Anisotropic diffusion theory

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Chapter from Seth's dissertation

The previous work in anisotropic diffusion has only considered a steady-state problem in an infinite medium [1, 2]. The new understanding of the AD method presented in this chapter provides a theoretical basis for using the AD method in time-dependent and nonlinear contexts, and it also addresses the heretofore unsolved problem of boundary conditions for the AD method.

1 Anisotropic transport equation

We begin by considering the gray transport equation with cross section frozen at some value σ (which could be σ^n for a semi-implicit formulation, or $\sigma^{n+1,(k)}$ if Picard iteration [3] is being used to converge the nonlinearities). The transport equation is:

$$\begin{aligned}\frac{1}{c}\frac{\partial\psi}{\partial t}(\boldsymbol{x},\boldsymbol{\Omega}) + \boldsymbol{\Omega}\cdot\nabla\psi(\boldsymbol{x},\boldsymbol{\Omega}) + \sigma(\boldsymbol{x})\psi(\boldsymbol{x},\boldsymbol{\Omega}) \\ = \frac{1}{4\pi}\sigma(\boldsymbol{x})ac[T(\boldsymbol{x})]^4 + \frac{1}{4\pi}q_r(\boldsymbol{x}) \equiv \frac{1}{4\pi}Q(\boldsymbol{x})\,, \\ x\in V, \boldsymbol{\Omega}\in 4\pi,\end{aligned} \tag{1a}$$

with incident radiation on some subset of the boundary, a Dirchlet boundary condition

$$\psi(\boldsymbol{x},\boldsymbol{\Omega}) = \psi^b(\boldsymbol{x},\boldsymbol{\Omega})\,, \quad \boldsymbol{x}\in\partial V_b,\ \boldsymbol{\Omega}\cdot\boldsymbol{n}<0, \tag{1b}$$

a reflecting boundary condition on the rest of the boundary,

$$\psi(\boldsymbol{x},\boldsymbol{\Omega}) = \psi(\boldsymbol{x},\boldsymbol{\Omega}_r)\,, \quad \boldsymbol{x}\in\partial V_r,\ \boldsymbol{\Omega}\cdot\boldsymbol{n}<0, \tag{1c}$$

The reflected angle on a boundary surface with outward normal $\boldsymbol{n}$ is just

$$\boldsymbol{\Omega}_r = \boldsymbol{\Omega} - 2(\boldsymbol{\Omega}\cdot\boldsymbol{n})\boldsymbol{n} \tag{2}$$

for incident angles, $\boldsymbol{\Omega}\cdot\boldsymbol{n}<0$.

1.1 Conservation equation

The particle (or radiation energy) conservation equation is the zeroth moment of the transport equation. Operating on Eq. (1a) by $\int_{4\pi}(\cdot)\,\mathrm{d}\Omega$ gives

$$\frac{1}{c}\frac{\partial\phi}{\partial t}(\boldsymbol{x}) + \boldsymbol{\nabla}\cdot\boldsymbol{J}(\boldsymbol{x}) + \sigma(\boldsymbol{x})\phi(\boldsymbol{x}) = \sigma(\boldsymbol{x})ac[T(\boldsymbol{x})]^4 + q_r(\boldsymbol{x}) = Q(\boldsymbol{x})\,, \quad \boldsymbol{x}\in V. \tag{3a}$$

As discussed in §**??**, the first two moments of the angular flux are the scalar flux $\phi = \int_{4\pi}\psi\,\mathrm{d}\Omega$ and the current $\boldsymbol{J} = \int_{4\pi}\boldsymbol{\Omega}\psi\,\mathrm{d}\Omega$. Equations (3) form the first piece of the "low-order" set of equations for the AD method. As in many approximate methods, we will be seeking some closure for this equation with an approximate representation of the exact current $\boldsymbol{J}$.

1.2 Anisotropic angular flux

Now we define the "anisotropic angular flux," which is the full angular flux with the isotropic component subtracted off:

$$\Psi(\boldsymbol{x},\boldsymbol{\Omega}) \equiv \psi(\boldsymbol{x},\boldsymbol{\Omega}) - \frac{1}{4\pi}\phi(\boldsymbol{x})\,. \tag{4}$$

This is equivalent to taking a spherical harmonic expansion of ψ, removing the $m = 0$ term, and reconstituting the remainder to form Ψ.

There are two important identities that the anisotropic angular flux satisfies by its definition: Its zeroth moment is identically zero:

$$\int_{4\pi} \Psi(\boldsymbol{x}, \boldsymbol{\Omega}) \, \mathrm{d}\Omega = \int_{4\pi} \psi \, \mathrm{d}\Omega - \frac{1}{4\pi} \int_{4\pi} \mathrm{d}\Omega \, \phi = \phi - \phi = 0 \,, \tag{5a}$$

and its first moment is the current:

$$\int_{4\pi} \boldsymbol{\Omega} \Psi(\boldsymbol{x}, \boldsymbol{\Omega}) \, \mathrm{d}\Omega = \int_{4\pi} \boldsymbol{\Omega} \psi \, \mathrm{d}\Omega - \frac{1}{4\pi} \int_{4\pi} \boldsymbol{\Omega} \, \mathrm{d}\Omega \, \phi = \boldsymbol{J} - \boldsymbol{0} = \boldsymbol{J}(\boldsymbol{x}) \,. \tag{5b}$$

1.2.1 Transport equation

The first step in deriving a transport equation for the anisotropic angular flux Ψ is to modify the particle conservation equation (3a). We move the $\boldsymbol{\nabla} \cdot \boldsymbol{J}$ term to the right hand side, multiply the equation by $\frac{1}{4\pi}$, and add $\frac{1}{4\pi} \boldsymbol{\Omega} \cdot \boldsymbol{\nabla} \phi$ to both sides:

$$\frac{1}{4\pi} \frac{1}{c} \frac{\partial}{\partial t} \phi + \frac{1}{4\pi} \boldsymbol{\Omega} \cdot \boldsymbol{\nabla} \phi + \frac{1}{4\pi} \sigma \phi = \frac{1}{4\pi} Q - \frac{1}{4\pi} \boldsymbol{\nabla} \cdot \boldsymbol{J} + \frac{1}{4\pi} \boldsymbol{\Omega} \cdot \boldsymbol{\nabla} \phi .$$

By making this change, we have taken an equation in $(\boldsymbol{x})$-space back to the higher-dimensional $(\boldsymbol{x}, \boldsymbol{\Omega})$-space. But there is a method in this madness: the left-hand side looks just like the left hand side of a transport equation for $\phi / 4\pi$ instead of ψ.

Subtracting this equation from the transport equation (1a) cancels the isotropic source on the right-hand side, yielding

$$\frac{1}{c} \frac{\partial}{\partial t} \left[\psi - \frac{1}{4\pi} \phi \right] + \boldsymbol{\Omega} \cdot \boldsymbol{\nabla} \left[\psi - \frac{1}{4\pi} \phi \right] + \sigma \left[\psi - \frac{1}{4\pi} \phi \right] = 0 + \frac{1}{4\pi} \boldsymbol{\nabla} \cdot \boldsymbol{J} - \frac{1}{4\pi} \boldsymbol{\Omega} \cdot \boldsymbol{\nabla} \phi .$$

Substituting Eq. (4) gives an exact transport equation for Ψ:

$$\begin{aligned} &\frac{1}{c} \frac{\partial}{\partial t} \Psi(\boldsymbol{x}, \boldsymbol{\Omega}) + \boldsymbol{\Omega} \cdot \boldsymbol{\nabla} \Psi(\boldsymbol{x}, \boldsymbol{\Omega}) + \sigma(\boldsymbol{x}) \Psi(\boldsymbol{x}, \boldsymbol{\Omega}) \\ &\qquad = \frac{1}{4\pi} \boldsymbol{\nabla} \cdot \boldsymbol{J}(\boldsymbol{x}) - \frac{1}{4\pi} \boldsymbol{\Omega} \cdot \boldsymbol{\nabla} \phi(\boldsymbol{x}) \,, \qquad x \in V, \ \boldsymbol{\Omega} \in 4\pi. \end{aligned} \tag{6}$$

No approximations have been made, but now instead of an isotropic source term on the right hand side, we have an anisotropic source term that depends on the unknowns ϕ and $\boldsymbol{J}$.

1.2.2 Incident boundary condition

Next, for specified incident radiation boundaries, we subtract $\phi / 4\pi$ from Eq. (1b):

$$\psi(\boldsymbol{x}, \boldsymbol{\Omega}) - \frac{1}{4\pi} \phi(\boldsymbol{x}) = \psi^b(\boldsymbol{x}, \boldsymbol{\Omega}) - \frac{1}{4\pi} \phi(\boldsymbol{x})$$

Substituting Eq. (4) into the left hand side gives a boundary condition for Ψ:

$$\Psi(\boldsymbol{x}, \boldsymbol{\Omega}) = \psi^b(\boldsymbol{x}, \boldsymbol{\Omega}) - \frac{1}{4\pi} \phi(\boldsymbol{x}) \,, \tag{7}$$

for $\boldsymbol{x} \in \partial V_b$, $\boldsymbol{\Omega} \cdot \boldsymbol{n} < 0$.

