). This is what we are going to tackle in the next lines.*

As explained before, system (11) is now linear and can be solved with an MC scheme. We here insist on the fact that it has the same structure as a multigroup transport equation (for neutronics for example, see [51, 52]): in this context, a  $P$ -truncated basis  $(\phi_0(v), \dots, \phi_P(v))^t$  is introduced and the solution  $u$  is decomposed on this basis  $\psi(x, t, \omega, v) \approx \sum_{k=0}^P u_k(x, t, \omega) \phi_k(v)$ . But in our case, there are  $M+1$  groups with  $M$  the number of different materials within the layers and the basis functions are analytical, given by  $\phi_0(v) = \delta_c(v)$  and  $(\phi_i(v) = \delta_{c_m, i}(v))_{i \in \{1, \dots, M\}}$ . To clarify this point, let us put forward the expression of the total and scattering opacities of linear system (11). It consists in recovering the equation whose solution is  $\psi(x, t, \omega, v) = I(x, t, \omega) \delta_c(v) + \sum_{i=1}^M e(x, t, \omega) \delta_{c_m, i}(v)$ .

For the sake of conciseness of the calculations, we assume that  $c_m$  can be continuously distributed even if in practice, it will have  $M+1$  discrete values specified by the characteristics of the different layers of the media, see section 4. Hence,  $\psi$  simplifies to  $\psi(x, t, \omega, v) = I(x, t, \omega) \delta_c(v) + e(x, t, \omega) \delta_{c_m}(v)$ . In the latter expression,  $\delta_{c_m}, \delta_c$  are such that

$$\int_{\{V\}} \delta_c(v) dv = \delta_{V, c} \text{ and } \int_{\{V\}} \delta_{c_m}(v) dv = \delta_{V, c_m},$$

where  $\delta_{V, k}$  is the Kronecker symbol<sup>3</sup> and  $\{V\}$  denotes the singleton  $V$ . In fact,  $v$  is nothing more than a velocity which can be  $c$  for photons or  $c_m$  for sensible heat. Let us now build the linear equation satisfied by  $\psi$ . Expression (11) can be rewritten (we drop the dependences for conciseness):

$$\begin{aligned} \partial_t(I\delta_c + e\delta_{c_m}) + v\omega \cdot \nabla(I\delta_c + e\delta_{c_m}) = & - (c\sigma_t I\delta_c + c\sigma_a \bar{\eta} e\delta_{c_m} + c_m \sigma_m e\delta_{c_m}) \\ & + \left( c\sigma_a \delta_c \bar{\eta} \int_{4\pi} e + c\sigma_a \delta_{c_m} \int_{4\pi} I + c_m \sigma_m \delta_{c_m} \int_{4\pi} P_m e + c\sigma_s \delta_c \int_{4\pi} I \right). \end{aligned}$$

It remains to make  $\psi$  appear in the collisional part. For the moment the integration is only over the angular distribution. Let us introduce the Kronecker symbols

$$\delta_{c_m, c}(v', v) = \delta_{c_m}(v') \delta_c(v) \quad \text{and} \quad \delta_{c, c_m}(v', v) = \delta_c(v') \delta_{c_m}(v).$$

We can then rewrite the above equation as:

$$\begin{aligned} \partial_t \psi + v\omega \cdot \nabla \psi + (c\sigma_t \delta_c(v) + c\sigma_a \bar{\eta} \delta_{c_m}(v) + c_m \sigma_m \delta_{c_m}(v)) \psi = \\ + \int_{\mathcal{V}} \int_{4\pi} [c\sigma_a \delta_{c, c_m}(v', v) + c\sigma_s \delta_{c, c}(v', v) + c\sigma_a \bar{\eta} \delta_{c_m, c}(v', v) + c_m \sigma_m P_m(v', v)] \psi(v', \omega') dv' d\omega', \end{aligned} \quad (12)$$

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<sup>3</sup>i.e. is such that  $\delta_{V, k} = 0$  if  $V \neq k$  and  $\delta_{V, k} = 1$  if  $V = k$ .

with  $\mathcal{V} = \{c_m, c\}$  a discrete set with only two elements. One can check that performing  $\int_{\{c\}} (12) dv$  allows recovering the transport equation of (11) and that  $\int_{\{c_m\}} (12) dv$  leads to the second equation. We can identify the scattering  $v\Sigma_s(v, v')$  and total  $v\Sigma_t(v)$  opacities to rewrite the system above under the general form:

$$\partial_t \psi + v\omega \nabla \psi + v\Sigma_t(v)\psi = \int_{\mathcal{V}} \int_{4\pi} v\Sigma_s(v', v)\psi(v', \omega') dv' d\omega'.$$

In the above expression, we have:

$$\begin{aligned} v\Sigma_t(v) &= c\sigma_t \delta_c(v) + c\sigma_a \bar{\eta} \delta_{c_m}(v) + c_m \sigma_m \delta_{c_m}(v), \\ v\Sigma_s(v', v) &= c\sigma_a \delta_{c, c_m}(v', v) + c\sigma_s \delta_{c, c}(v', v) + c\sigma_a \bar{\eta} \delta_{c_m, c}(v', v) + c_m \sigma_m P_m(v', v). \end{aligned}$$

Let us rewrite the scattering part as  $v\Sigma_s(v)P_s(v', v) = v\Sigma_s(v', v)$ . By doing so, we introduce  $P_s$ , the probability of being scattered with velocity  $v$ , incoming with velocity  $v'$ : it is mainly used for a backward resolution. This implies

$$\begin{aligned} v\Sigma_s(v) &= \int v\Sigma_s(v', v) dv', \\ &= \int [c\sigma_a \delta_{c, c_m}(v', v) + c\sigma_s \delta_{c, c}(v', v) + c\sigma_a \bar{\eta} \delta_{c_m, c}(v', v) + c_m \sigma_m P_m(v', v)] dv', \\ &= (c\sigma_s + c\sigma_a \bar{\eta}) \delta_c(v) + (c\sigma_a + c_m \sigma_m) \delta_{c_m}(v). \end{aligned}$$

By definition of  $P_s$  we have:

$$\begin{aligned} P_s(v', v) &= \frac{v\Sigma_s(v', v)}{v\Sigma_s(v)}, \\ &= \frac{[c\sigma_a \delta_{c, c_m}(v', v) + c\sigma_s \delta_{c, c}(v', v) + c\sigma_a \bar{\eta} \delta_{c_m, c}(v', v) + c_m \sigma_m P_m(v', v)]}{(c\sigma_s + c\sigma_a \bar{\eta}) \delta_c(v) + (c\sigma_a + c_m \sigma_m) \delta_{c_m}(v)}. \end{aligned}$$

