Transport approximations in partially diffusive media

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Summary. This paper concerns the analysis of approximations of transport equations in diffusive media. Firstly, we consider a variational formulation for the first-order transport equation that has the correct diffusive behavior in the limit of small mean free paths. The associated bilinear form is shown to be coercive on a classical Hilbert space in transport theory with a constant of coercivity independent of the mean free path. This allows us to obtain the diffusion approximation of transport as an orthogonal projection onto a subspace of functions that are independent of the angular variable. Similarly, projections onto functions that are independent of the angular variable only in subsets of the full domain can be interpreted as a transport-diffusion coupling method. Convergence results based on averaging lemmas and error estimates are presented. Secondly, we address the problem of extended non-scattering layers or filaments surrounded by highly scattering media and derive generalized diffusion equations to model transport in such geometries.

1 Introduction

The solution of linear transport equations of Boltzmann type describing the phase-space density of particles, is of interest in many applications ranging from neutron transport in nuclear reactor physics [14] and photon transport in human tissues to wave propagation in highly heterogeneous media [10, 18, 31]. Among the many deterministic methods available [23], several numerical schemes have been obtained recently by using a variational framework. Variational methods have a long history in transport theory, both in the analytical and numerical approaches of source term and eigenvalue transport problems. A very short and incomplete list of bibliographical references includes [8, 11, 14, 30, 32]. Although variational methods that involve *symmetric* positive definite forms have been known for a long time in the even-parity formulation of transport (see e.g. [1, 23, 27]), their derivations for the first-order Boltzmann equation are more recent [7, 24, 25, 26].

Among the variational formulations involving a symmetric positive definite form over a Hilbert space defined in [7, 25], some enjoy the property that the constant of coercivity is independent of the transport mean free path, which measures (locally) the main distance between successive interactions of the particles with the underlying media. This property ensures that discretizations of solutions of the variational problem are accurate in the transport regime, characterized by mean free paths comparable to the typical length of variation of the geometrical components of the transport equation, as well as in the diffusive regime, characterized by much smaller mean free paths. For references on the approximation of transport by diffusion, see e.g. [12, 19].

We consider in this paper the SAAF (Self-adjoint angular flux) method presented in [26] and characterized explicitly in [7] as a variational method equivalent to the solution of the first-order transport equation. We show that the symmetric bilinear form associated to the variational problem has indeed a constant of coercivity independent of the mean free path over a Hilbert space that is also defined independently of the mean free path.

One of the main advantages of symmetric variational formulations is that approximations of the solutions can be obtained by orthogonal projection (with respect to the bilinear form and onto a subspace of the considered Hilbert space). This is analyzed in detail in [24, 25] in the framework of first-order system least squares (FOSLS). In this paper we show that the diffusion approximation of transport may be obtained as such an orthogonal projection (this already appears in [26]) and show that the error between the transport and the diffusion equations are linear in the mean free path (and

quadratic in certain circumstances) as expected. The use of the variational formulation in conjunction with averaging lemmas allows us to obtain that the above error converges to zero in the limit of small mean free paths even when the limiting solution is not very regular. The advantage of the proposed method is that there is no need to construct any scaling transformation as in [24] or adding any terms accounting for boundary conditions as in [25] as both can be deduced directly from the variational formulation.

In many applications, the mean free path will be small (compared to variations of the geometrical environment) in certain areas but not necessarily in the whole domain. A possible numerical approach consists then of solving the diffusion approximation where it is valid and the transport equation elsewhere. The main difficulty is then to couple both models at their common interface. Such a coupling was considered in the even-parity formulation of transport in [5]. See [16, 22, 33, 34] for additional references on the coupling problem. We consider here the transport-diffusion coupling as the orthogonal projection of the exact transport solution onto the subspace of the underlying Hilbert space of functions that depend only on the spatial variable in the diffusive domain but depend on both the spatial and angular variables in the rest of the domain. We also show the convergence of the coupled transport-diffusion solution (with appropriate error estimates) to the exact transport solution when diffusion is valid on the domain treated by the diffusion equation. It is interesting to observe that the first-order transport equation is not exactly satisfied on the transport area (as opposed to the case where the full domain is modeled by transport as mentioned earlier; see [7]). Rather the coupling involves a second-order transport equation in the transport area. This exemplifies the influence of the boundary and interface conditions in the variational formulation of first-order transport.

Many more details on the full discretization of the transport equation using variational approaches can be found in [24, 25, 26]. We do not consider the discretization problem here except for a brief remark in section 2.7.

For general geometries of embedded domains where the diffusion approximation does not hold, the coupling mentioned above may be a useful alternative to solving the full transport equations. In certain situations however, a more macroscopic model can be derived. Initiated by the analysis of clear layers in optical tomography [13], generalized diffusion models have been derived in [4, 6] to account for the propagation of photons along straight lines in non-scattering clear layers. In this paper we generalize the analysis to non-scattering filaments in three dimensional geometries and obtain new generalized diffusion models. Possible applications in which similar models may be useful include γ ray propagation in astrophysics and radiation in atmospheric clouds.

The rest of the paper is structured as follows. Section 2 presents the variational formulation of the first-order transport equation. General symmetric scattering operators are considered in the two-dimensional model only where the decomposition over spherical harmonics is particularly simple as shown in section 2.1. The variational formulation in the diffusive regime and its main properties are presented in section 2.2. The diffusion approximation is derived in section 2.3 and analyzed in the spherical harmonics expansion in section 2.4. Convergence results and error estimates are given in sections 2.5 and 2.6. The transport-diffusion coupling is addressed in section 3. Seen as an orthogonal projection in section 3.1 the resulting local equations are show in section 3.2. Finally error estimates are given in section 3.3. The derivation of generalized diffusion models to account for thin non-scattering inclusions is addressed in section 4.

2 Variational formulation for transport

We start with the steady-state transport equation written in the form

$$\begin{array}{ll} \boldsymbol{\omega}\cdot\nabla u + Gu = q, & X = \Omega\times V \\ u = g, & \Gamma_- = \{(\mathbf{x},\boldsymbol{\omega})\in\partial\Omega\times V,\ \boldsymbol{\omega}\cdot\boldsymbol{\nu}(\mathbf{x})<0\}. \end{array} \tag{1}$$

Here $u(\mathbf{x},\boldsymbol{\omega})$ is the particle density in phase space, $q(\mathbf{x},\boldsymbol{\omega})$ is a volume source term, $g(\mathbf{x},\boldsymbol{\omega})$ is a boundary source term, $\Omega\subset\mathbb{R}^n$ for $n=2$ or $n=3$ is the spatial domain, $\boldsymbol{\nu}(\mathbf{x})$ is its outward unit normal at $\mathbf{x}\in\partial\Omega$, and $V=S^{n-1}$ is the unit sphere in the monogroup-approximation of transport. As usual Γ_- denotes the set of incoming conditions. The operator G is defined as

$$Gu(\mathbf{x},\boldsymbol{\omega}) = \sigma(\mathbf{x})u(\mathbf{x},\boldsymbol{\omega}) - \int_{S^{n-1}} k(\mathbf{x},\boldsymbol{\omega}'-\boldsymbol{\omega})u(\mathbf{x},\boldsymbol{\omega}')d\mu(\boldsymbol{\omega}'). \tag{2}$$

The integration measure is the normalized Lebesgue measure so that $\mu(S^{n-1}) = 1$. The total absorption $\sigma(\mathbf{x})$ and the scattering coefficient $k(\mathbf{x}, \boldsymbol{\omega}' - \boldsymbol{\omega})$ are positive bounded functions. The scattering coefficient satisfies $k(\mathbf{x}, \mathbf{v}) = k(\mathbf{x}, -\mathbf{v})$ and is sufficiently small so that G is a symmetric positive definite operator on $L^2(S^{n-1})$ with bounded inverse G^{-1}.

We now consider the variational formulation presented in [7] and mentioned in [26]. We first recast the equation as

$$\begin{aligned} &G^{-1}(\boldsymbol{\omega} \cdot \nabla u) + u = G^{-1}(q), && X \\ &u = g, && \Gamma_-. \end{aligned} \tag{3}$$

We now multiply the first equation above by $\boldsymbol{\omega} \cdot \nabla v$ for a smooth test function $v(\mathbf{x}, \boldsymbol{\omega})$ and integrate over X to get:

$$\int_X G^{-1}(\boldsymbol{\omega} \cdot \nabla u)\boldsymbol{\omega} \cdot \nabla v \; dp - \int_X \boldsymbol{\omega} \cdot \nabla u v \; dp + \int_{\partial\Omega \times V} uv\boldsymbol{\omega} \cdot \boldsymbol{\nu} \; dq = \int_X G^{-1}(q)\boldsymbol{\omega} \cdot \nabla v \; dp.$$

Here, $dp = d\mathbf{x}d\mu(\boldsymbol{\omega})$ and $dq = d\sigma(\mathbf{x})d\mu(\boldsymbol{\omega})$, where $d\sigma(\mathbf{x})$ is the surface measure on $\partial\Omega$. Upon using the transport equation (1) we recast the above equality as finding $u \in W$ such that

$$a(u, v) = L(v), \qquad \forall v \in W, \tag{4}$$

where

$$\begin{aligned} a(u, v) &= \int_X \Big(G^{-1}(\boldsymbol{\omega} \cdot \nabla u)\boldsymbol{\omega} \cdot \nabla v + Guv \Big) dp + \int_{\Gamma_+} uv\boldsymbol{\omega} \cdot \boldsymbol{\nu} \; dq, \\ L(v) &= \int_X \Big(G^{-1}(q)\boldsymbol{\omega} \cdot \nabla v + qv \Big) dp + \int_{\Gamma_-} gv|\boldsymbol{\omega} \cdot \boldsymbol{\nu}| \; dq \\ W &= \big\{ u \in L^2(X), \quad \boldsymbol{\omega} \cdot \nabla u \in L^2(X), \quad u_{\Gamma_\pm} \in L^2(\Gamma_\pm; |\boldsymbol{\omega} \cdot \boldsymbol{\nu}| dq) \big\}. \end{aligned} \tag{5}$$

The set $\Gamma_+ = \{(\mathbf{x}, \boldsymbol{\omega}) \in \partial\Omega \times V, \; \boldsymbol{\omega} \cdot \boldsymbol{\nu}(\mathbf{x}) > 0\}$. It is easy to verify that with our assumptions on G, $a(u, v)$ is a continuous, coercive, and symmetric bilinear form on the Hilbert space W (equipped with its natural norm) [12] and that L is continuous in the same sense. The above equation (4) thus admits a unique solution by the Lax-Milgram theory.

2.1 Harmonic decomposition

It is interesting to analyze the above variational formulation using the spherical harmonics decomposition. We concentrate on the two dimensional case $n = 2$ so that the velocity space $V = S^1$ is the unit circle. Generalizations to $n = 3$ using "classical" spherical harmonics are straightforward though more tedious computationally [25, 26]. In this setting, directions are parameterized by $\boldsymbol{\omega} = (\cos\theta, \sin\theta)$ for $0 \le \theta < 2\pi$. We identify $u(\boldsymbol{\omega}) \equiv u(\theta)$.

Define the harmonic decomposition

$$\mathcal{F}u(n) = \hat{u}_n = \frac{1}{2\pi} \int_0^{2\pi} e^{-in\theta} u(\boldsymbol{\omega}) d\theta(\boldsymbol{\omega}), \qquad \mathcal{F}^{-1}\hat{u}(\theta) = u(\theta) = \sum_{n \in \mathbb{Z}} e^{in\theta} \hat{u}_n. \tag{6}$$

In this basis, the operator G may be written as a (diagonal) Fourier multiplier:

$$G = \mathcal{F}^{-1}(\sigma - k_n)\mathcal{F}, \tag{7}$$

where the coefficients σ and k_n are such that $|k_n| < k_0 < \sigma$ for $|n| \ge 1$. Also, since G is a real-valued operator, we verify that $k_{-n} = \bar{k}_n$, where the upper bar denotes complex conjugation. Because G is symmetric, we have here $k_{-n} = k_n$ real-valued. The above decomposition means that $Ge^{in\theta} = (\sigma - k_n)e^{in\theta}$ and implies that

$$G^{-1} = \mathcal{F}^{-1}(\sigma - k_n)^{-1}\mathcal{F}. \tag{8}$$

We also verify the following convenient expression for the differential operator

$$\boldsymbol{\omega} \cdot \nabla = e^{i\theta}\partial + e^{-i\theta}\bar{\partial}, \qquad \partial = \frac{1}{2}\Big(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y} \Big), \quad \bar{\partial} = \frac{1}{2}\Big(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y} \Big). \tag{9}$$

This implies that $\widehat{(\boldsymbol{\omega}\cdot\nabla v)}_n = \partial\hat{v}_{n-1} + \bar{\partial}\hat{v}_{n+1}$. We finally identify $\mathbf{x} = (x, y)$ with $z = x + iy$ in the complex plane.

