Diffusion Boundary Conditions in Flatland Geometry

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INTRODUCTION

"Flatland" is a fictional two-dimensional universe in which particles are constrained to exist and travel in a 2-D plane [1]. Because the flatland phase space is (x, y, ω) with *one* angular variable (the azimuthal ω), rather than the standard 2-D (x, y, μ, ω) with *two* angular variables (the polar cosine μ and the azimuthal ω), flatland is a computationally simpler testing ground that retains the complexity of multidimensional geometry. For this reason, flatland has recently been used in the development and testing of multi-D transport methods [2, 3, 4].

Previous work has shown that the 3-D diffusion coefficient $\frac{1}{3\sigma}$ differs from the flatland diffusion coefficient $\frac{1}{2\sigma}$, but accurate boundary conditions for the flatland diffusion equations have not been derived. An accurate diffusion boundary condition is needed for benchmarking new transport methods against diffusion solutions. Thus, in the following we *(i)* derive "Marshak" and "variational" boundary conditions for the flatland diffusion equation, and *(ii)* demonstrate their accuracy via numerical simulations.

ANALYSIS

The steady-state, monoenergetic transport equation is

$$\boldsymbol{\Omega} \cdot \boldsymbol{\nabla}\psi + \sigma\psi = \frac{c\sigma}{\gamma_0} \int_{\Omega} \psi \, \mathrm{d}\Omega + \frac{q}{\gamma_0} \quad \boldsymbol{x} \in V, \ \boldsymbol{\Omega} \in \Omega\,, \tag{1}$$

where the direction vector $\boldsymbol{\Omega}$, the unit "sphere" Ω, and the constant γ_0 depend on whether the geometry is flatland or 2-D. We consider a specified incident boundary condition:

$$\psi(\boldsymbol{x}, \boldsymbol{\Omega}) = \psi^b(\boldsymbol{x}, \boldsymbol{\Omega})\,, \quad \boldsymbol{x} \in \partial V, \ \boldsymbol{\Omega} \cdot \boldsymbol{n} < 0\,. \tag{2}$$

In 2-D geometry, $\boldsymbol{\Omega} = \sqrt{1-\mu^2} \cos\omega \boldsymbol{i} + \sqrt{1-\mu^2} \sin\omega \boldsymbol{j}$; and in flatland, $\boldsymbol{\Omega} = \cos\omega \boldsymbol{i} + \sin\omega \boldsymbol{j}$. The domain of angular integration Ω in 2-D is $-1 \le \mu \le 1$, $0 \le \omega < 2\pi$; in flatland, it is $0 \le \omega < 2\pi$. These lead to the different angular moments

$$\gamma_m = \int_{\Omega} |\boldsymbol{\Omega} \cdot \boldsymbol{i}|^m \, \mathrm{d}\Omega\,. \tag{3}$$

In 2-D, $\gamma_0 = 4\pi$, $\gamma_1 = 2\pi$, and $\gamma_2 = \frac{4\pi}{3}$. In flatland, $\gamma_0 = 2\pi$, $\gamma_1 = 4$, and $\gamma_2 = \pi$. The differences between these values lead to different diffusion coefficients and different boundary conditions.

Under the assumption that ψ is linear in angle, the first angular moment of the transport equation can be reduced to Fick's law, expressed using the identities of Eq. (3):

$$\boldsymbol{J}(\boldsymbol{x}) = -\frac{\gamma_2}{\gamma_0} \frac{1}{\sigma(\boldsymbol{x})} \boldsymbol{\nabla}\phi(\boldsymbol{x}) \equiv -D(\boldsymbol{x}) \boldsymbol{\nabla}\phi(\boldsymbol{x})\,. \tag{4}$$

In 2-D and 3-D, $\gamma_2/\gamma_0 = (4\pi/3)/(4\pi) = 1/3$; however, in flatland, $\gamma_2/\gamma_0 = \pi/(2\pi) = 1/2$. Thus, $D = \frac{1}{3\sigma}$ in 2-D but $D = \frac{1}{2\sigma}$ in flatland.

Fick's law and the linear-in-angle approximation give the following diffusion approximation to the angular flux:

$$\psi(\boldsymbol{x}, \boldsymbol{\Omega}) = \frac{1}{\gamma_0} \left(\phi(\boldsymbol{x}) - \frac{1}{\sigma(\boldsymbol{x})} \boldsymbol{\Omega} \cdot \boldsymbol{\nabla}\phi(\boldsymbol{x}) \right). \tag{5}$$