The above expression can be considerably simplified by noticing that

$$\text{for } v = c_m, \quad P_s(c_m, v') = \frac{c\sigma_a \delta_c(v') + c_m \sigma_m P_m(v', c_m)}{(c\sigma_a + c_m \sigma_m)}, \quad \text{for } v = c, \quad P_s(c, v') = \frac{\sigma_s \delta_c(v') + \sigma_a \bar{\eta} \delta_{c_m}(v')}{\sigma_s + \sigma_a \bar{\eta}},$$

so that  $P_s$  resumes to

$$P_s(v, v') = \delta_{c_m}(v) \frac{c\sigma_a \delta_c(v') + c_m \sigma_m P_m(v', c_m)}{(c\sigma_a + c_m \sigma_m)} + \delta_c(v) \frac{\sigma_s \delta_c(v') + \sigma_a \bar{\eta} \delta_{c_m}(v')}{\sigma_s + \sigma_a \bar{\eta}}.$$

Now, we are interested in a direct resolution of (11) on time step  $[t^n, t^n + \Delta t]$ . In other words, we need (cf. [53]) to characterise the total and scattering opacities of the adjoint form of (11). It is given by

$$-\partial_t \psi - v\omega \cdot \nabla \psi + v\Sigma_t(v)\psi = \int_{\mathcal{V}} \int_{4\pi} v\Sigma_S(v', v)\psi(v', \omega') dv' d\omega', \quad (13)$$

where

$$v\Sigma_S(v, v') = v\Sigma_S(v)P_S(v, v') = v'\Sigma_s(v')P_s(v, v').$$

In the previous expression,  $P_S$  is the probability of being scattered from velocity  $v$  toward velocity  $v'$ : it is used for a direct resolution. Then we have

$$\begin{aligned}
v\Sigma_S(v) &= \int_{\mathcal{V}} v' \Sigma_s(v') P_s(v, v') dv', \\
&= \int_{\mathcal{V}} ((c\sigma_s + c\sigma_a \bar{\eta}) \delta_c(v') + (c\sigma_a + c_m \sigma_m) \delta_{c_m}(v')) \times \\
&\quad \left( \delta_{c_m}(v') \frac{c\sigma_a \delta_c(v') + c_m \sigma_m P_m(v', c_m)}{(c\sigma_a + c_m \sigma_m)} + \delta_c(v') \frac{c\sigma_s \delta_c(v) + c\sigma_a \bar{\eta} \delta_{c_m}(v)}{c\sigma_s + c\sigma_a \bar{\eta}} \right) dv' \\
&= (c\sigma_a + c\sigma_s) \delta_c(v) + (c\sigma_a \bar{\eta} + c_m \sigma_m) \delta_{c_m}(v) = c\sigma_t \delta_c(v) + (c\sigma_a \bar{\eta} + c_m \sigma_m) \delta_{c_m}(v) = \Sigma_t(v).
\end{aligned}$$

Few calculations, similar to the one already performed to identify  $P_S$ , show that:

$$P_S(v, v') = \delta_{c_m}(v) \frac{c_m \sigma_m P_m(v', c_m) + c\sigma_a \bar{\eta} \delta_c(v')}{c\sigma_a \bar{\eta} + c_m \sigma_m} + \delta_c(v) \frac{\sigma_s \delta_c(v') + \sigma_a \delta_{c_m}(v')}{\sigma_s + \sigma_a}.$$

With the above calculations, we identified the direct and adjoint opacities for (11) to be revisited as a 2-group linear transport equation (13). By selecting  $\bar{\eta}$  as

- $\bar{\eta} = \eta^n$ , we use the SMC for the radiative counterpart as in [25],
- $\bar{\eta} = \eta^{n+1}$ , we use the ISMC for the radiative counterpart as in [23].

In practice, in the next calculations, the ISMC solver is used. It natively degenerates toward SMC when the problem is not stiff and allows taking (stably) larger time steps than SMC for stiffer or stationary problems.

#### 4. Choosing $c_m, \sigma_m, P_m$ with respect to $\kappa, \rho c_v$

Until now, we mainly explained how the coupled system (8) can be solved consistently, with Poissonian paths, independently of the choice of  $c_m, \sigma_m, P_m$ . Our aim now is to make some particular choices for the solution of system (8) to coincide with the solution of system (1). For this, we rely on the fact that in the diffusion limit [22] characterised by  $c_m \sim \infty$  and  $c_m \sigma_m \sim \infty$ , system (8) tends toward

$$\begin{cases} \frac{1}{c} \partial_t I + \omega \cdot \nabla I + \sigma_t I = \sigma_a B(T_m) + \sigma_s \int_{4\pi} I \frac{d\omega'}{4\pi}, \\ \partial_t E(T_m) - \nabla \cdot \left( \frac{c_m}{3\sigma_m} \nabla E(T_m) \right) = \int_{4\pi} c\sigma_a \left( \frac{I}{4\pi} - B(T_m) \right) d\omega'. \end{cases} \quad (14)$$

The above system must be compared to

$$\begin{cases} \frac{1}{c} \partial_t I + \omega \cdot \nabla I + \sigma_t I = \sigma_a B(T_m) + \sigma_s \int_{4\pi} I \frac{d\omega'}{4\pi}, \\ \partial_t E(T_m) - \nabla \cdot \left( \frac{\kappa}{\rho c_v} [\nabla E(T_m) - E(T_m) \nabla \ln(\rho c_v)] \right) = \int_{4\pi} c\sigma_a \left( \frac{I}{4\pi} - B(T_m) \right) d\omega', \end{cases} \quad (15)$$

which corresponds to system (1) in which the change of variable  $T_m = \frac{E}{\rho c_v}$  has been performed in the spatial operator:  $\nabla T_m$  in (1) has been replaced by  $\nabla \frac{E}{\rho c_v}$ .

We now aim at choosing  $c_m, \sigma_m, P_m$  with respect to  $\kappa, \rho c_v$  for the solution of system (14) to coincide with the solution of system (15). In order to constrain our choices, let us distinguish between two situations, using the fact that we rely on constant-per-cell conductivities and heat capacities:

- (\*) within a cell,  $\frac{c_m}{3\sigma_m}$  must be close to  $\frac{\kappa}{\rho c_v} = D$  and a particle "sees" a homogeneous media.
- (\*\*)  $c_m, \sigma_m, P_m$  must be able to take into account the term  $-D\nabla \ln(\rho c_v)$  which is non-zero only when a particle crosses an interface between two media with different heat capacities.

For condition (\*) to be satisfied, we need to make sure that, additionally to having

$$\begin{aligned} c_m &\sim \infty, \\ c_m \sigma_m &\sim \infty, \end{aligned} \tag{16}$$

we must satisfy

$$D = \frac{c_m}{3\sigma_m} \text{ leading to } \sigma_m = \frac{c_m}{3D}. \tag{17}$$

With the above expression, we can define  $c_m$  and  $\sigma_m$  up to a scaling factor  $f$  such that  $c_m = \tilde{c}_m f$  and  $\sigma_m = \tilde{\sigma}_m f$  with  $f \gg 1$  "large enough". We will see in section 6 what "large enough" must be in practice.