1.2.3 Reflecting boundary condition

Likewise with a reflecting boundary, subtract $\phi/4\pi$ from Eq. (1b):

$$\begin{aligned} \psi(\boldsymbol{x},\boldsymbol{\Omega}) - \frac{1}{4\pi}\phi(\boldsymbol{x}) &= \psi(\boldsymbol{x},\boldsymbol{\Omega} - 2(\boldsymbol{\Omega}\cdot\boldsymbol{n})\boldsymbol{n}) - \frac{1}{4\pi}\phi(\boldsymbol{x})\,. \\ \Psi(\boldsymbol{x},\boldsymbol{\Omega}) &= \Psi(\boldsymbol{x},\boldsymbol{\Omega}_r) \end{aligned} \tag{8}$$

for $\boldsymbol{x} \in \partial V_r$, $\boldsymbol{\Omega}\cdot\boldsymbol{n} < 0$.

1.2.4 Initial condition

Finally, to get an initial condition for the anisotropic angular flux, we multiply the low-order initial condition, Eq. (**??**), by $1/4\pi$ and subtract it from the initial condition for the angular flux, Eq. (**??**):

$$\begin{aligned} \psi(\boldsymbol{x},\boldsymbol{\Omega},0) - \frac{1}{4\pi}\phi(\boldsymbol{x},0) &= \psi^i(\boldsymbol{x},\boldsymbol{\Omega} - \frac{1}{4\pi}\phi^i(\boldsymbol{x}) \\ \Psi(\boldsymbol{x},\boldsymbol{\Omega},0) &=\equiv \Psi^i(\boldsymbol{x},\boldsymbol{\Omega})\,, \end{aligned} \tag{9}$$

for $\boldsymbol{x} \in V$, $\boldsymbol{\Omega} \in 4\pi$.

Equations (6), (7), (8), and (9) comprise a full description of the "anisotropic" component of the angular angular flux. Even though they involve unknowns, they are exact.

A later discussion section, §4.5, describes how Fick's law can be derived from the anisotropic angular flux equations by using the linearly anisotropic approximation $\Psi \approx \frac{3}{4\pi}\boldsymbol{\Omega}\cdot\boldsymbol{J}$, but we shall instead use the anisotropic transport equations to derive a new approximation to Ψ that yields an expression distinct from but analogous to Fick's law.

2 Anisotropic diffusion

The anisotropic diffusion approximation is derived by manipulating the anisotropic transport equation and assuming that the gradients and anisotropy of the solution are small. Some care must be taken in deriving a suitable boundary condition, because we desire a simple expression for $\boldsymbol{J}$ that only depends on the low-order unknown ϕ and some other function of space and angle that does not depend on ψ or its moments.

2.1 Modification for boundary condition treatment

In order to formulate transport-matched boundary conditions, we separate Ψ into an internal solution $\tilde{\Psi}$ and a boundary layer solution Ψ_{bl}:

$$\Psi(\boldsymbol{x},\boldsymbol{\Omega}) = \tilde{\Psi}(\boldsymbol{x},\boldsymbol{\Omega}) + \Psi_{\text{bl}}(\boldsymbol{x},\boldsymbol{\Omega})\,. \tag{10}$$

The internal transport equation is just like Eq. (7):

$$\begin{aligned} &\frac{1}{c}\frac{\partial}{\partial t}\tilde{\Psi}(\boldsymbol{x},\boldsymbol{\Omega}) + \boldsymbol{\Omega}\cdot\nabla\tilde{\Psi}(\boldsymbol{x},\boldsymbol{\Omega}) + \sigma(\boldsymbol{x})\tilde{\Psi}(\boldsymbol{x},\boldsymbol{\Omega}) \\ &\qquad = \frac{1}{4\pi}\nabla\cdot\boldsymbol{J}(\boldsymbol{x}) - \frac{1}{4\pi}\boldsymbol{\Omega}\cdot\nabla\phi(\boldsymbol{x}) \equiv \hat{Q}(\boldsymbol{x},\boldsymbol{\Omega})\,, \qquad x \in V,\ \boldsymbol{\Omega} \in 4\pi. \end{aligned} \tag{11a}$$

However, we will define incident boundary conditions for this internal solution to be

$$\tilde{\Psi}(\boldsymbol{x},\boldsymbol{\Omega}) = -\zeta(\boldsymbol{x},\boldsymbol{\Omega})\boldsymbol{\Omega}\cdot\nabla\phi(\boldsymbol{x}) \equiv \tilde{\Psi}^b(\boldsymbol{x},\boldsymbol{\Omega}) \tag{11b}$$

for $\boldsymbol{x} \in \partial V_b$, $\boldsymbol{\Omega} \cdot \boldsymbol{n} < 0$. The function ζ, which lives on the boundary for incident directions, is yet to be determined. This seemingly odd boundary condition will be justified later.

The reflecting boundary condition is just like Eq. (8):

$$\tilde{\Psi}(\boldsymbol{x}, \boldsymbol{\Omega}) = \tilde{\Psi}(\boldsymbol{x}, \boldsymbol{\Omega}_r) \equiv \tilde{\Psi}^b(\boldsymbol{x}, \boldsymbol{\Omega}) \tag{11c}$$

for $\boldsymbol{x} \in \partial V_r$, $\boldsymbol{\Omega} \cdot \boldsymbol{n} < 0$.

Finally, the internal solution contains the same initial condition as Eq. (9):

$$\tilde{\Psi}(\boldsymbol{x}, \boldsymbol{\Omega}, 0) = \Psi^i(\boldsymbol{x}, \boldsymbol{\Omega})\,. \tag{11d}$$

The corresponding transport equation for Ψ_{bl} are defined to satisfy the transport equations for Ψ using the definition in Eq. (10). It has the same left-hand side as Eq. (7) but no internal source:

$$\frac{1}{c}\frac{\partial}{\partial t}\Psi_{\text{bl}}(\boldsymbol{x}, \boldsymbol{\Omega}) + \boldsymbol{\Omega} \cdot \boldsymbol{\nabla}\Psi_{\text{bl}}(\boldsymbol{x}, \boldsymbol{\Omega}) + \sigma(\boldsymbol{x})\Psi_{\text{bl}}(\boldsymbol{x}, \boldsymbol{\Omega}) = 0\,, \tag{12a}$$

for $x \in V$, $\boldsymbol{\Omega} \in 4\pi$. The incident boundary condition accounts for the true incident boundary source as well as the ζ term we introduced:

$$\Psi_{\text{bl}}(\boldsymbol{x}, \boldsymbol{\Omega}) = \psi^b(\boldsymbol{x}, \boldsymbol{\Omega}) - \frac{1}{4\pi}\phi(\boldsymbol{x}) + \zeta(\boldsymbol{x}, \boldsymbol{\Omega})\boldsymbol{\Omega} \cdot \boldsymbol{\nabla}\phi(\boldsymbol{x}) \equiv \Psi^b_{\text{bl}}(\boldsymbol{x}, \boldsymbol{\Omega})\,. \tag{12b}$$

For $\boldsymbol{x} \in \partial V_r$, the boundary layer solution is reflecting:

$$\Psi_{\text{bl}}(\boldsymbol{x}, \boldsymbol{\Omega}) = \Psi_{\text{bl}}(\boldsymbol{x}, \boldsymbol{\Omega}_r)\,. \tag{12c}$$

Finally, because $\tilde{\Psi}$ accounts for the initial condition, the initial condition for Ψ_{bl} is zero: Eq. (9):

$$\Psi_{\text{bl}}(\boldsymbol{x}, \boldsymbol{\Omega}, 0) = 0\,. \tag{12d}$$

If we add Eqs. (12) to Eqs. (11), we recover the anisotropic transport equation. However, unlike the original transport equation, Eqs. (11) and (12) allow us to formulate boundary conditions for the anisotropic diffusion method.

