# Further Development of the Elliptic PDE Formulation of The $P_N$-Approximation and its Marshak Boundary Conditions

Michael F. Modest*,

School of Engineering, University of California,

Merced, CA 95343, USA

February 20, 2012

**Abstract**

The expansion of the radiative transfer equation (RTE) into spherical harmonics results in the $P_N$-approximation, consisting of $(N + 1)^2$ simultaneous, first-order partial differential equations (PDEs). This system of equations is generally solved subject to a set of so-called Marshak's boundary conditions, although some ambiguity exists in multi-dimensional media, for which the set provides more than the necessary number of conditions. In recent work Modest has shown that the general 3D $P_N$-approximation can be formulated as a set of $N(N + 1)/2$ second-order, elliptic PDEs, using the original set of Marshak's conditions, and which can be solved with standard PDE solution packages. In this paper the Marshak boundary conditions are reexamined in the light of the elliptic formulation, culminating in a self-consistent set of $= N(N + 1)/2$ conditions along the boundary of the enclosure. The elliptic set of PDEs is reformulated and reduced considerably by limiting considerations to isotropic scattering. As an example the 2D $P_3$-approximation is extracted, and sample 2D $P_1$, $P_3$ and $P_5$ computations are compared with Monte Carlo results.

Keywords: *Radiative heat transfer, radiative transfer equation, spherical harmonics method, $P_N$-method, Marshak conditions.*

## Nomenclature

$D^n_{mm'}$ Wigner function

*mmodest@ucmerced.edu

| | |
|---|---|
| $I$ | Radiative Intensity, W/m$^2$sr |
| $I_n^m$ | Intensity coefficient function, W/m$^2$sr |
| $\mathscr{L}$ | Differential operator, – |
| $\hat{\mathbf{n}}$ | Unit normal vector |
| $P_n^m$ | Associated Legendre polynomial |
| $q_n$ | Net radiative flux (normal to surface), W/m$^2$ |
| $\hat{\mathbf{s}}$ | Unit direction vector |
| $Y_n^m$ | Spherical harmonic |

*Greek symbols*

| | |
|---|---|
| $\alpha, \beta, \gamma$ | Euler rotation angles, – |
| $\beta$ | Extinction coefficient, m$^{-1}$ |
| $\delta$ | Surface rotation angle, – |
| $\Delta$ | Rotation tensor, – |
| $\epsilon$ | Surface emittance, – |
| $\kappa$ | Absorption coefficient, m$^{-1}$ |
| $\theta$ | Polar angle, – |
| $\mu$ | $\equiv \cos\theta$, – |
| $\sigma_s$ | Scattering coefficient, m$^{-1}$ |
| $\tau$ | Optical coordinate, – |
| $\omega$ | Single scattering albedo, – |
| $\Omega$ | Solid angle, sr |

*Subscripts*

| | |
|---|---|
| $b$ | blackbody |
| $s$ | surface |

# 1 Introduction

The radiative transfer equation (RTE) is an integro-differential equation in five independent variables (three in space and two in direction), which is exceedingly difficult to solve. Several approximate methods have been developed over time. Among these approximate methods the *Spherical Harmonics Method* (SHM), the *Discrete Ordinates Method* or the *Finite Volume Method,* and the *Monte Carlo Method* are presently used most frequently [1]. Both the *Spherical Harmonics Method* and DOM/FVM approximate the directional variation of the radiative intensity. However, the DOM employs a discrete representation of the directional variation with integrals over total solid angle $4\pi$ obtained via numerical quadrature, while the SHM captures the directional distribution of intensity by expressing it into a series of spherical harmonics. The DOM/FVM method is relatively simple to implement, but has several drawbacks, such as the fact that an iterative solution is required in the presence of scattering media or reflecting surfaces. In addition, its convergence is known to slow down for optically thick media. Furthermore, DOM may suffer ray effects and possibly false scattering due to its angular discretization [2]. The *Spherical Harmonics Method* has several advantages over other approximate methods: first, it converts the integro-differential RTE into relatively simple partial differential equations, similar to DOM/FVM. Secondly, in this method the spatial and directional dependencies are completely decoupled, allowing independent choices for spatial and directional accuracy, without suffering detrimental ray effects.