**Remark 2.** *It is important noting that the Poissonian approach we suggest introduces  $f$  as a numerical parameter (which echoes  $\Delta t$  for Brownian paths). One important feature of  $f$  is that convergence of (10) toward (1) is ensured as  $f \rightarrow \infty$ , see [54].*

Constraints (16) and (17) are enough to satisfy (\*). But *they are not for the second condition (\*\*)* to hold: the difficulty comes from the fact that at the interface between two phases,  $D\nabla \ln(\rho c_v)$  is not defined. We suggest relying on the preservation of some physical invariant at the interface, namely the *continuity of temperature*, in order to impose additional constraints on  $c_m, \sigma_m$  with respect to  $\rho c_v$ . For this, let us consider a configuration at equilibrium (i.e. for  $t \rightarrow \infty$  for example), without radiative transfer: in other words, in the case we have  $\sigma_a = \sigma_s = \sigma_t = 0$ . In this case, (8) degenerates towards

$$\begin{cases} \partial_t I + c\omega \cdot \nabla I = 0, \\ \partial_t e + c_m \omega \cdot \nabla e + c_m \sigma_m e = c_m \sigma_m \int \int_{4\pi} P_m e \frac{d\omega'}{4\pi} dc'_m, \\ \text{with } E(T_m(x, t)) = \iiint e(x, t, \omega, c_m) d\omega dc_m. \end{cases} \tag{18}$$

In this configuration, photons are not anymore coupled with sensible heat. Let us integrate with respect to both  $\omega, c_m$  to get

$$\begin{cases} \partial_t E(x, t) + \int \int c_m \omega \cdot \nabla e = 0, \\ \text{with } E(T_m(x, t)) = \iiint e(x, t, \omega, c_m) d\omega dc_m. \end{cases} \tag{19}$$

In an infinite medium, we must be able to recover the fact that independently of  $\kappa$ , as  $t \rightarrow \infty$ , we must have a homogeneous temperature

$$T_m(x, t) = T_m, \forall x \in \Omega, t \rightarrow \infty.$$

Let us now consider two<sup>4</sup> materials next to each other, with different densities and heat capacities. Note that such test-case has already been studied in order to enforce constraints in numerical methods in for similar problems, see [40]. We have

$$E(x) = \rho(x)c_v(x)T_m(x) = \rho(x)c_v(x)T_m,$$

which means that even if  $T_m$  is constant as  $t \rightarrow \infty$ ,  $E$  may suffer a jump just because  $x \rightarrow \rho(x)c_v(x)$  suffers a jump due to the presence of two layers of different materials. Let us consider we have material 1 and material 2 in presence, then we must have

$$T_m = \frac{E_1}{\rho_1 c_{v,1}} = \frac{E_2}{\rho_2 c_{v,2}}.$$

This means that equilibrium imposes an additional constraint on the flux at the interface between the two materials for equilibrium to remain fulfilled. Indeed, let us come back to (19) with additional hypothesis that  $t \rightarrow \infty$ , we then have

$$\int \int c_m \omega \cdot \nabla e(x, \omega, c_m) d\omega dc_m = 0.$$

Let us integrate the above equation on two half spaces  $\Omega = \Omega_1 \cup \Omega_2$

$$\begin{aligned} \int_{\Omega} \int \int c_m \omega \cdot \nabla e(x, \omega, c_m) d\omega dc_m dx &= 0, \\ \int c_m \int \int_{\partial\Omega_1 \cup \partial\Omega_2} \omega \cdot n(x) e(x, \omega, c_m) dx d\omega dc_m &= 0, \end{aligned}$$

where  $n$  is the normal to the boundary  $\partial\Omega = \partial\Omega_1 \cup \partial\Omega_2$ . We obtain

$$\begin{aligned} \int c_m \int \int_{\partial\Omega_1} \omega \cdot n_1(x) e_1(\omega, c_m) dx d\omega dc_m + \int c_m \int \int_{\partial\Omega_2} \omega \cdot n_2(x) e_2(\omega, c_m) dx d\omega dc_m &= 0, \\ \int c_m \int \int_{\partial\Omega_1 \cap \partial\Omega_2} \omega \cdot n(x) e_1(\omega, c_m) dx d\omega dc_m = \int c_m \int \int_{\partial\Omega_2 \cap \partial\Omega_1} \omega \cdot n(x) e_2(\omega, c_m) dx d\omega dc_m. \end{aligned}$$

Furthermore, in the equilibrium diffusion limit,  $e$  is isotropic (i.e.  $e(x, t, \omega, c_m) = e(x, t, c_m)$ ) leading to

$$\frac{1}{4} \int c_m e_1(c_m) dc_m = \frac{1}{4} \int c_m e_2(c_m) dc_m.$$

The last equation can be reinterpreted as such: for equilibrium to be fulfilled, the mean with respect to the velocity of  $c_m e(c_m)$  must be equal in all the materials. There are several ways to make sure

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<sup>4</sup>The generalisation to  $M$  materials is almost straightforward but the intuition is easier to get with only two.

this equality holds. Let us introduce the asymptotic expression ( $t \rightarrow \infty$ ) into the previous equation to get

$$\begin{aligned}\frac{1}{4} \int c_m E_1 dc_m &= \frac{1}{4} \int c_m E_2 dc_m, \\ \frac{1}{4} \int c_m \rho_1 c_{v,1} T_m dc_m &= \frac{1}{4} \int c_m T_m \rho_2 c_{v,2} dc_m, \\ \int c_m \rho_1 c_{v,1} dc_m &= \int c_m \rho_2 c_{v,2} dc_m.\end{aligned}$$

In the next lines, we take  $dc_m = \delta_{c_{m,1}}(c_m)dc_m$  in material 1 and  $dc_m = \delta_{c_{m,2}}(c_m)dc_m$  in material 2, i.e. we enforce the relation quite naively by making sure that the average velocities  $c_{m,1}$  and  $c_{m,2}$  in each materials verify

$$c_{m,1} \rho_1 c_{v,1} = c_{m,2} \rho_2 c_{v,2}.$$

More elaborated strategies may present nicer properties but this kind of study is beyond the scope of this paper. In practice, for  $M$  materials (or  $N$  cells), we will have

$$\forall i \in \{1, \dots, M\}, c_{m,i} \rho_i c_{v,i} = \tilde{c}_m f. \quad (20)$$

It is easy to check that the last equation is compatible with the previous ones given by (16)–(17). Finally, it remains to choose  $P_m$ . In practice, we choose to take

$$P_m(x, v, v') = \delta_{c_{m,i}}(v) \mathbf{1}_{\Omega_i}(x). \quad (21)$$

In other words, a sensible heat MC particle incoming in medium  $\Omega_i$  has velocity  $c_{m,i}$  after its first collision in  $\Omega_i$  and if enough collisions are made, its average values within the material will get closer and closer to  $c_{m,i}$ .

