Specular reflective boundary conditions for Discrete Ordinate Methods in Periodic or Symmetric Geometries

Jian Cai*, Michael F. Modest†

* Assistant Professor, University of Wyoming, Laramie, WY 82071, USA
† Shaffer and George Professor of Engineering, University of California, Merced, CA 95343, USA
E-mail: jcai@uwyo.edu, mmodest@ucmerced.edu

Abstract. In simulations of periodic or symmetric geometries, computational domains are reduced by imaginary boundaries that present the symmetry conditions. In Photon Monte Carlo methods, this is achieved by imposing specular reflective boundary conditions for the radiative intensity. In this work, a similar specular reflective boundary condition is developed for Discrete Ordinate Methods. The effectiveness of the new boundary condition is demonstrated by multiple numerical examples including plane symmetry and axisymmetry.

1. Introduction
Periodic and symmetric geometries are frequently encountered in engineering applications. Examples of such geometries include periodic structures, plane symmetry and axisymmetry. In the simulations of these problems, flow variables are solved for only a section of the domain. The computational domain is separated from the rest by imaginary boundaries, upon which symmetric constraints as opposed to physical conditions are applied.

While the symmetry constraints may be easily expressed into mathematical formulas for scalar and vector fields as frequently performed in CFD simulations, they present challenges for radiative intensities. This is because the radiative intensities are functions of both spatial and directional coordinates [1]. Plane and rotational symmetric conditions are complicated by the additional directional variations. As an example, scalar flow variables in an axisymmetric problem are only functions of radial and axial locations that fit into two-dimensional cylindrical coordinates. In flow solvers designed for only three-dimensional coordinates, a wedge geometry that has only one layer of cells in the azimuthal direction may be employed. Symmetry conditions are imposed on the imaginary wedge planes. However, even in these axisymmetric problems, the radiative intensities are still three-dimensional, i.e., light propagation is not limited to the plane formed by radial and axial direction vectors. Such issues are also observed in Photon Monte Carlo (PMC) methods for radiative transfer. In PMC methods, the wedge planes may be treated as specular reflective boundary conditions, i.e., a ray hitting the wedge plane is reflected back into the computational domain like hitting a perfect mirror.

When applying Discrete Ordinate Methods [1, 2] to axisymmetric simulations, three methods are typically employed. In the first method, the Radiative Transfer Equations (RTE) are solved for ordinate intensities in a full three-dimensional axisymmetric domain, as in Ref. [3, 4]. This method cannot take advantage of symmetry to reduce computational cost. In the second method, the RTEs are formulated in cylindrical coordinates directly as in Ref. [5–7]. However, this approach requires a different implementation of the equations. In the third method, a reduced mesh based on symmetry is used to discretize the RTE formulated for Cartesian coordinates [8, 9]. Axisymmetry is enforced by special treatment of the wedge boundaries. This method simplifies the implementations of RTEs, because the same solver and discretization method are used for both reduced geometry or the full three-dimensional case.
dimensional geometry. However, the resulting new wedge boundaries require different treatment from that employed for scalar or vector partial differential equations.

In this work, a specular reflective boundary condition is proposed for Discrete Ordinate Methods in recognition of the fact that the ordinates have similarities to rays in Photon Monte Carlo methods. The specular reflective boundary conditions are expressed as mathematical boundary conditions for the first-order partial differential equations that govern spatial variations of each ordinate depending on the spatial relationship between the surface normal and the ordinate directions. The proposed method makes a theoretical contribution to radiation solution methods and provides potential reduction in computational cost for symmetric geometries.

2. Theoretical background

2.1. Discrete Ordinate Methods

In this section, the Discrete Ordinate Methods for solving Radiative Transfer Equation are briefly reviewed. The presentation focuses only on necessary content for the new development as opposed to completeness. Discussions will be limited to nonscattering participating media, because the treatment of scattering is not essential to this work and does not impose new technical difficulties. Readers are referred to [1] for more comprehensive discussions and [2] for a review of recent developments.

The Radiative Transfer Equation (RTE) for a radiatively participating medium with emission and absorption is a first order partial differential equation:

$$\hat{s} \cdot \nabla_x I(x, \hat{s}) = \kappa I_b(x) - \kappa I(x, \hat{s})$$

(1)

where $x$ is the spatial coordinate, $\hat{s}$ is a unit direction vector, $\kappa$ is the absorption coefficient, $I$ the radiative intensity and $I_b$ the blackbody intensity (or Planck function). The subscript $x$ of the gradient operator $\nabla$ emphasizes that the gradient is respect to spatial coordinates only.