2.2 Integral transport equation

The integral transport equation is formulated [4] by taking the right-hand side of a transport equation to be a known quantity, then integrating along the characteristic ray $\boldsymbol{\Omega}$, accumulating particles born along the ray and attenuating by collisions during their flight. Instead of considering the integral transport equation for ψ, we invert Eqs. (11) to express $\tilde{\Psi}$ as an integral:

$$\begin{aligned}\tilde{\Psi}(\boldsymbol{x}, \boldsymbol{\Omega}) = {} & \tilde{\Psi}^b(\boldsymbol{x} - s_b\boldsymbol{\Omega}, \boldsymbol{\Omega})\,\mathrm{e}^{-\tau(\boldsymbol{x}, \boldsymbol{x} - s_b\boldsymbol{\Omega})}U(ct - s_b) \\ & + \Psi^i(\boldsymbol{x} - ct\boldsymbol{\Omega}, \boldsymbol{\Omega})\,\mathrm{e}^{-\tau(\boldsymbol{x}, \boldsymbol{x} - ct\boldsymbol{\Omega})}U(s_b - ct) \\ & + \int_0^{s_b}\left[\hat{Q}(\boldsymbol{x} - s\boldsymbol{\Omega}, \boldsymbol{\Omega})\right]\mathrm{e}^{-\tau(\boldsymbol{x}, \boldsymbol{x} - s\boldsymbol{\Omega})}\,\mathrm{d}s\,.\end{aligned} \tag{13a}$$

Here, $U(v)$ is the Heaviside function, unity for $v \geq 0$ and zero otherwise. The optical thickness of the medium between points $\boldsymbol{x}$ and $\boldsymbol{x}'$ along direction $\boldsymbol{\Omega} = (\boldsymbol{x}' - \boldsymbol{x}) / \left\|\boldsymbol{x}' - \boldsymbol{x}\right\|$ is

$$\tau(\boldsymbol{x}, \boldsymbol{x}') = \int_0^{\|\boldsymbol{x} - \boldsymbol{x}'\|}\sigma(\boldsymbol{x} - s\boldsymbol{\Omega})\,\mathrm{d}s\,. \tag{13b}$$

The quantity s_b is the distance to the boundary along $-\boldsymbol{\Omega}$ from $\boldsymbol{x}$.

For brevity, we write Eq. (13a) as a sum of linear operators, each of which corresponds to the local contribution of a nonlocal particle source:

$$\begin{aligned}\tilde{\Psi}(\boldsymbol{x},\boldsymbol{\Omega}) &\equiv \mathcal{I}_b\left[\tilde{\Psi}^b\right] + \mathcal{I}_i\left[\Psi^i\right] + \mathcal{I}_v\left[\hat{Q}\right]\\ \tilde{\Psi}(\boldsymbol{x},\boldsymbol{\Omega}) &\equiv -\mathcal{I}_b\left[\zeta\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi\right]_{\partial V_b} + \mathcal{I}_b\left[\tilde{\Psi}(\boldsymbol{x},\boldsymbol{\Omega}_r)\right]_{\partial V_r} + \mathcal{I}_i\left[\Psi^i\right]\\ &\quad + \mathcal{I}_v\left[\frac{1}{4\pi}\boldsymbol{\nabla}\cdot\boldsymbol{J}\right] - \mathcal{I}_v\left[\frac{1}{4\pi}\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi\right].\end{aligned} \tag{14}$$

No approximations or assumptions at all have been made yet. As a result, the inverse equation (13a) still contains the unknowns ϕ and $\boldsymbol{J}$ (as well as the exiting anisotropic current on any reflecting boundaries), and the local value of $\tilde{\Psi}$ depends on the global value of those unknowns.

Our goal is to make reasonable approximations to this equation that yield a low-order approximation to $\boldsymbol{J} = \int_{4\pi}\boldsymbol{\Omega}\tilde{\Psi}\,\mathrm{d}\Omega$ that depends only on local unknowns and certain coefficients that can be calculated without any a priori *knowledge of the exact solution.*

2.3 Asymptotic ansatz and expansions

To simplify the integral transport equation (14), it is necessary to make some approximations. We make an ansatz that the spatial gradients of the angular flux are weak, the angular flux varies slowly in time, and the solution is mildly (but not necessarily linearly) anisotropic:

$$\psi = O(1), \qquad \boldsymbol{\nabla}\psi = O(\epsilon), \qquad \frac{1}{c}\frac{\partial}{\partial t} = O(\epsilon^2), \qquad \int_{4\pi}\boldsymbol{\Omega}\psi\,\mathrm{d}\Omega = O(\epsilon). \tag{15}$$

The contribution from $\boldsymbol{\nabla}\cdot\boldsymbol{J}$ is $O(\epsilon^2)$, as the term contains an $O(\epsilon)$ derivative as well as the $O(\epsilon)$ radiation current. The assumption about the speed of light being very large means that the contribution from the initial condition is $O(\epsilon^2)$.

To derive the anisotropic diffusion method, we first discard the $O(\epsilon^2)$ terms that appear in Eq. (14):

$$\tilde{\Psi} \approx -\mathcal{I}_b\left[\zeta\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi\right]_{\partial V_b} + \mathcal{I}_b\left[\tilde{\Psi}(\boldsymbol{\Omega}_r)\right]_{\partial V_r} - \mathcal{I}_v\left[\frac{1}{4\pi}\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi\right] + O(\epsilon^2) \tag{16}$$

The ansatz about the gradients allows the nonlocal variables in Eq. (13a) to be expanded about the local spatiotemporal point:

$$\phi(\boldsymbol{x}-s\boldsymbol{\Omega}) \sim \phi(\boldsymbol{x}) - s\left(\frac{1}{c}\frac{\partial}{\partial t} + \boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\right)\phi(\boldsymbol{x}) + O(\epsilon^2) \sim \phi(\boldsymbol{x}) + O(\epsilon)\,. \tag{17}$$

This Taylor series will enable, to leading order, the conversion of nonlocal quantities inside the operators $\mathcal{I}[\cdot]$ to local quantities.

2.4 Approximating the streaming term

The streaming term in Eq. (16) is (see Eq. (13a)):

$$-\mathcal{I}_v\left[\frac{1}{4\pi}\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi(\boldsymbol{x})\right] = \int_0^{\|\boldsymbol{x}-\boldsymbol{x}_b\|}\left[-\frac{1}{4\pi}\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi(\boldsymbol{x}-s\boldsymbol{\Omega},t)\right]\mathrm{e}^{-\tau(\boldsymbol{x},\boldsymbol{x}-s\boldsymbol{\Omega})}\,\mathrm{d}s$$

This integral describes the contribution from the volumetric source along $\boldsymbol{\Omega}$, evaluated at a prior point in time (t, the point along s at which a particle would travel to $\boldsymbol{x}$ at time t), attenuated by the medium along the way (the $\mathrm{e}^{-\tau}$ factor).

We now make our first approximation by expanding the distant $\phi(\boldsymbol{x}-s\boldsymbol{\Omega})$ about the local $\phi(\boldsymbol{x})$ using Eq. (17). Thus,

$$\nabla\phi(\boldsymbol{x}-s\boldsymbol{\Omega}) = \nabla\phi(\boldsymbol{x}) + \nabla O(\epsilon) = \nabla\phi(\boldsymbol{x}) + O(\epsilon^2).$$

The expansion is a good approximation if ϕ is smooth, especially because the $\mathrm{e}^{-\tau}$ term exponentially attenuates the non-local components of the Taylor series as s increases, assuming $\sigma \neq 0$ along the ray $\boldsymbol{\Omega}$.

We can now move the unknown ϕ outside the integral, because it is no longer a function of s:

$$\begin{aligned} -\mathcal{I}_v\left[\frac{1}{4\pi}\boldsymbol{\Omega}\cdot\nabla\phi(\boldsymbol{x})\right] &\approx \int_0^{\|\boldsymbol{x}-\boldsymbol{x}_b\|}\left[-\frac{1}{4\pi}\boldsymbol{\Omega}\cdot\nabla\tilde{\phi}(\boldsymbol{x})\right]\mathrm{e}^{-\tau(\boldsymbol{x},\boldsymbol{x}-s\boldsymbol{\Omega})}\,\mathrm{d}s \\ &= -\int_0^{\|\boldsymbol{x}-\boldsymbol{x}_b\|}\left[\frac{1}{4\pi}\right]\mathrm{e}^{-\tau(\boldsymbol{x},\boldsymbol{x}-s\boldsymbol{\Omega})}\,\mathrm{d}s\,\boldsymbol{\Omega}\cdot\nabla\phi(\boldsymbol{x}) \\ &= -\mathcal{I}_v\left[\frac{1}{4\pi}\right]\boldsymbol{\Omega}\cdot\nabla\phi(\boldsymbol{x})\,. \end{aligned} \tag{18}$$

2.5 Approximating the incident boundary term

The incident boundary term in Eq. (16) is

$$-\mathcal{I}_b\left[\zeta\boldsymbol{\Omega}\cdot\nabla\phi\right]_{\partial V_b} = -\left[\zeta(\boldsymbol{x}-s_b\boldsymbol{\Omega},\boldsymbol{\Omega})\boldsymbol{\Omega}\cdot\nabla\phi(\boldsymbol{x}-s_b\boldsymbol{\Omega})\right] \times \mathrm{e}^{-\tau(\boldsymbol{x},\boldsymbol{x}-s_b\boldsymbol{\Omega})}U(ct-s_b)\,.$$

It accounts for particles that start their life at a specified incident boundary inside the current time step and stream along $\boldsymbol{\Omega}$, attenuated by $\mathrm{e}^{-\tau}$ along their path. As the optical thickness between $(\boldsymbol{x})$ and the boundary increases, this term vanishes exponentially fast.