To sum up, given some material physical quantities  $(\kappa_i, \rho_i, c_{v,i})_{i \in \{1, \dots, M\}}$ , we choose  $\forall i \in \{1, \dots, M\}$

$$\begin{cases} c_{m,i} = \frac{\tilde{c}_m f}{\rho_i c_{v,i}}, \\ \sigma_i = \frac{c_{m,i}}{3D_i} = \frac{\tilde{c}_m f}{3D_i \rho_i c_{v,i}}, \\ P_i(x, v, v') = \delta_{c_{m,i}}(v) \mathbf{1}_{\Omega_i}(x). \end{cases} \quad (22)$$

Parameter  $f$  is the only *numerical* parameter and it guarantees the convergence of (10) toward (1) as it tends to infinity. It must be used in order to satisfy condition (16). It must be acknowledged that satisfying condition (16) may lead to computationally intensive calculations as the larger  $f$  is, the stiffer  $\sigma_m$  is and the more frequent the collisions and the longer the calculations are for an MC resolution. In the numerical section 6, we will see that despite the previous con, the strategy remains interesting.

We finally insist on the fact that other choices could be made for  $\sigma_m$ . For example, one could introduce a dependence of  $\sigma_m$  with respect to  $v$ . For example in order to enforce a collision as soon as possible when a sensible heat MC particle enters medium  $\Omega_m$  with velocity  $c_{m'}$  with  $m' \neq m$  (incoming from another medium  $\Omega_{m'}$ ), we can imagine an opacity of the form

$$\sigma_m(v) = \sigma_m \delta_{c_m}(v) + \frac{1}{\epsilon} (1 - \delta_{c_m}(v)), \text{ with } \epsilon \sim 0.$$

This topic may be the scope of further studies aiming at accelerating our new solver. For the moment, we remain with the simple choices (22) and show that they already allow significant improvements (section 6).

## 5. Revisiting the Brownian paths resolutions

Having the previous compatibility results in mind, it is possible to revisit the Brownian paths resolution. The Brownian paths ensure condition (\*) is satisfied. It remains to work on condition (\*\*) which was ensured *via* constraints on the velocities of the particles, see (20). The velocity of particles has no sense for Brownian particles. But displacements can be compared and the same analysis at equilibrium holds. With this in mind, let us compare a Brownian displacements and a Poissonian one: a Brownian displacement on time step  $\Delta t$  is proportional to  $\sqrt{2D\Delta t}$ . On this same time step, the equivalent velocity is :

$$c_m \propto \sqrt{\frac{2D}{\Delta t}}. \quad (23)$$

Let us now apply the same conditions on the velocities as in the previous case, i.e.  $c_{m,1}\rho_1c_{v,1} = c_{m,2}\rho_2c_{v,2}$ , we then get :

$$\sqrt{\frac{2\kappa_1}{\rho_1c_{v,1}\Delta t_1}}\rho_1c_{v,1} = \sqrt{\frac{2\kappa_2}{\rho_2c_{v,2}\Delta t_2}}\rho_2c_{v,2} \implies \frac{\Delta t_1}{\Delta t_2} = \frac{\kappa_1\rho_1c_{v,1}}{\kappa_2\rho_2c_{v,2}}. \quad (24)$$

In other words, the ratio of the time steps is the ratio of the squared effusivities. Now introduce a reference time step  $\Delta t_{ref}$ : the velocity condition for continuity at the boundary translates into a condition on the time steps used in each subdomains as

$$\kappa_i\rho_i c_{v,i}\Delta t_{ref} = \Delta t_i, \forall i \in \{1, \dots, M\}. \quad (25)$$

In the next section, this numerical strategy will be studied as well as the transport (Poissonian) one. We will see that the previous simple analogy leads to efficient corrections of the Brownian path. Convergence as  $\Delta t_{ref} \rightarrow 0$  will even be observed.

## 6. Numerical results

In this section, we apply the material of the previous sections to several test-cases. In section 6.1, we begin by revisiting the benchmarks of section 1, which motivated our study, but with the strategies described in section 3–4 and 5. The results are presented in sections 6.1.1 and 6.1.2. The benchmark of section 6.1.1 (with constant diffusivities for which we have an analytical solution) studies the convergence speed of the phonon model with respect to  $f$ . The benchmark of section 6.1.2 allows focusing on conditions (16)–(17) for the phonon model resolution and on condition (25) for the Brownian one in the case of a discontinuous conductivity  $x \rightarrow \kappa(x)$ . In section 6.1.3, we consider a problem without conductivity jump but with discontinuous  $\rho c_v$ . In section 6.2, we test both of our suggested strategies for the resolution of the full system (1) *in the equilibrium diffusion limit* for photons *and* phonons, in layered media (discontinuous conductivities – section 6.2.1 – volumic heat capacity – section 6.2.3 – or both at the same time – section 6.2.3): these test-cases are convenient because obtaining a reference solution *in the equilibrium diffusion limit* is quite easy with a deterministic solver. Finally, in section 6.3, we consider some fully coupled physics with transparent media in which radiative transfer cannot be approximated with the diffusion model.

In the next sections, the resolution strategy described in sections 3–4 is referred to as the *kinetic* solver or the solution with *Poissonian paths*. The strategy consisting in Brownian paths *with the time step corrections described in section 5* is referred to as the *diffusive* solver or the solution with *Brownian paths*.

### 6.1. Uncoupled benchmarks in layered media: with only diffusion for material temperature

In this section, we revisit the benchmarks of section 1 but with the new resolution strategies described in sections 3–4 and 5. We focus on the resolution of the diffusion equation for material temperature (not yet coupled to radiative transfer):

$$\partial_t E(x, t) - \nabla \cdot (\kappa(x) \nabla T_m(x, t)) = 0,$$

with  $\partial_t E(x, t) = \partial_t E(T_m(x, t)) = \rho(x)c_v(x)\partial_t T_m(x, t)$ . The test-case of section 6.1.1 considers constant  $\kappa$ ,  $\rho c_v$  and studies the sensitivity of  $f$  (Poissonian) and to  $\Delta t_{ref}$  (Brownian) on this simple benchmark. In section 6.1.2, we focus on a problem with discontinuous  $x \mapsto \kappa(x)$  and in section 6.1.3, on a problem with discontinuous  $x \mapsto \rho(x)c_v(x)$ .