With this notation, we verify that the transport equation is equivalent to

$$\Big(e^{i\theta}\partial + e^{-i\theta}\bar{\partial}\Big)u + Gu = q \tag{10}$$

with appropriate boundary conditions. In the Fourier domain this is nothing but

$$\partial\hat{u}_{n-1} + \bar{\partial}\hat{u}_{n+1} + (\sigma - k_n)\hat{u}_n = \hat{q}_n, \qquad \Omega\times\mathbb{Z}. \tag{11}$$

Recall the Parseval relation $\int_{S^1} uvd\mu = \sum_{n\in\mathbb{Z}}\hat{u}_n\overline{\hat{v}_n} = \sum_{n\in\mathbb{Z}}\hat{u}_n\hat{v}_{-n}$ since u and v are real-valued functions. The variational formulation (4) still holds with $a(u,v)$ and $L(v)$ recast as:

$$\begin{aligned} a(u,v) &= \int_\Omega \sum_{n\in\mathbb{Z}} \Big(\frac{1}{a-k_n}(\partial\hat{u}_{n-1} + \bar{\partial}\hat{u}_{n+1})(\partial\hat{v}_{-n-1} + \bar{\partial}\hat{v}_{-n+1}) + (\sigma - k_n)\hat{u}_n\hat{v}_{-n}\Big)d\mu(z) \\ &\quad + \int_{\Gamma_+} uv\boldsymbol{\omega}\cdot\boldsymbol{\nu}\, dq, \\ L(v) &= \int_\Omega \sum_{n\in\mathbb{Z}} \Big(\frac{1}{a-k_n}\hat{q}_n(\partial\hat{v}_{-n-1} + \bar{\partial}\hat{v}_{-n+1}) + \hat{q}_n\hat{v}_{-n}\Big)d\mu(z) + \int_{\Gamma_-} gv|\boldsymbol{\omega}\cdot\boldsymbol{\nu}|\, dq. \end{aligned} \tag{12}$$

The above formulae prove very useful in the analysis of the transport solution in the diffusive regime.

2.2 Variational formulation in the diffusive regime

We now consider the regime of high collisions and small absorption. This regime is characterized by replacing G, q and g by [12]

$$\begin{aligned} G_\varepsilon u(\mathbf{x},\boldsymbol{\omega}) &= \frac{1}{\varepsilon}\int_{S^{n-1}} k(\mathbf{x},\boldsymbol{\omega}'-\boldsymbol{\omega})\big(u(\mathbf{x},\boldsymbol{\omega}) - u(\mathbf{x},\boldsymbol{\omega}')\big)d\mu(\boldsymbol{\omega}') + \varepsilon\sigma_a u, \\ q_\varepsilon &= \varepsilon q, \qquad g_\varepsilon = \varepsilon g. \end{aligned} \tag{13}$$

Here g_ε is of order ε to avoid the presence of boundary layers at the leading order [12] (we will see below that a term of order $\varepsilon^{1/2}$ rather than ε would have been sufficient). We recast $G_\varepsilon = \varepsilon^{-1}Q + \varepsilon\sigma_a$, where σ_a is uniformly bounded from below by a positive constant so that G_ε^{-1} is bounded on $L^2(X)$ though not uniformly in ε. The local first-order transport equation (1) reads in this regime:

$$\boldsymbol{\omega}\cdot\nabla u_\varepsilon + G_\varepsilon u_\varepsilon = \varepsilon q. \tag{14}$$

We recast (4) in this regime as finding $u\in W$ such that

$$a_\varepsilon(u,v) = L_\varepsilon(v), \qquad \forall v\in W, \tag{15}$$

where

$$\begin{aligned} a_\varepsilon(u,v) &= \int_X \Big((\varepsilon G_\varepsilon)^{-1}(\boldsymbol{\omega}\cdot\nabla u)\boldsymbol{\omega}\cdot\nabla v + \varepsilon^{-1}G_\varepsilon(u)v\Big)dp + \frac{1}{\varepsilon}\int_{\Gamma_+} uv\boldsymbol{\omega}\cdot\boldsymbol{\nu}\, dq, \\ L_\varepsilon(v) &= \int_X \Big(G_\varepsilon^{-1}(q)\boldsymbol{\omega}\cdot\nabla v + qv\Big)dp + \int_{\Gamma_-} gv|\boldsymbol{\omega}\cdot\boldsymbol{\nu}|\, dq. \end{aligned} \tag{16}$$

We now derive some properties of the above variational formulation and the above bilinear form that make them attractive theoretically and computationally. We first assume that G_ε is invertible (in $L^2(V)$) with inverse given by

$$G_\varepsilon^{-1}u = \frac{1}{\varepsilon\sigma_a}\bar{u} + \varepsilon H_\varepsilon u, \qquad \overline{H_\varepsilon u} = 0, \tag{17}$$

where $H_\varepsilon u$ is a symmetric and bounded operator in $L^2(X)$ with norm bounded by $\alpha^{-1} < \infty$, and $\bar{u} = \int_{S^{n-1}} u(\boldsymbol{\omega})d\mu(\boldsymbol{\omega})$ is the angular average of u. This property holds when G_ε is decomposed over spherical harmonics; see for instance (37) and (41) below. This allows us to recast (16) as

$$
\begin{aligned}
a_\varepsilon(u,v) &= \int_X \Big(\frac{1}{\varepsilon^2 \sigma_a} \overline{\boldsymbol{\omega}\cdot\nabla u}\ \overline{\boldsymbol{\omega}\cdot\nabla v} + H_\varepsilon(\boldsymbol{\omega}\cdot\nabla u)\boldsymbol{\omega}\cdot\nabla v + \frac{G_\varepsilon}{\varepsilon} uv \Big) dp + \frac{1}{\varepsilon}\int_{\Gamma_+} uv\boldsymbol{\omega}\cdot\boldsymbol{\nu}\ dq \\
L_\varepsilon(v) &= \int_X \Big(\frac{1}{\varepsilon\sigma_a} \overline{\boldsymbol{\omega}\cdot\nabla v} + \varepsilon H_\varepsilon(\boldsymbol{\omega}\cdot\nabla v) + v \Big) q\ dp + \int_{\Gamma_-} gv\boldsymbol{\omega}\cdot\boldsymbol{\nu}\ dq.
\end{aligned}
\tag{18}
$$

Let us assume that Q and H_ε are coercive on $L^2(X)$ with coercivity constants α and σ_0^{-1}, respectively, in the sense that:

$$
(Qu,u) \geq \alpha \|u\|^2, \qquad (H_\varepsilon u, u) \geq \frac{1}{\sigma_0}\|u\|^2. \tag{19}
$$

Here $\|f\|$ is the $L^2(X)$ norm of f. These are reasonable assumptions when G_ε can be diagonalized in the basis of spherical harmonics; see (37) and (41) below. Let us also assume that the absorption $0 < \sigma_{a1} \leq \sigma_a(\mathbf{x}) \leq \sigma_{a0}$ on Ω. We then verify that

$$
\frac{1}{\sigma_0}\|\boldsymbol{\omega}\cdot\nabla u_\varepsilon\|^2 + \frac{1}{\varepsilon^2\sigma_{a0}}\|\overline{\boldsymbol{\omega}\cdot\nabla u_\varepsilon}\|^2 + \frac{\alpha}{\varepsilon^2}\|u_\varepsilon - \overline{u_\varepsilon}\|^2 + \sigma_{a1}\|u_\varepsilon\|^2 + \frac{1}{\varepsilon}\|u_{\varepsilon|\Gamma_+}\|_b^2 \leq a_\varepsilon(u_\varepsilon, u_\varepsilon). \tag{20}
$$

Here $\|f\|_b$ denotes the $L^2(\Gamma_\pm; |\boldsymbol{\omega}\cdot\boldsymbol{\nu}|dq)$ norm of f defined on $\Gamma_\pm$. This implies that a_ε is coercive on W with constant of coercivity *independent* of ε. The constant of coercivity also depends on the scattering kernel only through the constants α and σ_0^{-1}.

It is also straightforward to observe that $a_\varepsilon(u,v)$ is continuous on $W\times W$, though with a continuity constant that depends on ε. In order to obtain a constant of continuity independent of ε, the Hilbert space may be equipped with a norm $\|\cdot\|_{W_\varepsilon}$ defined as the (square root of the) left-hand side of (20); this is in essence the norm introduced in [24]. On W_ε (i.e., W equipped with $\|\cdot\|_{W_\varepsilon}$) the form a_ε is coercive and continuous with constants of coercivity and continuity independent of ε (see also section 2.7). The source term is also bounded on W_ε with a constant independent of ε, and bounded on W with a constant that depends on ε:

$$
|L_\varepsilon(u_\varepsilon)| \lesssim \frac{\varepsilon}{\alpha}\|\boldsymbol{\omega}\cdot\nabla u_\varepsilon\|\|q\| + \frac{1}{\varepsilon\sigma_{a1}}\|\bar{q}\|\|\overline{\boldsymbol{\omega}\cdot\nabla u_\varepsilon}\| + \|q\|\|u_\varepsilon\| + \|u_{\varepsilon|\Gamma_+}\|_b\|g\|_b. \tag{21}
$$

The notation $a \lesssim b$ stands for $a \leq Cb$ for some constant C independent of ε. We deduce from the constraints on a_ε and L_ε that the unique solution u_ε of the variational formulation (15) satisfies the (a priori) estimate

$$
\|\boldsymbol{\omega}\cdot\nabla u_\varepsilon\| + \frac{1}{\varepsilon}\|\overline{\boldsymbol{\omega}\cdot\nabla u_\varepsilon}\| + \|u_\varepsilon\| \lesssim \|q\| + \sqrt{\varepsilon}\|g\|_b. \tag{22}
$$

This implies that

$$
|L_\varepsilon(u_\varepsilon)| \lesssim \|q\|^2 + \varepsilon\|g\|_b^2, \tag{23}
$$

so that from (20),

$$
\|u_\varepsilon - \bar{u}_\varepsilon\|_{L^2(X)} \lesssim \sqrt{\alpha}(\varepsilon\|q\| + \varepsilon^{3/2}\|g\|_b). \tag{24}
$$

To summarize we have the following result:

Lemma 1. *Provided that* (19) *holds, the unique solution* u_ε *of* (15) *verifies that*

$$
\|\boldsymbol{\omega}\cdot\nabla u_\varepsilon\| + \|u_\varepsilon\| + \frac{1}{\varepsilon}\|\overline{\boldsymbol{\omega}\cdot\nabla u_\varepsilon}\| + \frac{1}{\varepsilon}\|u_\varepsilon - \bar{u}_\varepsilon\|_{L^2(X)} + \frac{1}{\sqrt{\varepsilon}}\|u_{\varepsilon|\Gamma_+}\|_b \lesssim \|q\| + \sqrt{\varepsilon}\|g\|_b \tag{25}
$$

provided that $q \in L^2(X)$ *and* $g \in L^2(\Gamma_-; |\boldsymbol{\omega}\cdot\boldsymbol{\nu}|dq)$. *We recognize the above left-hand side as* $\|u_\varepsilon\|_{W_\varepsilon}$.

Least-Square formulation.

