# Boundary Conditions for the Anisotropic Diffusion Approximation

*Seth R. Johnson, Edward W. Larsen*

*Department of Nuclear Engineering & Radiological Sciences, University of Michigan, Ann Arbor, MI, 48109*
*sethrj@umich.edu, edlarsen@umich.edu*

## INTRODUCTION

Recently, an anisotropic diffusion (AD) equation has been derived that uses transport-calculated AD coefficients to inexpensively but accurately model particle transport, particularly in voided channels, where standard diffusion theory breaks down [**?**, **?**, **?**]. However, these derivations did not address boundary conditions; numerical simulations to test the equations used heuristic boundary conditions.

Here we present a new derivation in which the AD equation and boundary conditions are both obtained systematically from an integral transport equation. Also, we numerically test the AD equation and the proposed boundary conditions on a "flatland" VHTR-like problem driven by a boundary source, and we demonstrate that the results are highly accurate.

## DERIVATION

We consider a 3-D, monoenergetic, steady-state transport equation with isotropic scattering and an isotropic source:

$$\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\psi(\boldsymbol{x},\boldsymbol{\Omega})+\sigma(\boldsymbol{x})\psi(\boldsymbol{x},\boldsymbol{\Omega})=\frac{\sigma_s(\boldsymbol{x})}{4\pi}\int_{4\pi}\psi(\boldsymbol{x},\boldsymbol{\Omega}')\,\mathrm{d}\Omega' + \frac{q(\boldsymbol{x})}{4\pi}\equiv\frac{1}{4\pi}Q(\boldsymbol{x})\,,\quad \boldsymbol{x}\in V,\ \boldsymbol{\Omega}\in 4\pi\,, \tag{1a}$$

with an incident flux boundary condition

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

Operating on Eq. (1a) by $\int_{4\pi}(\cdot)\,\mathrm{d}\Omega$ gives the particle conservation equation

$$\boldsymbol{\nabla}\cdot\boldsymbol{J}(\boldsymbol{x})+\sigma(\boldsymbol{x})\phi(\boldsymbol{x})=Q(\boldsymbol{x})\,,\quad \boldsymbol{x}\in V\,. \tag{2}$$

Adding $\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi$ to both sides of Eq. (2), dividing the resulting equation by $4\pi$, and subtracting from Eq. (1a), the isotropic scattering and extraneous sources cancel. Then, defining $\Psi(\boldsymbol{x},\boldsymbol{\Omega})\equiv\psi(\boldsymbol{x},\boldsymbol{\Omega})-\frac{1}{4\pi}\phi(\boldsymbol{x})$, we get

$$\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\Psi(\boldsymbol{x},\boldsymbol{\Omega})+\sigma(\boldsymbol{x})\Psi(\boldsymbol{x},\boldsymbol{\Omega})=\tfrac{1}{4\pi}\boldsymbol{\nabla}\cdot\boldsymbol{J}(\boldsymbol{x})-\tfrac{1}{4\pi}\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi(\boldsymbol{x})\,. \tag{3a}$$

Subtracting $\phi/4\pi$ from Eq. (1b) gives the boundary condition

$$\Psi(\boldsymbol{x},\boldsymbol{\Omega})=\psi^b(\boldsymbol{x},\boldsymbol{\Omega})-\tfrac{1}{4\pi}\phi(\boldsymbol{x})\,,\quad \boldsymbol{x}\in\partial V,\ \boldsymbol{\Omega}\cdot\boldsymbol{n}<0\,. \tag{3b}$$

The transport solution $\psi$ satisfies these equations exactly. Also, $\Psi$ satisfies the identities

$$\int_{4\pi}\Psi(\boldsymbol{x},\boldsymbol{\Omega})\,\mathrm{d}\Omega=0\quad\text{and}\quad\int_{4\pi}\boldsymbol{\Omega}\Psi(\boldsymbol{x},\boldsymbol{\Omega})\,\mathrm{d}\Omega=\boldsymbol{J}(\boldsymbol{x})\,. \tag{4}$$

To proceed, we write $\Psi$ as the sum of an "interior" solution $\tilde\Psi$ and a "boundary layer" solution $\Psi_{\mathrm{bl}}$:

$$\Psi(\boldsymbol{x},\boldsymbol{\Omega})=\tilde\Psi(\boldsymbol{x},\boldsymbol{\Omega})+\Psi_{\mathrm{bl}}(\boldsymbol{x},\boldsymbol{\Omega})\,. \tag{5}$$

