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Letters to the Editor

Comments on "A Comparison of Angular Difference Schemes for One-Dimensional Spherical Geometry S_N Equations": The Validity of the Discrete Ordinates Method in Spherical Geometry

The discrete ordinates method in spherical geometry with central symmetry was revisited recently with a new approach that retains the structure of the original boundary value problem in two respects: the angular parameters and its consequential starter flux.[1] The angular parameters approximate the angular derivative and are constrained to the condition of constant flux in the asymptotic region. The starter flux is needed to initiate the solution of N equations in $N + 1$ unknowns that are generated with the angular parameters.[2]

The new approach relaxes the asymptotic condition of the angular parameters. It is sufficient to assume an isotropic flux at the center of the sphere. This assumption was justified by observing that if we multiply the equation

$$\left\{\mu \partial_r \psi + \frac{\eta^2}{r} \partial_\mu \psi\right\} + \sigma\psi = Q \tag{1}$$

by r, then, according to the argument in Ref. 1, all the terms of the equation vanish at the center. Here, ∂_r is the tensor symbol of the derivative with respect to r; $\eta = (1 - \mu^2)^{1/2}$; the braces quantity is the divergence, also known as the streaming term; and the other terms have the usual meanings. The result of this multiplication is an isotropic flux at the center inferred from $\eta^2 \partial_\mu \psi_{r=0} = 0$ without further justifications.[1]

The divergence term is singular at $r = 0$. It yields a flux in $1/r^2$; its spatial derivative varies as $1/r^3$, whether the sphere is vacuum or any other material, with or without a source. Therefore, whether or not rQ vanishes at the center, neither $r\psi$ nor $r\partial_r \psi$ vanishes at $r = 0$, which invalidates the argument for the assumption of an isotropic flux at the center.

We realize that Eq. (1) is the linearized form of the transport equation; that is, it is not valid at the center. It is difficult to justify the hypothesis of an isotropic flux at $r = 0$. On the other hand, if we legitimize the multiplication by r in the manner suggested in Ref. 1, the resulting isotropic flux at the center is only one contribution to the physical flux. The contributions from collisions and source emission are yet to be accounted for in order to obtain the integral flux at the center. There is nothing we are aware of that inhibits collision and emission at a point in a continuum, including the center.

Equation (1) defines a boundary value problem completely specified by one natural boundary condition at the surface: the boundary flux ψ_R, where R is the radius of the sphere. If we impose an additional boundary condition descriptive of the nature of the flux at the center, such as the isotropic flux suggested in Ref. 1, we will be solving a boundary value problem of our own that may not necessarily be representative of the actual flow of neutrons in the sphere. It was shown that if we do not impose a condition on the nature of the flux at $r = 0$, the spatial derivative is always negative, and ψ is a function of μ there; that is, the solution is anisotropic at the center.[3] Indeed, the coefficient μ of $\partial_r \psi$ guarantees that ψ is always anisotropic at the center, except in vacuum.

It was shown that if the flux is needed only for calculating the reaction rate in the sphere and the neutron flow across the surface, the singularity of the flux at the center can be bypassed. This can be done by shifting the spatial variable so that the new variable is $\vartheta = a + r$, where a is any positive number smaller, equal to, or larger than the radius R and r varies on $[0, R]$. The integral over the volume of the now ϑ-sphere produces the exact reaction rate in the R-sphere, under the conditions of validity of the linearized transport equation.[3]

The other shortcoming of the discrete ordinates of Ref. 1 is the starter flux. It is inherited from the original formulation of the discrete ordinates. This is in effect a redundant boundary condition on the angular domain; the angular boundary condition is already contained in the boundary flux ψ_R.

The starter flux is taken to be the solution of the transport equation in slab geometry by simply setting $\mu = -1 \Leftrightarrow \eta = 0$ in Eq. (1). This practice is not appropriate for this class of equations. The angular derivative of Eq. (1) couples the fluxes in different directions. If we remove it from the equation, then we will be solving a boundary value problem different from the one defined by the original equation. A good approximation for the starter flux should be consistent with $1/r^2$ flux. It could be the case that a plane geometry starter flux is a reasonable approximation in a large sphere for $r \sim R$; it is unlikely to be the case in the interior of the sphere and certainly not in the proximity of the center. It was shown that it is possible to construct a set of discrete ordinates that is closed, without necessitating a starter flux if unnormalized circular functions are used.[3]

Now, we address the following question: Can we retain the angular parameters of the discrete ordinates and start the solution with a starter flux in $1/r^2$, assuming we have a reasonable approximate prescription for that flux? The short answer in general is no. The angular parameters are evaluated from a recursion relation conditioned by a constant asymptotic flux.[2] The $1/r^2$ flux is not constant anywhere in a finite sphere, and therefore, it is not consistent with the structure of the angular parameters.