Let us introduce the operator

$$
\mathcal{L}_\varepsilon = (\varepsilon G_\varepsilon)^{-1/2}(\boldsymbol{\omega}\cdot\nabla + G_\varepsilon). \tag{26}
$$

Using the divergence theorem on $\nabla\cdot(uv\boldsymbol{\omega}) = (\boldsymbol{\omega}\cdot\nabla u)v + u\boldsymbol{\omega}\cdot\nabla v$, we verify that

$$
a_\varepsilon(u,v) = (\mathcal{L}_\varepsilon u, \mathcal{L}_\varepsilon v) + \frac{1}{\varepsilon}\langle u, v\rangle, \tag{27}
$$

where $(\cdot,\cdot)$ is the usual inner product on $L^2(X)$ and $\langle\cdot,\cdot\rangle$ is the inner product on $L^2(\Gamma_-,|\boldsymbol{\omega}\cdot\boldsymbol{\nu}|dq)$. We also have

$$L_\varepsilon(v)=(q_\varepsilon,\mathcal{L}_\varepsilon v)+\langle g,v\rangle,\qquad q_\varepsilon=\varepsilon^{1/2}G_\varepsilon^{-1/2}(q). \tag{28}$$

Since G_ε, whence a_ε, is symmetric, the variational formulation (15) is equivalent to minimizing the functional:

$$\arg\min_{v\in W}\frac{1}{2}a_\varepsilon(v,v)-L_\varepsilon(v), \tag{29}$$

which is also equivalent to minimizing the following least-square problem

$$\arg\min_{u\in W}\frac{1}{2}\|\mathcal{L}_\varepsilon u-q_\varepsilon\|^2_{L^2(X)}+\frac{1}{2\varepsilon}\|u-\varepsilon g\|^2_{L^2(\Gamma_-;|\boldsymbol{\omega}\cdot\boldsymbol{\nu}|dq)}, \tag{30}$$

as can easily be verified.

We have thus recast solving the transport solution as minimizing the least-square problem associated to a variational form a_ε that is W-coercive with constant of coercivity independent of ε. The boundary conditions are also accounted for in a variational sense as the functions in the space W need not satisfy the boundary conditions exactly. These very important properties are a central element in the numerical methods developed in [24, 25], which are based on Galerkin projections; see also section 2.7. Note that the scaling operator S used in the above references is replaced in our analysis by $(\varepsilon G_\varepsilon)^{-1/2}$. The method developed in this paper may thus be seen as a case of first-order system least-squares (FOSLS) [24, 25].

Because of (20), Galerkin methods, which are orthogonal projections onto subspaces of W with respect to the bilinear form a_ε, provide lower-dimensional approximations that are expected to be valid both in the transport regime ($\varepsilon\sim 1$) and the diffusive regime ($\varepsilon\ll 1$) as in [24, 25]. We now consider two Galerkin methods, which are not discretizations of the transport solution, but rather projections onto smaller subsets of W that are physically relevant in the diffusive regime. The first method consists of projecting the transport solution onto functions that only depend on space and not on the angular variable. The resulting diffusion approximation is analyzed in the rest of this section. In the next section we project the transport solution onto functions that depend on the spatial variable only in parts of the domain. This allows us to couple the diffusion approximation to the full transport solution in regions where diffusion may not be valid.

2.3 Diffusion by orthogonal projection

We want to use the above variational formulation to deduce the limit of the transport solution in the diffusion limit. Diffusion is characterized by high scattering and small absorption. High scattering implies that the initial directional content of the particles is quickly lost through interactions. It is therefore reasonable to assume that $u(\mathbf{x},\boldsymbol{\omega})$ does not depend on $\boldsymbol{\omega}$ in a first approximation. Such a condition is easy to implement in a variational setting: we orthogonally (with respect to $a_\varepsilon(\cdot,\cdot)$) project the solution u of (4) onto functions that depend only on $\mathbf{x}$. Let us define

$$W_D=\big\{f\in W,\,f=f(\mathbf{x})\big\}\equiv H^1(\Omega),\quad W_{D\varepsilon}^\perp=\big\{f\in W,\,a_\varepsilon(f,v)=0\;\forall v\in W_D\big\}. \tag{31}$$

We verify that $W=W_D\oplus W_{D\varepsilon}^\perp$ since $a_\varepsilon(\cdot,\cdot)$ is an inner product on W [5]. Then the orthogonal projection Π_ε of W to W_D for the inner product $a_\varepsilon(u,u)$ allows us to define the "diffusion" solution

$$U_\varepsilon=\Pi_\varepsilon u_\varepsilon, \tag{32}$$

where u_ε is the solution to (15). By definition, we have that U_ε is the solution in W_D of

$$a_\varepsilon(U_\varepsilon,v)=L_\varepsilon(v),\qquad v\in W_D. \tag{33}$$

We may recast the above equation as

$$\begin{aligned}&\int_\Omega\Big(D_\varepsilon\nabla U\cdot\nabla V+\sigma_aUV\Big)d\mathbf{x}+\int_{\partial\Omega}c_n\frac{1}{\varepsilon}UV\,d\sigma(\mathbf{x})\\&=\int_\Omega\Big[\Big(\int_{S^{n-1}}G_\varepsilon^{-1}(q)\boldsymbol{\omega}d\mu(\boldsymbol{\omega})\Big)\cdot\nabla V+qV\Big]d\mathbf{x}+\int_{\Gamma_-}gV|\boldsymbol{\omega}\cdot\boldsymbol{\nu}|\;dq,\end{aligned}$$

for all $V \in W_D$, where

$$\begin{aligned} D_\varepsilon &= \int_{S^{n-1}} (\varepsilon G_\varepsilon)^{-1}(\boldsymbol{\omega}) \otimes \boldsymbol{\omega} d\mu(\boldsymbol{\omega}) \\ c_n &= \frac{1}{2}\int_{S^{n-1}} |\boldsymbol{\omega}\cdot\boldsymbol{\nu}| d\mu(\boldsymbol{\omega}). \end{aligned} \tag{34}$$

We verify that $c_2 = \frac{2}{\pi}$ and that $c_3 = \frac{1}{2}$. After classical integrations by parts, this means that U_ε is the solution of the following diffusion equation:

$$\begin{aligned} &-\nabla\cdot D_\varepsilon \nabla U_\varepsilon + \sigma_a U_\varepsilon = q - \nabla\cdot\Big(\int_{S^{n-1}} G_\varepsilon^{-1}(q)\boldsymbol{\omega} d\mu(\boldsymbol{\omega})\Big) \\ &\boldsymbol{\nu}\cdot D_\varepsilon\nabla U_\varepsilon + \frac{c_n}{\varepsilon} U_\varepsilon = J(\mathbf{x}) \equiv \int_{\boldsymbol{\omega}\cdot\boldsymbol{\nu}<0} g(\mathbf{x},\boldsymbol{\omega})|\boldsymbol{\omega}\cdot\boldsymbol{\nu}| d\mu(\boldsymbol{\omega}). \end{aligned} \tag{35}$$

Here we assume that q vanishes at the domain boundary $\partial\Omega$ to simplify. This is consistent with our choice of incoming conditions of size εg as $O(1)$ source terms at the domain boundary result in boundary layer analyses that we do not want to dwell into here; see [12].

It remains to understand whether the solution U_ε, which is obviously uniquely defined, is uniformly bounded in $H^1(\Omega)$ and to obtain an error estimate for $u_\varepsilon - U_\varepsilon$ and for similar diffusion approximations of u_ε.

Let us first consider the simpler case where scattering is isotropic, which implies that

$$G_\varepsilon u = \frac{k_0}{\varepsilon}(u - \bar{u}) + \varepsilon\sigma_a u, \tag{36}$$

where $\bar{u} = \int_{S^{n-1}} u(\boldsymbol{\omega}) d\mu(\boldsymbol{\omega})$ and where $k_0(\mathbf{x}) = k(\mathbf{x}, \boldsymbol{\omega} - \boldsymbol{\omega}')$. In this context we verify that

$$G_\varepsilon^{-1} u = \frac{1}{\varepsilon}\frac{k_0}{\sigma_a\sigma_\varepsilon}\bar{u} + \frac{\varepsilon}{\sigma_\varepsilon} u, \qquad \sigma_\varepsilon = k_0 + \varepsilon^2\sigma_a. \tag{37}$$

Assuming that $q = \bar{q}$ and that $g \equiv 0$ to simplify, this implies that the transport equation takes the form

$$\begin{aligned} &\int_X \Big[\Big(\frac{1}{\sigma_\varepsilon}\boldsymbol{\omega}\cdot\nabla u + \frac{1}{\varepsilon^2}\frac{k_0}{\sigma_a\sigma_\varepsilon}\overline{\boldsymbol{\omega}\cdot\nabla u}\Big)\boldsymbol{\omega}\cdot\nabla v + \frac{k_0}{\varepsilon^2}(u-\bar{u})v + \sigma_a uv\Big] dp \\ &+\frac{1}{\varepsilon}\int_{\Gamma_+} uv\boldsymbol{\omega}\cdot\boldsymbol{\nu}\, dq \;=\; \int_X q\Big(\frac{\boldsymbol{\omega}\cdot\nabla v}{\varepsilon\sigma_a} + v\Big) dp. \end{aligned} \tag{38}$$

Upon choosing u and v in W_D in the above equation, we find the variational formulation for U_ε:

$$\int_\Omega \Big(\frac{1}{n\sigma_\varepsilon}\nabla U\cdot\nabla V + \sigma_a UV\Big) d\mathbf{x} + \frac{1}{\varepsilon} c_n \int_{\partial\Omega} UV d\sigma = \int_\Omega qV\, d\mathbf{x}. \tag{39}$$

This is nothing but the variational formulation of (35) with the diffusion coefficient given by $D_\varepsilon = (n\sigma_\varepsilon)^{-1}$ as usual and the right-hand side given by $q(\mathbf{x})$. We thus obtain the classical diffusion equation [19].

2.4 Harmonic decomposition and diffusion approximation

The generalization of the derivation of the above diffusion solution to arbitrary scattering kernels is relatively straightforward as long as G_ε^{-1} can be explicitly characterized. We restrict ourselves here to the two-dimensional case with scattering kernel of convolution type and use explicitly the variational form written in the harmonic basis. Within this context and in the diffusive regime, G_ε is given by

$$G_\varepsilon = \mathcal{F}^{-1}\Big(\frac{k_0 - k_n}{\varepsilon} + \varepsilon\sigma_a\Big)\mathcal{F}. \tag{40}$$

We recall that the Fourier transform is considered in the angular variable only. The inverse of G_ε is then

$$G_\varepsilon^{-1} = \mathcal{F}^{-1}\frac{\varepsilon}{k_0 - k_n + \varepsilon^2\sigma_a}\mathcal{F} \equiv \mathcal{F}^{-1}\frac{\varepsilon}{\sigma_\varepsilon - k_n}\mathcal{F} \tag{41}$$

where $\sigma_\varepsilon = k_0 + \varepsilon^2 \sigma_a$, This yields (37) when $k_n = 0$ for $|n| \geq 1$ and (17) in general, where $H_\varepsilon u$ is a bounded operator in $L^2(X)$. Let us introduce the spectral gap of Q:

$$\alpha = \min_{n \geq 1, \mathbf{x} \in \Omega} (k_0(\mathbf{x}) - k_n(\mathbf{x})) > 0, \tag{42}$$

and the minimum of σ_ε:

$$\sigma_0 = \min_{\mathbf{x} \in \Omega} \sigma_\varepsilon(\mathbf{x}) > 0. \tag{43}$$

We then verify that the coercivity constraints (19) are verified.