The interior transport equation is just like Eq. (3a):

$$\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\tilde\Psi(\boldsymbol{x},\boldsymbol{\Omega})+\sigma(\boldsymbol{x})\tilde\Psi(\boldsymbol{x},\boldsymbol{\Omega})=\frac{1}{4\pi}\boldsymbol{\nabla}\cdot\boldsymbol{J}(\boldsymbol{x})-\frac{1}{4\pi}\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi(\boldsymbol{x})\,. \tag{6a}$$

We define incident boundary conditions for $\tilde\Psi$ to be

$$\tilde\Psi(\boldsymbol{x},\boldsymbol{\Omega})=-\zeta(\boldsymbol{x},\boldsymbol{\Omega})\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi(\boldsymbol{x})\equiv\tilde\Psi^b(\boldsymbol{x},\boldsymbol{\Omega})\,, \tag{6b}$$

where $\zeta$ is a to-be-determined function on the boundary. The boundary layer solution complements the interior solution, but is expected to tend to zero rapidly with distance from the outer boundary. Its transport equation has no internal source, and its boundary condition is Eq. (6b) subtracted from Eq. (3b):

$$\Psi_{\mathrm{bl}}(\boldsymbol{x},\boldsymbol{\Omega})=\psi^b(\boldsymbol{x},\boldsymbol{\Omega})-\frac{1}{4\pi}\phi(\boldsymbol{x})+\zeta(\boldsymbol{x},\boldsymbol{\Omega})\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi(\boldsymbol{x})\,. \tag{7}$$

Integrating along a characteristic ray transforms the differential equation (6a) and its boundary condition (6b) into an integral transport equation [**?**]:

$$\begin{aligned}\tilde\Psi(\boldsymbol{x},\boldsymbol{\Omega})&=\tilde\Psi^b(\boldsymbol{x}-s_b\boldsymbol{\Omega},\boldsymbol{\Omega})\,\mathrm{e}^{-\tau(\boldsymbol{x},\boldsymbol{x}-s_b\boldsymbol{\Omega})}\\&\quad+\int_0^{s_b}\Big[\tfrac{1}{4\pi}\boldsymbol{\nabla}\cdot\boldsymbol{J}(\boldsymbol{x}-s\boldsymbol{\Omega},\boldsymbol{\Omega})\\&\qquad-\tfrac{1}{4\pi}\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi(\boldsymbol{x}-s\boldsymbol{\Omega},\boldsymbol{\Omega})\Big]\mathrm{e}^{-\tau(\boldsymbol{x},\boldsymbol{x}-s\boldsymbol{\Omega})}\,\mathrm{d}s\end{aligned} \tag{8a}$$

$$\equiv-\mathcal{I}_b[\zeta\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi]+\mathcal{I}_v\Big[\tfrac{1}{4\pi}\boldsymbol{\nabla}\cdot\boldsymbol{J}\Big]-\mathcal{I}_v\Big[\tfrac{1}{4\pi}\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi\Big]\,. \tag{8b}$$

Here $\tau(\boldsymbol{x},\boldsymbol{x}')$ is the optical distance between points $\boldsymbol{x}$ and $\boldsymbol{x}'$ along the direction $\boldsymbol{\Omega}=(\boldsymbol{x}'-\boldsymbol{x})/\,\|\boldsymbol{x}'-\boldsymbol{x}\|$, and $s_b$ is the distance to the boundary along $-\boldsymbol{\Omega}$ from $\boldsymbol{x}$.

Now we assume that the spatial gradients of the angular flux are weak, and the solution is mildly (but not necessarily linearly) anisotropic:

$$\psi=O(1),\qquad\boldsymbol{\nabla}\psi=O(\epsilon),\qquad\int_{4\pi}\boldsymbol{\Omega}\psi\,\mathrm{d}\Omega=O(\epsilon). \tag{9}$$

Then $\boldsymbol{\nabla}\cdot\boldsymbol{J}=O(\epsilon^2)$, and the second term in Eq. (8b) is neglected. We also expand the nonlocal variables in Eq. (8a) about the local spatial point:

$$\phi(\boldsymbol{x}-s\boldsymbol{\Omega})\sim\phi(\boldsymbol{x})-s\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi(\boldsymbol{x})+O(\epsilon^2)\sim\phi(\boldsymbol{x})+O(\epsilon)\,. \tag{10}$$