#### 6.1.1. Constant diffusivities ( $D_1 = D_2$ ) for heat conduction (no coupling with radiative transfer)

In this section, we revisit the simple test-case of section 1 (simple case  $D_1 = D_2$ ). We quantitatively exploit the fact that an analytical solution is available and we study the convergence rate of the kinetic strategy toward the equilibrium diffusion limit. Figure 2 presents the results obtained with the kinetic solver (left column) and the diffusive one (right column) on the constant diffusivity benchmark. The results are displayed in terms of temperature profiles  $x \mapsto T_m(x, t = 10^{-2})$ . Note that the profiles  $x \mapsto \kappa(x)$  and  $x \mapsto \rho(x)c_v(x)$  are also displayed (the scales for them are on the right vertical axis). For the Brownian paths (right), to reach census, i.e. final time  $t = 10^{-2}$ , each

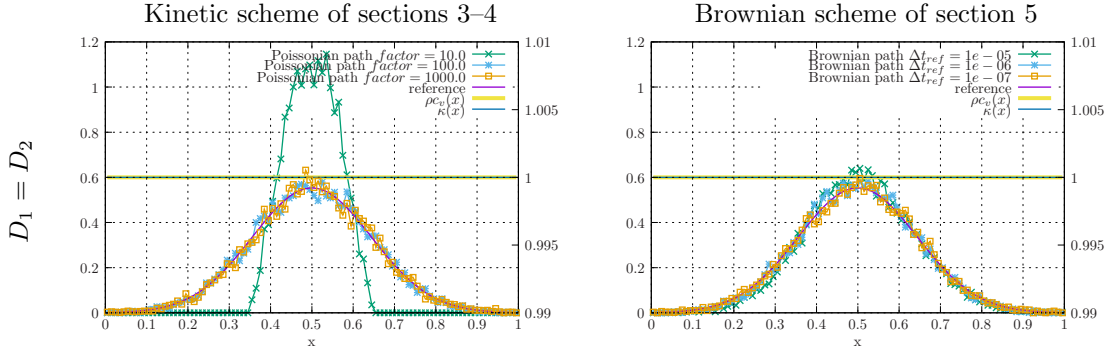


Figure 2: Results in terms of temperature profiles  $x \mapsto T_m(x, t = 10^{-2})$  obtained with the kinetic solver (left column) and the diffusive one (right column) on the constant diffusivity benchmark of section 1.

#### MC particle encounters

- $10^2$  collisions for  $\Delta t_{ref} = 10^{-5}$ ,
- $10^3$  collisions for  $\Delta t_{ref} = 10^{-6}$ ,
- $10^4$  collisions for  $\Delta t_{ref} = 10^{-7}$ .

As soon as  $\Delta t_{ref} \leq 10^{-6}$ , equivalent to each particle performing more than 1000 collisions, the results show a good agreement. The top left picture of figure 2 displays the results obtained with the Poissonian paths for three values of the factor  $f \in \{10^1, 10^2, 10^3\}$ . For  $f = 10^1$ , the equilibrium diffusion limit is not reached and the results are similar to the ones we obtain for transport in a semi transparent medium. As soon as  $f \geq 100$ , the results are in agreement with the reference.



Figure 3 presents some more quantitative results: it displays the evolutions of the errors obtained with the Poissonian and Brownian methods with respect to the number of scattering events

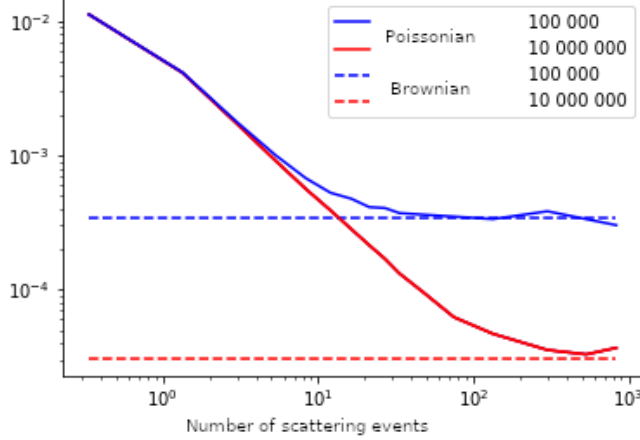


Figure 3: Behaviour of the errors with respect to  $N_{MC}$  and  $f$  for the Poissonian path and to  $N_{MC}$  and  $\Delta t_{ref}$  for the Brownian one in terms of total scattering events.

(related to  $f$  for the Poissonian strategy and to  $\Delta t_{ref}$  for the Brownian one) for two different MC discretisations (respectively  $N_{MC} = 10^5$  and  $N_{MC} = 10^7$ ).

On figure 3, we can see that the error for the Brownian method does not depend on the number of scattering events (related to  $\Delta t_{ref}$ ) but rather more directly on the number of MC particles used to solve the problem. The convergence with respect to  $\Delta t_{ref}$  is fast. On another hand, for the Poissonian method, by increasing  $f$ , the number of scattering events increases, the diffusive regime is better and better captured and the error tends toward the one obtained with the Brownian scheme, dictated by the number of MC particles  $N_{MC}$ . The convergence seems to be of order 1 with respect to the number of scattering events. As a matter of fact, when the errors match, the two solvers are in exactly the same conditions (same  $N_{MC}$ , same time step, same number of cells and even same accuracies) and their run times are the almost the same.

### 6.1.2. Discontinuous conductivities ( $\kappa_1 \neq \kappa_2$ and $\rho_{v,1} = \rho_{v,2}$ ) for heat conduction (no coupling with radiative transfer)

In this section, we revisit the test-case of section 1 for which  $x \mapsto \kappa(x)$  is discontinuous. It is given by  $x \mapsto \kappa(x) = 10 \times \mathbf{1}_{[0, \frac{1}{2}]}(x) + 1 \times \mathbf{1}_{[\frac{1}{2}, 1]}(x)$ . For this test-case,  $x \mapsto \rho(x)c_v(x) = 1, \forall x \in [0, 1]$ . We tackle it with the material of the previous sections 3–4 and section 5.

Figure 4 presents the results obtained with the kinetic solver (left column) and the diffusive one (right column) on the discontinuous conductivity  $x \mapsto \kappa(x)$  benchmark of section 1. The results are displayed in terms of temperature profiles  $x \mapsto T_m(x, t = 10^{-2})$ . Note that the profiles  $x \mapsto \kappa(x)$  and  $x \mapsto \rho(x)c_v(x)$  are also displayed (the scales for them are on the right vertical axis).

The solutions are obtained in the same numerical settings:  $N_x = 100$  cells,  $N_{MC} = 10^6$ . The two resolution strategies give satisfactory results as soon as  $f = 10^2$  for the kinetic solver and  $\Delta t = 10^{-6}$  for the diffusion one. For both cases of figure 4, the new strategies we suggest in this paper are satisfactory.

