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Asymptotic diffusion limit of the symbolic Monte-Carlo method for the transport equation

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Abstract

We use asymptotic analysis to study the diffusion limit of the Symbolic Implicit Monte-Carlo (SIMC) method for the transport equation. For standard SIMC with piecewise constant basis functions, we demonstrate mathematically that the solution converges to the solution of a wrong diffusion equation. Nevertheless a simple extension to piecewise linear basis functions enables to obtain the correct solution. We present numerical examples which illustrate the analysis.

AMS: 65C05; 85A25

Keywords: Monte-Carlo method; Radiative transfer

1. Introduction

Let us consider the following model transport equation for function $(x, \vec{\Omega}) \to u(x, \vec{\Omega})$:

$$\begin{cases} \vec{\Omega} \cdot \vec{\nabla} u + \sigma_t u = \frac{\sigma_s}{4\pi} \int_{\mathscr{S}_2} u \, d\vec{\Omega} + Q, \\ u(x, \vec{\Omega}) = g, \quad x \in \Gamma, \ \vec{\Omega} \cdot \vec{n} < 0 \end{cases} \tag{1}$$

for x in some bounded domain $\mathscr{D}$ whose boundary is Γ and $\vec{\Omega}$ is in the unit sphere $\mathscr{S}_2$ ($\vec{n} = \vec{n}(x)$ denotes the exterior normal vector to Γ at point x). Here σ_a is the absorption cross-section, σ_s the scattering cross-section and $\sigma_t = \sigma_s + \sigma_a$ the total cross-section, u the intensity.

This equation can be used as a model equation for neutron transport but we have in mind radiative transfer applications. In this case the mean free path may be very small compared to some macroscopic length scale. Following [4,10], it is then customary to introduce some small parameter ε and to scale cross-sections as

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$$\sigma_{\rm t} \to \frac{\sigma_{\rm t}}{\varepsilon}, \quad \sigma_{\rm a} \to \varepsilon\sigma_{\rm a}, \quad Q \to \varepsilon Q, \tag{2}$$

so that Eq. (1) becomes

$$\vec{\Omega}\cdot\vec{\nabla}u + \frac{\sigma_{\rm t}}{\varepsilon}u = \left(\frac{\sigma_{\rm t}}{\varepsilon} - \sigma_{\rm a}\right)\frac{1}{4\pi}\int_{\mathscr{S}_2} u\,{\rm d}\vec{\Omega} + \varepsilon Q. \tag{3}$$

It is well known [5] that the limit of u at the zeroth order in ε is solution of

$$\begin{cases} -\vec{\nabla}\cdot\frac{1}{3\sigma_{\rm t}}\vec{\nabla}u + \sigma_{\rm a}u = Q, \\ u(x,\vec{\Omega}) = \frac{1}{2\pi}\int_{\vec{\Omega}\cdot\vec{n}<0}\frac{\sqrt{3}}{2}|\vec{\Omega}\cdot\vec{n}|H(|\vec{\Omega}\cdot\vec{n}|)g(\vec{\Omega}), \quad x\in\Gamma, \end{cases} \tag{4}$$

where $H(\mu)$ is Chandrasekhar's function [11].

In this paper, we are interested in studying numerical schemes for system (1) which have the so-called diffusion limit property, i.e. which gives a correct discretization of the diffusion equation (4) when the scaling (2) is applied. A large amount of theoretical work has already been done to design deterministic methods having the diffusion limit. Examples of such methods are the linear discontinuous finite element method, the linear characteristic method and the SCB method [1,6,7]. They are able to treat, at the same time, opaque and transparent regions. But they are still not widely used in three-dimensional problems because of the number of cells involved in such calculations.

On the other end, Monte-Carlo methods are used in three dimensions for a long time because of their simplicity and their ability to treat complex geometries. But an analysis of their behavior in optically thick regions, i.e. when scaling (2) applies is still missing. Our goal is to apply the same kind of analysis that has been performed for deterministic methods to a particular Monte-Carlo method: the Symbolic Monte-Carlo method (SIMC) [3,9]. It consists in solving system

$$\begin{cases} \vec{\Omega}\cdot\vec{\nabla}u + \sigma_{\rm t}u = \sigma_{\rm t}\Phi, \\ -\sigma_{\rm s}\frac{1}{4\pi}\int_{\mathscr{S}_2} u\,{\rm d}\vec{\Omega} + \sigma_{\rm t}\Phi = Q, \end{cases} \tag{5}$$

which is equivalent to (1) (with same boundary condition). In the SIMC method, after space discretization the matrix which gives $\sigma_{\rm t}\frac{1}{4\pi}\int_{\mathscr{S}_2} u\,{\rm d}\vec{\Omega}$, as a function of Φ in the first equation of (5), is computed. Replacing $\sigma_{\rm s}\frac{1}{4\pi}\int_{\mathscr{S}_2} u\,{\rm d}\vec{\Omega}$ in the second equation of (5) leads to a linear system whose solution is Φ. One can prove the equivalence, for this model equation, of the collision probability method [2] and the SIMC method. But the SIMC method is mostly used for photonics to solve

$$\begin{cases} \frac{\partial u}{\partial t} + \vec{\Omega}\cdot\vec{\nabla}u + \sigma_{\rm t}u = \sigma_{\rm t}\Phi, \\ \gamma\frac{\partial\Phi}{\partial t} - \sigma_{\rm t}\frac{1}{4\pi}\int_{\mathscr{S}_2} u\,{\rm d}\vec{\Omega} + \sigma_{\rm t}\Phi = Q. \end{cases} \tag{6}$$

The second equation in (6) is the electronic energy equation where Φ is the electronic temperature and γ the calorific capacity. This system takes a form analogous to (5) after discretizing $\partial\Phi/\partial t$ implicitly in time

$$\begin{cases} \frac{\partial u}{\partial t} + \vec{\Omega}\cdot\vec{\nabla}u + \sigma_{\rm t}u = \sigma_{\rm t}\Phi, \\ -\sigma_{\rm t}\frac{1}{4\pi}\int_{\mathscr{S}_2} u\,{\rm d}\vec{\Omega} + (\sigma_{\rm t} + \frac{\gamma}{\Delta t})\Phi = Q + \gamma\frac{\Phi_0}{\Delta t}. \end{cases} \tag{7}$$

Thus, all the conclusions we can draw from the study of the SIMC method for solving (5) can be also applied for solving (7). In radiation hydrodynamics problems, because of the complexity of the geometries which can change in time and the dependency in time of u, the coefficients of the matrix are approximated by using a particle method. In contrast, the collision probability method is mostly used in the field of neutronics. The equation which is solved is generally the steady state neutronics equation. Thus, the calculation of the probability of collisions can be performed analytically.

We are concerned with the behavior of the SIMC method in optically thick regions. In such a region, only the particles which travel between cells contribute to the matrix. It follows that a large amount of particles are necessary to yield meaningful results. The question which arises is? If the number of particles is sufficient to compute the matrix accurately, does the linear system correspond to a consistent discretization of the diffusion equation. In other words, do we solve the right equation in the opaque region? We prove in this paper that the original method gives a wrong solution in those regions and we improve the SIMC method to obtain a consistent discretization of the diffusion equation. The difficulty of obtaining the correct diffusion behavior with a Monte-Carlo method has been known for a long time (see [8] for a recent contribution): we present a rigorous analysis of this weakness.

The paper is organized as follows. In the next section, we describe the Symbolic Monte-Carlo method for piecewise constant basis functions as it was first introduced in [3,9] and how it can be extended to more general basis functions. Then, we perform an asymptotic analysis on the numerical schemes to study the diffusion limit. Finally, we illustrate the theoretical results with numerical simulations for one- and two-dimensional geometry and present some numerical issues.

2. Extension of SIMC

In this section, we recall the main features of SIMC and describe its extension to higher order elements. For simplicity, we first assume that the incoming intensity g is zero.

Let $u(x,\vec{\Omega})$ where $x \in \mathscr{D}$ and $\vec{\Omega} \in \mathscr{S}_2$ be the solution of the transport equation:

$$\begin{cases} \vec{\Omega} \cdot \vec{\nabla} u + \sigma_{\mathrm{t}} u = \sigma_{\mathrm{t}} \Phi, \\ -\sigma_{\mathrm{s}} \tilde{u} + \sigma_{\mathrm{t}} \Phi = Q, \end{cases} \tag{8}$$

where $\tilde{u}(x) = (1/4\pi) \int_{\mathscr{S}_2} u(x,\vec{\Omega})\, \mathrm{d}\vec{\Omega}$. In the SIMC method, we generally look only for the integrated intensity $\tilde{u}$: the angular variation of the solution of the transport equation is of little interest. Suppose the domain $\mathscr{D}$ is discretized into N cells $(T_i)_{i\in(1,N)}$ and that we have defined basis functions $(\chi_i^l(x))_{l\in(1,L)}$ for each cell T_i such that

$$\sum_{l=1}^{L} \chi_i^l(x) = \mathbb{1}_{x\in T_i}, \quad \chi_i^l(x)\chi_{i'}^{l'}(x) = 0 \quad \text{for } i \neq i'.$$

We can express Φ as

$$\Phi(x) = \sum_{i,l} \phi_i^l \chi_i^l(x). \tag{9}$$

We approximate (8) by the following system:

$$\begin{cases} \vec{\Omega} \cdot \vec{\nabla} u + \sigma_{\mathrm{t}} u = \sigma_{\mathrm{t}} \Phi, \\ \langle -\sigma_{\mathrm{s}} \tilde{u} + \sigma_{\mathrm{t}} \Phi - Q, \chi_i^l \rangle = 0 \quad \forall i \in (1,N),\ \forall l \in (1,L), \end{cases} \tag{10}$$

where $\langle , \rangle$ is the scalar product in $L^2(\mathscr{D})$, i.e. we look for a weak solution of system (8) in a discontinuous finite element space. For simplicity, throughout the paper, we will use the same notation for the exact solution u and the approximate solution. Thanks to the linearity of (10) with respect to Φ, the solution of (10) can be expressed as

$$u(x,\vec{\Omega}) = \sum_{i,l} \phi_i^l u_i^l(x,\vec{\Omega}), \tag{11}$$

where function $u_i^l(x,\vec{\Omega})$ is solution of

$$\begin{cases} \vec{\Omega}\cdot\vec{\nabla}u_i^l + \sigma_t u_i^l = \sigma_t \chi_i^l, \\ u_i^l(x,\vec{\Omega}) = 0, \quad x\in\Gamma,\ \vec{\Omega}\cdot\vec{n} < 0. \end{cases} \tag{12}$$

The boundary condition is equivalent to $u_i^l(x,\vec{\Omega}) = 0,\ x\in\Gamma_i,\ \vec{\Omega}\cdot\vec{n}<0$ where Γ_i is the boundary of cell T_i. Putting expansions Eqs. (9), (11) into system (10) leads to

$$\begin{cases} \vec{\Omega}\cdot\vec{\nabla}u_i^l + \sigma_t u_i^l = \sigma_t \chi_i^l, \\ \sum_{i,l}(b_{i,i'}^{l,l'} - a_{i,i'}^{l,l'})\phi_i^l = \langle Q, \chi_{i'}^{l'}\rangle \quad \forall i'\in(1,N),\ \forall l'\in(1,L), \\ u_i^l(x,\vec{\Omega}) = 0, \quad x\in\Gamma,\ \vec{\Omega}\cdot\vec{n}<0, \end{cases} \tag{13}$$

where we have denoted $a_{i,i'}^{l,l'} = \langle\sigma_s\tilde{u}_i^l, \chi_{i'}^{l'}\rangle$ and $b_{i,i'}^{l,l'} = \langle\sigma_t\chi_i^l, \chi_{i'}^{l'}\rangle$.

The system (13) is solved in three steps. First, we look for solution of Eqs. (12) for all indices (i,l). Actually, because we do not look for a detailed description in angle of u_i^l but only for the integrated quantity $a_{i,i'}^{l,l'}$, a particle method is well appropriate (see below). Then, knowing the matrices $\mathscr{A} = (a_{i,i'}^{l,l'})_{1\leqslant i,i'\leqslant N, 1\leqslant l,l'\leqslant L}$ and $\mathscr{B} = (b_{i,i'}^{l,l'})_{1\leqslant i,i'\leqslant N, 1\leqslant l,l'\leqslant L}$, we solve the linear system whose unknowns are ϕ_i^l

$$\sum_{i,l}(b_{i,i'}^{l,l'} - a_{i,i'}^{l,l'})\phi_i^l = \langle Q, \chi_{i'}^{l'}\rangle \quad \forall i', l'. \tag{14}$$

This gives Φ by (9) and finally we deduce $\tilde{u} = (\sigma_t\Phi - Q)/\sigma_s$.

If instead of $\tilde{u}$ some other quantity G is needed (such as $u(x,\vec{\Omega})$ for some particular point x_0 and some particular direction $\vec{\Omega}_0$), it is necessary to compute during the tracking of the particles the linear operator which relies G to Φ: once Φ is known G is simply obtained by a scalar product.

Taking into account a non-zero boundary condition g simply leads to the introduction of a second auxiliary function u_b, solution of

$$\begin{cases} \vec{\Omega}\cdot\vec{\nabla}u_b + \sigma_t u_b = 0, \\ u_b(x,\vec{\Omega}) = g, \quad x\in\Gamma,\ \vec{\Omega}\cdot\vec{n}<0, \end{cases} \tag{15}$$

and the right-hand term of linear system (14) $\langle Q, \chi_{i'}^{l'}\rangle$ is replaced by $\langle Q + \sigma_s u_b, \chi_{i'}^{l'}\rangle$ (see [9] for details).

In the original SIMC method, Φ was supposed to be constant by cell for each cell T_i, i.e. $L = 1$ and $\chi_i^1(x) = \mathbb{1}_{x\in T_i}$. In the improved SIMC method, Φ is supposed to be piecewise linear for each cell and discontinuous:

- For one-dimensional problems, there are two basis functions on each cell

  $$T_i = [x_{i-1/2}, x_{i+1/2}] : \chi_i^1(x) = \frac{x_{i+1/2} - x}{x_{i+1/2} - x_{i-1/2}} \quad \text{and} \quad \chi_i^2(x) = \frac{x - x_{i-1/2}}{x_{i+1/2} - x_{i-1/2}}.$$

  Thus, ϕ_i^1 is the value of Φ in the cell T_i for $x_{i-1/2}$ and ϕ_i^2 the value for $x_{i+1/2}$.
- For two-dimensional problems, we choose triangular cells and there are three basis functions on each cell T. Basis function χ_i^l is the polynomial of degree one in x, y whose value is 1 on the vertex l and 0 on the others and ϕ_i^l is the value of Φ on this vertex.
- For three-dimensional problems, cells are tetrahedrons, there are four basis function for each cell. Basis function χ_i^l is the polynomial of degree one in x, y, z whose value is 1 on the vertex l and 0 on the others and ϕ_i^l is the value of Φ on this vertex.

For completeness, we briefly describe the particle method which is used for computing the matrices $\mathscr{A}$ and $\mathscr{B}$.