Now we apply the Taylor series expansion from Eq. (17) to ϕ, but not to ζ:

$$\nabla\phi(\boldsymbol{x}-s_b\boldsymbol{\Omega}) \approx \nabla\phi(\boldsymbol{x}) + O(\epsilon^2)\,,$$

and we discard the $O(\epsilon^2)$ term. Now we have

$$\begin{aligned} -\mathcal{I}_b\left[\zeta\boldsymbol{\Omega}\cdot\nabla\phi\right]_{\partial V_b} &\approx -\left[\zeta(\boldsymbol{x}-s_b\boldsymbol{\Omega},\boldsymbol{\Omega})\right]\mathrm{e}^{-\tau(\boldsymbol{x},\boldsymbol{x}-s_b\boldsymbol{\Omega})}U(ct-s_b)\boldsymbol{\Omega}\cdot\nabla\phi \\ &= -\mathcal{I}_b[\zeta]_{\partial V_b}\,\boldsymbol{\Omega}\cdot\nabla\phi(\boldsymbol{x})\,. \end{aligned} \tag{19}$$

2.6 Approximating the reflecting boundary term

For a moment, let us consider a problem without reflecting boundaries, so $\partial V_b = \partial V$. At this point, Eq. (16) has been reduced to

$$\begin{aligned} \tilde{\Psi} &= -\mathcal{I}_b\left[\zeta\boldsymbol{\Omega}\cdot\nabla\phi\right] + \mathcal{I}_i\left[\Psi^i\right] + \mathcal{I}_v\left[\frac{1}{4\pi}\nabla\cdot\boldsymbol{J}\right] - \mathcal{I}_v\left[\frac{1}{4\pi}\boldsymbol{\Omega}\cdot\nabla\phi\right] \\ &\approx -\mathcal{I}_b[\zeta]\,\boldsymbol{\Omega}\cdot\nabla\phi - \mathcal{I}_v\left[\frac{1}{4\pi}\right]\boldsymbol{\Omega}\cdot\nabla\phi\,. \end{aligned}$$

Now the decision to choose the particular form for the boundary condition in Eq. (11b) is clear: under the systematic approximations made so far, the internal solution $\tilde{\Psi}$ can be written

$$\tilde{\Psi}(\boldsymbol{x},\boldsymbol{\Omega}) = -\left\{\mathcal{I}_b[\zeta] + \mathcal{I}_v\left[\frac{1}{4\pi}\right]\right\}\boldsymbol{\Omega}\cdot\nabla\phi \equiv -f(\boldsymbol{x},\boldsymbol{\Omega})\boldsymbol{\Omega}\cdot\nabla\phi(\boldsymbol{x})\,.$$

Let us assume that an approximation to the reflecting boundary condition can be made that, in the general case with mixed reflecting and incident boundaries, also allows us to write

$$\tilde{\Psi}(\boldsymbol{x},\boldsymbol{\Omega}) \approx -f(\boldsymbol{x},\boldsymbol{\Omega})\boldsymbol{\Omega}\cdot\nabla\phi(\boldsymbol{x}) .$$

Substituting this approximation into the reflecting boundary term in Eq. (14) yields

$$\begin{aligned}\mathcal{I}_b\big[\tilde{\Psi}(\boldsymbol{\Omega}_r)\big]_{\partial V_r} &= \big[\tilde{\Psi}(\boldsymbol{x}-s_b\boldsymbol{\Omega},\boldsymbol{\Omega}_r)\big]\,\mathrm{e}^{-\tau(\boldsymbol{x},\boldsymbol{x}-s_b\boldsymbol{\Omega})}U(ct-s_b)\\ &= \big[-f(\boldsymbol{x}-s_b\boldsymbol{\Omega},\boldsymbol{\Omega}_r)\boldsymbol{\Omega}_r\cdot\nabla\phi(\boldsymbol{x}-s_b\boldsymbol{\Omega})\big]\,\mathrm{e}^{-\tau(\boldsymbol{x},\boldsymbol{x}-s_b\boldsymbol{\Omega})}U(ct-s_b) .\end{aligned}$$

First, we expand $\boldsymbol{\Omega}_r$ using Eq. (2).

$$\begin{aligned}\mathcal{I}_b\big[\tilde{\Psi}(\boldsymbol{\Omega}_r)\big]_{\partial V_r} &= -\mathcal{I}_b\big[f(\boldsymbol{x}-s_b\boldsymbol{\Omega},\boldsymbol{\Omega}_r)\,(\boldsymbol{\Omega}-2(\boldsymbol{\Omega}\cdot\boldsymbol{n})\boldsymbol{n})\cdot\nabla\phi(\boldsymbol{x}-s_b\boldsymbol{\Omega})\big]\\ &= -\mathcal{I}_b\big[f(\boldsymbol{x}_b,\boldsymbol{\Omega})\boldsymbol{\Omega}\cdot\nabla\phi(\boldsymbol{x}_b)\big]+\mathcal{I}_b\big[f(\boldsymbol{x}_b,\boldsymbol{\Omega})2(\boldsymbol{\Omega}\cdot\boldsymbol{n})\boldsymbol{n}\cdot\nabla\phi(\boldsymbol{x}_b)\big] .\end{aligned}$$

On a reflecting boundary at any point $\boldsymbol{x}_b$, the exact angular flux satisfies $\boldsymbol{n}\cdot\nabla\psi = 0$, which also means $\boldsymbol{n}\cdot\nabla\phi = 0$. Thus, the second term is zero.

$$\mathcal{I}_b\big[\tilde{\Psi}(\boldsymbol{\Omega}_r)\big]_{\partial V_r} = -\mathcal{I}_b\big[f\boldsymbol{\Omega}\cdot\nabla\phi\big] .$$

Now, just like in the incident boundary situation, we apply the Taylor series expansion from Eq. (17) to ϕ but not to f:

$$\mathcal{I}_b\big[\tilde{\Psi}(\boldsymbol{\Omega}_r)\big]_{\partial V_r} \approx -\big[f(\boldsymbol{x}-s_b\boldsymbol{\Omega},\boldsymbol{\Omega}_r)\big]\,\mathrm{e}^{-\tau(\boldsymbol{x},\boldsymbol{x}-s_b\boldsymbol{\Omega})}U(ct-s_b)\boldsymbol{\Omega}\cdot\nabla\phi(\boldsymbol{x}) ,$$

or, in the more simplified form,

$$\mathcal{I}_b\big[\tilde{\Psi}(\boldsymbol{\Omega}_r)\big]_{\partial V_r} \approx -\mathcal{I}_b\big[f(\boldsymbol{\Omega}_r)\big]_{\partial V_r}\boldsymbol{\Omega}\cdot\nabla\phi(\boldsymbol{x}) . \tag{20}$$

This has the same form as the other approximations to the term. This is crucial to forming the anisotropic diffusion approximation.

2.7 Completed approximation to the anisotropic angular flux

Substituting Eqs. (18), (19), and (20) into Eq. (16) gives a nearly complete approximation to the anisotropic angular flux:

$$\tilde{\Psi} \approx -\mathcal{I}_b[\zeta]_{\partial V_b}\boldsymbol{\Omega}\cdot\nabla\phi - \mathcal{I}_b\big[f(\boldsymbol{\Omega}_r)\big]_{\partial V_r}\boldsymbol{\Omega}\cdot\nabla\phi - \mathcal{I}_v\left[\frac{1}{4\pi}\right]\boldsymbol{\Omega}\cdot\nabla\phi$$

$$\tilde{\Psi} = -\left\{\mathcal{I}_b[\zeta]_{\partial V_b} + \mathcal{I}_b\big[f(\boldsymbol{\Omega}_r)\big]_{\partial V_r} + \mathcal{I}_v\left[\frac{1}{4\pi}\right]\right\}\boldsymbol{\Omega}\cdot\nabla\phi \tag{21}$$

$$\tilde{\Psi}(\boldsymbol{x},\boldsymbol{\Omega}) = -f(\boldsymbol{x},\boldsymbol{\Omega})\boldsymbol{\Omega}\cdot\nabla\phi(\boldsymbol{x}) . \tag{22}$$

The exciting part of this representation is in the interpretation of

$$f(\boldsymbol{x},\boldsymbol{\Omega}) \equiv \mathcal{I}_b[\zeta]_{\partial V_b} + \mathcal{I}_b\big[f(\boldsymbol{\Omega}_r)\big]_{\partial V_r} + \mathcal{I}_v\left[\frac{1}{4\pi}\right] .$$

Converting this from an integral transport representation back to a differential transport equation, we see that f is the solution of a purely absorbing transport equation with a uniform, isotropic source:

$$\boldsymbol{\Omega}\cdot\nabla f(\boldsymbol{x},\boldsymbol{\Omega}) + \sigma f(\boldsymbol{x},\boldsymbol{\Omega}) = \frac{1}{4\pi} , \quad x \in V,\ \boldsymbol{\Omega} \in 4\pi , \tag{23a}$$

with to-be-determined boundary conditions,

$$f(\boldsymbol{x},\boldsymbol{\Omega}) = \zeta(\boldsymbol{x},\boldsymbol{\Omega}) , \quad \boldsymbol{x} \in \partial V_b,\ \boldsymbol{\Omega}\cdot\boldsymbol{n} < 0 . \tag{23b}$$

and with reflecting boundary conditions where the physical problem is reflecting,

$$f(\boldsymbol{x},\boldsymbol{\Omega}) = f(\boldsymbol{x},\boldsymbol{\Omega}_r) , \quad \boldsymbol{x} \in \partial V_r,\ \boldsymbol{\Omega}\cdot\boldsymbol{n} < 0 . \tag{23c}$$

We have applied the approximation that $\frac{1}{c}\frac{\partial}{\partial t} = O(\epsilon^2)$ to turn the transport equation for f into a steady-state equation, and we have accordingly restricted ζ to a function constant within the time step.