It is instructive at this point to examine the problem in a different representation. Consider a sphere of radius R with isotropic and uniformly distributed boundary flux ψ_R. Assume further that the sphere is vacuum; the expressions are simple and equally instructive as in any other sphere. If we convert the divergence into an ordinary derivative along the trajectory of a neutron as it is done in Eq. (1), then Eq. (1) becomes $\partial_s \psi = 0$, and its solution is $\psi_s = \psi_R$. At first sight, this identity suggests the scalar flux is constant in r. This is not necessarily correct; the scalar flux is obtained as a line integral on an arc on the surface of the sphere. Therefore, whether or not ψ_s is constant, the limits of integration must be explicit in r. This is the case in earnest in the medium exterior to a sphere when its radiance is ψ_R. Then, we will have

$$\varphi_r \propto \int_{\mu_0}^{+1} \psi_s \, d\mu \ , \quad r \geq R \ , \tag{2}$$

where $\mu_0 = (1 - R^2/r^2)^{1/2}$ (Ref. 1). If the medium is vacuum and the radiance is isotropic and uniformly distributed, then

$$\varphi_r \propto \psi_R [1 - (1 - R^2/r^2)^{1/2}] \ . \tag{3}$$

This solution and the one obtained with discrete ordinates of Ref. 3 are numerically congruent $\forall r \geq R$. This result shows that the ∂_s representation is compatible with the formal divergence representation in the exterior of a radiating sphere. The two representations reproduce the same physical quantity, the scalar flux φ. It is not so in the interior of the sphere. There, we would have

$$\varphi_r \propto \int_{-1}^{+1} \psi_s \, d\mu \ , \quad r \leq R \ . \tag{4}$$

That is, the scalar flux is uniform in the interior of our sphere. A closer look at this result reveals that Eq. (4) is a statement of self-denial.

Indeed, if the flux is uniform in the sphere, then its value is the same at the center and at the surface. Now, by recognizing that the flux at the center is the contribution from neutrons normal to the surface, let ψ_R be the normal flux. Then, the total number of normal neutrons is $N = 4\pi R^2 \psi_R = 4\pi \epsilon^2 \psi_\epsilon$, where ϵ is the radius of a concentric sphere. Clearly, the normal flux $\psi_{\epsilon \to 0}$ is different from the normal flux ψ_R, which denies the validity of Eq. (4).

It appears that the flux ψ_s is a kernel for the general solution for Eq. (1). The line integral of the kernel yields the general solution for the scalar flux if at least one limit of integration is explicit in r. This happened to be the case in the exterior but not in the interior of the sphere.

We conclude from the forgoing that the ∂_s representation is not a valid boundary value problem of neutron transport in the interior of a sphere. Consequently, a discrete ordinates solution that is designed to compare with the solution in ∂_s representation in the interior of a sphere represents a boundary value problem different from the problem of flow of neutrons in spheres.

Charles H. Aboughantous

Louisiana State University
Department of Physics and Astronomy
Baton Rouge, Louisiana 70803
E-mail: abough@rouge.phys.lsu.edu

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Reply to "Comments on 'A Comparison of Angular Difference Schemes for One-Dimensional Spherical Geometry S_N Equations'": The Validity of the Discrete Ordinates Method in Spherical Geometry

Discussing the one-dimensional transport equation in spherical geometry[1]

$$r\mu \frac{\partial \psi}{\partial r} + (1 - \mu^2) \frac{\partial \psi}{\partial \mu} + r\sigma(r)\psi(r,\mu) = rS(r,\mu) \ , \tag{1}$$

Aboughantous objects to the argument that if rS vanishes at $r = 0$, then $r\psi$ and $r(\partial\psi/\partial r)$ also vanish at $r = 0$ so that $\partial\psi/\partial\mu = 0$ and the angular flux is constant in angle or isotropic at the center of such spheres. He incorrectly believes that because the divergence form of the transport streaming operator contains a $1/r^2$ term, the angular flux of all solutions has this behavior at the origin, and thus, the angular flux there is not isotropic. He ignores the analytic solutions [Eqs. (3), (4), and (5) in Ref. 2] that satisfy Eq. (1) and its boundary condition and are finite and isotropic at the center of the sphere. To "cure" his self-created problem, he proposes shifting the radial coordinate to avoid his postulated singularity at the center. This ignores the fact that solutions are independent of coordinate representations.

Neutral particles are assumed to travel in straight lines, and as Davison shows,[3] at any point in a medium the angular flux is the sum of contributions from scattering, from sources and from incoming boundary particles back along a straight line in the direction of motion. At the center of a one-dimensional sphere, these contributions are the same in every direction, so that unless there are singular sources at the center, the angular flux is a constant or isotropic. Conversely, in this situation, if the angular flux at the center is not isotropic, the sphere is not one-dimensional.

Aboughantous also objects to using Eq. (1) with $\mu = -1$ to determine initial values for the angular flux in angular finite difference approximations. He says that removing this angular derivative term from the equation results in solving a different boundary value problem. Also, fixated on a $1/r^2$ angular flux, he says the initial value flux should have this form. The angular derivative in Eq. (1) expresses the fact that usually as a particle moves in a straight line through a sphere, its μ coordinate changes. But, this is not true if the particle is moving straight into or straight out of the sphere, that is, with $\mu = -1$ or $\mu = +1$. And, Eq. (1) with these values has no singularity at $r = 0$.

Finally, Aboughantous says, "We realize that Eq. (1) is the linearized form of the transport equation; that is, it is not valid at the center." If true, this would be news to many generations of researchers in the field. This statement is indicative of the merit of his comments.

Kaye D. Lathrop

Stanford Linear Accelerator Center—SLAC
Mail Stop 7
2575 Sand Hill Road
Menlo Park, CA 94025
E-mail: klathrop@independence.net

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