With this explicit form for G_ε, the terms of the variational equation (15) now take the form

$$\begin{aligned} a_\varepsilon(u,v) &= \int_\Omega \sum_{n \in \mathbb{Z}} \Big[\frac{1}{k_0 - k_n + \varepsilon^2 \sigma_a} \widehat{(\boldsymbol{\omega} \cdot \nabla u)}_n \widehat{(\boldsymbol{\omega} \cdot \nabla v)}_{-n} + \Big(\frac{k_0 - k_n}{\varepsilon^2} + \sigma_a \Big) \hat{u}_n \hat{v}_{-n} \Big] d\mathbf{x} \\ &\quad + \varepsilon^{-1} \int_{\Gamma_+} uv \boldsymbol{\omega} \cdot \boldsymbol{\nu} \, dq, \\ L_\varepsilon(v) &= \int_\Omega \sum_{n \in \mathbb{Z}} \Big[\frac{\varepsilon \hat{q}_n \widehat{(\boldsymbol{\omega} \cdot \nabla v)}_{-n}}{k_0 - k_n + \varepsilon^2 \sigma_a} + \hat{q}_n \hat{v}_{-n} \Big] d\mathbf{x} + \int_{\Gamma_-} gv |\boldsymbol{\omega} \cdot \boldsymbol{\nu}| \, dq. \end{aligned} \tag{44}$$

The generalization of (39) to more general scattering terms may easily be carried out thanks to the above formulae. Indeed, U and V belong to W_D if and only if all their Fourier coefficients $\hat{U}_n$ and $\hat{V}_n$ vanish for $|n| \geq 1$. As a result, U is the unique solution to the following variational problem

$$\begin{aligned} &\int_\Omega \Big(\frac{\partial \hat{U}_0 \bar{\partial} \hat{V}_0 + \bar{\partial} \hat{U}_0 \partial \hat{V}_0}{k_0 - k_1 + \varepsilon^2 \sigma_a} + \sigma_a \hat{U}_0 \hat{V}_0 \Big) d\mathbf{x} + \frac{c_2}{\varepsilon} \int_{\partial\Omega} UV d\sigma \\ &= \int_\Omega \Big(\varepsilon \frac{\hat{q}_1 \bar{\partial} \hat{V}_0 + \hat{q}_{-1} \partial \hat{V}_0}{k_0 - k_1 + \varepsilon^2 \sigma_a} + \hat{q}_0 \hat{V}_0 \Big) d\mathbf{x} + \int_{\partial\Omega} V \Big(\int_{\boldsymbol{\omega} \cdot \boldsymbol{\nu} < 0} g(\mathbf{x}, \boldsymbol{\omega}) |\boldsymbol{\omega} \cdot \boldsymbol{\nu}| d\mu(\boldsymbol{\omega}) \Big) d\sigma. \end{aligned} \tag{45}$$

We have used here the symmetry of G implying that $k_{-1} = k_1$. We denote by $\hat{q}_{-1} = \frac{1}{2}(q_x + i q_y)$ and identify it with the vector $\mathbf{q} = (q_x, q_y)$ in Cartesian coordinates. The above variational formulation shows that U is the (weak) solution in W_D of the following diffusion equation:

$$\begin{aligned} &-\nabla \cdot D_\varepsilon \nabla U + \sigma_a U = \overline{q} - \varepsilon \nabla \cdot D_\varepsilon \mathbf{q}, \qquad \Omega \\ &D_\varepsilon \frac{\partial U}{\partial n} + \frac{c_2}{\varepsilon} U = J, \qquad \partial\Omega. \end{aligned} \tag{46}$$

The diffusion coefficient is given by

$$D_\varepsilon = \frac{1}{2(\sigma_\varepsilon - k_1)} = \frac{1}{2(k_0 - k_1 + \varepsilon^2 \sigma_a)}. \tag{47}$$

This is the usual expression for the diffusion coefficient.

Remark 1. The property that the constant of coercivity of a_ε is independent of the mean free path ε is very important to obtain the diffusion solution by orthogonal projection. Consider for instance the transport problem

$$T_\varepsilon u_\varepsilon \equiv \frac{1}{\varepsilon} \boldsymbol{\omega} \cdot \nabla u_\varepsilon + \frac{1}{\varepsilon} G_\varepsilon u_\varepsilon = q(\mathbf{x}) \quad \text{ in } X, \qquad u_\varepsilon = 0 \quad \text{ on } \Gamma_-, \tag{48}$$

and the variational formulation: find u_ε such that

$$\tilde{a}_\varepsilon(u_\varepsilon, v) = (w_\varepsilon T_\varepsilon u_\varepsilon, T_\varepsilon v) = (q, w_\varepsilon T_\varepsilon v), \quad \forall v \in W. \tag{49}$$

Here $w_\varepsilon(\mathbf{x})$ is a weight function that could take the value 1 as in the introduction in [24] or σ_ε^{-1} as in [7]. The above problem is equivalent to (48) for w_ε uniformly bounded from above and below by positive constants as is shown in [7]. This results from the fact that $\tilde{a}_\varepsilon(u_\varepsilon, v)$ is coercive on W. However the constant of coercivity is not independent of ε. The equivalence between (48) and (49) thus somewhat degrades as $\varepsilon \to 0$. The consequence is that (49) becomes inaccurate in the diffusive regime with dire consequences when it comes to discretizations as pointed out in [24]. The same consequence arises when

the natural orthogonal projection $\tilde{\Pi}_\varepsilon$ of u_ε onto W_D is considered. Assuming that G_ε is isotropic as in (36) to simplify, we obtain that $\tilde{U}_\varepsilon = \tilde{\Pi}_\varepsilon u_\varepsilon$ solves the equation

$$-\nabla \cdot \frac{w_\varepsilon}{n} \nabla \tilde{U}_\varepsilon + w_\varepsilon \sigma_a^2 \tilde{U}_\varepsilon = w_\varepsilon \sigma_a q, \qquad \text{in } \Omega. \tag{50}$$

Here $n = 2, 3$ is the spatial dimension. Although the local equilibrium $\tilde{U}_\varepsilon \approx \sigma_a^{-1} q$ is verified in the limit of very strong absorption and sources, the diffusion tensor is not correct, independently of the choice of the weight w_ε. This indicates that variational formulations of the form (49) should not be used in the diffusive regime and should be replaced by (4) or by rescaled formulations as in [24].

2.5 Convergence result and error estimates

Let $u_\varepsilon(\mathbf{x}, \boldsymbol{\omega})$ be the solution of the transport equation (15) and $U_\varepsilon = \Pi_\varepsilon u_\varepsilon$ the diffusion approximation solution of (33). Define $\delta u_\varepsilon = u_\varepsilon - U_\varepsilon$. We first show that δu_ε converges to 0 in W as $\varepsilon \to 0$. The proof is similar to that in [5].

Thanks to the orthogonal projection, we first obtain that $\delta u_\varepsilon \in W_{D\varepsilon}^\perp$. Consequently, we have

$$a_\varepsilon(\delta u_\varepsilon, \delta u_\varepsilon) = a_\varepsilon(u_\varepsilon, \delta u_\varepsilon) = L_\varepsilon(\delta u_\varepsilon).$$

We then deduce from (20) and (21) that

$$\|\delta u_\varepsilon\|_W + \frac{1}{\varepsilon} \|\delta u_\varepsilon - \overline{\delta u_\varepsilon}\| \lesssim \|q\| + \sqrt{\varepsilon} \|g\|_b.$$

Since δu_ε is uniformly bounded in W, which is a Hilbert space with a unit ball compact for the weak topology, we deduce the existence of a subsequence of δu_ε converging to w. However the subsequence of $\overline{\delta u_\varepsilon}$ converges to the same limit so that $w = \overline{w} \in W_D$. This implies that

$$a_\varepsilon(\delta u_\varepsilon, w) = 0.$$

Upon passing to the limit in the above expression, we find that

$$\int_\Omega \Big(\frac{1}{k_0 - k_1} \Big| \widehat{(\boldsymbol{\omega} \cdot \nabla w)}_1 \Big|^2 + \sigma_a |w|^2 \Big) d\mathbf{x} = 0$$

and that $w_{|\partial\Omega} = 0$. This implies that $w = 0$, whence that δu_ε converges to 0. Note that all we have used to get this convergence result is that $\|q\|$ and $\|g\|_b$ are bounded (in the L^2-sense).

In order to obtain error estimates for δu_ε, additional regularity of the solutions and source terms is required. Let us recall (18):

$$\begin{aligned} a_\varepsilon(u, v) &= \int_X \Big(\frac{1}{\varepsilon^2 \sigma_a} \overline{\boldsymbol{\omega} \cdot \nabla u}\ \overline{\boldsymbol{\omega} \cdot \nabla v} + H_\varepsilon(\boldsymbol{\omega} \cdot \nabla u) \boldsymbol{\omega} \cdot \nabla v + \frac{G_\varepsilon}{\varepsilon} uv \Big) dp + \frac{1}{\varepsilon} \int_{\Gamma_+} uv \boldsymbol{\omega} \cdot \boldsymbol{\nu}\ dq, \\ L_\varepsilon(v) &= \int_X \Big(q - \boldsymbol{\omega} \cdot \nabla \frac{\overline{q}}{\varepsilon \sigma_a} - \varepsilon \boldsymbol{\omega} \cdot \nabla H_\varepsilon(q) \Big) v\ dp + \int_{\Gamma_-} gv \boldsymbol{\omega} \cdot \boldsymbol{\nu}\ dq, \end{aligned} \tag{51}$$

assuming that q vanishes on $\partial\Omega$ to simplify. We split the source term as

$$\begin{aligned} L_\varepsilon &= L_0 + L_1, \\ L_0(v) &= \int_X qv\ dp - \int_X \varepsilon \boldsymbol{\omega} \cdot \nabla H_\varepsilon(q) v\ dp + \int_{\Gamma_-} gv \boldsymbol{\omega} \cdot \boldsymbol{\nu}\ dq, \\ L_1(v) &= \int_X -\boldsymbol{\omega} \cdot \nabla \frac{\overline{q}}{\varepsilon \sigma_a} v\ dp. \end{aligned} \tag{52}$$

The term appearing in $L_1(v)$ is of order ε^{-1} and cannot be estimated from the variational formulation. In order to estimate it explicitly, we define W_1 as the subspace of W of functions $u(\mathbf{x}, \boldsymbol{\omega})$ such that $\hat{u}_n(\mathbf{x}) = 0$ for $|n| \neq 1$. This is thus the Hilbert space of functions linear in $\boldsymbol{\omega}$. Let $\Pi_{1\varepsilon}$ be the orthogonal projection of W onto W_1 with respect to $a_\varepsilon(\cdot, \cdot)$. We define $U_{1\varepsilon} = \Pi_{1\varepsilon} u_\varepsilon$, i.e.,

$$a_\varepsilon(U_{1\varepsilon}, V_1) = L_\varepsilon(V_1), \qquad \forall V_1 \in W_1. \tag{53}$$

Thanks to the two terms of order ε^{-2} in a_ε in (51), we verify that

$$\|U_{1\varepsilon}\| + \|\boldsymbol{\omega}\cdot\nabla U_{1\varepsilon}\| \lesssim \varepsilon\|q\|_W + \varepsilon^{3/2}\|g\|_b. \tag{54}$$

In what follows, we need a similar estimate for the following solution:

$$a_\varepsilon(\tilde U_{1\varepsilon}, V_1) = L_1(V_1), \qquad \forall V_1 \in W_1. \tag{55}$$

We verify as above that

$$\|\tilde U_{1\varepsilon}\| + \|\boldsymbol{\omega}\cdot\nabla \tilde U_{1\varepsilon}\| \lesssim \varepsilon\|\nabla\overline{q}\| + \varepsilon^{3/2}\|g\|_b. \tag{56}$$

In order to estimate the error coming from the source term $L_0(v)$, we define $\psi_{2\varepsilon}$ as

$$\begin{aligned} \big((\varepsilon G_\varepsilon)\psi_{2\varepsilon}, v\big) &= L_0(v) - a_\varepsilon(U_\varepsilon, v), \qquad \forall v \in W \\ \overline{\psi_{2\varepsilon}} &= 0. \end{aligned} \tag{57}$$

Here $(\cdot,\cdot)$ is the usual inner product of $L^2(X)$. We verify that $\psi_{2\varepsilon}$ is well-posed and is given by

$$\begin{aligned} \psi_{2\varepsilon}(\mathbf{x},\boldsymbol{\omega}) = H_\varepsilon\Big(&\boldsymbol{\omega}\cdot\nabla H_\varepsilon(\boldsymbol{\omega})\cdot\nabla U_\varepsilon - \nabla\cdot D_\varepsilon\nabla U_\varepsilon \\ &+\varepsilon\boldsymbol{\omega}\cdot\nabla H_\varepsilon(q) - 2D_\varepsilon\varepsilon\nabla\cdot\mathbf{q}\Big). \end{aligned} \tag{58}$$

The term within brackets in the above expression is mean zero by construction so that all equalities in (57) are verified. Let us now decompose the exact solution as

$$u_\varepsilon = u_{0\varepsilon} + u_{1\varepsilon}, \qquad a_\varepsilon(u_{k\varepsilon}, v) = L_k(v), \qquad \forall v \in W,\ k = 0, 1. \tag{59}$$