For each cell i, we solve (12) at the same time for all $l \in \{1, L\}$. The source term is sampled with P particles in each cell, their direction Ω_p is uniform on $\mathscr{S}_2$ and their birth place $x_p(0)$ uniform on T_i. The sample may be random or deterministic. To each particle p is associated a weight $\omega_p(0) = (1/P)\sigma_t V_i$, where V_i is the volume of the cell i. Actually, each particle represents L particles whose weights are $\omega_p^l(0) = \omega_p(0)\chi_i^l(x_p(0))$. This particle is called a *symbolic* particle because we do not know at this stage its "true" weight $\omega_p^l \phi_i^l$. During the sampling, we compute by Monte-Carlo integration the scalar products $b_{i,i'}^{l,l'}$

$$b_{i,i'}^{l,l'} = \frac{1}{P}\sigma_t V_i \sum_p \chi_i^l(x_p(0))\chi_{i'}^{l'}(x_p(0)).$$

Each particle p travels at unit speed with direction Ω_p through the mesh. When a distance l_p is traveled in cell $T_{i'}$, the weight is decreased by the attenuation factor $e^{-\sigma_t l_p}$ and the matrix estimator $a_{i,i'}^{l,l'}$ is incremented:

$$\begin{aligned} &\omega_p \to \omega_p e^{-\sigma_t l_p}, \\ &a_{i,i'}^{l,l'} \to a_{i,i'}^{l,l'} + \omega_p \textstyle\int_0^{l_p} \sigma_t \chi_{i'}^{l'}(x_p(s)) e^{-\sigma_t s}\, ds. \end{aligned}$$

Notice that the sum of all contributions to the matrix term is just the loss of weight of the particle p

$$\omega_p \sum_{l'=1}^{L} \int_0^{l_p} \sigma_t \chi_{i'}^{l'}(x_p(s))\sigma_t e^{-\sigma_t s}\, ds = \omega_p(1 - e^{-\sigma_t l_p}).$$

We can compute analytically the increment for $a_{i,i'}^{l,l'}$. Supposing that the particle p travels from A to B through T_i, we obtain

$$\begin{aligned} \int_0^{l_p} \sigma_t \chi_{i'}^{l'}(A + \vec{\Omega}_p s) e^{-\sigma_t s}\, ds &= [-e^{-\sigma_t s}\chi_{i'}^{l'}(A + \vec{\Omega}_p s)]_0^{l_p} + \int_0^{l_p} \vec{\Omega}_p \cdot \vec{\nabla}\chi_{i'}^{l'}(A + \vec{\Omega}_p s) e^{-\sigma_t s}\, ds, \\ &= -\chi_{i'}^{l'}(B) e^{-\sigma_t l_p} + \chi_{i'}^{l'}(A) + \frac{1 - e^{-\sigma_t l_p}}{\sigma_t} \vec{\Omega}_p \cdot \vec{\nabla}\chi_{i'}^{l'}, \end{aligned}$$

where we have used the fact that $\nabla \chi_{i'}^{l'}$ is a constant vector for each cell T_i. For different kind of cells a numerical integration would be necessary.

3. Diffusion limit of SIMC

In this section, we study the diffusion limit of SIMC, first for standard SIMC (i.e. basis functions are piecewise constant) and then for extended SIMC (i.e. basis functions are piecewise linear). The technique, which was first introduced in [4], consists in performing an asymptotic analysis of the numerical scheme under the scaling (2). Let u^ε be the solution of the scaled numerical scheme. We will obtain the numerical scheme satisfied by u^ε to first order with respect to ε. If this is a correct discretization of the diffusion equation (4) then we will say that SIMC has the diffusion limit.

Notice that all expansions that will be presented are formal expansions and that we will not give any bounds on high order error terms.

In this section, we will restrict ourselves to zero-boundary conditions.

We begin with the following lemma which will be used throughout this section.

Lemma 1. *Let Γ be the part of the boundary of some cell and $\mathscr{S}'$ some subdomain of $\mathscr{S}_2$. Let F and L be two bounded non-negative functions defined on $\Gamma \times \mathscr{S}'$ and consider the integral*

$$\mathrm{CT}(\varepsilon) = \int_\Gamma \mathrm{d}\gamma \int_{\mathscr{S}'} \mathrm{d}\vec{\Omega} F(\gamma, \vec{\Omega}) \exp\left(-\frac{\sigma_{\mathrm{t}} L(\gamma, \vec{\Omega})}{\varepsilon} \right).$$

(i) *For one-dimensional problems, if there exists some constant $c > 0$ such that $L(\gamma, \vec{\Omega}) > c$ for all $(\gamma, \vec{\Omega})$: then $CT(\varepsilon)$ goes exponentially to zero as ε goes to zero.*
(ii) *In dimension D ($D = 2$ or $D = 3$), if $L(\gamma, \vec{\Omega})$ is zero only for some γ_0 and $L(\gamma, \vec{\Omega}) \sim C_0(\vec{\Omega})|\gamma - \gamma_0|$ for γ close to γ_0: then*

$$\mathrm{CT}(\varepsilon) = C\left(\frac{\varepsilon}{\sigma_{\mathrm{t}}}\right)^{D-1} + \mathrm{O}(\varepsilon^D)$$

for some constant C

$$\left(C = |\Gamma| \int_{\mathscr{S}' \cap \{C_0(\vec{\Omega}) < \infty\}} \frac{F(\gamma_0, \vec{\Omega})}{C_0(\vec{\Omega})} \, \mathrm{d}\vec{\Omega} \textit{ in two dimensions} \right).$$

$L(\gamma, \vec{\Omega})$ is the distance from point γ on the boundary Γ to another point γ' on Γ such that $\overrightarrow{\gamma'\gamma}$ is collinear with $\vec{\Omega}$. CT will be called a corner term.

Proof. In one-dimensional problem, we have, for some positive constant c,

$$0 < \mathrm{CT}(\varepsilon) < \int_{\mathscr{S}'} f(\mu) \mathrm{e}^{-\frac{\sigma_{\mathrm{t}} c}{\varepsilon|\mu|}} \, \mathrm{d}\mu$$

and this term is obviously exponentially decaying.

In two dimensions, we introduce a parametric coordinate $\gamma(s)$ on Γ such that $\gamma(0) = \gamma_0$. Then

$$\mathrm{CT}(\varepsilon) = |\Gamma| \int_0^1 \mathrm{d}s \int_{\mathscr{S}'} F(\gamma(s), \vec{\Omega}) \exp\left(-\frac{\sigma_{\mathrm{t}} L(\gamma(s), \vec{\Omega})}{\varepsilon} \right) \mathrm{d}\vec{\Omega}.$$

Since $L(\gamma, \vec{\Omega})$ is zero only for γ_0 there exists some positive values $L_0 > 0$ and $s_0 > 0$ such that for $s > s_0$ we have $L(\gamma(s), \vec{\Omega}) > L_0$. We deduce that

$$\begin{aligned}\mathrm{CT}(\varepsilon) &= |\Gamma| \int_0^{s_0} \mathrm{d}s \int_{\mathscr{S}'} F(\gamma(s), \vec{\Omega}) \exp\left(-\frac{\sigma_{\mathrm{t}} C_0(\vec{\Omega})|\gamma(s) - \gamma_0|}{\varepsilon} \right) \mathrm{d}\vec{\Omega} + \mathrm{O}(\mathrm{e}^{-\frac{1}{\varepsilon}}) \\ &= |\Gamma| \int_{\mathscr{S}'} F(\gamma_0, \vec{\Omega}) \left(\int_0^{s_0} \exp\left(-\frac{\sigma_{\mathrm{t}} C_0(\vec{\Omega}) s}{\varepsilon} \right) \mathrm{d}s \right) \mathrm{d}\vec{\Omega}(1 + \mathrm{O}(s_0)) + \mathrm{O}(\mathrm{e}^{-\frac{1}{\varepsilon}}).\end{aligned}$$

Integrating by parts we have

$$\int_0^{s_0} \exp\left(-\frac{\sigma_{\mathrm{t}} C_0(\vec{\Omega}) s}{\varepsilon} \right) \mathrm{d}s \sim \frac{\varepsilon}{\sigma_{\mathrm{t}} C_0(\vec{\Omega})} + \mathrm{O}\left(\frac{\varepsilon}{s_0}\right),$$

hence

$$\mathrm{CT}(\varepsilon) \sim |\Gamma| \frac{\varepsilon}{\sigma_t} \int_{\mathscr{S}' \cap \{C_0(\vec{\Omega}) < \infty\}} \frac{F(\gamma_0, \vec{\Omega})}{C_0(\vec{\Omega})} \, \mathrm{d}\vec{\Omega}.$$

In three dimensions, we introduce a parametric coordinate $\gamma(s,t)$ on Γ such that $\gamma(0,0) = \gamma_0$. This leads to

$$\mathrm{CT}(\varepsilon) \sim C' \int_{\mathscr{S}'} F(\gamma_0, \vec{\Omega}) \left(\int_0^{s_0} \int_0^{t_0} \exp\left(- \frac{\sigma_t C_0(\vec{\Omega}) \sqrt{s^2 + t^2}}{\varepsilon} \right) \mathrm{d}s \, \mathrm{d}t \right) \mathrm{d}\vec{\Omega}$$

for some constant C' coming from the change of variable. Using polar coordinates, we obtain

$$\int_0^{s_0} \int_0^{t_0} \exp\left(- \frac{\sigma_t C_0(\vec{\Omega}) \sqrt{s^2 + t^2}}{\varepsilon} \right) \mathrm{d}s \, \mathrm{d}t \sim \frac{2\pi\varepsilon^2}{\sigma_t C_0(\vec{\Omega})}$$

and we conclude as in the two-dimensional case. □

3.1. Standard SIMC

In this case, we denote $\chi_i^l(x) = \chi_i(x) = \mathbb{1}_{x \in T_i}$. We shall prove the following proposition.

Proposition 1. *At the lowest order with respect to* ε, u^ε *is solution of the linear system*

$$\left(\frac{1}{4} \int_{\Gamma_i} \mathrm{d}\gamma \right) u_i^\varepsilon - \frac{1}{4} \sum_{i'} \int_{\Gamma_i^{i'}} \mathrm{d}\gamma u_{i'}^\varepsilon = \varepsilon \langle Q, \chi_i \rangle, \tag{16}$$

where $u^\varepsilon = \sum_i u_i^\varepsilon \chi$, Γ_i *is the boundary of cell* T_i *and* $\Gamma_i^{i'}$ *is the common edge of adjacent cells* T_i *and* T_i'.

We deduce immediately from this result that standard SIMC does not satisfy the diffusion limit property because (16) is not a correct discretization of the diffusion equation (4) (with zero boundary condition).

Proof. Using the scaling (2), linear system (14) becomes

$$\sum_i (b_{i,i'}^\varepsilon - a_{i,i'}^\varepsilon) \phi_i^\varepsilon = \varepsilon \langle Q, \chi_{i'} \rangle, \tag{17}$$

with

$$b_{i,i'}^\varepsilon = \frac{\langle \sigma_t \chi_i, \chi_{i'} \rangle}{\varepsilon} = \delta_i^{i'} \frac{\sigma_t}{\varepsilon} V_i,$$
$$a_{i,i'}^\varepsilon = \left(\frac{\sigma_t}{\varepsilon} - \varepsilon \sigma_a \right) \langle \tilde{u}_i^\varepsilon, \chi_{i'} \rangle$$

and u_i^ε is solution of

$$\begin{cases} \vec{\Omega} \cdot \vec{\nabla} u_i^\varepsilon + \frac{\sigma_t}{\varepsilon} u_i^\varepsilon = \frac{\sigma_t}{\varepsilon} \chi_i, \\ u_i^\varepsilon(x, \vec{\Omega}) = 0, \quad x \in \Gamma_i, \ \vec{\Omega} \cdot \vec{n} < 0. \end{cases} \tag{18}$$

We integrate this equation with respect to $\vec{\Omega}$ and take the scalar product with $\chi_{i'}$

$$\frac{\sigma_t}{\varepsilon}\langle \tilde{u}_i^\varepsilon, \chi_{i'}\rangle = \frac{\sigma_t}{\varepsilon}\langle \chi_i, \chi_{i'}\rangle - \frac{1}{4\pi}\int_{\Gamma_{i'}} d\gamma \int_{\mathscr{S}_2} d\vec{\Omega}(\vec{\Omega}\cdot\vec{n}) u_i^\varepsilon(\gamma, \Omega). \tag{19}$$

We shall now replace u_i^ε by its expression. Eq. (18) reduces to an ordinary differential equation which has to be solved along each characteristic starting from the boundary Γ with direction Ω. We will consider four distinct cases:

(1) $T_i = T_{i'}$. For $x \in T_i$, we have

$$u_i^\varepsilon(x, \vec{\Omega}) = \int_0^{l_i(x,\vec{\Omega})} \frac{\sigma_t}{\varepsilon} \exp\left\{ -\frac{\sigma_t}{\varepsilon}(l_i(x,\vec{\Omega}) - s)\right\} \chi_i(x - \vec{\Omega}s)\, ds, \tag{20}$$

where the point $x - \vec{\Omega} l_i(x,\vec{\Omega})$ is at the intersection of the boundary Γ_i of T_i with the half-line starting from x with direction $-\vec{\Omega}$ (see Fig. 1) and $l_i(x,\vec{\Omega})$ is the distance between x and the boundary Γ_i in the direction Ω. In order to simplify the notations we shall only write l_i instead of $l_i(x,\vec{\Omega})$ (this simplification will be made throughout the paper). With $\chi_i(x) = \mathbb{1}_{x\in T_i}$, we obtain

$$u_i^\varepsilon(x, \vec{\Omega}) = 1 - e^{-\frac{\sigma_t}{\varepsilon} l_i}. \tag{21}$$

We notice that $u_i^\varepsilon(\gamma, \vec{\Omega}) = 0$ for $\gamma \in \Gamma_i$ and $\vec{\Omega}\cdot\vec{n} < 0$ so that replacing u_i by its expression (21) into (19), we obtain

$$\begin{aligned}\frac{\sigma_t}{\varepsilon}\langle \tilde{u}_i^\varepsilon, \chi_i\rangle &= \frac{\sigma_t}{\varepsilon}\langle \chi_i, \chi_i\rangle - \frac{1}{4\pi}\int_{\Gamma_i} d\gamma \int_{\vec{\Omega}\cdot\vec{n}>0} d\vec{\Omega}(\vec{\Omega}\cdot\vec{n})(1 - e^{-\frac{\sigma_t}{\varepsilon} l_i}) \\ &= \frac{\sigma_t}{\varepsilon}\langle \chi_i, \chi_i\rangle - \frac{1}{4}\int_{\Gamma_i} d\gamma + \mathrm{CT}(\varepsilon)\end{aligned}$$

with

$$\mathrm{CT}(\varepsilon) = \frac{1}{4\pi}\int_{\Gamma_i} d\gamma \int_{\vec{\Omega}\cdot\vec{n}>0} d\Omega(\vec{\Omega}\cdot\vec{n}) e^{-\frac{\sigma_t}{\varepsilon} l_i}.$$

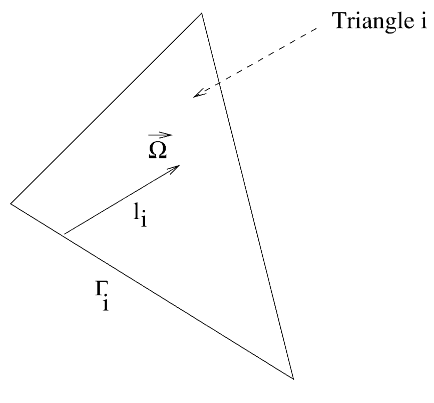

Fig. 1.