On the other hand, like all methods, the SHM also has a number of drawbacks. The lowest-order $P_N$-approximation, the $P_1$-approximation, has enjoyed great popularity because of its relative simplicity and compatibility with standard solution methods [1], but performs poorly in the optically thin limit and other nonisotropic radiative intensity fields. However, errors due to nonisotropy generated from surface emission can be mitigated using the modified differential approximation approach [3, 4]. Mathematical complexity increases rapidly if higher-order $P_N$-approximations for multi-dimensional geometry are desired. Consequently, only a few and very limited multi-dimensional formulations of higher order have been presented [5, 6], as reviewed by Yang and Modest [7].

Recently, Modest and Yang [8] have shown how the $(N + 1)^2$ first-order PDEs of the general three-dimensional $P_N$-approximation can be condensed into a set of $N(N + 1)/2$ second-order, elliptic PDEs, which are compatible with, and can be embedded into, standard commercial codes. By allowing for spatially varying absorption and anisotropic scattering this leaves the set of equations in rather complex form, making it difficult to apply to actual problems. While no medium is a true isotropic scatterer, the vast majority of calculations in scattering media are limited isotropic scattering, perhaps by removing forward scattering peaks to reduce computational complexity, or simply because accurate knowledge of the phase function is not available. It is the purpose of the present paper to further reduce the complexity of the elliptic $P_N$-formulation by limiting the problem to isotropic scattering (but with spatially varying absorption and scattering coefficients), considering the fact that very few practical calculations are ever carried out for anisotropic scattering. In addition, a self-consistent set of $N(N+1)/2$ boundary conditions will be extracted from the Marshak set, which contains $(N + 2)(N + 1)/2$ elements, eliminating an ambiguity, which has existed since first formulated by Marshak in 1947 [9]. Finally, as an example, the 2D $P_3$-approximation will be extracted, consisting of $(N+1)^2/4$ equations and boundary conditions, and results for $P_1$-, $P_3$ and $P_5$-approximations will be compared with those from a Monte Carlo code.

## 2 Mathematical Formulation

We have shown in our preliminary work [8] how the spherical harmonics approach can be formulated for general three-dimensional media with spatially varying properties, and how—after eliminating odd-numbered harmonics—this can be reduced to a set of $N(N+1)/2$ coupled elliptic PDEs in terms of spatial coefficients $I_n^m$ of even spherical harmonics ($n$ even). For convenience of the reader a few of the basic steps of the procedure are repeated here. For the complete development and the lengthy set of the governing equations and boundary conditions the original reference [8] should be consulted. The set contains a number of tensors, such as $\mathbf{ss1}_n^{m,m'}$, eight in all, each with $n, m, m' = 0, 1, \ldots N$, which are combined with elliptic operators and the $I_n^m$ of even spherical harmonics to form the set of $P_N$-equations. This development will be continued here to further simplify the $N(N+1)/2$ equations for the case of isotropic scattering. Similarly, boundary condition for the general $P_N$-method will be simplified for the isotropic scattering case.

Following Davison [5], we may express the intensity field $I(\vec{\tau}, \hat{\mathbf{s}})$ in terms of an infinite series[1]

$$I(\vec{\tau}, \hat{\mathbf{s}}) = \sum_{n=1}^{N} \sum_{m=-n}^{n} I_n^m(\vec{\tau}) Y_n^m(\hat{\mathbf{s}}), \tag{1}$$

where $\vec{\tau}$ is a location vector using optical coordinates based on the extinction coefficient $\beta$, i.e., $d\vec{\tau} = \beta d\vec{x}$, with $\vec{x}$ being the position vector, and $\hat{\mathbf{s}}$ is a unit direction vector originating at $\vec{\tau}$. In Eq. (1) the $I_n^m(\vec{\tau})$ are location-dependent coefficient functions associated with a given spherical harmonic $Y_n^m(\hat{\mathbf{s}})$, while directional dependency of the intensity field is resolved in terms of a series of integral-degree real spherical harmonics defined as [10]

$$Y_n^m(\theta, \psi) = \begin{cases} \cos(m\psi) P_n^m(\cos\theta), & \text{for} \quad m \geq 0, \\ \sin(m\psi) P_n^m(\cos\theta), & \text{for} \quad m < 0, \end{cases} \tag{2}$$

and $P_n^m(\cos\theta)$ are *associated Legendre polynomials*, given by

$$P_n^m(\mu) = (-1)^m \frac{(1-\mu^2)^{|m|/2}}{2^n n!} \frac{d^{n+|m|}}{d^{n+|m|}\mu} (\mu^2 - 1)^n. \tag{3}$$

Here $\theta$ and $\psi$ are the polar and azimuthal angles defining the direction of the unit vector $\hat{\mathbf{s}}$. Based on the

[1]Note that, for convenience, the notation for $I_n^m$ used here differs by a factor of $4\pi$ from that used in [8].

orthogonality of spherical harmonics over the solid angle of $4\pi$, we have

$$\int_{4\pi} [Y_n^m(\theta,\psi)]^2 \, d\Omega = \frac{(n+|m|)!}{(n-|m|)!} \frac{2\pi(1+\delta_{m,0})}{(2n+1)}, \tag{4}$$

where $\delta_{m,0}$ is Kronecker's delta.