We introduce the following decompositions:

$$u_{0\varepsilon} = U_\varepsilon + \varepsilon^2\psi_{2\varepsilon} + \delta_{0\varepsilon}, \qquad u_{1\varepsilon} = \tilde U_{1\varepsilon} + \delta_{1\varepsilon}, \tag{60}$$

and estimate both terms $\delta_{k\varepsilon}$ for $k = 0, 1$. We start with $k = 0$ and obtain from the transport equation $a_\varepsilon(u_{0\varepsilon}, \delta_{0\varepsilon}) - L_0(\delta_{0\varepsilon}) = 0$ that

$$\begin{aligned} &a_\varepsilon(\delta_{0\varepsilon},\delta_{0\varepsilon}) = -\varepsilon^2\Big(a_\varepsilon(\psi_{2\varepsilon},\delta_{0\varepsilon}) - \frac{1}{\varepsilon^2}\big((\varepsilon G_\varepsilon)\psi_{2\varepsilon},\delta_{0\varepsilon}\big)\Big) \\ &= -\varepsilon^2\Big(\int_X\Big(\frac{1}{\varepsilon^2\sigma_a}\overline{\boldsymbol{\omega}\cdot\nabla\psi_{2\varepsilon}}\ \overline{\boldsymbol{\omega}\cdot\nabla\delta_{0\varepsilon}} + H_\varepsilon(\boldsymbol{\omega}\cdot\nabla\psi_{2\varepsilon})\boldsymbol{\omega}\cdot\nabla\delta_{0\varepsilon}\Big)dp + \frac{1}{\varepsilon}\int_{\Gamma_+}\psi_{2\varepsilon}\delta_{0\varepsilon}\boldsymbol{\omega}\cdot\boldsymbol{\nu}\ dq\Big). \end{aligned}$$

By the Cauchy-Schwarz inequality, this implies that

$$a_\varepsilon(\delta_{0\varepsilon},\delta_{0\varepsilon}) \lesssim \|\overline{\boldsymbol{\omega}\cdot\nabla\psi_{2\varepsilon}}\|\|\overline{\boldsymbol{\omega}\cdot\nabla\delta_{0\varepsilon}}\| + \varepsilon^2\|\boldsymbol{\omega}\cdot\nabla\psi_{2\varepsilon}\|\|\boldsymbol{\omega}\cdot\nabla\delta_{0\varepsilon}\| + \varepsilon\|\psi_{2\varepsilon|\Gamma_+}\|_b\|\delta_{0\varepsilon|\Gamma_+}\|_b.$$

We verify that $\|\overline{\boldsymbol{\omega}\cdot\nabla\psi_{2\varepsilon}}\| \lesssim \varepsilon$ thanks to its expression in (58). This shows that provided that q and U_ε, whence $\psi_{2\varepsilon}$, are sufficiently regular, we obtain that

$$a_\varepsilon^{1/2}(\delta_{0\varepsilon},\delta_{0\varepsilon}) \lesssim \varepsilon\|\psi_{2\varepsilon|\Gamma_+}\|_b + \varepsilon^2\big(\|\boldsymbol{\omega}\cdot\nabla\psi_{2\varepsilon}\| + \varepsilon^{-1}\|\overline{\boldsymbol{\omega}\cdot\nabla\psi_{2\varepsilon}}\|\big). \tag{61}$$

This implies for instance that

$$\|u_{0\varepsilon} - U_\varepsilon\|_W \lesssim \varepsilon. \tag{62}$$

It remains to address the term $u_{1\varepsilon} = \tilde U_{1\varepsilon} + \delta_{1\varepsilon}$. We verify that

$$\begin{aligned} &a_\varepsilon(\tilde U_{1\varepsilon},\delta_{1\varepsilon}) = \int_X\Big(\frac{1}{\varepsilon^2\sigma_a}\overline{\boldsymbol{\omega}\cdot\nabla\tilde U_{1\varepsilon}}\ \overline{\boldsymbol{\omega}\cdot\nabla\delta_{1\varepsilon}} + H_\varepsilon(\boldsymbol{\omega}\cdot\nabla\tilde U_{1\varepsilon})\boldsymbol{\omega}\cdot\nabla\delta_{1\varepsilon} + \frac{G_\varepsilon}{\varepsilon}\tilde U_{1\varepsilon}\delta_{1\varepsilon}\Big)dp \\ &+\frac{1}{\varepsilon}\int_{\Gamma_+}\tilde U_{1\varepsilon}\delta_{1\varepsilon}\boldsymbol{\omega}\cdot\boldsymbol{\nu}\ dq = L_1(\delta_{1\varepsilon}) + \int_X H_\varepsilon(\boldsymbol{\omega}\cdot\nabla\tilde U_{1\varepsilon})\boldsymbol{\omega}\cdot\nabla\delta_{1\varepsilon}dp \\ &= a_\varepsilon(u_{1\varepsilon},\delta_{1\varepsilon}) + \int_X H_\varepsilon(\boldsymbol{\omega}\cdot\nabla\tilde U_{1\varepsilon})\boldsymbol{\omega}\cdot\nabla\delta_{1\varepsilon}dp, \end{aligned}$$

because $\overline{\boldsymbol{\omega}\cdot\nabla v}$ depends only on $\hat v_{\pm1}$ and $\tilde U_{1\varepsilon}\delta_{1\varepsilon} = \Pi_{1\varepsilon}(\tilde U_{1\varepsilon}\delta_{1\varepsilon})$. Now however, $\|H_\varepsilon(\boldsymbol{\omega}\cdot\nabla\tilde U_{1\varepsilon})\| \lesssim \varepsilon$ thanks to (56). This implies that

$$a_\varepsilon(\delta_{1\varepsilon},\delta_{1\varepsilon}) \lesssim \varepsilon\|\delta_{1\varepsilon}\|_W \lesssim \varepsilon^2. \tag{63}$$

In summary we have proved using a variational approach that:

Theorem 1. *Let u_ε and U_ε be the transport and diffusion solutions. Then we have*

$$\|u_\varepsilon - U_\varepsilon\|_W \lesssim \varepsilon, \tag{64}$$

provided that the source term q and the solution U are sufficiently regular.

How regular the solution U and source term q need to be can be explicitly read off the previous formulae. We do not dwell on the details.

2.6 Better error estimates in infinite domains

The accuracy of order $O(\varepsilon)$ cannot be improved in general; see *e.g.* [12]. Indeed, we know that in the presence of boundaries, boundary layer terms need be accounted for by other means than volume asymptotic expansions and diffusion-like approximations. We refer *e.g.* to [3] for two-dimensional numerical simulations quantifying the role of the boundary layers.

In the absence of boundaries however, i.e., when $\Omega = \mathbb{R}^2$, the above method provides more accurate approximations of the transport solution than $O(\varepsilon)$. Indeed we verify from (61) that

$$\|u_{0\varepsilon} - U_\varepsilon\|_W \lesssim \varepsilon^2. \tag{65}$$

The same type of variational arguments (based on explicit test functions similar to $\psi_{2\varepsilon}$) allows us to show that

$$\|u_{1\varepsilon} - \tilde{U}_{1\varepsilon}\|_W \lesssim \varepsilon^2$$

as well, which accounts for the source term $-(\varepsilon\sigma_a)^{-1}\boldsymbol{\omega}\cdot\nabla\overline{q}$. This type of estimates hinges on the fact that $u_{0\varepsilon}$ only involves polynomials that are even in θ (in the sense that $\hat{u_{0\varepsilon}}_n = 0$ for n odd) whereas $u_{1\varepsilon}$ only involves odd polynomials in θ as can been seen from the variational formulations (12) and (44). We finally observe, as is done in the Appendix, that

$$\tilde{U}_{1\varepsilon}(\mathbf{x},\boldsymbol{\omega}) = -\varepsilon H_\varepsilon(\boldsymbol{\omega})\cdot\nabla U_\varepsilon(\mathbf{x}), \tag{66}$$

up to terms that can be estimated to be of order $O(\varepsilon^2)$. In the absence of boundaries, whence of boundary layers, we therefore obtain the following classical result:

$$u_\varepsilon(\mathbf{x},\boldsymbol{\omega}) = U_\varepsilon(\mathbf{x}) - \varepsilon H_\varepsilon(\boldsymbol{\omega})\cdot\nabla U_\varepsilon(\mathbf{x}) + O(\varepsilon^2), \tag{67}$$

which can be shown to be equivalent to the expression

$$u_\varepsilon(\mathbf{x},\boldsymbol{\omega}) = U_\varepsilon(\mathbf{x}) - \frac{\varepsilon}{k_0 - k_1}\boldsymbol{\omega}\cdot\nabla U_\varepsilon(\mathbf{x}) + O(\varepsilon^2). \tag{68}$$

Here the error terms are $O(\varepsilon^2)$ for the $\|\cdot\|_W$ norm for instance.

2.7 A remark on discretizations in the diffusive regime

The variational formulation (15) for transport allows us to easily construct discretizations of the transport solution u_ε by Galerkin approximation. Indeed let W_h be a discrete subspace of W. We may then define Π_h as the orthogonal projection onto W_h for the inner product $a_\varepsilon(\cdot,\cdot)$. Denoting by $u_h = \Pi_h u_\varepsilon$, we have the equivalent characterization:

$$a_\varepsilon(u_h, v) = L_\varepsilon(v), \qquad \forall v \in W_h. \tag{69}$$

Let us equip W with the norm $\|\cdot\|_{W_\varepsilon}$ whose square is defined on the left-hand side of (20). For this norm, a_ε is not only coercive but also continuous with constants independent of ε as we noted earlier. Céa's lemma [9] then implies that

$$\|u_\varepsilon - u_h\|_{W_\varepsilon} \leq C \min_{v\in W_h} \|u_\varepsilon - v\|_{W_\varepsilon}, \tag{70}$$

where C is independent of ε. The error estimate then becomes an approximation theory problem as in [24, 25], where the main difficulty arises because the W_ε norm depends on ε. Although it was more

convenient to equip W with its natural norm in the analysis of diffusion approximations, it is natural to introduce the norm $\|\cdot\|_{W_\varepsilon}$ in the analysis of discretizations (as in [24, 25]).

In the numerical solution of transport problems, it is very often useful to obtain discretizations that behave well in the diffusive regime. This is not always satisfied and is usually characterized by ensuring that the diffusive limit of the discretized transport equation is indeed a consistent discretization of the diffusion equation [15, 20, 21]. We note here the following corollary of orthogonal projections:

$$\Pi_h \Pi_\varepsilon = \Pi_\varepsilon \Pi_h. \tag{71}$$

This asserts that discretizing and taking the diffusive limit are commuting operations so that indeed the discretization of the diffusion limit is indeed the same as the $\varepsilon \to 0$ limit of the discretized transport equation.

3 Transport-diffusion coupling

We want to generalize the results obtained in the preceding section to the physical situation where the diffusive regime is valid in large parts of the domain but not everywhere. We refer to [5] for possible applications, which typically include large domains compared to the mean free path so that the diffusion approximation holds everywhere except for localized areas where the scattering or absorption coefficients may vary too fast.

3.1 Orthogonal projection

A plausible solution to this issue consists of solving the diffusion equation where it is valid and the transport equation elsewhere. It thus remains to find a method that couples both equations at the interface separating their domains of definition. As was shown in [5] in the simplified setting of the even-parity formulation of the transport equation, orthogonal projection is a natural approach when a variational formulation is available.

Let Ω be the physical domain and $\Omega_{\rm di}$ and $\Omega_{\rm tr}$ a non-overlapping partition of Ω. We denote by γ the common interface shared by $\Omega_{\rm di}$ and $\Omega_{\rm tr}$ and assume that it does not overlap with $\partial\Omega$. We denote by $\boldsymbol{\nu}_{\rm di}(\mathbf{x})$ the outward normal to $\Omega_{\rm di}$ at $\mathbf{x} \in \gamma$. Since the diffusion approximation is valid on $\Omega_{\rm di}$ by assumption, we expect the transport solution $u(\mathbf{x}, \boldsymbol{\omega})$ to depend only on $\mathbf{x}$ on $\Omega_{\rm di}$, but to depend on the full phase-space variables $\mathbf{x}, \boldsymbol{\omega}$ on $\Omega_{\rm tr}$. This justifies the introduction of the following spaces

$$W_C = \big\{ f \in W,\ f = f(\mathbf{x}) \text{ on } \Omega_{\rm di} \big\}, \quad W_{C\varepsilon}^{\perp} = \{ f \in W,\ a_\varepsilon(f, v) = 0\ \forall v \in W_C \big\}. \tag{72}$$

Let now $\Pi_{C\varepsilon}$ be the orthogonal (for a_ε) projector onto the Hilbert subspace W_C of W. For u_ε the solution of the transport solution of (15) we then define the *coupled transport-diffusion* solution as

$$u_{C\varepsilon} = \Pi_{C\varepsilon} u_\varepsilon. \tag{73}$$

Variationally, this means that

$$a_\varepsilon(u_{C\varepsilon}, v) = L_\varepsilon(v) \quad \forall v \in W_C. \tag{74}$$

Because a_ε is an inner product on W, whence on W_C, the above solution is uniquely defined.