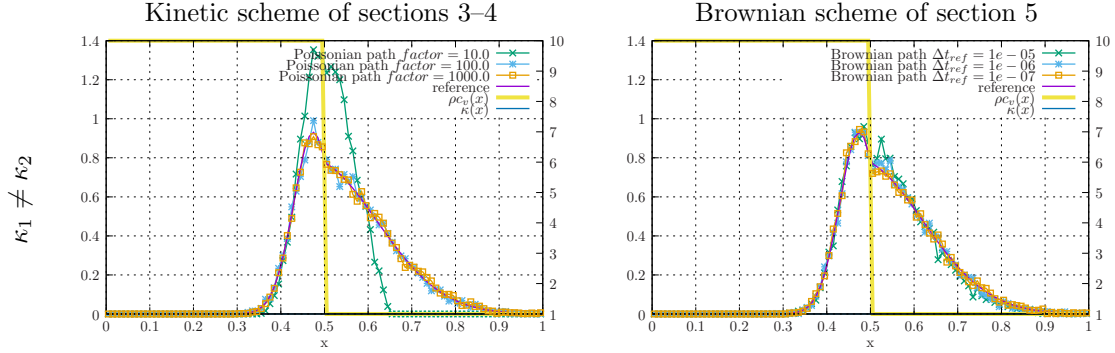


Figure 4: Results in terms of temperature profiles  $x \mapsto T_m(x, t = 10^{-2})$  obtained with the kinetic solver (left column) and the diffusive one (right column) on the discontinuous conductivity  $x \mapsto \kappa(x)$  benchmark of section 1.

### 6.1.3. Discontinuous density/volumic heat capacity ( $\kappa_1 = \kappa_2$ and $\rho c_{v,1} \neq \rho c_{v,2}$ ) for heat conduction (no coupling with radiative transfer)

In this section, we present some results on a benchmark for which there are discontinuities for  $x \mapsto \rho(x)c_v(x)$  but not for  $x \mapsto \kappa(x)$ . We take  $x \mapsto \kappa(x) = 1, \forall x \in [0, 1]$  and  $x \mapsto \rho(x)c_v(x) = 10^{-1} \times \mathbf{1}_{[0, \frac{1}{2}]}(x) + 1 \times \mathbf{1}_{[\frac{1}{2}, 1]}(x)$ . Once again, as a reference, we rely on the solution provided by a deterministic solver.

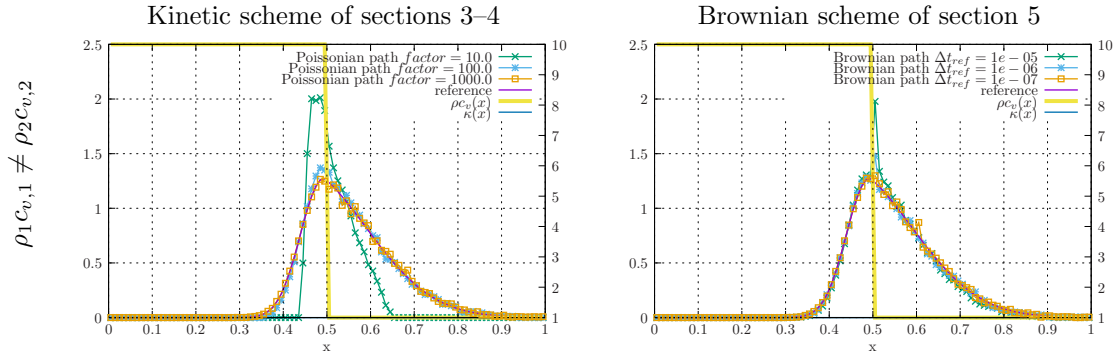


Figure 5: Results in terms of temperature profiles  $x \mapsto T_m(x, t = 10^{-2})$  obtained with the kinetic solver (left column) and the diffusive one (right column) on a benchmark with discontinuous  $x \mapsto \rho(x)c_v(x)$ .

The results are displayed in figure 5. For the Poissonian numerical strategy (left), as soon as the numerical parameter is well chosen ( $f \gg 1$ ), the exact solution is captured. The factor  $f$  must be equal to  $10^4$  for accurate restitutions. The new Brownian strategy also allows capturing efficiently this problem even if a spike at  $x = \frac{1}{2}$ , i.e. at the interface between the two material is observable for the coarse values of  $\Delta t_{ref}$ . We insist on the fact that the numerical parameters  $N_x = 100$  and  $N_{MC} = 10^6$  are the same for both resolution strategies: similar levels of noise are qualitatively observable.

## 6.2. Coupled benchmark (resolution of system (1)) in the equilibrium diffusion limit in layered media

In this section, we solve the full system (1) coupling radiative transfer and the diffusion equation for material temperature in layered media but *in the equilibrium diffusion limit*, i.e. in opaque materials for photons. In such conditions [55, 56, 57], the solution of (1) coincides with the solution of

$$\partial_t (E(T_m(x, t)) + aT_m^4(x, t)) - \nabla \cdot \left( \kappa(x) \nabla T_m(x, t) + \frac{c}{3\sigma_a(x)} \nabla (aT_m^4(x, t)) \right) = 0 \quad (26)$$

with Dirichlet boundary conditions  $T_m = 0$  and the same Heaviside initial condition as in the example of section 1. In order to solve the above model, we rely on a deterministic solver.

### 6.2.1. Resolution of system (1) in the equilibrium diffusion limit in layered media (discontinuous $\kappa$ )

In this section, we suggest considering a test problem with a full coupling between radiative transfer and diffusion in a layered material in the *equilibrium diffusion limit*. The solution of (1) in this regime coincides with the solution of (26). The characteristics of the test-case are summed up in table 1. We insist on the fact that these test-cases are more numerical than physical: we take

$\Omega = [0, 1]$	$\Omega_1 = [0, \frac{1}{2}]$	$\Omega_1 = [\frac{1}{2}, 1]$
$\kappa(x)$	$10^{-1}$	1
$\rho(x)c_v(x)$	1	1
$\sigma_a(x)$	5000	5000
$\sigma_s(x)$	0	0

Table 1: Characteristics of the benchmark of section 6.2.1

$c = 5000$  for the speed of light and  $a = 1$  for the radiative constant. In practice, for the numerical parameters, we take  $\Delta t = 10^{-4}$ ,  $N_x = 100$  and  $N_{MC} = 10^6$  for both computations. The initial condition is given by  $T_m(x, t = 0) = 2 \times \mathbf{1}_{[0.45, 0.55]}(x)$ . The final time  $t_f = 5 \times 10^{-3}$  has been chosen so that the solutions do not interact significantly with the boundary in order to avoid additional difficulties which would be beyond the scope of this paper.

Figure 6 displays the results in terms of temperature profiles  $x \mapsto T_m(x, t_f = 5 \times 10^{-3})$ . They are obtained with both strategies suggested in this paper, compared to a reference solution given by a deterministic code solving (26). Once again, even in this coupled context, the two numerical strategies we suggest in this paper allow recovering the reference solution as soon as  $f$  and  $\Delta t_{ref}$  are fine enough.