2.8 Approximate current

Now we have an equation for the local angle-dependent anisotropic angular flux as a separable function of this simple transport equation f and the scalar angular flux ϕ. We desire a simple low-order equation that provides a closure for the unknown current $\boldsymbol{J}$ in the radiation conservation equation (3a).

To get such a closure, we recall the property from Eq. (5b) that the first moment of the anisotropic angular flux is the current. We therefore apply this identity to our approximate anisotropic angular flux from Eq. (22):

$$\begin{aligned}
\boldsymbol{J}(\boldsymbol{x}) &= \int_{4\pi} \boldsymbol{\Omega}\tilde{\Psi}(\boldsymbol{x},\boldsymbol{\Omega})\,\mathrm{d}\Omega \\
&= -\left[\int_{4\pi} \boldsymbol{\Omega}\boldsymbol{\Omega} f(\boldsymbol{x},\boldsymbol{\Omega})\,\mathrm{d}\Omega\right]\cdot\boldsymbol{\nabla}\phi(\boldsymbol{x}) \\
&= -\mathbf{D}(\boldsymbol{x})\cdot\boldsymbol{\nabla}\phi(\boldsymbol{x}) .
\end{aligned} \tag{24}$$

This resembles "Fick's law," but instead of a scalar diffusion coefficient, the anisotropic diffusion method has a diffusion *tensor*, $\mathbf{D}$, the second angular moment of f:

$$\mathbf{D}(\boldsymbol{x}) \equiv \int_{4\pi} \boldsymbol{\Omega}\boldsymbol{\Omega} f(\boldsymbol{x},\boldsymbol{\Omega})\,\mathrm{d}\Omega . \tag{25}$$

Just as with Fick's law for diffusion, it is substituted into the time-dependent conservation equation to provide a simple approximate equation for the scalar angular flux:

$$-\boldsymbol{\nabla}\cdot\mathbf{D}\phi + \sigma\phi = \sigma a c T^4 + q_r .$$

3 Boundary conditions

In this section, we use the boundary layer equations (12) to address the connected issues of appropriate boundary conditions for the low-order anisotropic diffusion equations and the boundary condition ζ used in the transport calculation for f.

3.1 Incident boundary conditions

A boundary layer analysis [citation needed] shows that the transport boundary layer, the solution of Eqs. (12), decays most rapidly if the solution of the approximate method satisfies the boundary condition

$$0 = \int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}<0} W(|\boldsymbol{\Omega}\cdot\boldsymbol{n}|)\Psi_{\mathrm{bl}}(\boldsymbol{x},\boldsymbol{\Omega})\,\mathrm{d}\Omega , \qquad \boldsymbol{x} \in \partial V_b . \tag{26}$$

W is related to Chandrasekhar's H-function [5] and is well-approximated by a simple polynomial [6]:

$$W(\mu) = \frac{\sqrt{3}}{2}\mu H(\mu) \approx \mu + \tfrac{3}{2}\mu^2 . \tag{27}$$

To recover the Marshak boundary condition, we could use $W(\mu) \approx 2\mu$.

Substituting Eq. (12b) into Eq. (26) gives the low-order boundary condition for anisotropic diffusion:

$$2\int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}<0} W(|\boldsymbol{\Omega}\cdot\boldsymbol{n}|)\psi^b(\boldsymbol{x},\boldsymbol{\Omega})\,\mathrm{d}\Omega = \phi(\boldsymbol{x}) - 2\int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}<0} W(|\boldsymbol{\Omega}\cdot\boldsymbol{n}|)\zeta(\boldsymbol{x},\boldsymbol{\Omega})\boldsymbol{\Omega}\,\mathrm{d}\Omega\cdot\nabla\phi(\boldsymbol{x}) . \tag{28}$$

3.1.1 Determining ζ

The unknown function $\zeta(\boldsymbol{x},\boldsymbol{\Omega})$ that lives on the boundary is a degree of freedom introduced at the beginning of the anisotropic diffusion derivation. It allowed us to formulate a specified boundary condition such that the effect of ζ could be embedded in the anisotropic diffusion tensor $\mathbf{D}$.

To make use of this degree of freedom, we decide to enforce on the boundary the truth from Eq. (5a),

$$\int_{4\pi} \Psi(\boldsymbol{x},\boldsymbol{\Omega})\,\mathrm{d}\Omega = 0 .$$

Note that our approximate $\tilde{\Psi}$ defined in Eq. (22) does not generally satisfy this identity:

$$\begin{aligned} 0 &\stackrel{?}{=} \int_{4\pi} \tilde{\Psi}(\boldsymbol{x},\boldsymbol{\Omega})\,\mathrm{d}\Omega \\ &\stackrel{?}{=} \int_{4\pi} f(\boldsymbol{x},\boldsymbol{\Omega})\boldsymbol{\Omega}\cdot\nabla\phi(\boldsymbol{x})\,\mathrm{d}\Omega \\ &\stackrel{?}{=} \int_{4\pi} \boldsymbol{\Omega} f(\boldsymbol{x},\boldsymbol{\Omega})\,\mathrm{d}\Omega\cdot\nabla\phi(\boldsymbol{x}) . \end{aligned}$$

This identity holds if f is an even function of $\boldsymbol{\Omega}$. One situation where this is the case happens many mean free paths away from internal material boundaries, where f is effectively a constant and therefore even.

On exterior source boundaries, because ζ is defined for incident directions and f is known for exiting directions, we can choose ζ such that f on the boundary is an even function under certain conditions.

Returning to the description of f on an incident boundary in Eq. (23b), we can say that

$$\int_{4\pi} \boldsymbol{\Omega} f(\boldsymbol{x},\boldsymbol{\Omega})\,\mathrm{d}\Omega = \int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}<0} \boldsymbol{\Omega}\zeta(\boldsymbol{x},\boldsymbol{\Omega})\,\mathrm{d}\Omega + \int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}>0} \boldsymbol{\Omega} f(\boldsymbol{x},\boldsymbol{\Omega})\,\mathrm{d}\Omega .$$

Now we set the left hand side to zero, demanding that Eq. (5a) be satisfied:

$$\int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}<0} \boldsymbol{\Omega}\zeta(\boldsymbol{x},\boldsymbol{\Omega})\,\mathrm{d}\Omega = -\int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}>0} \boldsymbol{\Omega} f(\boldsymbol{x},\boldsymbol{\Omega})\,\mathrm{d}\Omega .$$

Making the substitution $\boldsymbol{\Omega} \to -\boldsymbol{\Omega}$ on the right hand side yields

$$\int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}<0} \boldsymbol{\Omega}\zeta(\boldsymbol{x},\boldsymbol{\Omega})\,\mathrm{d}\Omega = \int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}<0} \boldsymbol{\Omega} f(\boldsymbol{x},-\boldsymbol{\Omega})\,\mathrm{d}\Omega . \tag{29}$$

If $f(\boldsymbol{\Omega})$ is azimuthally symmetric about $\boldsymbol{n}$, then f is only a function of the cosine angle between $\boldsymbol{\Omega}$ and $\boldsymbol{n}$:

$$f(\boldsymbol{\Omega}) = \hat{f}(\boldsymbol{\Omega}\cdot\boldsymbol{n}) .$$

Now recall the definition of a reflecting boundary from Eq. (2),

$$\boldsymbol{\Omega}_r = \boldsymbol{\Omega} - 2(\boldsymbol{\Omega}\cdot\boldsymbol{n})\boldsymbol{n}\,.$$

Dotting the reflected vector with the normal vector $\boldsymbol{n}$,

$$\boldsymbol{\Omega}_r\cdot\boldsymbol{n} = \boldsymbol{\Omega}\cdot\boldsymbol{n} - 2(\boldsymbol{\Omega}\cdot\boldsymbol{n})\boldsymbol{n}\cdot\boldsymbol{n} = -\boldsymbol{\Omega}\cdot\boldsymbol{n}\,.$$

Thus,

$$\hat{f}(\boldsymbol{\Omega}_r\cdot\boldsymbol{n}) = \hat{f}(-\boldsymbol{\Omega}\cdot\boldsymbol{n})$$

and

$$f(\boldsymbol{\Omega}_r) = f(-\boldsymbol{\Omega})\,. \tag{30}$$

Therefore, if f is azimuthally symmetric about $\boldsymbol{n}$ on the boundary, Eq. (29) can be written

$$\int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}<0} \boldsymbol{\Omega}\zeta(\boldsymbol{x},\boldsymbol{\Omega})\,\mathrm{d}\Omega = \int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}<0} \boldsymbol{\Omega} f(\boldsymbol{x},\boldsymbol{\Omega}_r)\,\mathrm{d}\Omega\,, \tag{31}$$

which is satisfied by

$$\zeta(\boldsymbol{x},\boldsymbol{\Omega}) = f(\boldsymbol{x},\boldsymbol{\Omega}_r)\,,\quad \boldsymbol{x}\in\partial V_b,\ \boldsymbol{\Omega}\cdot\boldsymbol{n}<0\,. \tag{32}$$

This is not the only definition that satisfies Eq. (31), but it straightforward and has the advantage that all half-space angular moments of ζ are equal to f, an identity that is used to derive Marshak-like boundary conditions later.