Using Lemma 1, we obtain

$$\begin{aligned} a^{\epsilon}_{i,i} &= \frac{\left(\frac{\sigma_t}{\varepsilon} - \varepsilon\sigma_a\right)}{\frac{\sigma_t}{\varepsilon}} \left(\frac{\sigma_t}{\varepsilon} \langle \chi_i, \chi_i \rangle - \frac{1}{4} \int_{\Gamma_i} \mathrm{d}\gamma + \mathrm{CT}(\varepsilon) \right) \\ &= \left(\frac{\sigma_t}{\varepsilon} - \varepsilon\sigma_a \right) V_i - \frac{1}{4} \int_{\Gamma_i} \mathrm{d}\gamma + \mathrm{CT}(\varepsilon) + \mathrm{O}(\varepsilon^2). \end{aligned}$$

Finally,

$$b^{\varepsilon}_{i,i'} - a^{\epsilon}_{i,i} = \frac{1}{4} \int_{\Gamma_i} \mathrm{d}\gamma + \varepsilon\sigma_a V_i + \mathrm{CT}(\varepsilon) + \mathrm{O}(\varepsilon^2). \tag{22}$$

(2) $i \neq i'$ and cells T_i and $T_{i'}$ have a common edge $\Gamma_i^{i'}$. For $x \in T_{i'}$, we have

$$u^{\varepsilon}_i(x, \vec{\Omega}) = u^{\varepsilon}_i(x_{\Gamma_i^{i'}}, \vec{\Omega}) \mathrm{e}^{-\frac{\sigma_t}{\varepsilon} l_{i'}}, \tag{23}$$

where the point $x_{\Gamma_i^{i'}}$ is at the intersection of the boundary $\Gamma_i^{i'}$ with the half-line starting from x with direction $-\Omega$ and $l_{i'} = l_{i'}(x, \Omega)$ is the distance between that point and x (see Fig. 2). Using (20), we get

$$u^{\varepsilon}_i(x, \vec{\Omega}) = (1 - \mathrm{e}^{-\frac{\sigma_t}{\varepsilon} l_i}) \mathrm{e}^{-\frac{\sigma_t}{\varepsilon} l_{i'}}, \tag{24}$$

where $l_i = l_i(x, \Omega)$ is the distance between $x_{\Gamma_i^{i'}}$ and the opposite boundary of T_i in the direction Ω. Using (19) and using the fact that $\langle \chi_i, \chi_{i'} \rangle = 0$ because $i \neq i'$ we obtain

$$\frac{\sigma_t}{\varepsilon} \langle \tilde{u}^{\varepsilon}_i, \chi_{i'} \rangle = -\frac{1}{4\pi} \int_{\Gamma_{i'}} \mathrm{d}\gamma \int_{\vec{\Omega}\cdot\vec{n} > 0} \mathrm{d}\vec{\Omega} (\vec{\Omega} \cdot \vec{n}) (1 - \mathrm{e}^{-\frac{\sigma_t}{\varepsilon} l_i}) \mathrm{e}^{-\frac{\sigma_t}{\varepsilon} l_{i'}} - \frac{1}{4\pi} \int_{\Gamma_{i'}} \mathrm{d}\gamma \int_{\vec{\Omega}\cdot\vec{n} < 0} \mathrm{d}\vec{\Omega} (\vec{\Omega} \cdot \vec{n}) (1 - \mathrm{e}^{-\frac{\sigma_t}{\varepsilon} l_i}) \mathrm{e}^{-\frac{\sigma_t}{\varepsilon} l_{i'}}. \tag{25}$$

When the direction $\vec{\Omega}$ is entering the cell ($\vec{\Omega} \cdot \vec{n} < 0$), we have $u^{\varepsilon}_i(\gamma, \vec{\Omega}) = 0$ except for $\gamma \in \Gamma_i^{i'}$ and then $l_{i'} = l_{i'}(\gamma, \vec{\Omega}) = 0$. When $\vec{\Omega}$ is leaving the cell ($\vec{\Omega} \cdot \vec{n} > 0$), we have $u^{\varepsilon}_i(\gamma, \vec{\Omega}) = 0$ except for $\gamma \in \Gamma_{i'} - \Gamma_i^{i'}$. Hence

$$\begin{aligned} \frac{\sigma_t}{\varepsilon} \langle \tilde{u}^{\varepsilon}_i, \chi_{i'} \rangle &= -\frac{1}{4\pi} \int_{\Gamma_{i'} - \Gamma_i^{i'}} \mathrm{d}\gamma \int_{\vec{\Omega}\cdot\vec{n} > 0} \mathrm{d}\vec{\Omega} (\vec{\Omega} \cdot \vec{n}) (1 - \mathrm{e}^{-\frac{\sigma_t}{\varepsilon} l_i}) \mathrm{e}^{-\frac{\sigma_t}{\varepsilon} l_{i'}} - \frac{1}{4\pi} \int_{\Gamma_i^{i'}} \mathrm{d}\gamma \int_{\vec{\Omega}\cdot\vec{n} < 0} \mathrm{d}\vec{\Omega} (\vec{\Omega} \cdot \vec{n}) (1 - \mathrm{e}^{-\frac{\sigma_t}{\varepsilon} l_i}) \\ &= \frac{1}{4} \int_{\Gamma_i^{i'}} \mathrm{d}\gamma + \mathrm{CT}_1(\varepsilon) + \mathrm{CT}_2(\varepsilon). \end{aligned} \tag{26}$$

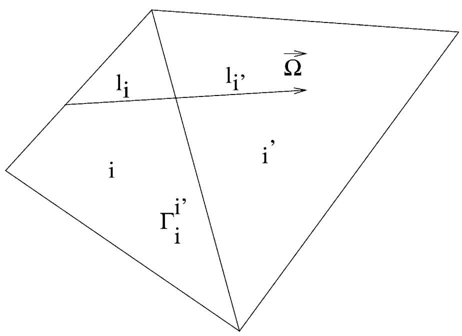

Fig. 2.

With

$$\mathrm{CT}_1(\varepsilon) = -\frac{1}{4\pi}\int_{\Gamma_{i'}-\Gamma_i^{i'}} \mathrm{d}\gamma \int_{\vec{\Omega}\cdot\vec{n}>0} \mathrm{d}\vec{\Omega}(\vec{\Omega}\cdot\vec{n})(1-\mathrm{e}^{-\frac{\sigma_t}{\varepsilon}l_i})\mathrm{e}^{-\frac{\sigma_t}{\varepsilon}l_{i'}},$$

$$\mathrm{CT}_2(\varepsilon) = +\frac{1}{4\pi}\int_{\Gamma_i^{i'}} \mathrm{d}\gamma \int_{\vec{\Omega}\cdot\vec{n}<0} \mathrm{d}\vec{\Omega}(\vec{\Omega}\cdot\vec{n})\mathrm{e}^{-\frac{\sigma_t}{\varepsilon}l_i}.$$

We can apply Lemma 1 to the corner terms CT_1 and CT_2. Finally,

$$\begin{aligned} a^{\epsilon}_{i,i'} &= \frac{\left(\frac{\sigma_t}{\varepsilon}-\varepsilon\sigma_a\right)}{\frac{\sigma_t}{\varepsilon}}\left(\frac{1}{4}\int_{\Gamma_i^{i'}}\mathrm{d}\gamma + \mathrm{CT}_1(\varepsilon) + \mathrm{CT}_2(\varepsilon)\right) \\ &= \frac{1}{4}\int_{\Gamma_i^{i'}}\mathrm{d}\gamma + \mathrm{CT}_1(\varepsilon) + \mathrm{CT}_2(\varepsilon) + \mathrm{O}(\varepsilon^2). \end{aligned}$$

(3) $i \neq i'$ and cells T_i and $T_{i'}$ have no common vertex. It is easy to see that $a^{\epsilon}_{i,i'}$ is exponentially decaying with respect to $\frac{1}{\varepsilon}$ so that we can neglect these contributions to the linear system.

(4) $i \neq i'$ and cells T_i and $T_{i'}$ have a common vertex but no common edge. Then $a^{\varepsilon}_{i,i'}$ itself is a corner term and Lemma 1 applies. For example, suppose that a cell T_j is adjacent to T_i and $T_{i'}$, then, for $x \in T_{i'}$, we have

$$u_i^{\varepsilon}(x,\vec{\Omega}) = \mathrm{e}^{-\frac{\sigma_t}{\varepsilon}l_{i'}}\mathrm{e}^{-\frac{\sigma_t}{\varepsilon}l_j}(1-\mathrm{e}^{-\frac{\sigma_t}{\varepsilon}l_i}),$$

thus $a^{\varepsilon}_{i,i'}$ is a corner term corresponding to particles emitted in T_i, crossing a distance $l_j = l_j(x,\vec{\Omega})$ in T_j and a distance then $l_{i'} = l_{i'}(x,\vec{\Omega})$ in $T_{i'}$ (Fig. 3):

$$a^{\varepsilon}_{i,i'} = -\frac{1}{4\pi}\int_{\vec{\Omega}\cdot\vec{n}<0}\mathrm{d}\vec{\Omega}\int_{\Gamma^j_{i'}}\mathrm{d}\gamma(\vec{\Omega}\cdot\vec{n})\mathrm{e}^{-\frac{\sigma_t}{\varepsilon}l_j}(1-\mathrm{e}^{-\frac{\sigma_t}{\varepsilon}l_i}) - \frac{1}{4\pi}\int_{\vec{\Omega}\cdot\vec{n}>0}\mathrm{d}\vec{\Omega}\int_{\Gamma_{i'}-\Gamma^j_{i'}}\mathrm{d}\gamma(\vec{\Omega}\cdot\vec{n})\mathrm{e}^{-\frac{\sigma_t}{\varepsilon}l_{i'}}\mathrm{e}^{-\frac{\sigma_t}{\varepsilon}l_j}(1-\mathrm{e}^{-\frac{\sigma_t}{\varepsilon}l_i}).$$

Linear system (14) can finally be rewritten as

$$\begin{aligned} &\left(\frac{1}{4}\int_{\Gamma_i}\mathrm{d}\gamma + \varepsilon\sigma_a V_i + \mathrm{CT}^i(\varepsilon)\right)\phi_i^{\varepsilon} - \frac{1}{4}\sum_{i',\ \text{common edge with } i}\int_{\Gamma_i^{i'}}\mathrm{d}\gamma\phi^{\varepsilon}_{i'} + \sum_{i'',\ \text{common vertex with } i}\mathrm{CT}^{i,i''}(\varepsilon)\phi^{\varepsilon}_{i''} + \mathrm{O}(\varepsilon^2) \\ &\quad = \varepsilon\langle Q,\chi_i\rangle, \end{aligned}$$

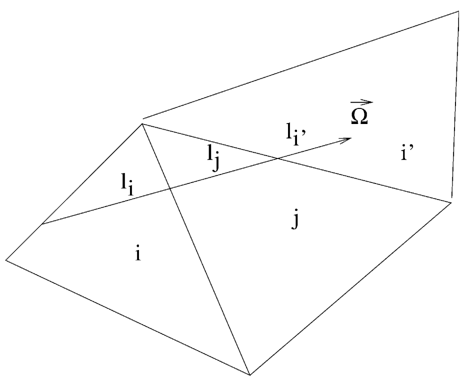

Fig. 3.

where $\mathrm{CT}^{i,i'}(\varepsilon)$ are corner terms. We now introduce the following formal expansion

$$\Phi^\varepsilon = \Phi^0 + \varepsilon\Phi^1 + \varepsilon^2\Phi^2 + \cdots,$$
$$\phi_i^\varepsilon = \phi_i^0 + \varepsilon\phi_i^1 + \varepsilon^2\phi_i^2 + \cdots \quad \forall i \in (1, N).$$

At the lowest order we obtain

$$\left(\frac{1}{4}\int_{\Gamma_i} \mathrm{d}\gamma\right)\phi_i^0 - \frac{1}{4}\sum_{i'}\int_{\Gamma_i^{i'}} \mathrm{d}\gamma\phi_{i'}^0 = 0.$$

We can easily prove that this linear system has a unique solution up to a constant. Consider the corresponding matrix $\mathscr{M} = (m_{ii'})$ with $m_{ii} = \frac{1}{4}\int_{\Gamma_i}\mathrm{d}\gamma$ and $m_{ii'} = -\frac{1}{4}\sum_{i'}\int_{\Gamma_i^{i'}}\mathrm{d}\gamma$. This is a singular matrix since $m_{ii} + \sum_{i'\neq i} m_{ii'} = 0$ but its kernel reduces to constant vectors: if v is a vector in the kernel then we have, for each component $v_i = \sum_{j\neq i}\alpha_{ij}v_j$ with $0 < \alpha_{ij} < 1$ so each component is in the interior convex set of the others which is not possible unless they are all equal.

We deduce that $\Phi^0 = 0$ since the Dirichlet boundary condition is $\Phi = 0$ at the boundary. At order ε we have

$$\left(\frac{1}{4}\int_{\Gamma_i} \mathrm{d}\gamma\right)\phi_i^1 - \frac{1}{4}\sum_{i'}\int_{\Gamma_i^{i'}} \mathrm{d}\gamma\phi_{i'}^1 = \langle Q, \chi_i\rangle - \sigma_\mathrm{a} V_i\phi_i^0 + \sum_{i'}\mathrm{CT}^{i,i'}(0)\phi_{i'}^0.$$

(corner terms actually only appear in two-dimensional problems and $\mathrm{CT}^{i,i'}(0) = \lim_{\varepsilon\to 0}(\mathrm{CT}^{i,i'}(\varepsilon)/\varepsilon)$). As $\phi_i^0 = 0$, equation for Φ_1 reduces to

$$\left(\frac{1}{4}\int_{\Gamma_i} \mathrm{d}\gamma\right)\phi_i^1 - \frac{1}{4}\sum_{i'}\int_{\Gamma_i^{i'}} \mathrm{d}\gamma\phi_{i'}^1 = \langle Q, \chi_i\rangle.$$

As $\Phi \sim \varepsilon\Phi_1$, we deduce that the equation satisfied by Φ at the lowest order is simply

$$\left(\frac{1}{4}\int_{\Gamma_i} \mathrm{d}\gamma\right)\phi_i - \frac{1}{4}\sum_{i'}\int_{\Gamma_i^{i'}} \mathrm{d}\gamma\phi_{i'} = \varepsilon\langle Q, \chi_i\rangle.$$

Second equation of the linear system with the scaling (2) writes as

$$\left(\frac{\sigma_\mathrm{t}}{\varepsilon} - \varepsilon\sigma_\mathrm{a}\right)u^\varepsilon - \frac{\sigma_\mathrm{t}}{\varepsilon}\Phi^\varepsilon = -\varepsilon Q$$

so that $u^\varepsilon = \Phi^\varepsilon + \mathrm{O}(\varepsilon^2)$ which ends the proof. □

For example, in one-dimensional geometry with uniform mesh, we obtain:

$$-\frac{1}{4}\phi_{i-1}^\varepsilon + \frac{1}{2}\phi_i^\varepsilon - \frac{1}{4}\phi_{i+1}^\varepsilon = \varepsilon Q\Delta x, \tag{27}$$

with $\phi = 1 = \phi_N = 0$ (zero boundary condition). This is a consistent discretization of

$$-\frac{\partial^2\Phi}{\partial x^2} = KQ,$$

with $K = 4\varepsilon/\Delta x$, instead of the correct equation

$$-\frac{1}{3(\sigma_\mathrm{s} + \sigma_\mathrm{a})}\frac{\partial^2\Phi}{\partial x^2} + \sigma_\mathrm{a}\Phi = Q.$$

3.2. Linear SIMC

Proposition 2. *At the lowest order with respect to* ε, u^ε *is solution of the linear system*

$$\sigma_{\mathrm{a}} \sum_{j'} \langle \xi_j, \xi_{j'} \rangle u^\varepsilon_{j'} + \frac{1}{3\sigma_{\mathrm{t}}} \sum_{j'} \langle \nabla \xi_j \cdot \nabla \xi_{j'} \rangle u^\varepsilon_{j'} = \langle Q, \xi_j \rangle, \tag{28}$$

where $u^\varepsilon = \sum_j u^\varepsilon_j \xi_j$, *and* ξ_j *is the piecewise linear function which value is* 1 *on vertex* γ_j *and 0 on other vertices.*

This is a correct discretization of the diffusion equation (4) (with zero boundary condition) with linear continuous finite elements: hence extended SIMC satisfies the diffusion limit property.