Marshak Boundary Condition

The Marshak boundary condition preserves the incident partial current on the boundary. It is derived by substituting the approximate diffusion angular flux from Eq. (5) into the boundary condition, Eq. (2), multiplying by $|\boldsymbol{\Omega} \cdot \boldsymbol{n}|$, and integrating over incident directions:

$$\int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}<0} |\boldsymbol{\Omega} \cdot \boldsymbol{n}| \, \psi^b \, \mathrm{d}\Omega = \int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}<0} |\boldsymbol{\Omega} \cdot \boldsymbol{n}| \, \frac{1}{\gamma_0} \left(\phi - \frac{1}{\sigma} \boldsymbol{\Omega} \cdot \boldsymbol{\nabla}\phi \right) \mathrm{d}\Omega\,.$$

Using the definitions in Eq. (3), we obtain the following general-geometry expression for the Marshak boundary condition:

$$\frac{2\gamma_0}{\gamma_1} \int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}<0} |\boldsymbol{\Omega} \cdot \boldsymbol{n}| \, \psi^b \, \mathrm{d}\Omega = \phi + \frac{\gamma_2}{\gamma_1} \frac{1}{\sigma} \boldsymbol{n} \cdot \boldsymbol{\nabla}\phi\,. \tag{6}$$

In 2-D, this evaluates to the standard Marshak boundary condition with extrapolation distance $\frac{\gamma_2}{\gamma_1} = \frac{2}{3}$, but in flatland it gives

$$\pi J^- = \phi + \frac{\pi}{4} \frac{1}{\sigma} \boldsymbol{n} \cdot \boldsymbol{\nabla}\phi = \phi + \frac{\pi}{2} D \boldsymbol{n} \cdot \boldsymbol{\nabla}\phi\,.$$

Thus, the flatland extrapolation distance of $\frac{\pi}{4} \approx 0.7854$ is about 18% longer than in 2-D. The underlying physical reason is that in 2-D, a greater fraction of particles travel at a steep angle to the x, y-plane, yielding a shorter extrapolation distance, i.e. a steeper slope for ϕ on the boundary.

Variational Boundary Condition

It is known that the Marshak boundary condition is heuristic and that a more accurate boundary condition for diffusion can be derived from an asymptotic matched boundary layer analysis [5]. However, a simpler method of deriving a more accurate (than Marshak) boundary condition is to use a variational analysis [5]. A shorter but equivalent analysis, adapted to flatland geometry, follows.

We consider a steady-state, homogeneous, purely scattering transport problem in a semi-infinite plane, $-\infty < x < \infty$, $0 < y < \infty$,

$$\boldsymbol{\Omega} \cdot \boldsymbol{\nabla}\psi + \sigma\psi = \frac{\sigma}{2\pi} \int_0^{2\pi} \psi \, \mathrm{d}\omega\,, \quad 0 \le \omega < 2\pi\,. \tag{7a}$$

It has a uniform incident boundary condition,

$$\psi(x, 0, \omega) = \psi^b(\omega)\,, \quad 0 \le \omega < \pi\,. \tag{7b}$$

Because neither the boundary condition nor σ varies in x, $\partial\psi/\partial x = 0$, and Eq. (7a) reduces to the one-dimensional flatland transport equation

$$\sin\omega \frac{\partial}{\partial y}\psi(y,\omega) + \sigma\psi(y,\omega) = \frac{\sigma}{2\pi}\int_0^{2\pi}\psi(y,\omega')\,\mathrm{d}\omega'\,, \tag{8}$$

which is *not* the 1-D planar geometry transport equation. We define the y components of the angular moments of ψ as

$$\phi_m(y) = \int_0^{2\pi}(\boldsymbol{\Omega}\cdot\boldsymbol{j})^m\psi(y,\omega)\,\mathrm{d}\omega = \int_0^{2\pi}(\sin\omega)^m\psi(y,\omega)\,\mathrm{d}\omega\,. \tag{9}$$

As $y \to \infty$, the angular flux ψ will approach a constant $\varphi/2\pi$, which gives $\phi_0(\infty) = \varphi$. Concordantly, $\phi_1(\infty) = 0$.

Operating on Eq. (8) by $\int_0^{2\pi}(\sin\omega)^m(\cdot)\,\mathrm{d}\omega$ gives the mth angular moment in the y direction:

$$\frac{\partial\phi_{m+1}}{\partial y} + \sigma\phi_m = \frac{\sigma}{2\pi}\phi_0\int_0^{2\pi}(\sin\omega)^m\,\mathrm{d}\omega\,. \tag{10}$$

For $m = 0$, the conservation equation, Eq. (10) evaluates to

$$\frac{\partial\phi_1}{\partial y} + \sigma\phi_0 = \frac{\sigma}{2\pi}\phi_0(2\pi) \quad\Longrightarrow\quad \frac{\partial\phi_1}{\partial y} = 0\,.$$

Thus $\phi_1(y)$ is a constant, and because $\phi_1(\infty) = 0$, that constant is zero.