In Discrete Ordinate Methods the directional variation of the radiative intensity is expressed by intensities on a set of prescribed directions, known as the ordinates. For each of the $n$ ordinates ($\hat{s}_i, i = 1, \ldots, n$), the corresponding intensity ($I_i = I(x, \hat{s}_i)$) is determined by solving the RTE for direction $\hat{s}_i$, i.e.,

$$\hat{s}_i \cdot \nabla I_i(x) = \kappa I_b(x) - \kappa I_i(x)$$

(2)

The resulting RTE is a first order partial differential equation and depends on spatial coordinates only. Each ordinate $\hat{s}_i$ has a directional quadrature weight $w_i$ such that a directional integral is converted into a sum over quadratures. In particular,

$$\int \Omega d\Omega = \sum_i w_i = 4\pi$$

(3)

$$\int \Omega I d\Omega = \sum_i I_i w_i = G$$

(4)

where $G$ is incident radiation.

2.2. Finite Volume Discretization

Equation (2) may be solved numerically by Finite Volume Methods, i.e., it is integrated within a cell before the Gauss theorem is used to convert differential operators into algebraic operations. For example, consider a cell $C$ with a volume $V_c$ enclosed by $m_f$ faces (Fig. 1). The RTE, Eq. (2), is integrated within this cell according to

$$\int_{V_c} \hat{s}_i \cdot \nabla I_i(x) dV = \int_{V_c} \kappa I_b(x)dV - \int_{V_c} \kappa I_i(x)dV.$$  

(5)

For the right-hand side, the cell-center values of radiative intensity ($I_{ic}$) and properties ($\kappa_c$) are defined such that

$$\int_{V_c} \kappa I_b(x)dV - \int_{V_c} \kappa I_i(x)dV = V_c \kappa_c (I_{ic} - I_{ic})$$

(6)
where $I_{bc}$ is the Planck function evaluated at the cell-valued thermodynamic state.

The left hand side is related to $I_i$ at the faces according to the Gauss theorem

$$\int_{V_c} \hat{s}_i \cdot \nabla I_i(x) \, dV = \int_{S_c} I_i(x) \hat{s}_i \cdot \hat{n}_f \, dA = \sum_f \int_{A_f} I_i(x) \hat{s}_i \cdot \hat{n}_f \, dA = \int \hat{s}_i \cdot \hat{n}_f \, dA = I_i \hat{s}_i \cdot \hat{n}_f$$ (7)

where $I_i$ is the intensity at face $f$, $A_f$ the surface area of face $f$, and $\hat{n}_f$ the surface normal of face $f$.

Further development is now required to express the face values $I_i$ in terms of $I_i$. When the face $f$ is an internal face, $I_i$ is usually expressed as a function of $I_i$ in the current cell ($I_{iC}$) and that in the neighbor cell ($I_{iN}$) that shares face $f$

$$I_{i f} = F(I_{iC}, I_{iN}, \hat{s}_i, \hat{n}_f). \quad (8)$$

The simplest scheme is an upwind scheme known as the step scheme, i.e.,

$$I_{i f} = F(I_{iC}, I_{iN}, \hat{s}_i, \hat{n}_f) = \begin{cases} I_{iC}, & \text{if } \hat{s}_i \cdot \hat{n}_f \geq 0 \\ I_{iN}, & \text{otherwise.} \end{cases} \quad (9)$$

However, when face $f$ is on a computational boundary, a boundary condition is needed to determine the value of $I_i$ on an ordinate $\hat{s}_i$ outgoing from the face. For physical boundaries with prescribed radiative properties, the intensity from the boundary is calculated from temperature, emittance and incoming intensities. For imaginary computational boundaries, a specular reflective boundary condition is commonly used with Photon Monte Carlo methods.

### 2.3. Specular reflective boundary condition

Light is reflected on a specular reflective boundary as if on a mirror, as shown in Fig. 2. The top half is within the computational domain, and is separated from the imaginary domain by a specular reflective boundary ($O0'$. The reflected direction ($\hat{s}_r$) of an incoming direction ($\hat{s}_i$) after hitting a face with a normal direction $\hat{n}_f$ is

$$\hat{s}_r = 2 \left( \hat{n}_f \cdot \hat{s}_i \right) \hat{n}_f - \hat{s}_i \quad (10)$$

Because of the reflective symmetry imposed by boundary, the intensities of the boundary cell ($C$) and its image ($C'$) are related by

$$I_{i C'} = I_{i C} \quad (11)$$
Figure 2. Reflective boundary condition. The boundary $OO'$ separates computational domain (shown above in solid lines) from its image (shown below in dashed lines). The cell centers are $C$ and its image $C'$. An incoming ordinate ($\hat{s}_i$) is reflected back to computational domain as $\hat{s}_r$. $\hat{s}_{i}'$ and $\hat{s}_{r}'$ are the images of the ordinates $\hat{s}_i$ and $\hat{s}_r$, correspondingly.

and the geometric constraints $\hat{s}_i' = \hat{s}_r$.