Proof. We will give the proof only in the two-dimensional case because this is the only one where corner terms matter: one and three-dimensional cases follow simply. We shall denote by $(\gamma_i^k)_{k=1,2,3}$ the three vertices of cell T_i: γ_i^l is the vertex such that $\chi_i^l(\gamma_i^l) = 1$.

Using the scaling (2), linear system (14) becomes

$$\sum_{i,l} (b^{\varepsilon,l,l'}_{i,i'} - a^{\varepsilon,l,l'}_{i,i'}) \phi^{\varepsilon,l}_i = \varepsilon \langle Q, \chi^{l'}_{i'} \rangle, \tag{29}$$

with

$$b^{\varepsilon,l,l'}_{i,i'} = \frac{\langle \sigma_{\mathrm{t}} \chi^l_i, \chi^{l'}_{i'} \rangle}{\varepsilon},$$
$$a^{\varepsilon,l,l'}_{i,i'} = \left(\frac{\sigma_{\mathrm{t}}}{\varepsilon} - \varepsilon \sigma_{\mathrm{a}} \right) \langle \tilde{u}^{\varepsilon,l}_i, \chi^{l'}_{i'} \rangle$$

and $u^{\varepsilon,l}_i$ is solution of

$$\begin{cases} \vec{\Omega} \cdot \vec{\nabla} u^{\varepsilon,l}_i + \frac{\sigma_{\mathrm{t}}}{\varepsilon} u^{\varepsilon,l}_i = \frac{\sigma_{\mathrm{t}}}{\varepsilon} \chi^l_i, \\ u^{\varepsilon,l}_i(x, \vec{\Omega}) = 0, \quad x \in \Gamma_i, \quad \vec{\Omega} \cdot \vec{n} < 0. \end{cases}$$

We integrate this equation with respect to $\vec{\Omega}$ and take the scalar product with $\chi^{l'}_{i'}$

$$\frac{\sigma_{\mathrm{t}}}{\varepsilon} \langle \tilde{u}^{\varepsilon,l}_i, \chi^{l'}_{i'} \rangle = \frac{\sigma_{\mathrm{t}}}{\varepsilon} \langle \chi^l_i, \chi^{l'}_{i'} \rangle + \frac{1}{4\pi} \int_{\mathscr{S}_2} \mathrm{d}\vec{\Omega} \langle \vec{\Omega} u^{\varepsilon,l}_i, \nabla \chi^{l'}_{i'} \rangle - \frac{1}{4\pi} \int_{\Gamma_{i'}} \mathrm{d}\gamma \int_{\mathscr{S}_2} \mathrm{d}\vec{\Omega} (\vec{\Omega} \cdot \vec{n}) u^{\varepsilon,l}_i(\gamma, \Omega) \chi^{l'}_{i'}(\gamma). \tag{30}$$

We shall now replace $u^{\varepsilon,l}_i$ by its expression. As before, we will consider four distinct cases:

(1) $T_i = T_{i'}$. We start from expression (20) which is still valid and perform an integration by parts, using the fact that $\nabla \chi^l_i$ is constant over triangle T_i

$$u^{\varepsilon,l}_i(x, \vec{\Omega}) = \chi^l_i(x) - \chi^l_i(x - \vec{\Omega} l_i) \mathrm{e}^{-\frac{\sigma_{\mathrm{t}}}{\varepsilon} l_i} - \frac{\varepsilon}{\sigma_{\mathrm{t}}} (\vec{\Omega} . \nabla \chi^l_i)(1 - \mathrm{e}^{-\frac{\sigma_{\mathrm{t}}}{\varepsilon} l_i}), \tag{31}$$

where the point $x - \vec{\Omega} l_i$ is at the intersection of the boundary Γ_i of T_i with the half-line starting from x with direction $-\vec{\Omega}$ (see Fig. 1). Replacing $u^{\varepsilon,l}_i$ by its expression into (30) we obtain

$$\begin{aligned} \frac{\sigma_t}{\varepsilon} \langle \tilde{u}^{\varepsilon,l}_i, \chi^{l'}_i \rangle = {} & \frac{\sigma_t}{\varepsilon} \langle \chi^l_i, \chi^{l'}_i \rangle + \frac{1}{4\pi} \int_{\mathscr{S}_2} \mathrm{d}\vec{\Omega} \langle \chi^l_i(x), \vec{\Omega} \cdot \nabla \chi^{l'}_i \rangle - \frac{1}{4\pi} \int_{\mathscr{S}_2} \mathrm{d}\vec{\Omega} \langle \chi^l_i(x - \vec{\Omega} l_i) e^{-\frac{\sigma_t}{\varepsilon} l_i}, \vec{\Omega} \cdot \nabla \chi^{l'}_i \rangle \\ & - \frac{1}{4\pi} \int_{\mathscr{S}_2} \mathrm{d}\vec{\Omega} \langle \frac{\varepsilon}{\sigma_t} (\vec{\Omega} \cdot \nabla \chi^l_i)(1 - e^{-\frac{\sigma_t}{\varepsilon} l_i}), \vec{\Omega} \cdot \nabla \chi^{l'}_i \rangle - \frac{1}{4\pi} \int_{\Gamma_i} \mathrm{d}\gamma \int_{(\vec{\Omega} \cdot \vec{n}) > 0} \mathrm{d}\vec{\Omega} (\vec{\Omega} \cdot \vec{n}) \chi^l_i(\gamma) \chi^{l'}_i(\gamma) \\ & + \frac{1}{4\pi} \int_{\Gamma_i} \mathrm{d}\gamma \int_{(\vec{\Omega} \cdot \vec{n}) > 0} \mathrm{d}\vec{\Omega} (\vec{\Omega} \cdot \vec{n}) \chi^{l'}_i(\gamma) \chi^l_i(\gamma - \vec{\Omega} l_i) e^{-\frac{\sigma_t}{\varepsilon} l_i} \\ & + \frac{1}{4\pi} \int_{\Gamma_i} \mathrm{d}\gamma \int_{(\vec{\Omega} \cdot \vec{n}) > 0} \mathrm{d}\vec{\Omega} (\vec{\Omega} \cdot \vec{n}) \frac{\varepsilon}{\sigma_t} (\vec{\Omega} \cdot \nabla \chi^l_i)(1 - e^{-\frac{\sigma_t}{\varepsilon} l_i}) \chi^{l'}_i(\gamma). \end{aligned} \tag{32}$$

We have used the fact that $u_i^{\varepsilon,l}(x,\vec{\Omega}) = 0$ on Γ_i for entering directions $(\vec{\Omega}\cdot\vec{n}) < 0$. We will now expand all the terms in the right-hand side of (32) with respect to ε. We denote by $I_1,\dots,I_7$ the seven terms appearing in the right-hand side of (32). We have

$$\int_{\mathscr{S}_2} \mathrm{d}\vec{\Omega}\vec{\Omega} = 0 \Rightarrow I_2 = 0.$$

As $\nabla\chi_i^{l'}$ is a constant vector, integral I_3 can be rewritten as

$$I_3 = -\frac{1}{4\pi}\int_{\mathscr{S}_2} \mathrm{d}\vec{\Omega}\vec{\Omega}\cdot\nabla\chi_i^{l'}\langle v^\varepsilon(x,\vec{\Omega})\rangle,$$

where v^ε is solution of the transport equation

$$\begin{cases} \vec{\Omega}\cdot\nabla v^\varepsilon + \frac{\sigma_t}{\varepsilon}v^\varepsilon = 0, \\ v^\varepsilon(x,\vec{\Omega}) = \chi_i^l(x), \quad x\in\Gamma_i,\ \vec{\Omega}\cdot\vec{n} < 0. \end{cases} \tag{33}$$

Integrating (33) on cell T_i, we obtain

$$\langle v^\varepsilon\rangle = -\frac{\varepsilon}{\sigma_t}\langle\vec{\Omega}\cdot\nabla v^\varepsilon\rangle = -\frac{\varepsilon}{\sigma_t}\int_{\Gamma_i}\mathrm{d}\gamma(\vec{\Omega}\cdot\vec{n})v^\varepsilon(\gamma,\vec{\Omega}).$$

Hence

$$I_3 = \frac{1}{4\pi}\frac{\varepsilon}{\sigma_t}\int_{\Gamma_i}\mathrm{d}\gamma\int_{\vec{\Omega}\cdot\vec{n}<0}\mathrm{d}\vec{\Omega}(\vec{\Omega}\cdot\nabla\chi_i^{l'})(\vec{\Omega}\cdot\vec{n})\chi_i^l(\gamma) + \frac{1}{4\pi}\frac{\varepsilon}{\sigma_t}\int_{\Gamma_i}\mathrm{d}\gamma\int_{\vec{\Omega}\cdot\vec{n}>0}\mathrm{d}\vec{\Omega}(\vec{\Omega}\cdot\nabla\chi_i^{l'})(\vec{\Omega}\cdot\vec{n})\chi_i^l(\gamma-\vec{\Omega}l_i)\mathrm{e}^{-\frac{\sigma_t}{\varepsilon}l_i},$$

which gives, using Lemma 1,

$$I_3 = \frac{\varepsilon}{6\sigma_t}\int_{\Gamma_i}(\vec{n}\cdot\nabla\chi_i^{l'})\chi_i^l(\gamma)\,\mathrm{d}\gamma + \mathrm{O}(\varepsilon^2).$$

Since $\mathrm{e}^{-\frac{\sigma_t}{\varepsilon}l_i}$ goes to zero as ε goes to zero, we can take the limit in the integral term of I_4:

$$\begin{aligned} I_4 &= -\frac{\varepsilon}{\sigma_t}\int_{\mathscr{S}_2}\langle(\vec{\Omega}\cdot\nabla\chi_i^l)\cdot(\vec{\Omega}\cdot\nabla\chi_i^{l'})\rangle\mathrm{d}\vec{\Omega} + \mathrm{O}(\varepsilon^2) \\ &= -\frac{\varepsilon}{3\sigma_t}\nabla\chi_i^l\cdot\nabla\chi_i^{l'}V_i + \mathrm{O}(\varepsilon^2). \end{aligned}$$

Integral I_5 can be computed

$$I_5 = -\frac{1}{4\pi}\int_{\Gamma_i}\mathrm{d}\gamma\int_{(\vec{\Omega}\cdot\vec{n})>0}\mathrm{d}\vec{\Omega}(\vec{\Omega}\cdot\vec{n})\chi_i^l(\gamma)\chi_i^{l'}(\gamma) = -\frac{1}{4}\int_{\Gamma_i}\mathrm{d}\gamma\chi_i^l(\gamma)\chi_i^{l'}(\gamma).$$

Integral I_6 is a corner term: we apply Lemma 1

$$I_6 = \frac{\varepsilon}{\sigma_t}\sum_{k=1}^{3}C_k\chi_i^l(\gamma_i^k)\chi_i^{l'}(\gamma_i^k) + \mathrm{O}(\varepsilon^2),$$

where C_k are some constant numbers and $(\gamma_i^k)_{k=1,2,3}$ are the three vertices of cell T_i. At last, taking the limit in the integral term of I_7 and using the lemma gives

$$I_7 \sim \frac{\varepsilon}{4\pi\sigma_t}\int_{\Gamma_i} \mathrm{d}\gamma \int_{(\vec{\Omega}\cdot\vec{n})>0} \mathrm{d}\vec{\Omega}(\vec{\Omega}\cdot n)(\vec{\Omega}\cdot\nabla\chi_i^l)\chi_i^{l'}(\gamma) + \mathrm{O}(\varepsilon^2)$$
$$\sim \frac{\varepsilon}{6\sigma_t}\int_{\Gamma_i} \mathrm{d}\gamma(\vec{n}\cdot\nabla\chi_i^l)\chi_i^{l'}(\gamma) + \mathrm{O}(\varepsilon^2).$$

Putting all these expansions together, Eq. (32) becomes

$$\frac{\sigma_t}{\varepsilon}\langle\tilde{u}_i^{\varepsilon,l},\chi_i^{l'}\rangle = \frac{\sigma_t}{\varepsilon}\langle\chi_i^l,\chi_i^{l'}\rangle - \frac{1}{4}\int_{\Gamma_i}\mathrm{d}\gamma\chi_i^l(\gamma)\chi_i^{l'}(\gamma) + \frac{\varepsilon}{\sigma_t}\left(\frac{1}{6}\int_{\Gamma_i}(\vec{n}\cdot\nabla\chi_i^{l'})\chi_i^l(\gamma)\,\mathrm{d}\gamma + \frac{1}{6}\int_{\Gamma_i}\mathrm{d}\gamma(\vec{n}\cdot\nabla\chi_i^l)\chi_i^{l'}(\gamma)\right) + \frac{\varepsilon}{\sigma_t}\left(-\frac{1}{3}\nabla\chi_i^l\cdot\nabla\chi_i^{l'}V_i + \sum_{k=1}^{3}C_k\chi_i^l(\gamma_i^k)\chi_i^{l'}(\gamma_i^k)\right) + \mathrm{O}(\varepsilon^2). \tag{34}$$

As basis functions χ_i^l are polynomial of degree one, we have the identity

$$\langle\nabla\chi_i^l\cdot\nabla\chi_i^{l'}\rangle = \int_{\Gamma_i}(\vec{n}\cdot\nabla\chi_i^{l'})\chi_i^l(\gamma)\,\mathrm{d}\gamma = \int_{\Gamma_i}(\vec{n}\cdot\nabla\chi_i^l)\chi_i^{l'}(\gamma)\,\mathrm{d}\gamma. \tag{35}$$

So Eq. (34) simply writes as

$$\frac{\sigma_t}{\varepsilon}\langle\tilde{u}_i^{\varepsilon,l},\chi_i^{l'}\rangle = \frac{\sigma_t}{\varepsilon}\langle\chi_i^l,\chi_i^{l'}\rangle - \frac{1}{4}\int_{\Gamma_i}\mathrm{d}\gamma\chi_i^l(\gamma)\chi_i^{l'}(\gamma) + \frac{\varepsilon}{\sigma_t}\sum_{k=1}^{3}C_k\chi_i^l(\gamma_i^k)\chi_i^{l'}(\gamma_i^k) + \mathrm{O}(\varepsilon^2). \tag{36}$$

We can now compute the matrix element $m_{i,i}^{\varepsilon,l,l'} = b_{i,i}^{\varepsilon,l,l'} - a_{i,i}^{\varepsilon,l,l'}$:

$$m_{i,i}^{\varepsilon,l,l'} = \frac{1}{4}\int_{\Gamma_i}\mathrm{d}\gamma\chi_i^l(\gamma)\chi_i^{l'}(\gamma) + \varepsilon\sigma_a\langle\chi_i^l,\chi_i^{l'}\rangle - \frac{\varepsilon}{\sigma_t}\sum_{k=1}^{3}C_k\chi_i^l(\gamma_i^k)\chi_i^{l'}(\gamma_i^k) + \mathrm{O}(\varepsilon^2). \tag{37}$$