Evaluating Eq. (10) for $m = 1$ and using $\phi_1 = 0$, we find

$$\frac{\partial\phi_2}{\partial y} + \sigma\phi_1 = \frac{\sigma}{2\pi}\phi_0(0) \quad\Longrightarrow\quad \frac{\partial\phi_2}{\partial y} = 0\,.$$

Thus ϕ_2 is also a constant. As $y \to \infty$, $\psi \to \varphi/2\pi$, so

$$\phi_2 = \int_0^{2\pi}(\sin\omega)^2\frac{\varphi}{2\pi}\,\mathrm{d}\omega = \frac{1}{2}\varphi\,.$$

Since $\phi_1 = 0$, we can add $\alpha\phi_1$ to the previous equation for any α:

$$\int_0^{2\pi}(\alpha\sin\omega + \sin^2\omega)\,\psi(y,\omega)\,\mathrm{d}\omega = \frac{\varphi}{2}\,.$$

At the boundary $y = 0$, $\psi = \psi^b$ for incident angles $0 \le \omega < \pi$.

The variational analysis in [5] reveals that certain trial functions allow an exiting angular distribution that is isotropic to second order, so we make the "variational" approximation that $\psi(0,\omega) = \psi^{\text{out}}$. The previous equation then yields

$$\int_0^{\pi}(\alpha\sin\omega + \sin^2\omega)\psi^b(\omega)\,\mathrm{d}\omega + \int_{\pi}^{2\pi}(\alpha\sin\omega + \sin^2\omega)\,\mathrm{d}\omega\psi^{\text{out}} = \frac{\varphi}{2}\,.$$

The value $\alpha = \pi/4$ eliminates the integral over outgoing directions and gives the following relation between moments of the incident angular flux and the magnitude of the angular flux as $y \to \infty$:

$$\int_0^{\pi}\left(\frac{\pi}{4}\sin\omega + \sin^2\omega\right)\psi^b(\omega)\,\mathrm{d}\omega = \frac{\varphi}{2}\,. \tag{11}$$

We wish our boundary condition to preserve the value of φ when the diffusion method is used, so we substitute the diffusion approximation, Eq. (5):

$$\begin{aligned}\varphi &= 2\int_0^{\pi}\left(\frac{\pi}{4}\sin\omega + \sin^2\omega\right)\psi^b(\omega)\,\mathrm{d}\omega\\ &= 2\int_0^{\pi}\left(\frac{\pi}{4}\sin\omega + \sin^2\omega\right)\left(\frac{1}{2\pi}\phi - \frac{1}{\sigma}\sin\omega\frac{\partial\phi}{\partial y}\right)\mathrm{d}\omega\\ &= \phi - \left(\frac{\pi}{8} + \frac{4}{3\pi}\right)\frac{1}{\sigma}\frac{\partial\phi}{\partial y}\,.\end{aligned}$$

In this problem, the boundary surface outer normal is $\boldsymbol{n} = -\boldsymbol{j}$. Replacing $\sin\omega$ with $-\boldsymbol{\Omega}\cdot\boldsymbol{n}$, we obtain the following flatland variational boundary condition:

$$\int_{\boldsymbol{\Omega}\cdot\boldsymbol{n}<0}\left[\frac{\pi}{2}\left|\boldsymbol{\Omega}\cdot\boldsymbol{n}\right| + 2(\boldsymbol{\Omega}\cdot\boldsymbol{n})^2\right]\psi^b(\boldsymbol{x},\boldsymbol{\Omega})\,\mathrm{d}\Omega = \phi(\boldsymbol{x}) - \left(\frac{\pi}{8} + \frac{4}{3\pi}\right)\frac{1}{\sigma}\boldsymbol{n}\cdot\boldsymbol{\nabla}\phi(\boldsymbol{x})\,. \tag{12}$$

Compared to the flatland Marshak boundary condition, Eq. (8), the variational boundary condition not only yields a different extrapolation distance $\frac{\pi}{8} + \frac{4}{3\pi} \approx 0.8171$ but also uses a different moment of the incident boundary flux.

NUMERICAL RESULTS

As a test problem, we consider a homogeneous flatland problem with a total cross section $\sigma = 1$ and scattering ratio $c = 0.99$. The spatial domain is the rectangle $0 \le x \le 2$, $0 \le y \le 10$, with reflecting boundaries on the left, right, and top sides. The bottom side has a specified unit-current incident flux; we consider three different angular distributions.

The first distribution is isotropic, $\psi^b(\omega) = \frac{1}{2}$. The second is a normally incident flux, with all particles entering perpendicular to the surface, $\psi^b(\omega) = \delta(\omega - \frac{\pi}{2})$. The third incident distribution is at a grazing angle, with $\psi^b(\omega) = 10\delta(\omega - \sin^{-1}.1)$.