A successful reflective boundary condition should reproduce the same surface value as the internal surface when the full geometry including the image is employed. In other words, this requires that for any outgoing ordinate $\hat{s}_r$, its intensity on the surface reads

$$I_{rf} = F(I_{iC}, I_{iC'}, \hat{s}_r, \hat{n}_f) = F(I_{iC}, I_{iC}, \hat{s}_r, \hat{n}_f)$$

(12)

Notice that Eq. (11) is employed to replace the cell-valued intensity in imaginary cells ($I_{iC'}$) with the intensity in boundary cells ($I_{iC}$).

Similarly, the equation for the boundary condition of the incoming ordinate $\hat{s}_i$ can be derived,

$$I_{if} = F(I_{iC}, I_{iC'}, \hat{s}_i, \hat{n}_f) = F(I_{iC}, I_{iC}, \hat{s}_i, \hat{n}_f)$$

(13)

When the simplest step (upwind) scheme (Eq. 9) is used, the above boundary conditions, Eqs. (12) and (13) can be simplified to

$$I_{rf} = I_{iC}$$

(14)

$$I_{if} = I_{iC}$$

(15)

These two equations suggest that when the step scheme is used, the boundary condition for incoming ordinates is zero gradient, while the boundary condition for the outgoing ordinate is fixed value of the cell value from the incoming ordinate before reflection. These simplified conditions for step scheme were also mentioned by [9]. However, for higher order spatial schemes, the boundary conditions are more complicated and involve cell values of both incoming and outgoing ordinates, as shown in Eqs. (12) and (13), respectively.
3. Results and discussion
In this section sample calculations are carried out to demonstrate the effects of specular reflective boundary conditions on Discrete Ordinate Methods solutions. The boundary condition may be used for periodic or symmetry geometries. In the first example, the consistency is demonstrated.

3.1. An axisymmetric and periodic example
An axisymmetric radiation problem is considered here to demonstrate that the proposed boundary condition produces identical results as those from the full geometry. A homogeneous emitting–absorbing medium is confined in an infinitely long cylindrical enclosure bounded by black and cold walls. The problem is one-dimensional in the radial direction, and has two symmetry conditions. One is along the azimuthal direction, the other one is along the axial direction. The problem therefore may be solved with four different geometries as shown in Fig. 3. Geometry A is a sufficiently long cylinder bounded by black and cold walls at both ends. The radial cross section at the center achieves the target solution asymptotically as the length of the cylinder increases. Specularly reflective boundary conditions, therefore, are not needed in this geometry. Geometry B has a wedge shape with one layer of cells along the azimuthal direction, and takes advantage of the axisymmetry of the problem. Both of the additional front and back surfaces require the specular reflective boundary condition. Geometry C has a pie shape with only one layer of cells along the axial direction. It utilizes axial periodicity, such that both up and down surfaces are specularly reflective. Finally, Geometry D utilizes both axial periodicity and axisymmetry, and has cells only along the radial direction. Specularly reflective boundaries are applied to front, back, top and bottom surfaces. Because the solution (e.g., incident radiation or radiative heat source) of this problem has only radial variations, a successful boundary condition for the reduced geometries should produce identical results in all four geometries.

In all four geometries, a cylindrical grid with uniform spacing along axial, radial and azimuthal directions is used to discretize the RTE. The wedge geometries (Geometry B and D) have a 10° angle. Geometry A and C have 36 azimuthal cells with 10° for each wedge. Geometry A and B have 100 uniform axial cells, and Geometry C and D have identical height corresponding to the cell height in Geometry A and B. A total of 72 ordinates (2 polar and 36 azimuthal directions) are employed. The choice of large number of azimuthal direction ensures that the reflected ordinate is within the set of ordinates. The radial direction is uniformly discretized into 1000 cells. The radius of the cylinder is 1 m, and the absorption coefficient is 1 cm$^{-1}$; emission is homogeneous.