## 2.1 RTE Transformation

The general equation of radiative transfer for a medium with constant index of refraction has the form [1]

$$\hat{\mathbf{s}} \cdot \nabla_\tau I + I = (1-\omega) I_b + \frac{\omega}{4\pi} \int_{4\pi} I(\hat{\mathbf{s}}') \Phi(\hat{\mathbf{s}} \cdot \hat{\mathbf{s}}') d\Omega', \tag{5}$$

where $\omega$ is the single scattering albedo. Augmentation of intensity due to in-scattering is calculated by the last term in the above equation, where $\Phi$ is the scattering phase function and describes the probability that a ray from direction $\hat{\mathbf{s}}'$ will be scattered into a certain direction, $\hat{\mathbf{s}}$. The intensity gradient, $\nabla_\tau$, along direction $\hat{\mathbf{s}}$ is written in terms of nondimensional optical coordinates with the extinction coefficient $\beta$.

Substituting Eq. (1) into the RTE, and collecting spherical harmonics of individual order, leads to a system of $(N+1)^2$ simultaneous first-order PDEs in the $I_n^m$ ($n = 0, 1, \ldots, N; -n \le m \le +n$). From this set the $I_n^m$ with odd $n$ may be eliminated, and after rather horrific algebra a set of $N(N+1)/2$ elliptic PDEs is obtained for even-order $I_n^m$ ($n = 0, 2, \ldots, N-1; -n \le m \le +n$). The full set of PDEs has been given in [8] and, because of their great length, will not be repeated here. Their essence is captured by noting that each equation contains many of the terms

$$\mathbf{pq}_{n,k}^{m,l} : \nabla_\tau \left( \frac{1}{\alpha} \nabla_\tau I_{n+k}^l \right); \quad k = -2, 0, +2; -(n+k) \le l \le +(n+k), \tag{6}$$

where the $\mathbf{pq}_{n,k}^{m,l}$ are constant-value coefficient tensors depending on $n, m, k$ and $l$, and $\alpha$ is a function of the anisotropy constants $A_i$ resulting from the expansion of the scattering phase function into a series of spherical harmonics [1]. This parameter reduces to a constant for the case of isotropic scattering. For anisotropic scattering the number of terms given by Eq. (6) is increased by one-third and some of the operators acting on the $I_n^m$ are nonsymmetric.

The tensor product form of the governing equations given in [8] may be eliminated in favor of more standard formulations, by defining a second-order operator

$$\mathscr{L}_{xy} = \frac{1}{\beta} \frac{\partial}{\partial x} \left( \frac{1}{\beta} \frac{\partial}{\partial y} \right), \tag{7}$$

etc. When also assuming isotropic scattering, some of the $\mathbf{pq}_{n,k}^{m,l}$ may be combined, resulting in all-symmetric operators. After more tedious algebra, not reproduced here, the set of governing equations given by Modest and Yang [8] may be restated as