### 6.2.2. Resolution of system (1) in the equilibrium diffusion limit in layered media (discontinuous $\rho c_v$ )

In this section, we suggest considering a test problem with a full coupling between radiative transfer and diffusion in a layered material in the *equilibrium diffusion limit*. The characteristics of the test-case are summed up in table 2. Once again, we take  $c = 5000$  for the speed of light and  $a = 1$  for the radiative constant and  $\Delta t = 10^{-4}$ ,  $N_x = 100$  and  $N_{MC} = 10^6$  for both computations. The initial condition is given by  $T_m(x, t = 0) = 2 \times \mathbf{1}_{[0.45, 0.55]}(x)$ . The final time is  $t_f = 1 \times 10^{-3}$ .

Figure 7 displays the results in terms of temperature profiles  $x \mapsto T_m(x, t_f = 10^{-3})$ . They are obtained with both strategies suggested in this paper, compared to a reference solution given

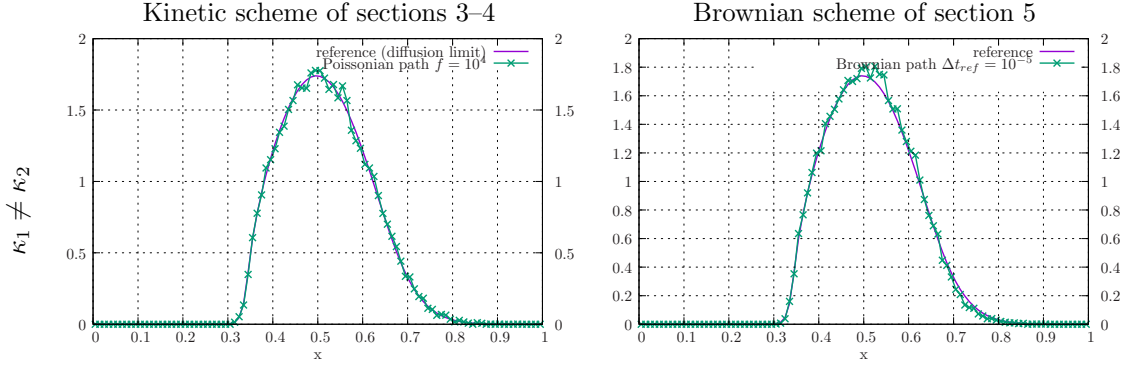


Figure 6: Spatial profile of the material temperature for two different solvers in the same configuration. The smooth curve comes from a deterministic simulation code solving the equilibrium diffusion limit for both radiative transfer and material conduction at time  $t_f = 5 \times 10^{-3}$ . The noisy curves are obtained from the phonon solver (left) and the corrected Brownian one (right).

$\Omega = [0, 1]$	$\Omega_1 = [0, \frac{1}{2}]$	$\Omega_1 = [\frac{1}{2}, 1]$
$\kappa(x)$	1	1
$\rho(x)c_v(x)$	10	1
$\sigma_a(x)$	5000	5000
$\sigma_s(x)$	0	0

Table 2: Characteristics of the benchmark of section 6.2.2

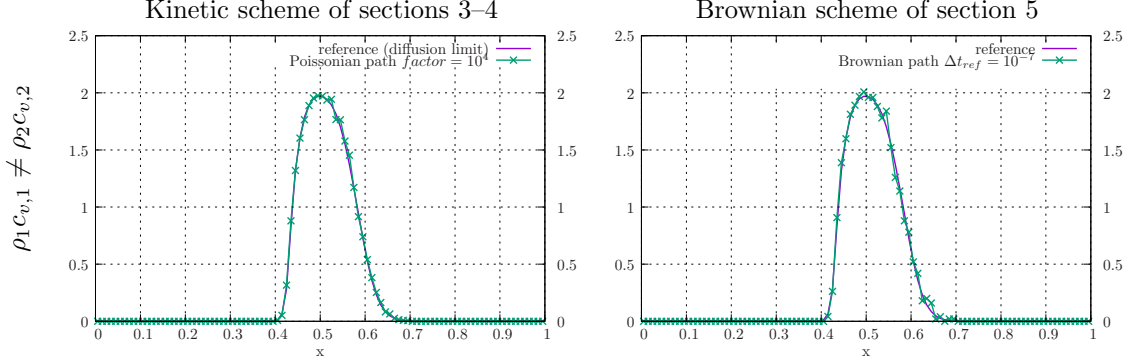


Figure 7: Spatial profile of the material temperature for two different solvers in the same configuration. The smooth curve comes from a deterministic simulation code solving the equilibrium diffusion limit for both radiative transfer and material conduction at time  $t_f = 10^{-3}$ . The noisy curves are obtained from the phonon solver (left) and the corrected Brownian one (right).

by a deterministic code solving (26). Once again, even in this coupled context, the two numerical strategies we suggest in this paper allow recovering the reference solution as soon as  $f$  and  $\Delta t_{ref}$  are fine enough.

6.2.3. Resolution of system (1) in the equilibrium diffusion limit in layered media (discontinuous  $\rho c_v$  and  $\kappa$ )

In this section, we consider a test-case which is a mix between the two previous ones in the sense that both  $x \mapsto \kappa(x)$  and  $x \mapsto \rho(x)c_v(x)$  are discontinuous. The characteristics of the test-case are summed up in table 3.

$\Omega = [0, 1]$	$\Omega_1 = [0, \frac{1}{2}]$	$\Omega_1 = [\frac{1}{2}, 1]$
$\kappa(x)$	$10^{-1}$	1
$\rho(x)c_v(x)$	10	1
$\sigma_a(x)$	5000	5000
$\sigma_s(x)$	0	0

Table 3: Characteristics of the benchmark of section 6.2.3

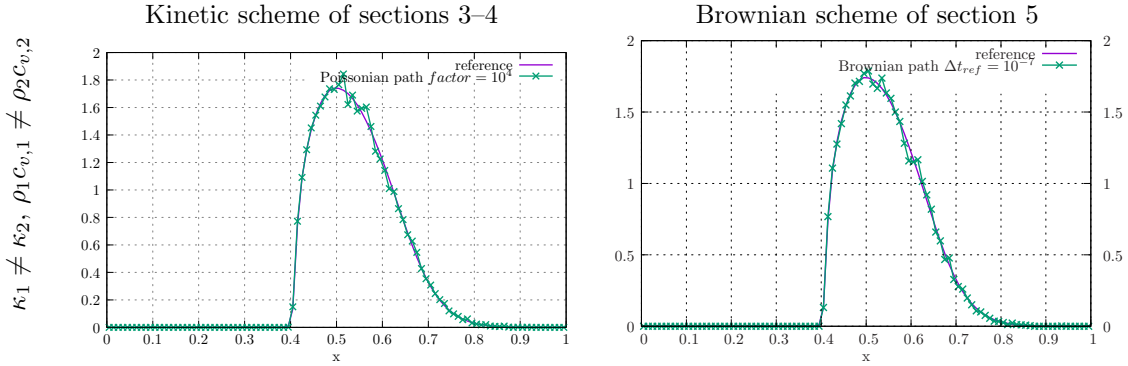


Figure 8: Spatial profile of the material temperature for two different solvers in the same configuration. The smooth curve comes from a deterministic simulation code solving the equilibrium diffusion limit for both radiative transfer and material conduction at time  $t_f = 5 \times 10^{-2}$ . The noisy curves are obtained from the phonon solver (left) and the corrected Brownian one (right).