Now the boundary condition for f in Eq. (23b) becomes

$$f(\boldsymbol{x},\boldsymbol{\Omega}) = f(\boldsymbol{x},\boldsymbol{\Omega}_r)\,,\quad \boldsymbol{x}\in\partial V_b,\ \boldsymbol{\Omega}\cdot\boldsymbol{n}<0\,. \tag{33}$$

This says that under the approximations, assumptions, and restrictions we made, the transport equation for f has reflecting boundaries everywhere, even where the physical problem does *not* have reflecting boundaries.

3.1.2 Low-order boundary conditions

With a definition for ζ in hand, we return to Eq. (28) and substitute Eq. (32):

$$2\int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}<0} W(|\boldsymbol{\Omega}\cdot\boldsymbol{n}|)\psi^b(\boldsymbol{\Omega})\,\mathrm{d}\Omega = \phi - 2\int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}<0} W(|\boldsymbol{\Omega}\cdot\boldsymbol{n}|)\boldsymbol{\Omega} f(\boldsymbol{\Omega}_r)\,\mathrm{d}\Omega\cdot\nabla\phi\,.$$

We can make the right-hand side clearer by expressing the integral over exiting values of f. Making the substitution $\boldsymbol{\Omega}\to-\boldsymbol{\Omega}$ in the integral:

$$\begin{aligned}
-2\int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}<0} W(|\boldsymbol{\Omega}\cdot\boldsymbol{n}|)\boldsymbol{\Omega} f(\boldsymbol{\Omega}_r)\,\mathrm{d}\Omega &= -2\int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}>0} W(|-\boldsymbol{\Omega}\cdot\boldsymbol{n}|)(-\boldsymbol{\Omega}) f(-\boldsymbol{\Omega}_r)\,\mathrm{d}\Omega \\
&= 2\int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}>0} W(\boldsymbol{\Omega}\cdot\boldsymbol{n})\boldsymbol{\Omega} f(-\boldsymbol{\Omega}_r)\,\mathrm{d}\Omega \\
&= 2\int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}>0} W(\boldsymbol{\Omega}\cdot\boldsymbol{n})\boldsymbol{\Omega} f(\boldsymbol{\Omega})\,\mathrm{d}\Omega\,.
\end{aligned}$$

The boundary condition on f from Eq. (33) in conjunction with Eq. (30) give the equality $f(-\boldsymbol{\Omega}_r) = f(\boldsymbol{\Omega})$.

The low-order, transport-consistent boundary condition for an incident source is therefore

$$2\int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}<0} W(|\boldsymbol{\Omega}\cdot\boldsymbol{n}|)\psi^b(\boldsymbol{x},\boldsymbol{\Omega})\,\mathrm{d}\Omega = \phi(\boldsymbol{x}) + 2\int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}>0} W(\boldsymbol{\Omega}\cdot\boldsymbol{n})\boldsymbol{\Omega} f(\boldsymbol{x},\boldsymbol{\Omega})\,\mathrm{d}\Omega\cdot\nabla\phi(\boldsymbol{x})\,. \tag{34}$$

This form has a particular advantage if we use the Marshak-like approximation that $W(\mu) \approx 2\mu$. Equation (34) becomes

$$
\begin{aligned}
2\int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}<0} [2\,|\boldsymbol{\Omega}\cdot\boldsymbol{n}|]\,\psi^b(\boldsymbol{\Omega})\,\mathrm{d}\Omega &= \phi + 2\int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}>0} [2\boldsymbol{\Omega}\cdot\boldsymbol{n}]\boldsymbol{\Omega} f(\boldsymbol{\Omega})\,\mathrm{d}\Omega\cdot\boldsymbol{\nabla}\phi \\
4\boldsymbol{J}^- &= \phi + 4\boldsymbol{n}\cdot\left[\int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}>0} \boldsymbol{\Omega}\boldsymbol{\Omega} f(\boldsymbol{\Omega})\,\mathrm{d}\Omega\right]\cdot\boldsymbol{\nabla}\phi\,.
\end{aligned}
$$

We chose the boundary condition on f to ensure that it is an even function of $\boldsymbol{\Omega}$ on the boundary. Therefore, the integrand on the right hand side is also an even function of $\boldsymbol{\Omega}$, so

$$
\begin{aligned}
4\boldsymbol{J}^- &= \phi + 4\boldsymbol{n}\cdot\left[\frac{1}{2}\int_{4\pi} \boldsymbol{\Omega}\boldsymbol{\Omega} f(\boldsymbol{\Omega})\,\mathrm{d}\Omega\right]\cdot\boldsymbol{\nabla}\phi\,. \\
4\boldsymbol{J}^- &= \phi + 2\boldsymbol{n}\cdot\int_{4\pi} \boldsymbol{\Omega}\boldsymbol{\Omega} f(\boldsymbol{\Omega})\,\mathrm{d}\Omega\cdot\boldsymbol{\nabla}\phi\,.
\end{aligned}
$$

The integral on the right hand side is the same as in Eq. (24), which defined the anisotropic diffusion tensor. Our Marshak-like boundary approximation is

$$4\boldsymbol{J}^-(\boldsymbol{x}) = \phi(\boldsymbol{x}) + 2\boldsymbol{n}\cdot\mathbf{D}(\boldsymbol{x})\cdot\boldsymbol{\nabla}\phi(\boldsymbol{x})\,. \tag{35}$$

This is entirely analogous to the standard diffusion Marshak boundary condition,

$$4\boldsymbol{J}^-(\boldsymbol{x}) = \phi(\boldsymbol{x}) + 2D(\boldsymbol{x})\boldsymbol{n}\cdot\boldsymbol{\nabla}\phi(\boldsymbol{x})\,.$$

3.2 Reflecting boundary conditions

A reflecting boundary, as described by Eq. (1c), implies

$$\boldsymbol{n}\cdot\boldsymbol{J}(\boldsymbol{x}) = 0\,. \tag{36}$$

Substituting Eq. (24), the first moment of the AD approximation to $\tilde{\Psi}$, we find

$$\boldsymbol{n}\cdot\mathbf{D}(\boldsymbol{x})\cdot\boldsymbol{\nabla}\phi(\boldsymbol{x}) = 0\,. \tag{37}$$

As noted before, the exact angular flux also satisfies

$$\boldsymbol{n}\cdot\boldsymbol{\nabla}\phi(\boldsymbol{x}) = 0\,. \tag{38}$$

This is only compatible with Eq. (37) when $\boldsymbol{n}$ is an eigenvector of $\mathbf{D}$:

$$\boldsymbol{n}\cdot\mathbf{D}(\boldsymbol{x}) = \lambda\boldsymbol{n}\,.$$

Interestingly, as shown in the discussion section, this is the case when f is azimuthally symmetric about $\boldsymbol{n}$, which is exactly the same situation demanded by the boundary condition for specified incident radiation.

Because an azimuthally symmetric f will satisfy both Eq. (36) and Eq. (38), and because we make that demand for the low-order incident boundary condition, we also choose to demand it for reflecting boundaries. Therefore the low-order AD reflecting boundary condition is

$$\boldsymbol{n}\cdot\boldsymbol{\nabla}\phi(\boldsymbol{x}) = 0\,. \tag{39}$$

4 Discussion

Even without numerical results for the anisotropic diffusion equations, a number of interesting and beneficial properties can be deduced from the low-order AD equations (3a), (24), (35), and (39); and from the transport equations for f, Eqs. (23a), (33), and (23c).