(2) $i \neq i'$ and cells T_i and $T_{i'}$ have a common edge $\Gamma_i^{i'}$. For $x \in T_{i'}$, we have

$$u_i^{\varepsilon,l}(x,\vec{\Omega}) = u_i^{\varepsilon,l}(x_{\Gamma_i^{i'}},\vec{\Omega})\mathrm{e}^{-\frac{\sigma_t}{\varepsilon}l_{i'}}, \tag{38}$$

where the point $x_{\Gamma_i^{i'}}$ is at the intersection of the boundary $\Gamma_i^{i'}$ with the half-line starting from x with direction $-\Omega$ and $l_{i'} = l_{i'}(x,\Omega)$ is the distance between that point and x (see Fig. 2). Using (31), we get

$$u_i^{\varepsilon,l}(x,\vec{\Omega}) = \mathrm{e}^{-\frac{\sigma_t}{\varepsilon}l_{i'}}\left(\chi_i^l(x-\vec{\Omega}l_{i'}) - \chi_i^l(x-\vec{\Omega}(l_i+l_{i'}))\mathrm{e}^{-\frac{\sigma_t}{\varepsilon}l_i} - \frac{\varepsilon}{\sigma_t}(\vec{\Omega}\cdot\nabla\chi_i^l)(1-\mathrm{e}^{-\frac{\sigma_t}{\varepsilon}l_i})\right). \tag{39}$$

Putting this expression into (30), we get, since $\langle\chi_i^l,\chi_{i'}^{l'}\rangle = 0$:

$$\begin{aligned}\frac{\sigma_t}{\varepsilon}\langle\tilde{u}_i^{\varepsilon,l},\chi_{i'}^{l'}\rangle = {} & \frac{1}{4\pi}\int_{\mathscr{S}'}\mathrm{d}\vec{\Omega}\langle\vec{\Omega}\mathrm{e}^{-\frac{\sigma_t}{\varepsilon}l_{i'}}\chi_i^l(x-\vec{\Omega}l_{i'}),\nabla\chi_{i'}^{l'}\rangle - \frac{1}{4\pi}\int_{\mathscr{S}'}\mathrm{d}\vec{\Omega}\langle\vec{\Omega}\mathrm{e}^{-\frac{\sigma_t}{\varepsilon}l_{i'}}\chi_i^l(x-\vec{\Omega}(l_i+l_{i'}))\mathrm{e}^{-\frac{\sigma_t}{\varepsilon}l_i},\nabla\chi_{i'}^{l'}\rangle \\ & - \frac{1}{4\pi}\int_{\mathscr{S}'}\mathrm{d}\vec{\Omega}\langle\vec{\Omega}\mathrm{e}^{-\frac{\sigma_t}{\varepsilon}l_{i'}}\frac{\varepsilon}{\sigma_t}(\vec{\Omega}\cdot\nabla\chi_i^l)(1-\mathrm{e}^{-\frac{\sigma_t}{\varepsilon}l_i}),\nabla\chi_{i'}^{l'}\rangle \\ & - \frac{1}{4\pi}\int_{\Gamma_{i'}}\mathrm{d}\gamma\int_{\mathscr{S}'}\mathrm{d}\vec{\Omega}(\vec{\Omega}\cdot\vec{n})\mathrm{e}^{-\frac{\sigma_t}{\varepsilon}l_{i'}}\chi_i^l(\gamma-\vec{\Omega}l_{i'})\chi_{i'}^{l'}(\gamma) \\ & + \frac{1}{4\pi}\int_{\Gamma_{i'}}\mathrm{d}\gamma\int_{\mathscr{S}'}\mathrm{d}\vec{\Omega}(\vec{\Omega}\cdot\vec{n})\mathrm{e}^{-\frac{\sigma_t}{\varepsilon}l_{i'}}\chi_i^l(\gamma-\vec{\Omega}(l_i+l_{i'}))\mathrm{e}^{-\frac{\sigma_t}{\varepsilon}l_i}\chi_{i'}^{l'}(\gamma) \\ & + \frac{1}{4\pi}\int_{\Gamma_{i'}}\mathrm{d}\gamma\int_{\mathscr{S}'}\mathrm{d}\vec{\Omega}(\vec{\Omega}\cdot\vec{n})\mathrm{e}^{-\frac{\sigma_t}{\varepsilon}l_{i'}}\frac{\varepsilon}{\sigma_t}(\vec{\Omega}\cdot\nabla\chi_i^l)(1-\mathrm{e}^{-\frac{\sigma_t}{\varepsilon}l_i})\chi_{i'}^{l'}(\gamma).\end{aligned} \tag{40}$$

Here $\mathscr{S}'$ is the subdomain of $\mathscr{S}_2$ which corresponds to directions coming from T_i, i.e. $\vec{\Omega}\cdot\vec{n}<0$ on $\Gamma_i^{i'}$ and $\vec{\Omega}\cdot\vec{n}>0$ on $\Gamma_{i'}-\Gamma_i^{i'}$. We denote by $I_1,\dots,I_6$ the six integrals appearing in the right-hand side of (40). We now expand these terms with respect to ε.

First integral writes as

$$I_1=\frac{1}{4\pi}\int_{\mathscr{S}'}\mathrm{d}\vec{\Omega}(\vec{\Omega}\cdot\nabla\chi_{i'}^{l'})\langle v^\varepsilon\rangle,$$

where v^ε is solution of system (33). Integrating this equation on cell $T_{i'}$, we get

$$\begin{aligned}I_1&=-\frac{\varepsilon}{\sigma_\mathrm{t}}\frac{1}{4\pi}\int_{\mathscr{S}'}\int_{\Gamma_{i'}}\mathrm{d}\gamma\,\mathrm{d}\vec{\Omega}(\vec{\Omega}\cdot\nabla\chi_{i'}^{l'})(\vec{\Omega}\cdot n)v^\varepsilon(\gamma,\vec{\Omega})\\&=-\frac{\varepsilon}{\sigma_\mathrm{t}}\frac{1}{4\pi}\int_{\vec{\Omega}\cdot\vec{n}<0}\int_{\Gamma_i^{i'}}\mathrm{d}\gamma\,\mathrm{d}\vec{\Omega}(\vec{\Omega}\cdot\nabla\chi_{i'}^{l'})(\vec{\Omega}\cdot n)\chi_i^l(\gamma)\\&\quad-\frac{\varepsilon}{\sigma_\mathrm{t}}\frac{1}{4\pi}\int_{\vec{\Omega}\cdot\vec{n}>0}\int_{\Gamma^{i'}-\Gamma_i^{i'}}\mathrm{d}\vec{\Omega}(\vec{\Omega}\cdot\nabla\chi_{i'}^{l'})(\vec{\Omega}\cdot n)\chi_i^l(\gamma-\vec{\Omega}l_{i'})\mathrm{e}^{-\frac{\sigma_\mathrm{t}}{\varepsilon}l_{i'}}.\end{aligned}$$

We can apply Lemma 1 to

$$\frac{1}{4\pi}\int_{\vec{\Omega}\cdot\vec{n}>0}\int_{\Gamma_{i'}-\Gamma_i^{i'}}\mathrm{d}\vec{\Omega}(\vec{\Omega}\cdot\nabla\chi_{i'}^{l'})(\vec{\Omega}\cdot n)\chi_i^l(\gamma-\vec{\Omega}l_{i'})\mathrm{e}^{-\frac{\sigma_\mathrm{t}}{\varepsilon}l_{i'}}$$

so that

$$I_1=-\frac{\varepsilon}{6\sigma_\mathrm{t}}\int_{\Gamma_i^{i'}}(\vec{n}\cdot\nabla\chi_{i'}^{l'})\chi_i^l(\gamma)+\mathrm{O}(\varepsilon^2).$$

Second integral writes as

$$I_2=-\frac{1}{4\pi}\int_{\mathscr{S}'}\mathrm{d}\vec{\Omega}(\vec{\Omega}\cdot\nabla\chi_{i'}^{l'})\langle w^\varepsilon\rangle,$$

where w^ε is solution of

$$\begin{cases}\vec{\Omega}\cdot\nabla w^\varepsilon+\frac{\sigma_\mathrm{t}}{\varepsilon}w^\varepsilon=0,\\ w^\varepsilon(x,\vec{\Omega})=\chi_i^l(x-\vec{\Omega}l_i)\mathrm{e}^{-\frac{\sigma_\mathrm{t}}{\varepsilon}l_i},\quad x\in\Gamma_i^{i'},\ \vec{\Omega}\cdot\vec{n}<0.\end{cases}\tag{41}$$

Integrating (41) on cell $T_{i'}$, we obtain, for direction Ω in $\mathscr{S}'$

$$\begin{aligned}I_2&=\frac{\varepsilon}{\sigma_\mathrm{t}}\frac{1}{4\pi}\int_{\vec{\Omega}\cdot\vec{n}<0}\int_{\Gamma_i^{i'}}\mathrm{d}\gamma\,\mathrm{d}\vec{\Omega}(\vec{\Omega}\cdot\nabla\chi_{i'}^{l'})\chi_i^l(\gamma-\vec{\Omega}l_i)\mathrm{e}^{-\frac{\sigma_\mathrm{t}}{\varepsilon}l_i}\mathrm{d}\gamma\\&\quad+\frac{\varepsilon}{\sigma_\mathrm{t}}\frac{1}{4\pi}\int_{\vec{\Omega}\cdot\vec{n}>0}\int_{\Gamma_{i'}-\Gamma_i^{i'}}\mathrm{d}\gamma\,\mathrm{d}\vec{\Omega}(\vec{\Omega}\cdot\nabla\chi_{i'}^{l'}\chi_i^l(\gamma-\vec{\Omega}(l_i+l_{i'}))\mathrm{e}^{-\frac{\sigma_\mathrm{t}}{\varepsilon}(l_i+l_{i'})}\,\mathrm{d}\gamma.\end{aligned}$$

So, using the lemma, $I_2=\frac{\varepsilon}{\sigma_\mathrm{t}}\mathrm{CT}(\varepsilon)=\mathrm{O}(\varepsilon^2)$. Since $\mathrm{e}^{-\frac{\sigma_\mathrm{t}}{\varepsilon}l_{i'}}$ goes to zero as ε goes to zero, we conclude immediately that $I_3=\mathrm{O}(\varepsilon^2)$. The fourth term is defined as

$$\begin{aligned}I_4&=-\frac{1}{4\pi}\int_{\vec{\Omega}\cdot\vec{n}<0}\int_{\Gamma_i^{i'}}\mathrm{d}\gamma\,\mathrm{d}\vec{\Omega}(\vec{\Omega}\cdot\vec{n})\chi_i^l(\gamma)\chi_{i'}^{l'}(\gamma)-\frac{1}{4\pi}\int_{\vec{\Omega}\cdot\vec{n}>0}\int_{\Gamma_{i'}-\Gamma_i^{i'}}\mathrm{d}\gamma\,\mathrm{d}\vec{\Omega}(\vec{\Omega}\cdot\vec{n})\chi_i^l(\gamma-\vec{\Omega}l_{i'})\chi_{i'}^{l'}(\gamma)\mathrm{e}^{-\frac{\sigma_\mathrm{t}}{\varepsilon}l_{i'}}\\&=\frac{1}{4}\int_{\Gamma_i^{i'}}\mathrm{d}\gamma\chi_i^l(\gamma)\chi_{i'}^{l'}(\gamma)-\frac{\varepsilon}{\sigma_\mathrm{t}}\Big(C_0\chi_i^l(\gamma_{i,i'}^0)\chi_{i'}^{l'}(\gamma_{i,i'}^0)+C_1\chi_i^l(\gamma_{i,i'}^1)\chi_{i'}^{l'}(\gamma_{i,i'}^1)\Big)+\mathrm{O}(\varepsilon^2),\end{aligned}$$

where $\gamma^0_{i,i'}$ and $\gamma^1_{i,i'}$ are the common vertices of T_i and $T_{i'}$ and C_0, C_1 two constant numbers. The fifth integral is defined as

$$
\begin{aligned}
I_5 = &\frac{1}{4\pi}\int_{\vec{\Omega}\cdot\vec{n}<0}\int_{\Gamma_i^{i'}} \mathrm{d}\gamma\,\mathrm{d}\vec{\Omega}(\vec{\Omega}\cdot\vec{n})\chi_i^l(\gamma-\vec{\Omega}l_i)\mathrm{e}^{-\frac{\sigma_t}{\varepsilon}l_i}\chi_{i'}^{l'}(\gamma)\\
&+\frac{1}{4\pi}\int_{\vec{\Omega}\cdot\vec{n}>0}\int_{\Gamma_{i'}-\Gamma_i^{i'}} \mathrm{d}\gamma\,\mathrm{d}\vec{\Omega}(\vec{\Omega}\cdot\vec{n})\chi_i^l(\gamma-\vec{\Omega}(l_{i'}+l_i))\chi_{i'}^{l'}(\gamma)\mathrm{e}^{-\frac{\sigma_t}{\varepsilon}(l_{i'}+l_i)}.
\end{aligned}
$$

The lemma applies to both parts and we deduce that

$$
I_5 = \frac{\varepsilon}{\sigma_t}\left(C_0'\chi_i^l(\gamma^0_{i,i'})\chi_{i'}^{l'}(\gamma^0_{i,i'}) + C_1'\chi_i^l(\gamma^1_{i,i'})\chi_{i'}^{l'}(\gamma^1_{i,i'})\right) + \mathrm{O}(\varepsilon^2).
$$

At last, we have, taking the limit in the integral

$$
\begin{aligned}
I_6 &= \frac{\varepsilon}{4\pi\sigma_t}\int_{\vec{\Omega}\cdot\vec{n}<0}\int_{\Gamma_i^{i'}} \mathrm{d}\gamma\,\mathrm{d}\vec{\Omega}(\vec{\Omega}\cdot\vec{n})(\vec{\Omega}\cdot\nabla\chi_i^l)\chi_{i'}^{l'}(\gamma) + \frac{\varepsilon}{4\pi\sigma_t}\int_{\vec{\Omega}\cdot\vec{n}>0}\int_{\Gamma_{i'}-\Gamma_i^{i'}} \mathrm{d}\gamma\,\mathrm{d}\vec{\Omega}(\vec{\Omega}\cdot\vec{n})(\vec{\Omega}\cdot\nabla\chi_i^l)\chi_{i'}^{l'}(\gamma)\mathrm{e}^{-\frac{\sigma_t}{\varepsilon}l_{i'}}\\
&= \frac{\varepsilon}{6\sigma_t}\int_{\Gamma_i^{i'}}(\vec{n}\cdot\nabla\chi_i^l)\chi_{i'}^{l'}(\gamma)\mathrm{d}\gamma + \mathrm{O}(\varepsilon^2).
\end{aligned}
$$

Putting all these expansions together, Eq. (40) becomes

$$
\begin{aligned}
\frac{\sigma_t}{\varepsilon}\langle\tilde{u}_i^{\varepsilon,l},\chi_{i'}^{l'}\rangle = &\frac{1}{4}\int_{\Gamma_i^{i'}}\mathrm{d}\gamma\chi_i^l(\gamma)\chi_{i'}^{l'}(\gamma) + \frac{\varepsilon}{\sigma_t}\left(-\frac{1}{6}\int_{\Gamma_i^{i'}}(\vec{n}\cdot\nabla\chi_{i'}^{l'})\chi_i^l(\gamma) + \frac{1}{6}\int_{\Gamma_i^{i'}}(\vec{n}\cdot\nabla\chi_i^l)\chi_{i'}^{l'}(\gamma)\right)\\
&-\frac{\varepsilon}{\sigma_t}\left(C_0\chi_i^l(\gamma^0_{i,i'})\chi_{i'}^{l'}(\gamma^0_{i,i'}) + C_1\chi_i^l(\gamma^1_{i,i'})\chi_{i'}^{l'}(\gamma^1_{i,i'})\right) + \mathrm{O}(\varepsilon^2).
\end{aligned}
$$

The matrix element is now given by

$$
\begin{aligned}
m_{i,i'}^{\varepsilon,l,l'} &= -\left(1-\varepsilon^2\frac{\sigma_a}{\sigma_t}\right)\frac{\sigma_t}{\varepsilon}\langle\tilde{u}_i^{\varepsilon,l},\chi_{i'}^{l'}\rangle\\
&= -\frac{1}{4}\int_{\Gamma_i^{i'}}\mathrm{d}\gamma\chi_i^l(\gamma)\chi_{i'}^{l'}(\gamma) - \frac{\varepsilon}{\sigma_t}\left(-\frac{1}{6}\int_{\Gamma_i^{i'}}(\vec{n}\cdot\nabla\chi_{i'}^{l'})\chi_i^l(\gamma) + \frac{1}{6}\int_{\Gamma_i^{i'}}(\vec{n}\cdot\nabla\chi_i^l)\chi_{i'}^{l'}(\gamma)\right)\\
&\quad-\frac{\varepsilon}{\sigma_t}\left(C_0\chi_i^l(\gamma^0_{i,i'})\chi_{i'}^{l'}(\gamma^0_{i,i'}) + C_1\chi_i^l(\gamma^1_{i,i'})\chi_{i'}^{l'}(\gamma^1_{i,i'})\right) + \mathrm{O}(\varepsilon^2).
\end{aligned}
\tag{42}
$$

(3) $i \neq i'$ and cells T_i and $T_{i'}$ have no common vertex.