$Y_n^m: \ n = 0, 2, \ldots, N-1, \ 0 \le m \le n:$

$$\sum_{k=1}^{3}\Bigg\{(\mathscr{L}_{xx}-\mathscr{L}_{yy})\left[(1+\delta_{m2})a_k^{nm}I_{n+4-2k}^{m-2}+\frac{\delta_{m1}}{2}c_k^{nm}I_{n+4-2k}^{m}+e_k^{nm}I_{n+4-2k}^{m+2}\right]$$
$$+(\mathscr{L}_{xz}+\mathscr{L}_{zx})\left[(1+\delta_{m1})b_k^{nm}I_{n+4-2k}^{m-1}+d_k^{nm}I_{n+4-2k}^{m+1}\right]$$
$$+(\mathscr{L}_{xy}+\mathscr{L}_{yx})\left[-(1-\delta_{m2})a_k^{nm}I_{n+4-2k}^{-(m-2)}+\frac{\delta_{m1}}{2}c_k^{nm}I_{n+4-2k}^{-m}+e_k^{nm}I_{n+4-2k}^{-(m+2)}\right]$$
$$+(\mathscr{L}_{yz}+\mathscr{L}_{zy})\left[-(1-\delta_{m1})b_k^{nm}I_{n+4-2k}^{-(m-1)}+d_k^{nm}I_{n+4-2k}^{-(m+1)}\right]$$
$$+(\mathscr{L}_{xx}+\mathscr{L}_{yy}-2\mathscr{L}_{zz})c_k^{nm}I_{n+4-2k}^{m}\Bigg\}+\left[f_n\mathscr{L}_{zz}-(1-\omega\delta_{0n})\right]I_n^m=-(1-\omega)I_b\delta_{0n} \tag{8a}$$

and

$Y_n^{-m}: \ n = 0, 2, \ldots, N-1, \ 1 \le m \le n:$

$$\sum_{k=1}^{3}\Bigg\{(\mathscr{L}_{xy}+\mathscr{L}_{yx})\left[(1+\delta_{m2})a_k^{nm}I_{n+4-2k}^{m-2}+\frac{\delta_{m1}}{2}c_k^{nm}I_{n+4-2k}^{m}-e_k^{nm}I_{n+4-2k}^{m+2}\right]$$
$$+(\mathscr{L}_{yz}+\mathscr{L}_{zy})\left[(1+\delta_{m1})b_k^{nm}I_{n+4-2k}^{m-1}-d_k^{nm}I_{n+4-2k}^{m+1}\right]$$
$$+(\mathscr{L}_{xx}-\mathscr{L}_{yy})\left[(1-\delta_{m2})a_k^{nm}I_{n+4-2k}^{-(m-2)}-\frac{\delta_{m1}}{2}c_k^{nm}I_{n+4-2k}^{-m}+e_k^{nm}I_{n+4-2k}^{-(m+2)}\right]$$
$$+(\mathscr{L}_{xz}+\mathscr{L}_{zx})\left[(1-\delta_{m1})b_k^{nm}I_{n+4-2k}^{-(m-1)}+d_k^{nm}I_{n+4-2k}^{-(m+1)}\right]$$
$$+(\mathscr{L}_{xx}+\mathscr{L}_{yy}-2\mathscr{L}_{zz})c_k^{nm}I_{n+4-2k}^{-m}\Bigg\}+\left[f_n\mathscr{L}_{zz}-1\right]I_n^{-m}=0 \tag{8b}$$

The necessary constants are listed in Table 1. For anisotropic scattering, not presented here, the constants for $k = 1$ and 3 undergo only minor changes, but for $k = 2$ [involving two different anisotropy constants $A_i$ from the expansion of the scattering phase function] the operators become nonsymmetric.

Since the orientation of the Cartesian coordinate system is arbitrary, one would expect to see Eq. (8) to show similar operators in $x$, $y$ and $z$. The reason that this is not the case is that the global direction angles $(\theta, \psi)$ and, thus, the results for $I_n^m$ are tied to the choice of the coordinate system, i.e., we may write

$$I(\mathbf{r}, \hat{\mathbf{s}}) = \sum_{n}^{N}\sum_{m=-n}^{n} I_n^m(\mathbf{r})Y_n^m(\hat{\mathbf{s}}) = \sum_{n}^{N}\sum_{m=-n}^{n} \bar{I}_n^m(\bar{\mathbf{r}})\bar{Y}_n^m(\hat{\mathbf{s}}), \tag{9}$$

where the barred values refer to a rotated coordinate system $(\bar{x}, \bar{y}, \bar{z})$.

## 2.2 Boundary Conditions

Equation set (8) consists of $N(N+1)/2$ simultaneous, elliptic PDEs, requiring $N(N+1)/2$ boundary conditions everywhere along the domain boundary, which must be determined from the general Marshak's condition,

$$\int_{\hat{\mathbf{n}}\cdot\hat{\mathbf{s}}>0} I(\tau_w, \hat{\mathbf{s}})\bar{Y}^m_{2i-1} d\Omega = \int_{\hat{\mathbf{n}}\cdot\hat{\mathbf{s}}>0} I_s(\tau_w, \hat{\mathbf{s}})\bar{Y}^m_{2i-1} d\Omega, \qquad i = 1, 2, ..., \frac{1}{2}(N+1), \text{all relevant}\, m, \tag{10}$$