We compare a transport method (Monte Carlo using 10^7 particles) with a finite difference diffusion implementation on a fine spatial grid. Figure 1, a line-out of the scalar flux ϕ_0 along $x = 1$ for the normally incident boundary, illustrates the differences between the methods. The diffusion approximation cannot reproduce the boundary layer that the true transport solution features, but the variational approximation to the flatland diffusion boundary condition allows the asymptotic diffusion solution to closely match the transport solution. The Marshak boundary does not.

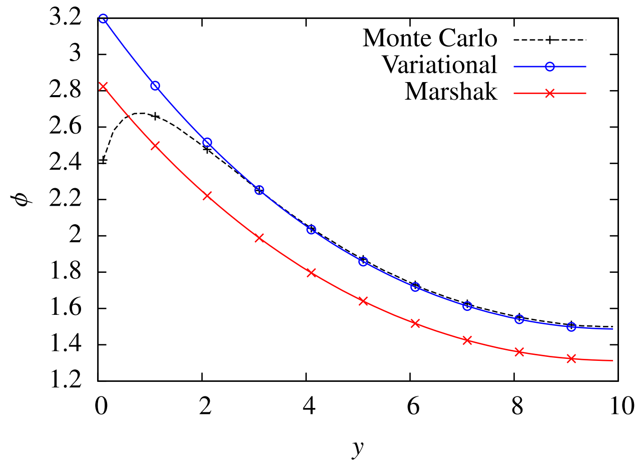

Fig. 1. Scalar flux with a normally incident boundary condition.

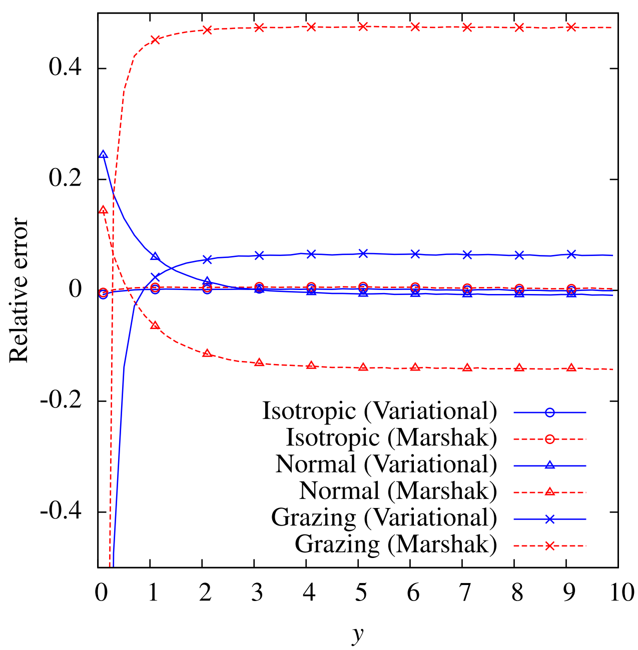

Fig. 2. Relative errors ($\phi/\phi_{MC} - 1$) of the three tested distributions.

Figure 2 quantitatively compares both "variational" and "Marshak" diffusion boundary conditions against the transport solution for all three incident distributions. As with the variational boundary condition for 3-D geometry, the flatland variational boundary condition gives an interior scalar flux accurate to within a few percent. The Marshak condition fails to limit to the transport solution except in the case of an isotropic boundary source, where only the extrapolation distance differs from the variational boundary condition.

CONCLUSIONS

We have derived and tested Marshak and variational boundary conditions for the diffusion approximation to the transport equation in flatland geometry.

The Marshak boundary condition, which uses $\pi \int_{\mathbf{\Omega}\cdot\boldsymbol{n}<0} |\mathbf{\Omega}\cdot\boldsymbol{n}|\, \psi^b \, d\Omega$, gives an extrapolation distance of about 0.7854. The variational boundary condition given in Eq. (12) uses $\int_{\mathbf{\Omega}\cdot\boldsymbol{n}<0} \left[\frac{\pi}{2}|\mathbf{\Omega}\cdot\boldsymbol{n}| + 2(\mathbf{\Omega}\cdot\boldsymbol{n})^2\right] \psi^b(\boldsymbol{x},\mathbf{\Omega})\, d\Omega$ with the extrapolation distance of about 0.8171. Numerical simulations show that the variational boundary condition is significantly more accurate than the Marshak condition, especially for anisotropic incident boundary fluxes ψ^b. Overall, the flatland Marshak and variational diffusion boundary conditions have accuracies comparable to their 3-D counterparts.

These results have application in the testing of numerical methods for multi-D transport problems. The flatland implementation of these methods is easier and less costly than in standard 2-D or 3-D geometries, and the results seen in flatland are strongly correlated to results in 2-D and 3-D.

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