It is easy to see that $a^{\epsilon}_{i,i'}$ is exponentially decaying with respect to $\frac{1}{\varepsilon}$ so that we can neglect these contributions to the linear system.

(4) $i \neq i'$ and cells T_i and $T_{i'}$ have a common vertex $\gamma_i^{i'}$ but no common edge. Then $a_{i,i'}^{\varepsilon,l,l'}$ itself is a corner term. Suppose for example that a cell T_j is adjacent to T_i and $T_{i'}$, then, for $x \in T_{i'}$, we have

$$
u_i^{\varepsilon,l}(x,\vec{\Omega}) = \mathrm{e}^{-\frac{\sigma_t}{\varepsilon}l_{i'}}\mathrm{e}^{-\frac{\sigma_t}{\varepsilon}l_j}\left(\chi_i^l(x-\vec{\Omega}(l_{i'}+l_j)) - \chi_i^l(x-\vec{\Omega}(l_{i'}+l_j+l_i))\mathrm{e}^{-\frac{\sigma_t}{\varepsilon}l_i} - \frac{\varepsilon}{\sigma_t}\vec{\Omega}\cdot\nabla\chi_i^l(1-\mathrm{e}^{-\frac{\sigma_t}{\varepsilon}l_i})\right).
$$

In this case $a_{i,i'}^{\varepsilon,l,l'}$ is a corner term corresponding to particles emitted in T_i, crossing a distance $l_j = l_j(x,\vec{\Omega})$ in T_j and a distance then $l_{i'} = l_{i'}(x,\vec{\Omega})$ in $T_{i'}$ (Fig. 3). It is easy to see, using Lemma 1, that

$$
a_{i,i'}^{\varepsilon,l,l'} \sim \frac{\varepsilon}{\sigma_t}C\chi_i^l(\gamma_i^{l'})\chi_{i'}^{l'}(\gamma_i^{l'}).
$$

Finally, neglecting the terms of order ε^2, the linear system for $\phi_i^{\varepsilon,l}$ writes as

$$\begin{aligned}
&\sum_{l'}\left(\frac{1}{4}\int_{\Gamma_i}\mathrm{d}\gamma\chi_i^l(\gamma)\chi_i^{l'}(\gamma)+\varepsilon\sigma_\mathrm{a}\langle\chi_i^l,\chi_i^{l'}\rangle-\frac{\varepsilon}{\sigma_\mathrm{t}}\sum_{k=1}^{3}C_k\chi_i^l(\gamma_i^k)\chi_i^{l'}(\gamma_i^k)\right)\phi_i^{\varepsilon,l'}\\
&\quad+\sum_{\Gamma_i^{i'},l'}\left(-\frac{1}{4}\int_{\Gamma_i^{i'}}\mathrm{d}\gamma\chi_i^l(\gamma)\chi_{i'}^{l'}(\gamma)-\frac{\varepsilon}{\sigma_\mathrm{t}}\left(\frac{1}{6}\int_{\Gamma_i^{i'}}(\vec{n}\cdot\nabla\chi_{i'}^{l'})\chi_i^l(\gamma)-\frac{1}{6}\int_{\Gamma_i^{i'}}(\vec{n}\cdot\nabla\chi_i^l)\chi_{i'}^{l'}(\gamma)\right)\right)\phi_{i'}^{\varepsilon,l'}\\
&\quad+\frac{\varepsilon}{\sigma_\mathrm{t}}\sum_{\gamma_{i,i''},l'}C_i^{i''}\chi_i^l(\gamma_{i,i''})\chi_{i''}^{l'}(\gamma_{i,i''})\phi_{i''}^{\varepsilon,l'}=\varepsilon\langle Q,\chi_i^l\rangle,
\end{aligned}\tag{43}$$

where $\sum_{\Gamma_i^{i'},l'}$ stands for the sum over common edges $\Gamma_i^{i'}$ of cells T_i and $T_{i'}$ and $\sum_{\gamma_{i,i''},l'}$ stands for the sum over common vertices between cells T_i and $T_{i''}$. We now introduce the following formal expansion

$$\begin{aligned}
&\Phi^\varepsilon=\Phi^0+\varepsilon\Phi^1+\varepsilon^2\Phi^2+\cdots,\\
&\phi_i^{\varepsilon,l}=\phi_i^{0,l}+\varepsilon\phi_i^{1,l}+\varepsilon^2\phi_i^{2,l}+\cdots\quad\forall i\in(1,N),\ \forall l.
\end{aligned}$$

At the lowest order we obtain

$$\sum_{l'}\frac{1}{4}\int_{\Gamma_i}\mathrm{d}\gamma\chi_i^l(\gamma)\chi_i^{l'}(\gamma)\phi_i^{0,l'}-\sum_{\Gamma_i^{i'},l'}\frac{1}{4}\int_{\Gamma_i^{i'}}\mathrm{d}\gamma\chi_i^l(\gamma)\chi_{i'}^{l'}(\gamma)\phi_{i'}^{0,l'}=0.\tag{44}$$

The solutions of this linear system are given by vectors ϕ_i^l corresponding to continuous functions, i.e. vectors such that $\phi_i^{0,l}=\phi_{i'}^{0,l'}$ when $\gamma_i^l=\gamma_{i'}^{l'}$. These vectors obviously satisfy system (44) since

$$\begin{aligned}
\int_{\Gamma_i}\mathrm{d}\gamma\chi_i^l(\gamma)\chi_i^{l'}(\gamma)&=\sum_{i'}\int_{\Gamma_i^{i'}}\mathrm{d}\gamma\chi_i^l(\gamma)\chi_i^{l'}(\gamma)\\
&=\sum_{i'}\int_{\Gamma_i^{i'}}\mathrm{d}\gamma\chi_i^l(\gamma)\chi_{i'}^{l'}(\gamma)
\end{aligned}$$

because $\chi_i^{l'}(\gamma)=\chi_{i'}^{l'}$ on $\Gamma_i^{i'}$. It also proves that ϕ_i^l is in the interior convex set of $\phi_{i'}^{l'}$ hence that all these values are equal.

At order ε we have

$$\begin{aligned}
&\sum_{l'}\frac{1}{4}\int_{\Gamma_i}\mathrm{d}\gamma\chi_i^l(\gamma)\chi_i^{l'}(\gamma)\phi_i^{1,l'}-\sum_{\Gamma_i^{i'},l'}\frac{1}{4}\int_{\Gamma_i^{i'}}\mathrm{d}\gamma\chi_i^l(\gamma)\chi_{i'}^{l'}(\gamma)\phi_{i'}^{1,l'}\\
&\quad=-\sigma_\mathrm{a}\sum_{l'}\langle\chi_i^l,\chi_i^{l'}\rangle\phi_i^{0,l'}-\frac{1}{6\sigma_\mathrm{t}}\sum_{\Gamma_i^{i'},l'}\left(-\int_{\Gamma_i^{i'}}(\vec{n}\cdot\nabla\chi_{i'}^{l'})\chi_i^l(\gamma)+\int_{\Gamma_i^{i'}}(\vec{n}\cdot\nabla\chi_i^l)\chi_{i'}^{l'}(\gamma)\right)\phi_{i'}^{0,l'}\\
&\quad\quad-\frac{1}{\sigma_\mathrm{t}}\sum_{\gamma_{i,i''}}C_i^{i''}\chi_i^l(\gamma_{i,i''})\chi_{i''}^{l'}(\gamma_{i,i''})\phi_{i''}^{0,l'}+\langle Q,\chi_i^l\rangle.
\end{aligned}$$

This system can be split into two systems

$$\begin{cases}
\sum_{l'}\frac{1}{4}\int_{\Gamma_i}\mathrm{d}\gamma\chi_i^l(\gamma)\chi_i^{l'}(\gamma)\phi_i^{1,l'}-\sum_{\Gamma_i^{i'},l'}\frac{1}{4}\int_{\Gamma_i^{i'}}\mathrm{d}\gamma\chi_i^l(\gamma)\chi_{i'}^{l'}(\gamma)\phi_{i'}^{1,l'}=0\\
\sigma_\mathrm{a}\sum_{l'}\langle\chi_i^l,\chi_i^{l'}\rangle\phi_i^{0,l'}+\frac{1}{6\sigma_\mathrm{t}}\sum_{\Gamma_i^{i'},l'}\left(-\int_{\Gamma_i^{i'}}(\vec{n}\cdot\nabla\chi_{i'}^{l'})\chi_i^l(\gamma)+\int_{\Gamma_i^{i'}}(\vec{n}\cdot\nabla\chi_i^l)\chi_{i'}^{l'}(\gamma)\right)\phi_{i'}^{0,l'}\\
+\frac{1}{\sigma_\mathrm{t}}\sum_{\gamma_{i,i''}}C_i^{i''}\chi_i^l(\gamma_{i,i''})\chi_{i''}^{l'}(\gamma_{i,i''})\phi_{i''}^{0,l'}=\langle Q,\chi_i^l\rangle.
\end{cases}\tag{45}$$

The first equation implies that Φ^1 is continuous (i.e. $\phi_i^{1,l} = \phi_{i'}^{1,l'}$ when $\gamma_i^l = \gamma_{i'}^{l'}$). The second equation will provide a consistent discretization of the diffusion equation. For a given vertex γ_j we add all the equations coming from cells i sharing vertex γ_j. For i, l such that $\gamma_i^l = \gamma_j$, we denote

$$\bar{\phi}_j = \bar{\phi}_{\gamma_j} = \phi_i^{0,l} \quad \text{and} \quad \xi_j = \xi_{\gamma_j} = \sum_{\gamma_i^l = \gamma_j} \chi_i^l.$$

We obtain

$$\sigma_{\mathrm{a}} \sum_{l', \gamma_i^l = \gamma_j} \langle \chi_i^l, \chi_i^{l'} \rangle \phi_i^{0,l'} + \frac{1}{6\sigma_{\mathrm{t}}} \sum_{\Gamma_i^{i'}, l', \gamma_i^l = \gamma_j} \left(- \int_{\Gamma_i^{i'}} (\vec{n} \cdot \nabla \chi_{i'}^{l'}) \chi_i^l(\gamma) + \int_{\Gamma_i^{i'}} (\vec{n} \cdot \nabla \chi_i^l) \chi_{i'}^{l'}(\gamma) \right) \phi_{i'}^{0,l'}$$
$$+ \frac{1}{\sigma_t} \sum_{\gamma_{i,i'} = \gamma_{j'}, \gamma_i^l = \gamma_j} C_i^{i'} \chi_i^l(\gamma_{i,i'}) \chi_{i'}^{l'}(\gamma_{i,i'}) \phi_{i'}^{0,l'} = \sum_{\gamma_i^l = \gamma_j} \langle Q, \chi_i^l \rangle.$$

In these sums index j is fixed and other indices l, l', i, i' and i'' take all possible values. We denote, respectively, by S_1, S_2, S_3 and S_4 these four sums. We have for the first sum

$$S_1 = \sigma_{\mathrm{a}} \sum_{l'} \langle \xi_j, \chi_i^{l'} \rangle \phi_i^{0,l'}.$$

The range of index l' corresponds to all vertices $\gamma_i^{l'}$ that are connected to γ_j so that finally

$$S_1 = \sigma_{\mathrm{a}} \sum_{\gamma_{j'}} \langle \xi_j, \xi_{j'} \rangle \bar{\phi}_{j'}.$$

Integration over edges can be separated into three parts (Fig. 4):

- The first part corresponds to indices l' such that $\gamma_i^l = \gamma_j,\ \gamma_{i'}^{l'} = \gamma_{j'},\ \Gamma_i^{i'} = \overrightarrow{\gamma_j \gamma_{j'}}$. In this case, the triangles i and i' have the edge $\overrightarrow{\gamma_j \gamma_{j'}}$ in common.
- The second part corresponds to indices l' such that $\gamma_i^l = \gamma_j, \gamma_{i'}^{l'} = \gamma_{j'}, \Gamma_i^{i'} \neq \overrightarrow{\gamma_j \gamma_{j'}}$ and there exists a vertex $\gamma_{j''}$ such that $\Gamma_i^{i'} = \overrightarrow{\gamma_{j''} \gamma_{j'}}$. In this case, the edge $\overrightarrow{\gamma_j \gamma_{j'}}$ belongs to i but not to i'.
- The third part corresponds to indices l' such that $\gamma_i^l = \gamma_j, \gamma_{i'}^{l'} = \gamma_{j'}, \Gamma_i^{i'} \neq \overrightarrow{\gamma_j \gamma_{j'}}$ and there exists a vertex $\gamma_{j'''}$ such that $\Gamma_i^{i'} = \overrightarrow{\gamma_j \gamma_{j'''}}$. In this case, the edge $\overrightarrow{\gamma_j \gamma_{j'}}$ belongs to i' but not to i.

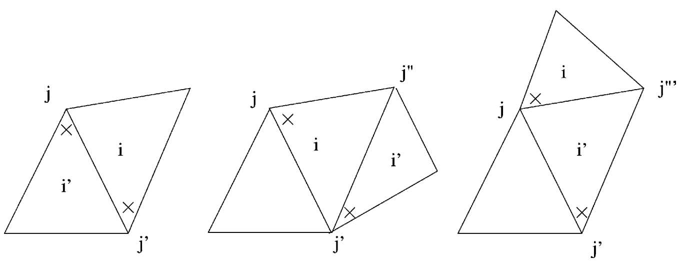

Fig. 4.