3.2 Local equations

The solution of (74) can directly be estimated numerically by Galerkin (orthogonal) projection onto finite dimensional subspaces. This is one of the main advantages of variational formulations [24, 25, 26]. It turns out that (74) does not seem to admit any simple "local" representation involving first-order and diffusion equations. In order to better exhibit the nature of the coupling at the interface γ, we introduce the notation

$$u_{\rm tr}(\boldsymbol{\omega}, \mathbf{x}) = u_{C\varepsilon|\Omega_{\rm tr}}(\boldsymbol{\omega}, \mathbf{x}), \qquad u_{\rm di}(\mathbf{x}) = u_{C\varepsilon|\Omega_{\rm di}}(\mathbf{x}) \tag{75}$$

for the solution $u_{C\varepsilon}$ of (74). Because $u_{C\varepsilon} \in W$, we directly obtain the continuity relation $u_{\rm tr}(\boldsymbol{\omega}, \mathbf{x}) = u_{\rm di}(\mathbf{x})$ for $\mathbf{x} \in \gamma$. The other relations are obtained as follows. We first observe that we may recast $a_\varepsilon(u,v) - L_\varepsilon(v)$ as

$$\begin{aligned} a_\varepsilon(u,v) - L_\varepsilon(v) &= \int_X \big(\boldsymbol{\omega}\cdot\nabla u + G_\varepsilon u - \varepsilon q\big)\frac{1}{\varepsilon}\big(I + G_\varepsilon^{-1}\boldsymbol{\omega}\cdot\nabla\big)v dp \\ &\quad + \int_{\Gamma_-} (g - \frac{u}{\varepsilon})v\boldsymbol{\omega}\cdot\boldsymbol{\nu} dq \\ &= \frac{1}{\varepsilon}\int_{(\Omega_{\rm di}\cup\Omega_{\rm tr})\times V} (I - \boldsymbol{\omega}\cdot\nabla G_\varepsilon^{-1})(\boldsymbol{\omega}\cdot\nabla u + G_\varepsilon u - \varepsilon q)v dp \\ &\quad + \int_{\gamma\times V} \big(\varepsilon G_\varepsilon\big)^{-1}\big(\boldsymbol{\omega}\cdot\nabla + G_\varepsilon\big)(u_{\rm di} - u_{\rm tr})\big)v\boldsymbol{\omega}\cdot\boldsymbol{\nu}_{\rm di} dq \\ &\quad + \frac{1}{\varepsilon}\int_{\partial X} (\boldsymbol{\omega}\cdot\nabla u + G_\varepsilon u - \varepsilon q)\boldsymbol{\omega}\cdot\boldsymbol{\nu} v dq + \int_{\Gamma_-}(g - \frac{u}{\varepsilon})v\boldsymbol{\omega}\cdot\boldsymbol{\nu} dq. \end{aligned} \tag{76}$$

Upon restricting the support of v on $\Omega_{\rm tr}$ and $\Omega_{\rm di}$, we find that $u_{\rm tr}$ and $u_{\rm di}$ satisfy the following equations

$$\begin{aligned} &(I - \boldsymbol{\omega}\cdot\nabla G_\varepsilon^{-1})(\boldsymbol{\omega}\cdot\nabla u_{\rm tr} + G_\varepsilon u_{\rm tr} - \varepsilon q) = 0, && \Omega_{\rm tr}\times V \\ &-\nabla\cdot D_\varepsilon\nabla u_{\rm di} + \sigma_a u_{\rm di} = \overline{q} - \varepsilon\nabla\cdot D_\varepsilon\mathbf{q}, && \Omega_{\rm di}. \end{aligned} \tag{77}$$

Once the volume source terms in (76) have vanished, we obtain the following boundary conditions on $\partial\Omega$:

$$\begin{aligned} &(\boldsymbol{\omega}\cdot\nabla u_{\rm tr} + G_\varepsilon u_{\rm tr} - \varepsilon q) + (g - u_{\rm tr}) = 0, && \Gamma_-\cap(\partial\Omega_{\rm tr}\times V) \\ &\boldsymbol{\omega}\cdot\nabla u_{\rm tr} + G_\varepsilon u_{\rm tr} - \varepsilon q = 0, && \Gamma_+\cap(\partial\Omega_{\rm tr}\times V) \\ &\boldsymbol{\nu}_{\rm di}\cdot D_\varepsilon\nabla u_{\rm di} + \frac{c_n}{\varepsilon}u_{\rm di} = J(\mathbf{x}), && \partial\Omega\cap\partial\Omega_{\rm di}. \end{aligned} \tag{78}$$

We observe that $G_\varepsilon(u_{\rm tr} - u_{\rm di}) = 0$ on γ since $u_{\varepsilon C} \in W$. The coupling condition on γ is then equivalent to:

$$\int_V \boldsymbol{\omega}\cdot\nabla u_{\rm tr}\boldsymbol{\omega}\cdot\boldsymbol{\nu}_{\rm di} d\mu(\boldsymbol{\omega}) = \boldsymbol{\nu}_{\rm di}\cdot D_\varepsilon\nabla u_{\rm di} \quad \text{ on } \gamma. \tag{79}$$

In the absence of coupling, i.e., when $\Omega_{\rm tr} = \Omega$, the above equations may be somewhat simplified on $\Omega_{\rm tr}$ as follows (see also [7]). Let $\varphi \in L^2(\Omega_{\rm tr}\times V)$ be an arbitrary test function and let us define $v \in W(\Omega_{\rm tr})$ as the solution to

$$\begin{aligned} &\boldsymbol{\omega}\cdot\nabla v + G_\varepsilon v = G_\varepsilon^{-1}\varphi, && \Omega_{\rm tr}\times V \\ &v = 0, && \Gamma_-(\Omega_{\rm tr}), \end{aligned} \tag{80}$$

where $\Gamma_\pm(\Omega_{\rm tr})$ and $W(\Omega_{\rm tr})$ are defined as $\Gamma_\pm$ and W with Ω replaced by $\Omega_{\rm tr}$. Classical transport theories [12] show that v is uniquely defined and belongs to $W(\Omega_{\rm tr})$. Upon multiplying the first equation in (77) by v and integrating by parts, we obtain using the second equation in (78) that

$$\int_{\Omega_{\rm tr}\times V}\big(\boldsymbol{\omega}\cdot\nabla u_{\rm tr} + G_\varepsilon u_{\rm tr} - \varepsilon q)\varphi dp + \int_{\gamma\times V} G_\varepsilon^{-1}\big(\boldsymbol{\omega}\cdot\nabla u_{\rm tr} + G_\varepsilon u_{\rm tr} - \varepsilon q\big)v\boldsymbol{\omega}\cdot\boldsymbol{\nu}_{\rm di} dq = 0. \tag{81}$$

When $\Omega_{\rm tr} = \Omega$ so that $\gamma = \emptyset$, the above formulation implies that

$$\boldsymbol{\omega}\cdot\nabla u_{\rm tr} + G_\varepsilon u_{\rm tr} - \varepsilon q = 0, \qquad \Omega_{\rm tr}\times V. \tag{82}$$

The above equality holds in the $L^2(\Omega_{\rm tr}\times V)$-sense, which implies that it holds almost everywhere. However, the variational formulation does not allow us to obtain that it also holds at the boundary of the domain, so that the first equation in (78) does not simplify. Only when regularity of the solution can be obtained, so that (82) holds in a stronger sense implying that it still holds at the domain boundary can one conclude that $u = g$ on Γ_-.

In the transport-diffusion coupling, the situation is more complicated as $\boldsymbol{\omega}\cdot\nabla u_{\rm tr} + G_\varepsilon u_{\rm tr} - \varepsilon q$ has no reason to vanish on $\Gamma_+(\Omega_{\rm tr})$. The first-order transport equation (82) then no longer holds and needs to be replaced by the equation for $u_{\rm tr}$ in (77). As in the even-parity formulation considered in [5], we obtain the coupling of the diffusion equation with the second-order transport equation, not the first-order transport equation. This further exemplifies the importance of the boundary conditions (or of the interface conditions in the transport-diffusion coupling) when using second-order variational formulations of first-order transport equations (see also [25, 26]).

3.3 Convergence and error estimates

The convergence results and error estimates are very similar to those for the diffusion approximation and the even-parity formulation developed in [5]. We outline the differences. Let u_ε be the transport solution, $u_{C\varepsilon}$ the coupled transport-diffusion solution, and $\delta u_\varepsilon = u_\varepsilon - u_{C\varepsilon}$. We obtain as before that $\delta u_\varepsilon \in W_{C\varepsilon}^\perp$ so that

$$a_\varepsilon(\delta u_\varepsilon, \delta u_\varepsilon) = a_\varepsilon(u_\varepsilon, \delta u_\varepsilon) = L_\varepsilon(\delta u_\varepsilon).$$

From (20) and (21), we still obtain that

$$\|\delta u_\varepsilon\|_W + \frac{1}{\varepsilon}\|\delta u_\varepsilon - \overline{\delta u_\varepsilon}\| \lesssim \|q\| + \sqrt{\varepsilon}\|g\|_b.$$

This implies the convergence of δu_ε to w (after possible extraction of a subsequence) and $w = \overline{w}$ so that $w \in W_C$; whence $a_\varepsilon(\delta u_\varepsilon, w) = 0$. Passing to the limit $\varepsilon \to 0$ in the above variational formulation yields that $w \equiv 0$.

In order to obtain convergence results, we still split L_ε as in (52). The contribution coming from L_1 is of order $O(\varepsilon)$ as before and we thus concentrate on the contribution from L_0. Let us define $\psi_{2\varepsilon}$ as

$$\begin{aligned} \big((\varepsilon G_\varepsilon)\psi_{2\varepsilon}, v\big) &= L_0(v) - a_\varepsilon(u_{C\varepsilon}, v), \qquad \forall v \in W \\ \overline{\psi_{2\varepsilon}} &= 0. \end{aligned} \tag{83}$$

We verify that $\psi_{2\varepsilon}$ is given by

$$\begin{aligned} \psi_{2\varepsilon}(\mathbf{x}, \boldsymbol{\omega}) = \chi_{\rm di}(\mathbf{x})\Big[H_\varepsilon\Big(&\boldsymbol{\omega}\cdot\nabla H_\varepsilon(\boldsymbol{\omega})\cdot\nabla u_{C\varepsilon} - \nabla\cdot D_\varepsilon\nabla u_{C\varepsilon} \\ &+\varepsilon\boldsymbol{\omega}\cdot\nabla H_\varepsilon(q) - 2D_\varepsilon\varepsilon\nabla\cdot\mathbf{q}\Big)\Big]. \end{aligned} \tag{84}$$

This is the main difference with respect to the diffusion case. Because the (second-order) transport solution is calculated on $\Omega_{\rm tr}$, the correction term only involves errors made on $\Omega_{\rm di}$. So when the coefficients σ_a and k_n wildly oscillate or do not have the correct behavior to justify the diffusion approximation on $\Omega_{\rm tr}$, they will generate errors only through the behavior of $u_{C\varepsilon}$, whence $\psi_{2\varepsilon}$, on $\Omega_{\rm di}$, where the validity of the diffusion approximation renders these errors much smaller.