Then the third term in Eq. (8b) simplifies to

$$
\begin{aligned}
-\mathcal{I}_v\left[\frac{1}{4\pi}\boldsymbol{\Omega}\cdot\nabla\phi(\boldsymbol{x})\right] &\approx \int_0^{\|\boldsymbol{x}-\boldsymbol{x}_b\|}\left[-\frac{1}{4\pi}\boldsymbol{\Omega}\cdot\nabla\phi(\boldsymbol{x})\right]\mathrm{e}^{-\tau(\boldsymbol{x},\boldsymbol{x}-s\boldsymbol{\Omega})}\,\mathrm{d}s \\
&= -\int_0^{\|\boldsymbol{x}-\boldsymbol{x}_b\|}\left[\tfrac{1}{4\pi}\right]\mathrm{e}^{-\tau(\boldsymbol{x},\boldsymbol{x}-s\boldsymbol{\Omega})}\,\mathrm{d}s\,\boldsymbol{\Omega}\cdot\nabla\phi(\boldsymbol{x}) \\
&= -\mathcal{I}_v\left[\tfrac{1}{4\pi}\right]\boldsymbol{\Omega}\cdot\nabla\phi(\boldsymbol{x}) + O(\epsilon^2)\,. \qquad (11)
\end{aligned}
$$

Similarly, the boundary term in Eq. (8b) becomes

$$
-\mathcal{I}_b[\zeta\boldsymbol{\Omega}\cdot\nabla\phi]_{\partial V_b} \approx -\mathcal{I}_b[\zeta]_{\partial V_b}\,\boldsymbol{\Omega}\cdot\nabla\phi(\boldsymbol{x}) + O(\epsilon^2)\,. \qquad (12)
$$

Substituting Eqs. (11) and (12) into Eq. (8b), and discarding $O(\epsilon^2)$ terms, we obtain

$$
\begin{aligned}
\tilde{\Psi}(\boldsymbol{x},\boldsymbol{\Omega}) &\approx -\mathcal{I}_b[\zeta]_{\partial V_b}\,\boldsymbol{\Omega}\cdot\nabla\phi - \mathcal{I}_v\left[\tfrac{1}{4\pi}\right]\boldsymbol{\Omega}\cdot\nabla\phi \\
&\equiv -f(\boldsymbol{x},\boldsymbol{\Omega})\boldsymbol{\Omega}\cdot\nabla\phi(\boldsymbol{x})\,. \qquad (13)
\end{aligned}
$$

Converting the $\mathcal{I}[\cdot]$ terms back into the differential form, we find that $f$ satisfies a purely absorbing transport equation with a uniform, unit isotropic source:

$$
\boldsymbol{\Omega}\cdot\nabla f(\boldsymbol{x},\boldsymbol{\Omega}) + \sigma(\boldsymbol{x})f(\boldsymbol{x},\boldsymbol{\Omega}) = \tfrac{1}{4\pi}\,, \quad x\in V,\ \boldsymbol{\Omega}\in 4\pi\,, \quad (14a)
$$

with a to-be-determined boundary condition:

$$
f(\boldsymbol{x},\boldsymbol{\Omega}) = \zeta(\boldsymbol{x},\boldsymbol{\Omega})\,, \quad \boldsymbol{x}\in\partial V,\ \boldsymbol{\Omega}\cdot\boldsymbol{n} < 0\,. \qquad (14b)
$$

We use the identity from Eq. (4) to get an expression for the current by taking the first moment of Eq. (13):

$$
\begin{aligned}
\boldsymbol{J}(\boldsymbol{x}) &= -\left(\int_{4\pi}\boldsymbol{\Omega}\boldsymbol{\Omega}f(\boldsymbol{x},\boldsymbol{\Omega})\,\mathrm{d}\Omega\right)\cdot\nabla\phi(\boldsymbol{x}) \\
&= -\mathbf{D}(\boldsymbol{x})\cdot\nabla\phi(\boldsymbol{x})\,. \qquad (15)
\end{aligned}
$$

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 $f$.

The unknown function $\zeta(\boldsymbol{x},\boldsymbol{\Omega})$, introduced at the beginning of the anisotropic diffusion derivation, allowed us to formulate a specified boundary condition in which the effect of $\zeta$ could be embedded in the anisotropic diffusion tensor $\mathbf{D}$. To make use of this degree of freedom, we enforce on the boundary the fact from Eq. (4) that the zeroth moment of $\Psi(\boldsymbol{x},\boldsymbol{\Omega})$ is zero. Applying the identity to Eq. (13) shows that for this to hold, we must have

$$
\int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}>0}\boldsymbol{\Omega}f(\boldsymbol{x},\boldsymbol{\Omega})\,\mathrm{d}\Omega = \int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}<0}(-\boldsymbol{\Omega})\zeta(\boldsymbol{x},\boldsymbol{\Omega})\,\mathrm{d}\Omega\,. \qquad (16)
$$