We have

$$S_2 = \frac{1}{6\sigma_t} \sum_{\gamma_{i'}^{l'}=\gamma_{j'},\gamma_i^l=\gamma_j} \left(-\int_{\overrightarrow{\gamma_j\gamma_{j'}}} (\vec{n}\cdot\nabla\chi_{i'}^{l'})\chi_i^l(\gamma) + \int_{\overrightarrow{\gamma_j\gamma_{j'}}} (\vec{n}\cdot\nabla\chi_i^l)\chi_{i'}^{l'}(\gamma) \right)\bar{\phi}_{j'}$$

(where i and i' are cells with common vertices γ_j and $\gamma_{j'}$ including the case $\gamma_j = \gamma_{j'}$)

$$+\frac{1}{6\sigma_t} \sum_{\gamma_{i'}^{l'}=\gamma_{j'},\gamma_i^l=\gamma_j} \left(-\int_{\overrightarrow{\gamma_{j''}\gamma_{j'}}} (\vec{n}\cdot\nabla\chi_{i'}^{l'})\chi_i^l(\gamma) + \int_{\overrightarrow{\gamma_{j''}\gamma_{j'}}} (\vec{n}\cdot\nabla\chi_i^l)\chi_{i'}^{l'}(\gamma) \right)\bar{\phi}_{j'}$$

(where i and i' are cells with common vertices $\gamma_{j''}$ and $\gamma_{j'}$)

$$+\frac{1}{6\sigma_t} \sum_{\gamma_{i'}^{l'}=\gamma_{j'},\gamma_i^l=\gamma_j} \left(-\int_{\overrightarrow{\gamma_{j'''}\gamma_{j}}} (\vec{n}\cdot\nabla\chi_{i'}^{l'})\chi_i^l(\gamma) + \int_{\overrightarrow{\gamma_{j'''}\gamma_{j}}} (\vec{n}\cdot\nabla\chi_i^l)\chi_{i'}^{l'}(\gamma) \right)\bar{\phi}_{j'}$$

(where i and i' are cells with common vertices $\gamma_{j'''}$ and γ_j).

We remark that $\chi_i^l = 0$ on $\overrightarrow{\gamma_{j''}\gamma_{j'}}$ and $\chi_{i'}^{l'} = 0$ on $\overrightarrow{\gamma_{j'''}\gamma_j}$. So we finally have

$$\begin{aligned} S_2 = {} & \frac{1}{6\sigma_t} \sum_{\gamma_{i'}^{l'}=\gamma_{j'},\gamma_i^l=\gamma_j} \left(-\int_{\overrightarrow{\gamma_j\gamma_{j'}}} (\vec{n}_i\cdot\nabla\chi_{i'}^{l'})\chi_i^l(\gamma) + \int_{\overrightarrow{\gamma_j\gamma_{j'}}} (\vec{n}_i\cdot\nabla\chi_i^l)\chi_{i'}^{l'}(\gamma) \right)\bar{\phi}_{j'} \\ & + \frac{1}{6\sigma_t} \sum_{\gamma_{i'}^{l'}=\gamma_{j'},\gamma_i^l=\gamma_j} \int_{\overrightarrow{\gamma_{j''}\gamma_{j'}}} (\vec{n}_i\cdot\nabla\chi_i^l)\chi_{i'}^{l'}(\gamma)\bar{\phi}_{j'} - \frac{1}{6\sigma_t} \sum_{\gamma_{i'}^{l'}=\gamma_{j'},\gamma_i^l=\gamma_j} \int_{\overrightarrow{\gamma_{j'''}\gamma_{j}}} (\vec{n}_i\cdot\nabla\chi_{i'}^{l'})\chi_i^l(\gamma)\bar{\phi}_{j'}, \end{aligned} \tag{46}$$

where index i on $\vec{n}_i$ reminds that n_i is exterior to cell T_i. We can identify $\langle\nabla\xi_j\cdot\nabla\xi_{j'}\rangle$ in this sum. For j' fixed ($j' \neq j$), we have

$$\langle\nabla\xi_j\cdot\nabla\xi_{j'}\rangle = \int_{T_i} \nabla\xi_j\cdot\nabla\xi_{j'}\,\mathrm{d}x + \int_{T_{i'}} \nabla\xi_j\cdot\nabla\xi_{j'}\,\mathrm{d}x,$$

where T_i is the cell $(\gamma_j, \gamma_{j'}, \gamma_{j''})$ and $T_{i'}$ is the cell $(\gamma_j, \gamma_{j'}, \gamma_{j'''})$. We have, for $\gamma_i^l = \gamma_j$ and $\gamma_i^{l'} = \gamma_j$

$$\begin{aligned} \int_{T_i} \nabla\xi_j\cdot\nabla\xi_{j'}\,\mathrm{d}x = {} & \frac{1}{2}\left(\int_{\overrightarrow{\gamma_j\gamma_{j'}}} (\vec{n}_i\cdot\nabla\chi_i^l)\chi_i^{l'}\mathrm{d}\gamma + \int_{\overrightarrow{\gamma_{j'}\gamma_{j''}}} (\vec{n}_i\cdot\nabla\chi_i^l)\chi_i^{l'}\mathrm{d}\gamma + \int_{\overrightarrow{\gamma_j\gamma_{j''}}} (\vec{n}_i\cdot\nabla\chi_i^l)\chi_i^{l'}\mathrm{d}\gamma \right) \\ & + \frac{1}{2}\left(\int_{\overrightarrow{\gamma_j\gamma_{j'}}} (\vec{n}_i\cdot\nabla\chi_i^{l'})\chi_i^l\mathrm{d}\gamma + \int_{\overrightarrow{\gamma_{j'}\gamma_{j''}}} (\vec{n}_i\cdot\nabla\chi_i^{l'})\chi_i^l\mathrm{d}\gamma + \int_{\overrightarrow{\gamma_j\gamma_{j''}}} (\vec{n}_i\cdot\nabla\chi_i^{l'})\chi_i^l\mathrm{d}\gamma \right). \end{aligned}$$

On $\overrightarrow{\gamma_j\gamma_{j''}}$, we have $\chi_i^{l'} = 0$, on $\overrightarrow{\gamma_j\gamma_{j'}}$, we have $\chi_i^{l'} = \chi_{i'}^{l'}$ and on $\overrightarrow{\gamma_{j'}\gamma_{j''}}$ we have $\chi_i^l = 0$ so

$$\begin{aligned} \int_{T_i} \nabla\xi_j\cdot\nabla\xi_{j'}\,\mathrm{d}x = {} & \frac{1}{2}\left(\int_{\overrightarrow{\gamma_j\gamma_{j'}}} (\vec{n}_i\cdot\nabla\chi_i^l)\chi_{i'}^{l'}\mathrm{d}\gamma + \int_{\overrightarrow{\gamma_{j'}\gamma_{j''}}} (\vec{n}_i\cdot\nabla\chi_i^l)\chi_i^{l'}\mathrm{d}\gamma \right) \\ & + \frac{1}{2}\left(\int_{\overrightarrow{\gamma_j\gamma_{j'}}} (\vec{n}_i\cdot\nabla\chi_i^{l'})\chi_{i'}^l\mathrm{d}\gamma + \int_{\overrightarrow{\gamma_j\gamma_{j''}}} (\vec{n}_i\cdot\nabla\chi_i^{l'})\chi_i^l\mathrm{d}\gamma \right). \end{aligned}$$

Similarly,

$$\int_{T_{i'}} \nabla\xi_j \cdot \nabla\xi_{j'}\, \mathrm{d}x = \frac{1}{2}\left(\int_{\overrightarrow{\gamma_j\gamma_{j'}}} (\vec{n}_{i'}\cdot\nabla\chi^l_{i'})\chi^{l'}_i \mathrm{d}\gamma + \int_{\overrightarrow{\gamma_{j'}\gamma_{j'''}}} (\vec{n}_{i'}\cdot\nabla\chi^l_{i'})\chi^{l'}_{i'}\mathrm{d}\gamma\right) + \frac{1}{2}\left(\int_{\overrightarrow{\gamma_j\gamma_{j'}}} (\vec{n}_{i'}\cdot\nabla\chi^{l'}_{i'})\chi^l_i \mathrm{d}\gamma + \int_{\overrightarrow{\gamma_j\gamma_{j'''}}} (\vec{n}_{i'}\cdot\nabla\chi^{l'}_{i'})\chi^l_{i'}\mathrm{d}\gamma\right).$$

Noticing that $\vec{n}_{i'} = -\vec{n}_i$ on $\overrightarrow{\gamma_j\gamma_{j'}}$, we put this expression into (46) and we obtain

$$S_2 = \frac{1}{3\sigma_t}\sum_{j'}\langle\nabla\xi_j\cdot\nabla\xi_{j'}\rangle\bar{\phi}j'.$$

The sum S_3 contains corner terms (we recall that these terms only appear in the two-dimensional case). To avoid lengthy calculations, we will only give a heuristic argument why they vanish. When adding all the contributions coming from a given vertex, due to the continuity of Φ^0 at vertices and the fact that $\chi^l_i(\gamma_j) = 1$ or 0, we find that

$$S_3 = \sum_{\gamma_{i,i'}=\gamma_{j'},\gamma^l_i=\gamma_j} C^{i'}_i\chi^l_i(\gamma_{i,i'})\chi^{l'}_{i'}(\gamma_{i,i'})\bar{\phi}_{j'} = \left(\sum_{\gamma_{i,i'}=\gamma_j} C^{i'}_i\right)\bar{\phi}_j.$$

Using Lemma 1, we are reduced to make a sum of the form

$$S = \sum_{i,i'}\int_{\mathscr{S}^{i'}_i}\frac{\vec{n}_i\cdot\vec{\Omega}}{C^{i'}_i(\vec{\Omega})}\,\mathrm{d}\vec{\Omega}.$$

When performing the sum over all cells (i,i') sharing vertex γ_j, the integration takes place over all sphere $\mathscr{S}_2$ and S vanishes.

Finally, we have immediately $S_4 = \langle Q,\xi_j\rangle$ and Φ^0 satisfies

$$\sigma_a\sum_{j'}\langle\xi_j,\xi_{j'}\rangle\bar{\phi}_{j'} + \frac{1}{3\sigma_t}\sum_{j'}\langle\nabla\xi_j\cdot\nabla\xi_{j'}\rangle\bar{\phi}_{j'} = \langle Q,\xi_j\rangle.$$

As $u^\varepsilon = \Phi^\varepsilon + \mathrm{O}(\varepsilon^2)$, this ends the proof. □

3.3. Boundary conditions for linear SIMC

So far, we have only considered zero boundary conditions. We should now extend previous results to arbitrary incoming fluxes. Actually it is not possible to perform a complete analysis and we have only obtained partial results. We describe now these results without proofs:

3.3.1. One-dimensional case

- If $\sigma_a = 0$, we obtain a correct discretization of the diffusion equation with Dirichlet boundary condition

$$\tilde{\phi}_0 = \int_0^1\left(\mu + \frac{3}{2}\mu^2\right)g(0,\mu)\,\mathrm{d}\mu \sim \int_0^1\frac{\sqrt{3}}{2}\mu H(\mu)g(0,\mu)\,\mathrm{d}\mu,$$

where $H(\mu)$ is the Chandrasekhar function. This is the case for radiative transfer problems.

- If $\sigma_a \neq 0$, we do not get the exact boundary condition: it would be necessary to lump some terms in the Monte-Carlo matrix.

3.3.2. Multidimensional case

In the simplest case where the incoming flux g is an isotropic function and g is continuous and piecewise linear on the boundary, we obtain the correct Dirichlet condition. In the most general case (i.e. non isotropic incoming flux), it does not seem possible to state a general result.

3.4. Choice of the basis functions

In the view of the asymptotic analysis, we have seen that the solution becomes continuous in the diffusion limit. Hence, we could use linear continuous basis function instead of a discontinuous one and obtain the same result. The benefit would be a smaller linear system and a reduced computational cost. However, in the general case, there is no reason to assume continuity of the solution and a discontinuous basis function is required as it is in deterministic transport methods.

4. Numerical results

4.1. ε problem test case

We first confirm the theoretical results presented in previous section. We consider the following pure scattering problem in one dimension:

$$\begin{cases} \mu\frac{\partial u^\varepsilon}{\partial x}+\frac{1}{\varepsilon}u^\varepsilon=\frac{1}{\varepsilon}\tilde{u}^\varepsilon+\varepsilon, & x\in(0,10),\ \mu\in(-1,1),\\ u^\varepsilon(0,\mu)=0 \quad \text{for } \mu>0, & u^\varepsilon(10,\mu)=0 \quad \text{for } \mu<0. \end{cases} \tag{47}$$

As ϵ goes to zero, we know that $\tilde{u}^\varepsilon$ tends to the solution U of the diffusion equation:

$$\begin{cases} -\frac{1}{3}\frac{\mathrm{d}^2U}{\mathrm{d}x^2}=1,\\ U(0)=0, \quad U(10)=0. \end{cases} \tag{48}$$

i.e. $U(x)=15x-(3/2)x^2$.

First, we compare the solutions for linear and constant SIMC with the exact solution of the diffusion equation in one-dimensional geometry. The mesh is composed of 100 cells of size $\Delta x=1$. We set $\varepsilon=0.01$ so that the optical depth of each cell is 10: this is large enough to apply the theoretical results.

In Fig. 5, we represent solution for constant SIMC, solution of the diffusion (48) and solution of the wrong diffusion limit problem

$$\begin{cases} -\frac{\mathrm{d}^2V^\varepsilon}{\mathrm{d}x^2}=\frac{4\varepsilon}{\Delta x},\\ V(0)=0, \quad V(10)=0. \end{cases} \tag{49}$$

As long as $\Delta x/\varepsilon$ is large enough, we observe that the Constant SIMC solution is much closer to V^ε than to U: this confirms the theoretical results.

In Fig. 6, we represent the linear SIMC solution and U: The agreement between the linear SIMC and U is correct but we observe fluctuations despite the large number of particles emitted in each cell (500,000): this is related to the difficulty of calculating the coefficients of the matrix accurately with a random choice. When performing the asymptotic analysis, we found that diffusion-like scheme appeared at order ε and that terms of order ε^{-1} and order ε^0 cancel. In the Monte-Carlo simulation, these terms cannot cancel exactly

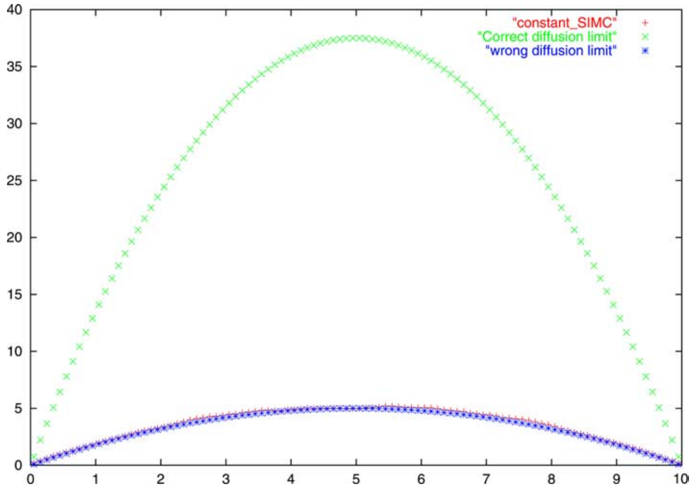

Fig. 5. Solution of constant SIMC, correct limiting diffusion solution, wrong limiting diffusion equation.