The rest of the derivation is then as in section 2.5. We obtain that δu_ε is of order ε in W provided that $\psi_{2\varepsilon}$ is sufficiently regular on $\Omega_{\rm di}$. Let us define W_{1C} as the subspace of W of functions $u(\mathbf{x}, \boldsymbol{\omega})$ such that $\hat{u}_n(\mathbf{x}) = 0$ for $|n| \neq 1$ on $\Omega_{\rm di}$. When the boundary conditions are treated with the transport equation so that $\psi_{2\varepsilon|\Gamma_+}$, and the corrector $u_{1C\varepsilon}$ given by the orthogonal projection of u_ε onto W_{1C} is added to $u_{C\varepsilon}$, we obtain an approximation of order ε^2 provided that $\psi_{2\varepsilon}$ is sufficiently regular as in [5].

4 Generalized diffusion models

When the diffusion approximation does not hold in an area relatively large compared to the transport mean free path but still small compared to the overall size of the domain, the transport-diffusion coupling presented above may be the only alternative to the more costly full transport solution. There are cases however where the area of invalidity of diffusion is sufficiently specific so that more macroscopic models may be defined. An example is the treatment of clear layers in optical tomography, where diffusion does not hold locally although modified (generalized) diffusion models can still be used efficiently. We refer to [4, 6] for the derivation of such a model and to [2, 3, 13, 17, 29] for additional references on the problem.

It is not clear how to derive the generalized diffusion models presented in [6] by purely variational means and orthogonal projections. Our objective in this section is rather to extend the models developed in [4, 6] to more general geometries of non-scattering inclusions. From the application's viewpoint, the main novelty of the following derivation is the treatment of narrow non-scattering tubes or filaments in three-dimensional geometry surrounded by highly scattering media. This may have applications in radiation problems in astrophysics and atmospheric cloud modeling. We consider non-scattering and non-absorbing inclusions to simplify the presentation although the results can be generalized to weakly scattering and absorbing media as in [4].

The framework we consider here is the following. Let Ω be a smooth compact domain in $\mathbb{R}^n$ and Ω_ε a smooth non-scattering subset of Ω. We consider the transport problem: find $u_\varepsilon \in W$ such that

$$\begin{array}{ll} \boldsymbol{\omega}\cdot\nabla u_\varepsilon + G_\varepsilon u_\varepsilon = \varepsilon q(\mathbf{x}), & \text{in } \Omega\backslash\Omega_\varepsilon \times V \\ \boldsymbol{\omega}\cdot\nabla u_\varepsilon = 0, & \text{in } \Omega_\varepsilon \times V \\ u_\varepsilon = 0, & \text{on } \Gamma_-. \end{array} \tag{85}$$

It is understood that the jump of u_ε across $\Sigma_\varepsilon = \partial\Omega_\varepsilon$ vanishes since $u_\varepsilon \in W$. We consider the case where G_ε is isotropic and given by (36) to simplify. The diffusion approximation holds in $\Omega\backslash\Omega_\varepsilon$ but not in Ω_ε. Because scattering and absorption are supposed to vanish in Ω_ε, the variational formulations defined in earlier sections need to be regularized (see [26] for more details on this problem). Yet independently of this issue, we claim that for specific forms of Ω_ε, there are simpler methods to approximate u_ε than the transport-diffusion coupling introduced in the previous section.

4.1 A non-local diffusion equation

We model Ω_ε as follows. Let Σ be a smooth (non self-intersecting) closed (to simplify) surface of co-dimension d in the $n-$dimensional domain Ω. Then Ω_ε is the subset of Ω of points that are sufficiently close to Σ:

$$\Omega_\varepsilon = \{\mathbf{x} \in \Omega; \quad d(\mathbf{x}, \Sigma) < L_\varepsilon\}, \tag{86}$$

where $d(\mathbf{x}, \Sigma)$ is the Euclidean distance from $\mathbf{x}$ to Σ and L_ε is a constant that depends on ε. We may thus parameterize Ω_ε as $\Sigma \times B_{L_\varepsilon}$, where B_{L_ε} is the $d-$ dimensional ball of radius L_ε, at least for sufficiently small L_ε.

Let $T_\mathbf{x}\Sigma$ be the $n-d$ dimensional vector space of vectors tangent to Σ at $\mathbf{x} \in \Sigma$ and $N_\mathbf{x}\Sigma$ the d dimensional vector space of vectors normal to Σ at $\mathbf{x} \in \Sigma$. The tangent and normal bundles $T\Sigma$ and $N\Sigma$ are as usual the unions of $T_\mathbf{x}\Sigma$ and $N_\mathbf{x}\Sigma$, respectively, where $\mathbf{x}$ runs over Σ. We also define $\mathbf{N}$ as the subset $(\mathbf{x}, \mathbf{n}(\mathbf{x})) \in N\Sigma$ such that $|\mathbf{n}| = 1$ and $\mathbf{N}_\mathbf{x}$ as the subset $\mathbf{n} \in N_\mathbf{x}\Sigma$ such that $|\mathbf{n}| = 1$. The latter set is isomorphic to the sphere S^{d-1}. It is the unit circle when Σ is a curve in three dimensions and is restricted to two points when Σ is a surface in three dimensions or a curve in two dimensions. We then realize that $\partial\Omega_\varepsilon = \Sigma + L_\varepsilon\mathbf{N}$ is a smooth co-dimension one surface for sufficiently small L_ε.

When L_ε is a positive constant independent of ε, it is shown in [4] that u_ε converges as $\varepsilon \to 0$ to the solution U of a diffusion equation on $\Omega\backslash\Omega_\varepsilon$ (which is in fact independent of ε) with the boundary condition on $\partial\Omega_\varepsilon$ that U is constant on $\partial\Omega_\varepsilon$ and the average of $\frac{\partial U}{\partial n}$ over $\partial\Omega_\varepsilon$ vanishes. This essentially means that nothing much happens inside Ω_ε. Because no scattering hampers the propagation of particles within Ω_ε, an equilibrium is reached which stipulates that u_ε is approximately constant in Ω_ε.

A more interesting regime may be obtained when L_ε is allowed to depend on ε. We assume that L_ε converges to 0 with ε. If L_ε converges too slowly to 0, then we are back to the case where the transport solution equilibrates to a constant inside Ω_ε. If L_ε converges too fast to 0, then the non-scattering inclusion is too small to have any effect and the approximate solution U_ε of u_ε becomes the solution of a diffusion equation with no inclusion. There is an intermediate regime where the physics is richer. Because $L_\varepsilon \ll 1$ in the regime of interest, we can assume that U_ε becomes constant on the $d-$dimensional cross-section $B_\mathbf{x} = \mathbf{x} + \tau L_\varepsilon \mathbf{N}_\mathbf{x}$ for $0 \le \tau \le 1$ as in [4]. This means that $U_\varepsilon(\mathbf{y})$ on $\partial\Omega_\varepsilon$ depends only on $\mathbf{x} \in \Sigma$, where $|\mathbf{x} - \mathbf{y}| = L_\varepsilon$ and generalizes the condition that the jump of U_ε across a co-dimension one surface vanishes as in [4].

Let us now consider the response operator $\mathcal{R}_\varepsilon$ on the non-scattering inclusion Ω_ε, which maps $u_{|\Gamma_-(\partial\Omega_\varepsilon)}$ to $u_{|\Gamma_+(\partial\Omega_\varepsilon)}$ solution of $\boldsymbol{\omega}\cdot\nabla u = 0$ in Ω_ε. Here, $\Gamma_\pm(\partial\Omega_\varepsilon) = \{(\mathbf{x}, \boldsymbol{\omega}) \in \partial\Omega_\varepsilon \times V, \pm\boldsymbol{\omega}\cdot\boldsymbol{\nu}(\mathbf{x}) > 0\}$. We also define $\Gamma_\pm(\mathbf{x}) = \{\boldsymbol{\omega} \in V, \pm\boldsymbol{\omega}\cdot\boldsymbol{\nu}(\mathbf{x}) > 0\}$ for $\mathbf{x} \in \partial\Omega_\varepsilon$ and note that $\partial B_\mathbf{x}$ for $\mathbf{x} \in \Sigma$ is the subset of $\partial\Omega_\varepsilon$ at a distance L_ε from $\mathbf{x}$. We decompose the response operator applied to functions U_ε as $\mathcal{R}_\varepsilon = \mathcal{R}_0 + \varepsilon\mathcal{R}_1$, where $\mathcal{R}_0$ maps $U_\varepsilon(\mathbf{x})$ on $\Gamma_-(\partial\Omega_\varepsilon)$ to $U_\varepsilon(\mathbf{x})$ on $\Gamma_+(\partial\Omega_\varepsilon)$. The correction $\varepsilon\mathcal{R}_1$ will be of order $O(\varepsilon)$ provided that L_ε is suitably chosen.

Following the same procedure as in [4], we obtain that an approximation U_ε of order $O(\varepsilon)$ of u_ε satisfies the following equation

$$\begin{aligned}
&-\nabla\cdot D_\varepsilon\nabla U_\varepsilon+\sigma_a U_\varepsilon=q, && \Omega\backslash\Omega_\varepsilon\\
&D_\varepsilon\frac{\partial U_\varepsilon}{\partial n}+\frac{c_n}{\varepsilon}U_\varepsilon=0, && \partial\Omega\\
&U_\varepsilon(\mathbf{x}+\tau L_\varepsilon\mathbf{n})=U_\varepsilon(\mathbf{x}),\quad (\tau,\mathbf{n})\in(0,1)\times\mathbf{N}_\mathbf{x}, && \mathbf{x}\in\Sigma\\
&\int_{\partial B_\mathbf{x}} D_\varepsilon\frac{\partial U_\varepsilon}{\partial n}d\sigma=\int_{\partial B_\mathbf{x}}\int_{\Gamma_+(\mathbf{x})}\boldsymbol{\omega}\cdot\boldsymbol{\nu}(\mathcal{R}_1U_\varepsilon)d\mu(\boldsymbol{\omega})d\sigma, && \mathbf{x}\in\Sigma.
\end{aligned}\tag{87}$$

The first two equations are the usual diffusion equation with boundary conditions on $\Omega\backslash\Omega_\varepsilon$ where the diffusion approximation is valid. The third equation indicates that the solution U_ε is constant on $B_\mathbf{x}$ for all $\mathbf{x}\in\Sigma$. The fourth equation, which is necessary to evaluate the latter constant, ensures the conservation of the particle current through the interface $\partial B_\mathbf{x}$ for each $\mathbf{x}\in\Sigma$. The left-hand side models ε^{-1} times the current coming into the non-scattering inclusion, while the right-hand side is ε^{-1} times the current going out of the non-scattering inclusion:

$$\int_{\partial B_\mathbf{x}\times V}\boldsymbol{\omega}\cdot\boldsymbol{\nu}v_\varepsilon dq=\int_{\partial B_\mathbf{x}}\int_{\Gamma_-(\mathbf{x})}\boldsymbol{\omega}\cdot\boldsymbol{\nu}U_\varepsilon dq+\int_{\partial B_\mathbf{x}}\int_{\Gamma_+(\mathbf{x})}\boldsymbol{\omega}\cdot\boldsymbol{\nu}\mathcal{R}_\varepsilon U_\varepsilon dq,$$

where v_ε solves $\boldsymbol{\omega}\cdot\nabla v_\varepsilon=0$ in Ω_ε and $v_\varepsilon=U_\varepsilon$ on $\Gamma_-(\partial\Omega_\varepsilon)$. Because $\mathcal{R}_0$ is the identity operator on functions of the form $U_\varepsilon(\mathbf{x})$, ε^{-1} times the transport current takes the form given on the right-hand side of the fourth equation in (87).

We thus obtain an equation for $U_\varepsilon(\mathbf{x})$, which is much less expensive to solve numerically than the full transport solution u_ε. Note however that the boundary conditions in the fourth equation of (87) are non-local and require us to estimate $\mathcal{R}_1$ explicitly. In the case where Σ is a co-dimension one surface, then $\partial B_\mathbf{x}$ and $\mathbf{N}_\mathbf{x}$ reduce to two points for $\mathbf{x}\in\Sigma$ and it is shown in [4] that (87) admits a unique solution for ε sufficiently small.

4.2 Generalized diffusion equation

It remains to find the value of L_ε for which $\mathcal{R}_1$ is indeed an $O(1)$ operator and to see whether the non-local conditions in (87) can be localized. Both questions are answered by the same asymptotic expansions as follows.