One way to satisfy this is to make $f$ an even function of $\boldsymbol{\Omega}$, $\zeta(\boldsymbol{\Omega}) = f(-\boldsymbol{\Omega})$. Furthermore, if $f$ is azimuthally symmetric about $\boldsymbol{n}$ on the boundary, then

$$
f(\boldsymbol{x},\boldsymbol{\Omega}) = \zeta(\boldsymbol{x},\boldsymbol{\Omega}) = f(\boldsymbol{x},\boldsymbol{\Omega}-2(\boldsymbol{n}\cdot\boldsymbol{\Omega})\boldsymbol{n})\,, \quad \boldsymbol{x}\in\partial V,\ \boldsymbol{\Omega}\cdot\boldsymbol{n}<0\,,
$$

which is a specular reflecting boundary condition for $f$.

Now we return to the boundary layer transport equation (7). A lengthy analysis shows that the transport boundary layer decays most rapidly if the solution of the approximate method satisfies the boundary condition

$$
0 = \int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}<0} W(|\boldsymbol{\Omega}\cdot\boldsymbol{n}|)\Psi_{\mathrm{bl}}(\boldsymbol{x},\boldsymbol{\Omega})\,\mathrm{d}\Omega\,, \qquad \boldsymbol{x}\in\partial V\,, \qquad (17)
$$

where $W(\mu)$ is well approximated by the simple polynomial $\mu + \frac{3}{2}\mu^2$ [**?**]. Applying Eq. (17) to Eq. (7), we find

$$
\begin{aligned}
&2\int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}<0} W(|\boldsymbol{\Omega}\cdot\boldsymbol{n}|)\psi^b(\boldsymbol{x},\boldsymbol{\Omega})\,\mathrm{d}\Omega \\
&\qquad = \phi(\boldsymbol{x}) - 2\int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}<0} W(|\boldsymbol{\Omega}\cdot\boldsymbol{n}|)\zeta(\boldsymbol{x},\boldsymbol{\Omega})\boldsymbol{\Omega}\,\mathrm{d}\Omega\cdot\nabla\phi(\boldsymbol{x})\,,
\end{aligned}
$$

or, rewriting the right hand side in terms of incident angles using $\zeta(\boldsymbol{\Omega}) = f(-\boldsymbol{\Omega})$,

$$
\begin{aligned}
&2\int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}<0} W(|\boldsymbol{\Omega}\cdot\boldsymbol{n}|)\psi^b(\boldsymbol{x},\boldsymbol{\Omega})\,\mathrm{d}\Omega \\
&\qquad = \phi(\boldsymbol{x}) + 2\int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}>0} W(\boldsymbol{\Omega}\cdot\boldsymbol{n})\boldsymbol{\Omega}f(\boldsymbol{x},\boldsymbol{\Omega})\,\mathrm{d}\Omega\cdot\nabla\phi(\boldsymbol{x})\,. \qquad (18)
\end{aligned}
$$

If instead we use $W(\mu) = 2\mu$, we obtain a less accurate Marshak-like boundary condition

$$
4J^-(\boldsymbol{x}) = \phi(\boldsymbol{x}) + 2\boldsymbol{n}\cdot\mathbf{D}(\boldsymbol{x})\cdot\nabla\phi(\boldsymbol{x})\,, \qquad (19)
$$

where $J^- \equiv \int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}<0}|\boldsymbol{\Omega}\cdot\boldsymbol{n}|\,\psi^b\,\mathrm{d}\Omega$ is the incident current.

## DISCUSSION

In a homogeneous medium, the reflecting boundary condition on $f$ gives a solution $f = 1/(4\pi\sigma)$, which gives the standard diffusion result $\mathbf{D} = \mathbf{I}/(3\sigma)$ and causes Eq. (18) to simplify to the transport-corrected diffusion boundary condition.

We chose a reflecting boundary to satisfy Eq. (16), but that is not the only possible choice. A white boundary (which has an isotropic incident distribution) also satisfies it, although that choice does not generally lead to Eqs. (18) and Eq. (19). However, a white boundary does have the property of leading to faster convergence of an $\mathrm{S}_N$ solution of $f$ when very few mean free paths separate two boundaries.