Figure 8 displays the results obtained with both strategies suggested in this paper, compared to a reference solution given by a deterministic code the diffusion limit for both radiative transfer and material diffusion. Even in this more complex case, the two strategies are in very good agreement with the reference solution.

6.3. Resolution of system (1) in semi-transparent layered media

In this last section, we revisit the test-case of the previous section but the materials of the two layers are now semitransparent to photons (see table 4). With this test-case, we want to insist on the importance of resorting to a transport model for photons in semitransparent material: for the sake of comparisons, we plot the solution obtained in this additional semitransparent medium for photons to the one obtained in the equilibrium diffusion limit with the same physical parameters as in table 4 and another one obtained by fitting the radiative conductivity for the solution of (26) to approximately match the one of (1). The speed of the photons is now  $c = 5$  and we still have  $a = 1$ . We once again have  $N_x = 100$ ,  $N_{MC} = 10^6$  and  $\Delta t = 10^{-4}$ .

$\Omega = [0, 1]$	$\Omega_1 = [0, \frac{1}{2}]$	$\Omega_1 = [\frac{1}{2}, 1]$
$\kappa(x)$	$10^{-1}$	1
$\rho(x)c_v(x)$	10	1
$\sigma_a(x)$	5	5
$\sigma_s(x)$	0	0

Table 4: Characteristics of the benchmark of section 6.3

Figure 9 displays four curves for each resolution strategies (the Poissonian on the left hand side and the Brownian on the right hand side):

- the first curve called the "equilibrium diffusion limit" is obtained by solving (26) with the values of table 4.
- The second and third curves are obtained with our MC solvers (independently of being Poissonian or Brownian):
  - $T_m(x, t)$  is the material temperature profile,
  - $T_r(x, t)$  is the radiative temperature computed from  $\int I(x, t, \omega, \nu) d\omega d\nu = aT_r^4(x, t)$
- The last curve is obtained by solving (26) but instead of relying on the physical quantities of table 4 in order to compute the radiative conductivity  $\kappa_{rad} = 3.333 \times 10^{-1}$ , we use a fitted radiative conductivity set to  $\kappa_{rad}^{fitted} = 3.333 \times 10^{-3}$ .

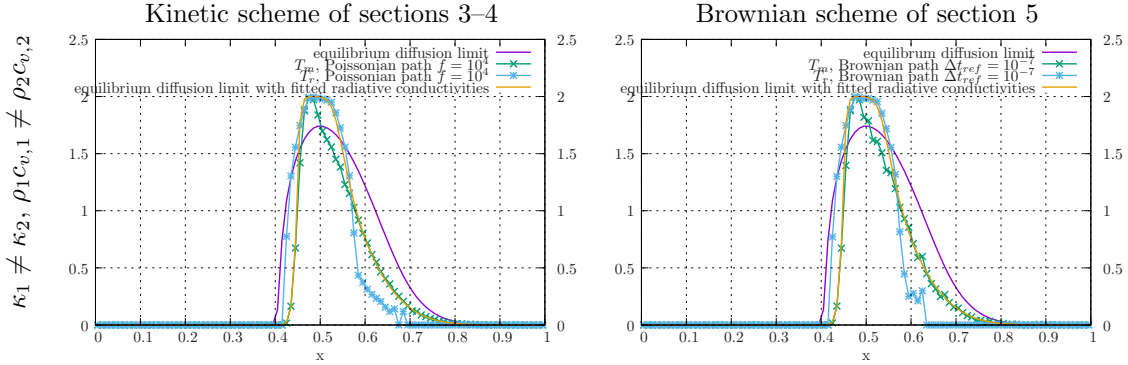


Figure 9: Spatial profile of the material temperature for two different solvers in the same configuration. The smooth curve comes from a deterministic simulation code solving the equilibrium diffusion limit for both radiative transfer and material conduction at time  $t = 10^{-2}$ . The noisy curves are obtained from the phonon solver (left) and the corrected Brownian one (right) but with radiative transfer in a semitransparent material.

First, on figure 9, we can see that with the physical parameters of table 4 and in this configuration, equilibrium is not fulfilled:  $T_m \neq T_r$  at some spatial locations. On the one hand, model (26) (with  $\kappa_{rad}$ ) predicts equilibrium and is far from both  $T_m$  and  $T_r$  profiles: the temperature is over-evaluated in the vicinities of the propagation fronts and under-estimated in the vicinity of the center of the domain. Model (26) with the fitted conductivity  $\kappa_{rad}^{fitted}$  on the other hand coincides with

$T_m$  and captures the vicinities of the propagation waves  $x \sim 0.70 - 0.80$  then coincides with  $T_r$  for  $x \in [0.45, 0.6]$  but under-estimates the temperature in the vicinity of  $x \sim 0.40 - 0.50$  which is driven by radiative transfer in a semitransparent medium.

## 7. Conclusion

In this paper, we tackle the problem of solving the conducto-radiative equation with a Monte-Carlo scheme (MC) in some layered media. From the observation that the resolution of the transport equation (valid in transparent media) in layered media with MC schemes is easy and the fact that the equilibrium diffusion limit is well captured by state-of-the-art MC schemes, we suggest modelling the sensible heat diffusion with a transport equation in a diffusive regime. The model is close to what is commonly called a *phonon model*. In order to capture the diffusion limit of material temperature (for the phonons), we suggest some additional model parameters for the velocities and opacities of phonons in the different layers (defined with respect to the conductivities, densities and heat capacities in the different layers). Those parameters are designed to both capture the diffusion limit and to preserve some physical invariants (continuity of temperature at the interface between materials) and ensure convergence. The model is efficient to reconstitute analytical and reference solutions in the equilibrium diffusion limit and can be safely used coupled with radiative transfer in transparent materials. From the analysis of the phonon model and by performing some analogies between Poissonian paths (which do not suffer jumps in material properties) and Brownian ones, we even suggest some original, quite simple and efficient corrections to the Brownian paths in layered media. In other words, two very different numerical strategies (Poissonian and Brownian) are suggested in this paper and both give very good results. The paper presents many numerical examples testifying of the relevance of the suggested numerical strategies in (transparent and opaque) layered media.

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