We first need to evaluate $\mathcal{R}_1U_\varepsilon(\mathbf{x}+L_\varepsilon\mathbf{n},\boldsymbol{\omega})$. For each $(\mathbf{x}+L_\varepsilon\mathbf{n},\boldsymbol{\omega})\in\Gamma_+(\mathbf{x})$, we have a unique $\mathbf{y}(\mathbf{x},\mathbf{n},\boldsymbol{\omega})\in\partial\Omega_\varepsilon\backslash\{\mathbf{x}+L_\varepsilon\mathbf{n}\}$ such that $\mathbf{x}+L_\varepsilon\mathbf{n}-\mathbf{y}=|\mathbf{x}+L_\varepsilon\mathbf{n}-\mathbf{y}|\boldsymbol{\omega}$, by following the characteristics of the operator $\boldsymbol{\omega}\cdot\nabla$. Let us define $\bar{\mathbf{x}}(\mathbf{x},\mathbf{n},\boldsymbol{\omega})$ as the closest point to $\mathbf{y}$ on Σ. Then we have

$$\mathcal{R}_1U_\varepsilon(\mathbf{x}+L_\varepsilon\mathbf{n},\boldsymbol{\omega})=\frac{1}{\varepsilon}\Big(U_\varepsilon\big(\bar{\mathbf{x}}(\mathbf{x},\mathbf{n},\boldsymbol{\omega})\big)-U_\varepsilon(\mathbf{x})\Big).\tag{88}$$

Assuming to simplify that Σ has positive curvature (in the sense that each curve in Σ has positive curvature), then $|\mathbf{x}-\bar{\mathbf{x}}|\ll 1$ when $L_\varepsilon\ll 1$. Let us define the tangent vector $\boldsymbol{\tau}(\boldsymbol{\omega})\in T_\mathbf{x}\Sigma$ such that $\bar{\mathbf{x}}$ is on the (unique) geodesic starting at $\mathbf{x}$ with direction $\boldsymbol{\tau}(\boldsymbol{\omega})$, and let $d(\mathbf{x},\bar{\mathbf{x}})$ be the geodesic distance (on Σ) between $\mathbf{x}$ and $\bar{\mathbf{x}}$. Geodesics are meant here with respect to the induced metric on Σ seen as a submanifold of $\mathbb{R}^n$ equipped with the Euclidean metric. Then we verify by Taylor expansion that

$$U_\varepsilon(\bar{\mathbf{x}})-U_\varepsilon(\mathbf{x})=\boldsymbol{\tau}(\boldsymbol{\omega})\cdot\nabla_\Sigma\Big(\frac{d^2(\mathbf{x},\bar{\mathbf{x}})}{2}\boldsymbol{\tau}(\boldsymbol{\omega})\cdot\nabla_\Sigma U_\varepsilon\Big)(\mathbf{x})+O(d^3(\mathbf{x},\bar{\mathbf{x}})).\tag{89}$$

Here ∇_Σ is the restriction (projection) of ∇ to $T_\mathbf{x}\Sigma$. We also define $\nabla_\Sigma^\perp$ as the restriction of ∇ to $N_\mathbf{x}\Sigma$. Neglecting the smaller-order term $O(d^3(\mathbf{x},\bar{\mathbf{x}}))$, we see that the operator $\mathcal{R}_1$ is now local in $\mathbf{x}$. Moreover, it will be of order $O(1)$ provided L_ε is chosen so that

$$\frac{1}{\varepsilon}\int_{\partial B_\mathbf{x}}\int_{\Gamma_+(\mathbf{x})}\boldsymbol{\omega}\cdot\boldsymbol{\nu}\boldsymbol{\tau}(\boldsymbol{\omega})\cdot\nabla_\Sigma\Big(\frac{d^2(\mathbf{x},\bar{\mathbf{x}})}{2}\boldsymbol{\tau}(\boldsymbol{\omega})\cdot\nabla_\Sigma U_\varepsilon\Big)(\mathbf{x})d\mu(\boldsymbol{\omega})d\sigma=\nabla_\Sigma\cdot D_\Sigma(\mathbf{x})\nabla_\Sigma U_\varepsilon(\mathbf{x})=O(1).\tag{90}$$

In other words, we want the (positive definite) second-order tensor $D_\Sigma(\mathbf{x})$, defined explicitly in (90) for a given geometry, to be of order $O(1)$.

Tedious calculations similar to those in [4] show that for an interface Σ of co-dimension $d\geq 1$ in a $n=2,3$ dimensional domain Ω, the domain Ω_ε must be characterized by a radius L_ε such that

$$L_\varepsilon^{d+1} |\ln L_\varepsilon| = O(\varepsilon). \tag{91}$$

The result probably holds for larger values of n although this was not considered in detail. In the physically interesting case $n = 3$, we therefore obtain that clear layers (where $d = 1$) of thickness $L_\varepsilon \approx \sqrt{\varepsilon}$ (neglecting logarithmic terms) and tubes (where $d = 2$) of radius $L_\varepsilon \approx \varepsilon^{1/3}$ will have an order $O(1)$ effect on the diffusion solution. The case of clear layers is treated in [4, 6]. In the case of a non-scattering tube, the limiting equation for U_ε as the thickness of the tube tends to 0 is thus given by the local generalized diffusion model:

$$\begin{aligned} &-\nabla \cdot D_\varepsilon \nabla U_\varepsilon + \sigma_a U_\varepsilon = q, && \Omega \backslash \Sigma \\ &D_\varepsilon \frac{\partial U}{\partial n} + \frac{c_n}{\varepsilon} U_n = 0, && \partial\Omega \\ &D_\varepsilon(\mathbf{x}) \lim_{\eta \to 0^+} \int_{\mathbf{N_x}} \boldsymbol{\theta} \cdot \nabla_\Sigma^\perp U_\varepsilon(\mathbf{x} + \eta\boldsymbol{\theta}) d\mu(\boldsymbol{\theta}) = -\nabla_\Sigma \cdot D_\Sigma(\mathbf{x}) \nabla_\Sigma U_\varepsilon, && \Sigma. \end{aligned} \tag{92}$$

It may be easier to understand the solution of the above equation by recasting it in a variational form: Find the unique solution $U \in H^1_\Sigma(\Omega)$ such that for all $V \in H^1_\Sigma(\Omega)$, we have:

$$\int_\Omega (D_\varepsilon \nabla U \cdot \nabla V + \sigma_a UV) d\mathbf{x} + \frac{c_n}{\varepsilon} \int_{\partial\Omega} UV d\sigma(\mathbf{x}) + \int_\Sigma D_\Sigma \nabla_\Sigma U \nabla_\Sigma V dl(\mathbf{x}) = \int_\Omega Vg d\mathbf{x}. \tag{93}$$

When $n = 3$ and $d = 2$, then $l(\mathbf{x})$ is the (one-dimensional) arclength along the curve Σ and ∇_Σ is nothing but $\frac{\partial}{\partial l}$. The Hilbert space $H^1_\Sigma(\Omega)$ is defined as the completion of the pre-Hilbert space of functions of class $\mathcal{C}^1$ on Ω such that $\langle U, U \rangle_\Sigma < \infty$, where the inner product $\langle \cdot, \cdot \rangle_\Sigma$ is defined as:

$$\langle U, V \rangle_\Sigma = \int_\Omega (\nabla U \cdot \nabla V + UV) d\mathbf{x} + \int_\Sigma \nabla_\Sigma U \nabla_\Sigma V dl(\mathbf{x}). \tag{94}$$

We know that $H^1_\Sigma(\Omega)$ is a Hilbert space [28] and that thanks to the uniform positiveness of D_ε, σ_a, and D_Σ on their domains of definition, the variational formulation (93) admits a unique solution by the Lax Milgram theory.

Note that functions in $H^1(\Omega)$, defined in (31) as the natural space for the classical diffusion approximation, do not necessarily admit traces on one-dimensional curves (though functions in $H^{1+\delta}(\Omega)$ do for all $\delta > 0$). This renders the use of the above completion argument necessary to construct $H^1_\Sigma(\Omega)$. This issue does not arise for (co-dimension one) surfaces as functions in $H^1(\Omega)$ indeed admit traces on surfaces. In any event, from the numerical viewpoint, we observe that the non-scattering filament is simply modeled by one additional integration over Σ in the variational formulation (93). This renders its numerical simulation rather straightforward and much less costly computationally than the full transport equation or the non-local diffusion model (87).

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A Local second-order equation and linear corrector

This appendix provides some useful calculations related to the variational formulations introduced in the text and sketches the derivation of the expression for the corrector of order ε. We first verify that by choosing a test function with support in Ω and by integrations by parts that the solution u_ε of (15) also solves

$$(I - \boldsymbol{\omega} \cdot \nabla G_\varepsilon^{-1})(\boldsymbol{\omega} \cdot \nabla u + G_\varepsilon u - \varepsilon q) = 0. \tag{95}$$

Let us introduce the shift operators

$$S_\pm = \mathcal{F}^{-1}\hat{S}_\pm\mathcal{F}, \qquad (\hat{S}_\pm\hat{u})_n = \hat{u}_{n\pm1}. \tag{96}$$

We then verify that

$$\boldsymbol{\omega}\cdot\nabla = \partial S_- + \bar{\partial}S_+.$$

Thanks to (40) and the above equalities, we deduce that (95) is equivalent to:

$$\begin{aligned} &-\Big[\partial\frac{\partial\hat{u}_{n-2}}{\sigma_\varepsilon-k_{n-1}} + \bar{\partial}\frac{\partial\hat{u}_n}{\sigma_\varepsilon-k_{n+1}} + \partial\frac{\bar{\partial}\hat{u}_n}{\sigma_\varepsilon-k_{n-1}} + \bar{\partial}\frac{\bar{\partial}\hat{u}_{n+2}}{\sigma_\varepsilon-k_{n+1}}\Big] + \frac{\sigma_\varepsilon-k_n}{\varepsilon^2}\hat{u}_n \\ &= \hat{q}_n - \varepsilon\Big[\partial\frac{\hat{q}_{n-1}}{\sigma_\varepsilon-k_{n-1}} + \bar{\partial}\frac{\hat{q}_{n+1}}{\sigma_\varepsilon-k_{n+1}}\Big]. \end{aligned} \tag{97}$$

Let u be the transport solution. The equation for its orthogonal projection over linear functions in the angular variable $\Pi_1 u$ is thus

$$-\Big[\partial\frac{\partial\hat{u}_{-1}}{\sigma_\varepsilon-k_0} + \bar{\partial}\frac{\partial\hat{u}_1}{\sigma_\varepsilon-k_2} + \partial\frac{\bar{\partial}\hat{u}_1}{\sigma_\varepsilon-k_0}\Big] + \frac{\sigma_\varepsilon-k_1}{\varepsilon^2}\hat{u}_1 = \hat{q}_1 - \varepsilon\Big[\partial\frac{\hat{q}_0}{\sigma_\varepsilon-k_0} + \bar{\partial}\frac{\hat{q}_2}{\sigma_\varepsilon-k_2}\Big].$$

Up to terms of smaller order that can be estimated, this is

$$-\Big[\partial\frac{\partial\hat{u}_{-1}}{\sigma_\varepsilon-k_0} + \partial\frac{\bar{\partial}\hat{u}_1}{\sigma_\varepsilon-k_0}\Big] + \frac{\sigma_\varepsilon-k_1}{\varepsilon^2}\hat{u}_1 = -\partial\frac{\hat{q}_0}{\varepsilon\sigma_a}.$$

We check that this is also the equation verified by

$$U_1 = -G_\varepsilon^{-1}(\boldsymbol{\omega}\cdot\nabla U_\varepsilon),$$

up to smaller-order terms, which may be written in the Fourier domain as

$$\widehat{(G_\varepsilon^{-1}(\boldsymbol{\omega}\cdot\nabla U_\varepsilon)}_1 = \varepsilon\frac{\partial\hat{U}_\varepsilon}{\sigma_\varepsilon-k_1},$$

where U_ε is the diffusion approximation. Therefore, the expression for the corrector is:

$$U_1(\mathbf{x},\boldsymbol{\omega}) = -\varepsilon H_\varepsilon(\boldsymbol{\omega})\cdot\nabla U_\varepsilon(\mathbf{x}). \tag{98}$$

This is the usual expression for the first-order corrector to the transport solution in the absence of boundaries.

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