The transport problem for $f$ does not need to store the full angular flux; it only needs to accumulate the components of the second angular moment. However, for development purposes, storing $f(\boldsymbol{x},\boldsymbol{\Omega})$ would allow the AD representation to the angular flux to be visualized as

$$
\psi_{\mathrm{AD}}(\boldsymbol{x},\boldsymbol{\Omega}) = \tfrac{1}{4\pi}\phi(\boldsymbol{x}) - f(\boldsymbol{x},\boldsymbol{\Omega})\boldsymbol{\Omega}\cdot\nabla\phi(\boldsymbol{x})\,.
$$

## NUMERICAL RESULTS

As a test problem, we consider a diffusive medium in flatland[1] on the domain $0 \le x \le 5$ and $0 \le y \le 10$, with a

[1] The low-order AD boundary conditions in flatland have different coefficients.

channel of unit width running vertically through the middle ($2.5 \le x \le 3.5$). The diffusive region has $\sigma = 1$ and $\sigma_s = 0.99$, and the channel has $\sigma = 0.01$ and $\sigma_s = 0.0099$. The problem has reflecting boundaries on the top, left, and right sides, and an incident boundary condition on the bottom. The geometry and cross sections are similar to Larsen and Trahan's VHTR problem [**?**].

The anisotropic diffusion equations and boundary conditions are implemented in the PyTRT transport code [**?**] using a finite difference scheme and executed with a very fine spatial grid. For comparison purposes, Monte Carlo and standard diffusion are also plotted. We compare the AD method using three different boundary conditions for $f$ on the bottom surface: a reflecting boundary, a white boundary, and a vacuum boundary. The vacuum boundary is not consistent with our theory but is shown to gauge how much $\phi$ is affected by the choice of $\zeta$.

Figure 1 shows a line-out of the scalar flux $\phi(2.5, y)$, along the center of the channel. Standard diffusion fails because $\sigma = 0.01$ leads to a very large diffusion coefficient, resulting in a nearly constant solution inside the channel. The anisotropic diffusion performs exceedingly well, and the white boundary condition for $f$ gives a better result than the reflecting boundary condition.

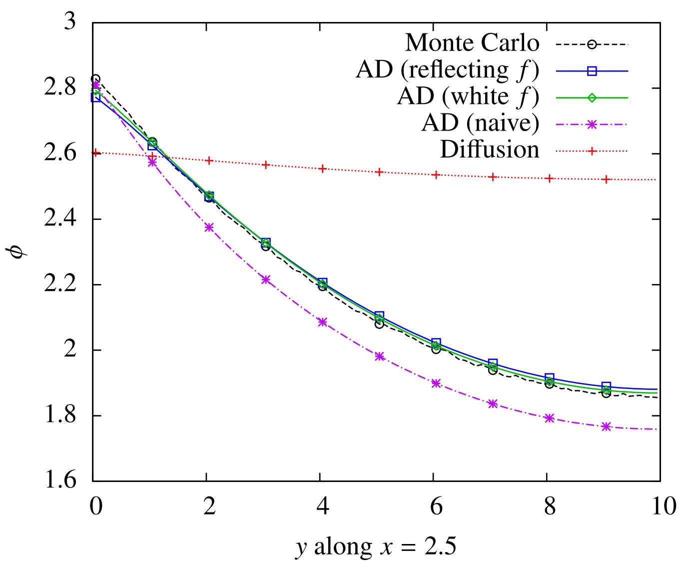


Fig. 1. Scalar flux along the centerline of the channel with an isotropic boundary condition at $y = 0$.

A close examination of the numerical solutions gives some insight into these results. AD does not exactly model the peak of freely streaming photons in the channel, but it does accurately approximate the angular flux shape driven by scattering from the diffusive regions along the edge of the channel. The standard linear-in-angle diffusion approximation does not accurately represent these features. Also, a reflecting boundary for $f$ produces a peak in $f$ along the channel, but a white boundary condition gives a more isotropic shape, better matching the incident isotropic boundary condition. This suggests that a more accurate way to satisfy Eq. (16) may be to have $\zeta$ take the shape of the true boundary condition. This will be examined in future work.

## CONCLUSIONS

We have presented a new derivation of the anisotropic diffusion (AD) approximation to the transport equation, yielding both the previously-known AD equation and new boundary conditions for this equation. The AD method requires that a purely-absorbing transport problem be solved to determine the anisotropic diffusion coefficients. Because of this, the AD approximation is more costly than standard diffusion, but much less costly than a transport simulation (Monte Carlo or deterministic). Numerical testing of a problem with two diffusive regions bordering an optically thin channel, driven by a surface source, show that the AD method is much more accurate than standard diffusion, with results comparable to Monte Carlo.

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