4.1 Transport calculation for f

The anisotropic diffusion tensors are calculated from the solution f of a transport problem:

$$\boldsymbol{\Omega} \cdot \nabla f(\boldsymbol{x}, \boldsymbol{\Omega}) + \sigma f(\boldsymbol{x}, \boldsymbol{\Omega}) = \frac{1}{4\pi}, \quad x \in V,\ \boldsymbol{\Omega} \in 4\pi,$$

and

$$f(\boldsymbol{x}, \boldsymbol{\Omega}) = f(\boldsymbol{x}, \boldsymbol{\Omega}_r), \quad \boldsymbol{x} \in \partial V,\ \boldsymbol{\Omega} \cdot \boldsymbol{n} < 0.$$

This is a purely absorbing transport problem with a unit isotropic source, reflecting boundary conditions, and the same cross section as the physical problem being simulated. It is steady-state, although it needs to be recalculated at every time step as σ^* changes.[1]

Because it is purely absorbing, if the boundaries are many mean free paths apart, an S_N solution of f will take just over one transport sweep to solve. The transport equation has no scattering source to converge. There is, however, a caveat because of the opposing reflecting boundaries. If two boundaries on opposite sides of the problem are separated by only a fraction of a mean free path (e.g., a voided channel), and a very fine angular quadrature set is used (one with ordinates that are nearly perpendicular to the boundary), then f will take many iterations to converge. However, because only the second angular moment of f is needed, an unconverged solution inside a small angular range will not affect the anisotropic diffusion tensor very much.

Another desirable property of f is that, because it is a steady-state solution, and because only the second moment $D^{ij} = \int_{4\pi} \Omega^i \Omega^j f \, \mathrm{d}\Omega$ needs to be calculated, the full angle-dependent solution does not need to be stored! This is a tremendous advantage: time-dependent transport typically requires the storage of the full angular flux, so computer memory is often a limiting factor.

If σ^* is a constant throughout the problem, then the solution is $f = 1/4\pi\sigma$. Taking the second moment of f then yields

$$\mathbf{D} = \frac{1}{4\pi\sigma} \int_{4\pi} \boldsymbol{\Omega}\boldsymbol{\Omega} \, \mathrm{d}\Omega = \frac{1}{3\sigma} \mathbf{I}.$$

Substituting this into the anisotropic Fick's law, Eq. (24), we recover the standard Fick's law:

$$\boldsymbol{J} = -\frac{1}{3\sigma} \nabla \phi.$$

In other words, for a homogeneous medium, the anisotropic diffusion method reduces to the standard diffusion method.

4.2 Properties of the anisotropic diffusion tensor

The diffusion tensor is defined in Eq. (25) to be

$$\mathbf{D}(\boldsymbol{x}) \equiv \int_{4\pi} \boldsymbol{\Omega}\boldsymbol{\Omega} f(\boldsymbol{x}, \boldsymbol{\Omega}) \, \mathrm{d}\Omega.$$

[1] The problem for f would also have to be recalculated at every iteration on the nonlinearities if the user wishes to converge $\sigma^* \to \sigma^{n+1}$.

Equivalently, the component in row i, column j of $\mathbf{D}$ is

$$D^{ij} = \int_{4\pi} \Omega^i \Omega^j f(\boldsymbol{x}, \boldsymbol{\Omega}) \, d\Omega \,, \tag{40}$$

where, for example, $i = x$ corresponds $\Omega^x = \boldsymbol{\Omega} \cdot \boldsymbol{i}$.

4.2.1 Limited magnitude

The standard diffusion coefficient is defined as

$$D(\boldsymbol{x}) = \frac{1}{3\sigma(\boldsymbol{x})} \,.$$

As $\sigma \to 0$ locally, $D \to \infty$.

Do I need to restate all of this? It has been covered partially in Larsen and Trahan's work [1].

4.2.2 Fick's law

TODO

4.2.3 Symmetric positive definiteness

From Eq. (40), $\mathbf{D}$ is clearly symmetric: $D^{ij} = D^{ji}$. Yet $\mathbf{D}$ is also symmetric positive definite (SPD), satisfying

$$\boldsymbol{a} \cdot \mathbf{D} \cdot \boldsymbol{a} > 0$$

for all non-zero, real vectors $\boldsymbol{a}$ [7]. To show this, we write

$$\begin{aligned} \boldsymbol{a} \cdot \mathbf{D} \cdot \boldsymbol{a} &= \boldsymbol{a} \cdot \left[\int_{4\pi} \boldsymbol{\Omega}\boldsymbol{\Omega} f(\boldsymbol{x}, \boldsymbol{\Omega}) \, d\Omega \right] \cdot \boldsymbol{a} \\ &= \int_{4\pi} (\boldsymbol{\Omega} \cdot \boldsymbol{a})(\boldsymbol{\Omega} \cdot \boldsymbol{a}) f(\boldsymbol{x}, \boldsymbol{\Omega}) \, d\Omega \,. \\ &= \int_{4\pi} (\boldsymbol{\Omega} \cdot \boldsymbol{a})^2 f(\boldsymbol{x}, \boldsymbol{\Omega}) \, d\Omega \,. \end{aligned}$$

Because the solution for f is strictly positive for all $\boldsymbol{\Omega} \in 4\pi$, and $(\boldsymbol{\Omega} \cdot \boldsymbol{a})^2$ is positive for non-zero $\boldsymbol{a}$, this integral will always be positive. Therefore, $\mathbf{D}$ is SPD.

4.2.4 Eigenvectors

As stated in §3.1.1, if $f(\boldsymbol{\Omega})$ is azimuthally symmetric about some unit vector $\boldsymbol{a}$, then f is only a function of the cosine angle between $\boldsymbol{\Omega}$ and $\boldsymbol{a}$:

$$f(\boldsymbol{\Omega}) = \hat{f}(\boldsymbol{\Omega} \cdot \boldsymbol{a}) \,.$$

If $\boldsymbol{a}$ is an eigenvector of $\mathbf{D}$, then

$$\mathbf{D} \cdot \boldsymbol{a} = \lambda \boldsymbol{a} \,,$$

where λ is a constant. Dotting Eq. (25) with $\boldsymbol{a}$ and omitting the $\boldsymbol{x}$ parameter for brevity, we find

$$\begin{aligned} \mathbf{D} \cdot \boldsymbol{a} &= \int_{4\pi} \boldsymbol{\Omega}\boldsymbol{\Omega} f(\boldsymbol{\Omega}) \, d\Omega \cdot \boldsymbol{a} \\ &= \int_{4\pi} (\boldsymbol{\Omega} \cdot \boldsymbol{a}) \boldsymbol{\Omega} f(\boldsymbol{\Omega}) \, d\Omega \,. \end{aligned}$$

If f is azimuthal about $\boldsymbol{a}$, then

$$\mathbf{D}\cdot\boldsymbol{a} = \int_{4\pi} (\boldsymbol{\Omega}\cdot\boldsymbol{a})\boldsymbol{\Omega}\hat{f}(\boldsymbol{\Omega}\cdot\boldsymbol{a})\,\mathrm{d}\Omega\,.$$

We change the angular coordinates so that $\boldsymbol{i} = \boldsymbol{a}$, which means $\boldsymbol{\Omega}\cdot\boldsymbol{a} = \mu$:

$$\mathbf{D}\cdot\boldsymbol{a} = \int_0^{2\pi}\int_{-1}^{1}(\mu)\left(\mu\boldsymbol{a} + \sqrt{1-\mu^2}\cos\theta\,\boldsymbol{u} + \sqrt{1-\mu^2}\sin\theta\,\boldsymbol{v}\right)\hat{f}(\mu)\,\mathrm{d}\mu\,\mathrm{d}\theta\,.$$

Because $\hat{f}$ is not a function of θ, the integrand is an odd function of θ, so the $\boldsymbol{u}$ and $\boldsymbol{v}$ components are zero.

$$\begin{aligned}\mathbf{D}\cdot\boldsymbol{a} &= 2\pi\int_{-1}^{1}\mu^2\hat{f}(\mu)\,\mathrm{d}\mu\,\boldsymbol{a}\\ &= \lambda\boldsymbol{a}\,.\end{aligned}$$

Thus, if f is azimuthally symmetric about $\boldsymbol{a}$, $\boldsymbol{a}$ is an eigenvector of $\mathbf{D}$.

Because $\mathbf{D}$ is SPD, its eigenvectors are orthogonal [7, p.173]. Therefore, if f is azimuthally symmetric about a cell's surface $\boldsymbol{n}$, then there will be no transverse leakage. The implication for implementation is that on the boundaries of the problem, under the assumptions used to derive the boundary condition for f which state that f is azimuthal about $\boldsymbol{n}$, only the derivative of ϕ along the normal matters. Boundary conditions for the AD method are therefore as simple to implement as those in standard diffusion.

4.3 Properties of the anisotropic diffusion method

The previous section showed that $\mathbf{D}$ is SPD. Therefore, many reasonable discretizations of the anisotropic diffusion equations will be SPD as well, allowing solution by the method of conjugate gradients [7]. This is in contrast to quasidiffusion or Variable Eddington Factor methods, which need more computationally expensive solvers.

4.4 Asymptotic ansatz

The anisotropic diffusion approximation for Ψ, as stated in Eq. (22),

$$\tilde{\Psi}(\boldsymbol{x},\boldsymbol{\Omega}) = -f(\boldsymbol{x},\boldsymbol{\Omega})\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi(\boldsymbol{x})\,,$$

is $O(\epsilon)$. The transport solution for f is $O(1)$; it is roughly the same magnitude as the cross section in the problem. $\boldsymbol{\nabla}\phi$ is $O(\epsilon)$. Multiplying the equation by $\boldsymbol{\Omega}$ and integrating yields an $O(1)$ diffusion tensor and the $O(\epsilon)$ gradient, so $\boldsymbol{J}$ is $O(\epsilon)$ like the ansatz supposes.