The solutions for normalized incident radiation ($G/4\pi I_0$) are compared in Fig. 4 with the exact results. Results from all four geometries overlap with each other, demonstrating the effectiveness of the proposed specular reflective boundary condition in dealing with both axisymmetric and periodic symmetries. The computational costs are 16720, 158, 15, and 2 seconds for Geometry A to D, respectively. A significant reduction of computational cost is achieved.
3.2. **Axisymmetric jet flame**

The specular reflective boundary condition is further applied to an axisymmetric jet diffusion flame solved on a wedge mesh similar to Geometry B in Fig. 3. The flame was derived from the methane–air partially premixed Sandia Flame D [10] by artificially quadrupling the jet diameter [11, 12] to make radiation in this small laboratory-scale flame appreciable. The wedge mesh has a $10^\circ$ opening angle. Time-averaged profiles are used for the radiation calculations. The same flame was previously employed to investigate the accuracy and efficiency of $k$-distribution methods and $P_N$ RTE solvers [13]. In this section the results from Discrete Ordinate Methods are reported. The spectral model is the full-spectrum $k$-distribution method assembled from a narrowband $k$-distribution database [14]. The polar direction is aligned with the axial direction. 36 azimuthal ordinates are employed so that reflected ordinates are also contained within the set of ordinates; the numbers of polar directions vary from 2 to 32.

The radiative heat flux divergence ($\nabla \cdot q$), i.e., the negative of the radiative heat source in the energy equations predicted by different DOM implementations are compared with PMC and $P_1$ at 1 m and 1.43 m above the nozzle in Figs. 5 and 6, respectively. Radiative emission is determined by the Optically Thin approximation (OT). The true radiative heat sources are determined by PMC coupled with a line-by-line spectral model. Identical trends are found at both downstream locations. The $P_1$ model recovers most of the non-gray self-absorption when coupled with the full-spectrum $k$-distributions. DOM with 2 polar ordinates overpredicts absorption, increasing the number of polar ordinates improves the accuracy only slightly, and the amount of improvement is small compared to the overall amount of self-absorption. Therefore, DOM results from different ordinate configurations appear very close.

3.3. **Conclusions**

In this work, a specular reflective boundary condition similar to that employed in Photon Monte Carlo method is proposed to reduce computational geometry by exploring periodicity or symmetry of the problem. The expression of the boundary condition depends on the spatial discretization scheme for the divergence term. For the simplest step scheme, the specular reflective boundary condition for ordinate intensity reduces to zero gradient (or fixed value) for incoming (or outgoing) directions relative to the boundary. Therefore, the intensity of outgoing ordinate at the boundary after reflection depends on the intensity of the incoming ordinate, but not vice versa. However, for higher order schemes the incoming
Figure 5. Radial scalar profiles (left) and prediction of radiative heat flux divergence (right) at 1 m above nozzle.

Figure 6. Radial scalar profiles (left) and prediction of radiative heat flux divergence (right) at 1.43 m above nozzle.

and outgoing ordinates are fully coupled. The consistency is demonstrated by a one-dimensional radial problem in a cylindrical coordinate that posses both axisymmetry and plane symmetry. The numerical example of a nongray axisymmetric jet flame solved on a wedge geometry with both radial and axial inhomogeneities is also provided.

[1] Modest M F 2013 Radiative Heat Transfer 3rd ed (New York: Academic Press)
[2] Coelho P J 2014 Journal of Quantitative Spectroscopy and Radiative Transfer 145 121 – 146
[3] Chiu E H, Raithby G D and Hughes P M J 1992 Journal of Thermophysics and Heat Transfer 6 605–611
[4] Moder J P, Chai J C, Parthasarathy G, Lee H S and Patankar S V 1996 Numerical Heat Transfer – Part B: Fundamentals 30 437–452
[5] Back S W and Kim M Y 1997 Numerical Heat Transfer – Part B: Fundamentals 31 313–326
[6] Fiveland W A 1982 ASME Paper 82-HT-20
[7] Murthy J Y and Mathur S R 1998 Numerical Heat Transfer – Part B: Fundamentals 33 397–416
[8] Mathur S R and Murthy J Y 1999 ASME Journal of Heat Transfer 121 357–364
[9] Kumar P and Eswaran V 2013 ASME Journal of Heat Transfer 125 124501
[10] Barlow R S and Frank J H 1998 Proceedings of the Combustion Institute 27 1087–1095
[11] Li G and Modest M F 2003 ASME Journal of Heat Transfer 125 831–838
[12] Wang A, Modest M F, Haworth D C and Wang L 2008 Journal of Quantitative Spectroscopy and Radiative Transfer 109 269–279
[13] Cai J, Marquez R and Modest M F 2014 ASME Journal of Heat Transfer 136 112702
[14] Cai J and Modest M F 2014 Journal of Quantitative Spectroscopy and Radiative Transfer 141 65–72