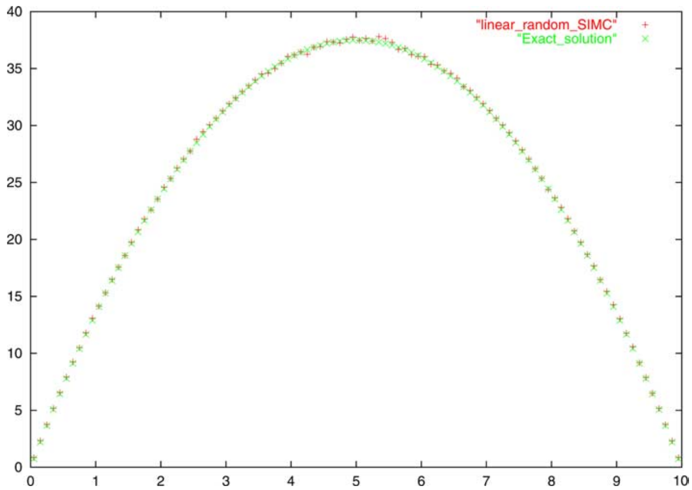

Fig. 6. Solution of linear SIMC and limiting diffusion solution.

and there is some remaining Monte-Carlo fluctuation which has to be of an order smaller than ε to obtain the diffusion solution. These fluctuations could be reduced by using adapted sampling of the emitted Monte-Carlo particles in each cell, for example we could sample Monte-Carlo particles for each basis function instead of each cell and use biasing of the position. Anyway, it would not be sufficient for very diffusive problems. Although the problem is one-dimensional, we can solve it on a two-dimensional triangular mesh $(x, y) \in (0, 10) \times (0, h)$ with symmetric boundary conditions for $y = 0$ and $y = h$. We took $h = \Delta x$ so that the aspect ratio of each triangle is of order 1. Results are displayed in Fig. 7: as expected from the theoretical analysis Constant SIMC results are wrong whereas Linear SIMC results are correct. We observe however larger fluctuations than for one-dimensional geometry.

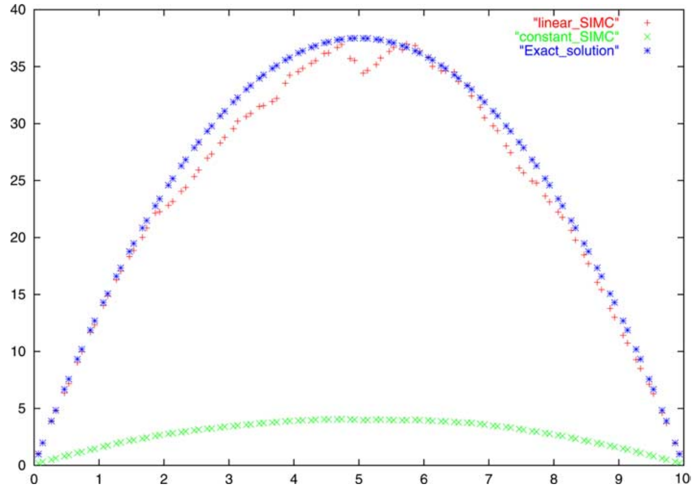

Fig. 7. Solution of linear SIMC, constant SIMC and limiting diffusion solution for two-dimensional mesh.

4.2. Larsen test case

This problem is presented in [7]. We solve

$$\begin{cases} \mu \frac{\partial u}{\partial x} + \sigma_t u = \sigma_s \tilde{u}, \quad x \in (0, 11), \ \mu \in (-1, 1), \\ u(0, \mu) = 1 \quad \text{for } \mu > 0, \quad u(11, \mu) = 0 \quad \text{for } \mu < 0, \\ \sigma_t = 2, \quad \sigma_s = 0, \ 0 \leqslant x < 1, \\ \sigma_t = 100, \quad \sigma_s = 100, \ 1 \leqslant x < 11. \end{cases} \tag{50}$$

First region $0 < x < 1$ is purely absorbing with a moderate absorption coefficient whereas second region $1 < x < 11$ is purely scattering with a large scattering coefficient. Hence particles coming from the left boundary do not suffer any scattering in the first region $x \in (0, 1)$ and their distribution becomes anisotropic at the interface $x = 1$. A boundary layer results at the interface between the two regions. There is no analytic solution to this problem so we used, as a reference, the solution given by a DSN calculation S16 on a very fine mesh.

Fig. 8 compares the reference solution with the solutions given by the linear SIMC method and the constant SIMC solution on a crude mesh (10 cells of size $\Delta x = 0.1$ for $0 < x < 1$ and 10 cells of size $\Delta x = 1$ for $1 < x < 11$). The results show that the linear SIMC method is very accurate in presence of a not resolved boundary layer except in the first cell in the opaque medium. The constant SIMC result is not as much accurate. This is not surprising since we have found that the anisotropy of the incident intensity in the opaque medium is not taken into account with this method.

With the constant SIMC method, the incident current ($\int_0^1 \mu u(1, \mu)\, \mathrm{d}\mu$) in the opaque medium determines entirely the value of $\tilde{u}$ inside the opaque medium.

4.3. Problems with non-isotropic incident flux

We solve

$$\begin{cases} \mu \frac{\partial u}{\partial x} + 100u = 100\tilde{u}, \quad x \in (0, 1), \ \mu \in (-1, 1), \\ u(0, \mu) = g(\mu) \quad \text{for } \mu > 0, \quad u(1, \mu) = 0 \quad \text{for } \mu < 0. \end{cases} \tag{51}$$

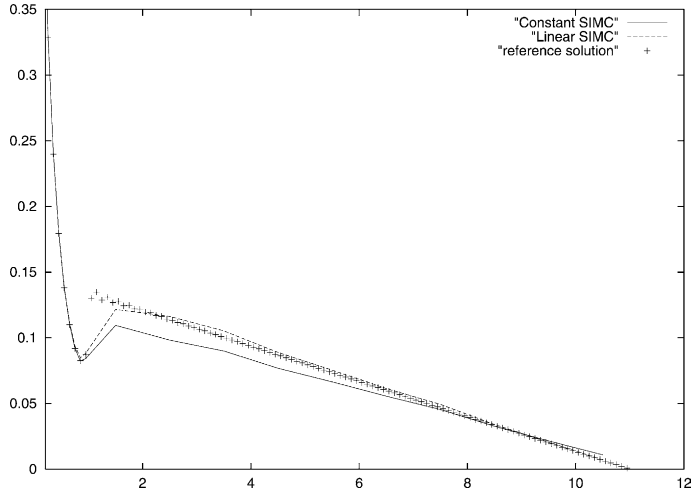

Fig. 8. Comparison between linear and constant SIMC solutions and reference solution.

The left boundary $\mu \mapsto g(\mu)$ condition is an anisotropic incident intensity:

- In the first case, it is an almost normal intensity (see Fig. 9)

$$g_l(\mu) = \delta(\mu - 1).$$

- In the second case, it is an almost grazing incident intensity (see Fig. 10)

$$g_l(\mu) = \delta(\mu - 1/100).$$

In the two cases, $g_l(\mu)$ is normalized so that $\int_0^1 \mu g_l(\mu)\, d\mu = 0.5$ is kept constant.

With these two cases, we want to verify our analysis of the boundary conditions in an opaque medium for the linear SIMC and the constant SIMC methods:

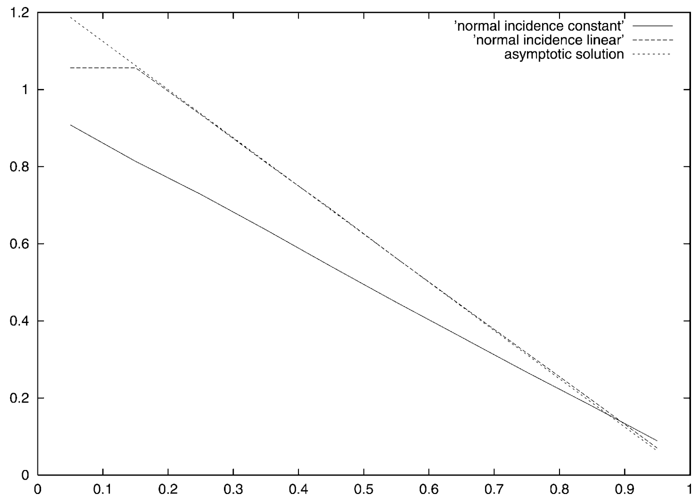

Fig. 9. Normal incident intensity problem, comparison between SIMC (linear and constant) and asymptotic one.

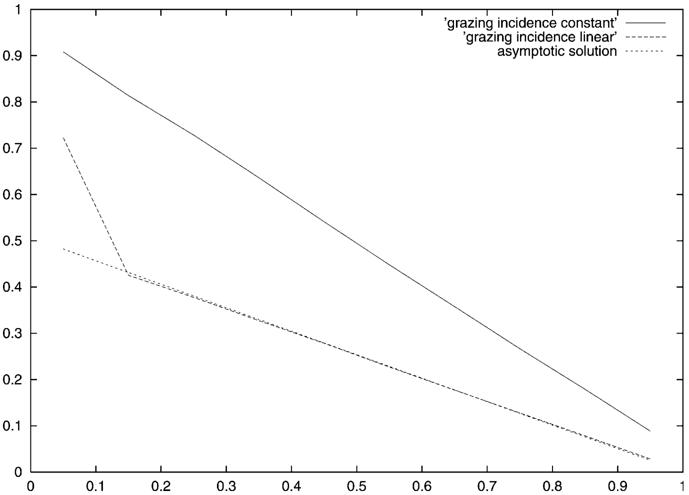

Fig. 10. Grazing incident intensity problem, comparison between SIMC (linear and constant) and asymptotic one.

- The linear SIMC method yields a very accurate boundary condition even if the boundary layer is unresolved $\Phi(0) = \int_0^1 (\mu + (3/2)\mu^2) g_l(\mu)\,\mathrm{d}\mu$.
- The constant SIMC method is accurate only if the medium is meshed at the mean free path scale. If the boundary layer is not resolved, the boundary condition is $\Phi(0) = \int_0^1 2\mu g_l(\mu)\,\mathrm{d}\mu$ that is $\Phi(0) = 1$.

We compare the SIMC results obtained on a crude mesh (10 cells between 0 and 1, optical thickness per cell 10) with the reference results given by the asymptotic diffusion equation: it is a linear function taking the values $y = 0$ at $x = 1$ and $y = \int_0^1 (\sqrt{3}/2)\mu H(\mu) g(0,\mu)\,\mathrm{d}\mu$ at $x = 0$ (it gives approximately the values $y = 1.25$ for the normal incidence case and $y = 0.5075$ for the grazing incidence case).

4.4. Error analysis

We wish now to discuss the benefits of linear SIMC versus constant SIMC in a transparent medium. In this case, away from the diffusion limit, constant SIMC is simply less accurate than linear SIMC due to the constant representation of the solution. We study the convergence of the method on a non-diffusive problem when the mesh size goes to zero.

We solve

$$\begin{cases} \mu \frac{\partial u}{\partial x} + \sigma_t u = \sigma_s \tilde{u} + Q(x), & x \in (0,1),\ \mu \in (-1,1), \\ u(0,\mu) = 0 \quad \text{for } \mu > 0, & u(1,\mu) = 0 \text{ for } \mu < 0, \\ \sigma_t = 14, \quad \sigma_s = 4, & 0 \leqslant x < 0.5, \\ \sigma_t = 1, \quad \sigma_s = 1, & 0.5 \leqslant x < 1 \\ Q(x) = 10 \quad \text{for } x \in (0.4, 0.6). \end{cases} \tag{52}$$

The problem is solved on a two-dimensional mesh with symmetric boundary conditions for $y = 0$ and $y = \Delta x$. The mesh size Δx varies from 0.1 to 0.0125. At each time the mesh size is divided by 2, we also multiply by 4 the number of particles tracked so that we keep the error due to Monte-Carlo fluctuations lower than the error due to spatial discretization (number of particles is set to 10^7 for $\Delta x = 0.1$). The reference solution is given by a DSN calculation on a very fine mesh. Fig. 11 compares the linear and constant SIMC solutions on the crudest mesh with the reference solution.

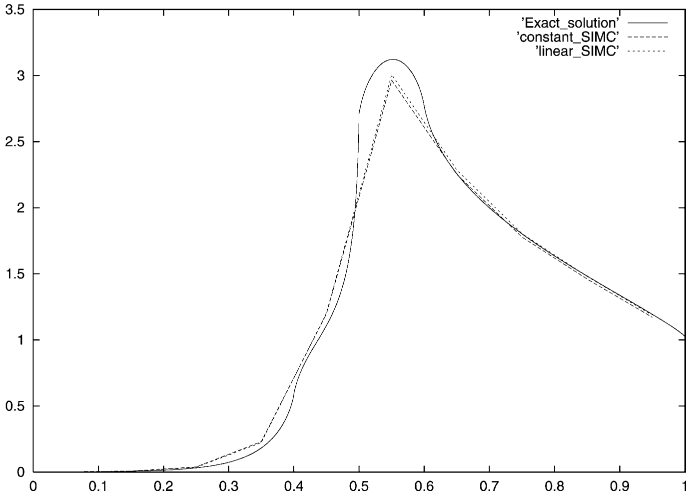

Fig. 11. Linear and constant SIMC, reference solution.

We now represent the L_1 error between SIMC solution and reference solution as a function of the mesh size (Fig. 12). We observe that the error goes to zero as the mesh size diminishes and that it is smaller for linear SIMC than for constant SIMC. We cannot directly conclude about the order of the method from this single example. It seems however that constant SIMC is of order one with respect to the mesh size.

The extra CPU time due to the linear SIMC method versus constant SIMC method is moderate. Actually the main part of time is spent during the tracking of particles which is the same in both methods: in constant SIMC method each particle has one single symbolic weight whereas in linear SIMC it represents 2, 3 or 4 weights (according to the dimension of the problem and number of degree of freedom in each cell). Hence, in this kind of non-diffusive problem, there is no clear benefit in using linear SIMC instead of constant SIMC (a little more accurate but a little more expensive): the situation is of course completely different for a diffusive problem.

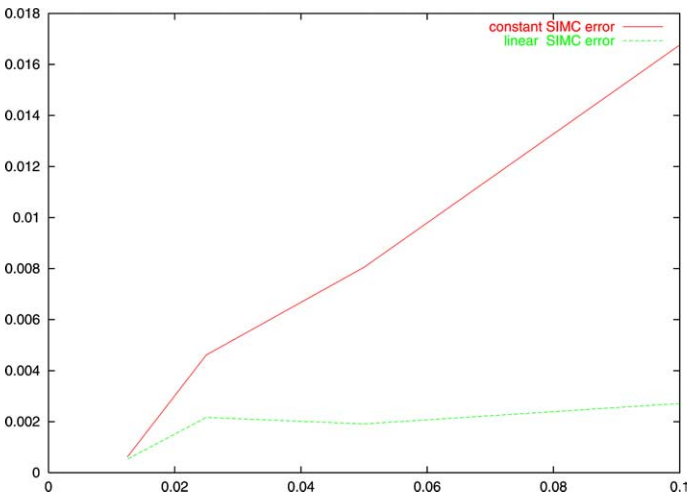

Fig. 12. L_1 error as a function of mesh size.

5. Conclusions

In this paper, we have analyzed and numerically demonstrated the behavior of the Symbolic Implicit Monte-Carlo method in opaque media. We have introduced an extension of standard SIMC method where the solution is linear in each cell instead of being constant.

We have proven that constant SIMC method does not possess the diffusion limit and that linear SIMC method does possess the diffusion limit. The limiting diffusion scheme is realized with the linear continuous finite element method. Analysis was performed in an arbitrary number of dimensions. The analysis of the boundary conditions is not complete. In the one-dimensional case, the asymptotic boundary condition is a very accurate approximation of the exact one. In higher dimensions, this result cannot be proven. However, we have proven the boundary condition is correct when incident intensity is isotropic.

Although the linear SIMC method is accurate in an opaque medium, it requires a huge number of Monte-Carlo particles. Otherwise large order Monte-Carlo fluctuations hide the correct solution. This is due to difficulty of calculating the coefficients of the diffusion matrix by the Monte-Carlo method. Hence cost could become prohibitive for a real application.

It could be possible to consider an improvement of the method which consists in computing analytically the matrix terms in diffusive regions. This would be equivalent to an hybrid Monte-Carlo Diffusion method.

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