Furthermore, as noted in the previous section, the diffusion tensor is continuous in space, and the solution for ϕ therefore has a smooth first derivative. This is compatible with the ansatz that $\boldsymbol{\nabla}\phi$ is $O(\epsilon)$.

4.5 Relating the anisotropic angular flux equation to diffusion

Let us return to Eq. (6). Instead of using the integral transport equation and the rest, we could approximate the anisotropic angular flux as a linear function in angle,

$$\Psi(\boldsymbol{x},\boldsymbol{\Omega}) \approx \frac{3}{4\pi}\boldsymbol{\Omega}\cdot\boldsymbol{J}(\boldsymbol{x})\,,$$

which corresponds to the P_1 approximation $\psi = \frac{1}{4\pi}(\phi + 3\boldsymbol{\Omega}\cdot\boldsymbol{J})$. It also satisfies the identities given in Eqs. (5): $\int_{4\pi}\Psi\,\mathrm{d}\Omega = 0$ and $\int_{4\pi}\boldsymbol{\Omega}\Psi\,\mathrm{d}\Omega = \boldsymbol{J}$.

For the interior, with function arguments omitted, Eq. (6) gives

$$\frac{1}{c}\frac{\partial}{\partial t}\left[\frac{3}{4\pi}\boldsymbol{\Omega}\cdot\boldsymbol{J}\right] + \boldsymbol{\Omega}\cdot\nabla\left[\frac{3}{4\pi}\boldsymbol{\Omega}\cdot\boldsymbol{J}\right] + \sigma\left[\frac{3}{4\pi}\boldsymbol{\Omega}\cdot\boldsymbol{J}\right] = \frac{1}{4\pi}\boldsymbol{\nabla}\cdot\boldsymbol{J} - \frac{1}{4\pi}\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi.$$

Taking the first moment of this equation and operating on it with $\int_{4\pi}\boldsymbol{\Omega}(\cdot)\,\mathrm{d}\Omega$ yields

$$\begin{aligned}\frac{3}{4\pi}\left(\int_{4\pi}\boldsymbol{\Omega\Omega}\,\mathrm{d}\Omega\right)\cdot\frac{1}{c}\frac{\partial}{\partial t}\boldsymbol{J} + \frac{3}{4\pi}\left(\int_{4\pi}\boldsymbol{\Omega\Omega\Omega}\,\mathrm{d}\Omega\right)\cdot\boldsymbol{\nabla}\cdot\boldsymbol{J} + \frac{3}{4\pi}\left(\int_{4\pi}\boldsymbol{\Omega\Omega}\,\mathrm{d}\Omega\right)\cdot\sigma\boldsymbol{J}& \\ = \frac{1}{4\pi}\left(\int_{4\pi}\boldsymbol{\Omega}\,\mathrm{d}\Omega\right)\boldsymbol{\nabla}\cdot\boldsymbol{J} - \frac{1}{4\pi}\left(\int_{4\pi}\boldsymbol{\Omega\Omega}\,\mathrm{d}\Omega\right)\cdot\boldsymbol{\nabla}\phi.&\end{aligned}$$

Now, basic vector identities [8] reduce the parenthesized quantities to very manageable expressions: $\int_{4\pi}\boldsymbol{\Omega\Omega}\,\mathrm{d}\Omega = \frac{4\pi}{3}\mathbf{I}$, and the odd multiples of $\boldsymbol{\Omega}$ integrated over the unit sphere are zero. Thus,

$$\frac{1}{c}\frac{\partial}{\partial t}\boldsymbol{J} + \sigma\boldsymbol{J} = -\frac{1}{3}\boldsymbol{\nabla}\phi.$$

This is the standard P_1 equation, although it was formulated in an admittedly very odd way.

Now if we neglect the time derivative using the quasi-static approximation [9], we recover Fick's law,

$$\boldsymbol{J}(\boldsymbol{x}) = -\frac{1}{3\sigma(\boldsymbol{x})}\boldsymbol{\nabla}\phi(\boldsymbol{x}).$$

5 Summary

The AD method approximates Eqs. (1) with a set of low-order equations for the scalar angular flux ϕ that use a diffusion coefficient calculated from a simple high-order transport equation. To derive the method, we performed the following steps:

1. Define the "anisotropic angular flux" as $\Psi = \psi - \frac{1}{4\pi}\phi$. The goal is to formulate an approximation to Ψ rather than to ψ.

2. Manipulate the radiation transport equation and conservation equation to get a differential transport equation for Ψ.

3. Split $\Psi \equiv \tilde{\Psi} + \Psi_{\mathrm{bl}}$. We will approximate $\tilde{\Psi}$ and use Ψ_{bl} to determine matched boundary conditions.

4. Transform the equation for $\tilde{\Psi}$ to an *integral* transport equation.

5. Assume $\psi = O(1)$, $\frac{1}{c}\frac{\partial}{\partial t} = O(\epsilon^2)$, $\boldsymbol{\nabla} = O(\epsilon)$, $\int_{4\pi}\boldsymbol{\Omega}(\cdot)\,\mathrm{d}\Omega = O(\epsilon)$.

6. Use Taylor series to approximate nonlocal unknowns with local unknowns, discarding small terms. This yields
$$\tilde{\Psi}(\boldsymbol{x},\boldsymbol{\Omega}) \approx -f(\boldsymbol{x},\boldsymbol{\Omega})\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi.$$

7. Apply the standard transport-matching procedure to Ψ_{bl} for vacuum or incident radiation boundary conditions. Use the identity $\int_{4\pi}\Psi\,\mathrm{d}\Omega = 0$ to find the boundary condition for f.

8. Take the first angular moment of $\tilde{\Psi}$ to get $\boldsymbol{J} = -\mathbf{D}\cdot\boldsymbol{\nabla}\phi$.

9. Substitute $\boldsymbol{J}$ into the time-dependent particle conservation equation to get time-dependent anisotropic diffusion.

The low order equation is the result of substituting the approximate Fick's law, Eq. (24) into Eq. (3a):

$$\frac{1}{c}\frac{\partial\phi}{\partial t}(\boldsymbol{x}) - \boldsymbol{\nabla}\cdot\mathbf{D}(\boldsymbol{x})\cdot\boldsymbol{\nabla}\phi(\boldsymbol{x}) + \sigma(\boldsymbol{x})\phi(\boldsymbol{x}) = \sigma(\boldsymbol{x})ac[T(\boldsymbol{x})]^4 + q_r(\boldsymbol{x}), \quad \boldsymbol{x}\in V.$$

From Eq. (**??**), it has an initial condition

$$\phi(\boldsymbol{x},0) = \phi^i(\boldsymbol{x}), \boldsymbol{x}\in V.$$

The incident source boundary condition with the simpler Marshak-like approximation from Eq. (35) is

$$4\boldsymbol{J}^-(\boldsymbol{x}) = \phi(\boldsymbol{x}) + 2\boldsymbol{n}\cdot\mathbf{D}(\boldsymbol{x})\cdot\boldsymbol{\nabla}\phi(\boldsymbol{x}). \quad \boldsymbol{x}\in\partial V_b.$$

The reflecting boundary condition from Eq. (39) is

$$\boldsymbol{n}\cdot\boldsymbol{\nabla}\phi(\boldsymbol{x}) = 0, \quad \boldsymbol{x}\in\partial V_r.$$

The diffusion tensor is defined in Eq. (25),

$$\mathbf{D}(\boldsymbol{x}) \equiv \int_{4\pi} \boldsymbol{\Omega}\boldsymbol{\Omega} f(\boldsymbol{x},\boldsymbol{\Omega})\,\mathrm{d}\Omega,$$

where f is the solution of a purely absorbing transport equation with an isotropic source of unit strength and reflecting boundary conditions, as described in Eqs. (23a), (33), and (23c):

$$\boldsymbol{\Omega}\cdot\boldsymbol{\nabla} f(\boldsymbol{x},\boldsymbol{\Omega}) + \sigma f(\boldsymbol{x},\boldsymbol{\Omega}) = \frac{1}{4\pi}, \quad x\in V,\ \boldsymbol{\Omega}\in 4\pi,$$

and

$$f(\boldsymbol{x},\boldsymbol{\Omega}) = f(\boldsymbol{x},\boldsymbol{\Omega}_r), \quad \boldsymbol{x}\in\partial V,\ \boldsymbol{\Omega}\cdot\boldsymbol{n} < 0.$$

These equations limit to the standard diffusion approximation in a homogeneous medium, but they do not make the diffusion approximation that ψ is linear in angle. We therefore expect the AD method to give much more accurate answers where ψ is a complex function of angle. Chapters **??** and **??** will put this expectation to the test.

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