where the $\bar{Y}^m_{2i-1}(\hat{\mathbf{s}})$ are expressed in terms of a local coordinate system, in which polar angle $\bar{\theta}$ is measured from the surface normal (i.e., $\cos\bar{\theta} = \hat{\mathbf{n}} \cdot \hat{\mathbf{s}}$), and azimuthal angle $\bar{\psi}$ is measured on the surface, as indicated in Fig. 1. The statement "all relevant $m$" rather than $-i \leq m \leq +i$ appears in Eq. (10) because, in general, it provides more boundary conditions than needed. For example, for a one-dimensional plane-parallel medium there is no azimuthal dependence, so that the only "relevant" value for $m$ is $m = 0$. This term leads to a single boundary condition on each surface for the $P_1$-approximation, two for the $P_3$-approximation, and so on. Unfortunately, Eq. (10) leads to too many boundary conditions in multi-dimensional situations. For example, for the $P_1$-approximation for a general three-dimensional medium without symmetry, Eq. (10) leads to three boundary conditions everywhere ($i = 1, m = 0, \pm 1$), while only one is needed. On intuitive grounds it was accepted practice to satisfy Eq. (10) for all $m$ for $i = 1, 2, \ldots, \frac{1}{2}(N-1)$, and for as many "relevant" $m$ as possible for $i = \frac{1}{2}(N+1)$. We will revisit this issue once we have cast the boundary conditions in terms of the $I^m_n$ of even spherical harmonics.

Equation (10) is cast in terms of a local coordinate system. Thus, in order to obtain a generic boundary condition for arbitrary geometries, the global spherical harmonics must be rotated into the local coordinate system. Such rotation, according to Euler's rotation theorem, may be described using three angles, which are called Euler angles. In the literature, there are several notation and rotation conventions for Euler angles. Here, the notation $(\alpha, \beta, \gamma)$ is used for three Euler angles following Varshalovichs *et al.*'s definition [11]. In Varshalovich's convention, as shown in Fig. 2, an arbitrary rotation is defined by Euler angles $(\alpha, \beta, \gamma)$, where the first rotation is by an angle $\alpha$ about the $z$-axis, the second is by an angle $\beta$ about the $y'$-axis, and the third is by an angle $\gamma$ about the $z'$-axis. As indicated in Fig. 2 all three rotations are, following the right-hand-rule, in counter-clockwise direction about the center axis. The three rotations can, in general, be carried out by (1) rotating $x$-$y$ so that $y'$ is perpendicular to $\hat{\mathbf{n}}$ ($\hat{\mathbf{n}} \cdot \hat{\mathbf{j}}' = 0$)

$$\hat{\mathbf{i}}' = \cos\alpha\hat{\mathbf{i}} + \sin\alpha\hat{\mathbf{j}};\ \hat{\mathbf{j}}' = -\sin\alpha\hat{\mathbf{i}} + \cos\alpha\hat{\mathbf{j}} \tag{11}$$

and

$$\tan\alpha = \frac{n_y}{n_x}, \tag{12}$$

(2) rotating $x'$-$z$ such that $z'$ becomes parallel to $\hat{\mathbf{n}}$, or

$$\hat{\mathbf{k}}' = \sin\beta\hat{\mathbf{i}}' + \cos\beta\hat{\mathbf{k}} \tag{13}$$

and $\hat{\mathbf{n}} \cdot \hat{\mathbf{k}}' = 1$ gives

$$(n_x \cos\alpha + n_y \sin\alpha)\sin\beta + n_z \cos\beta = 1. \tag{14}$$

(3) The third rotation is arbitrary and serves to place the local $\bar{x}$-$\bar{y}$-coordinates into convenient locations. For example, to perform the transformation indicated in Fig. 1 (with the global $z$-axis pointing toward the reader), the local surface normal is determined as

$$\hat{\mathbf{n}} = -\sin\delta\hat{\mathbf{i}} + \cos\delta\hat{\mathbf{j}} + 0\hat{\mathbf{k}}, \tag{15}$$

and the first rotation angle $\alpha$ follows from

$$\tan\alpha = -\tan\delta, \text{ or } \alpha = \delta \pm \frac{\pi}{2}. \tag{16}$$

If we choose $\alpha = \delta - \pi/2$ ($y'$ points into the indicated $\bar{x}$-direction), the second rotation angle becomes

$$\left[-\sin\delta\cos\left(\delta - \frac{\pi}{2}\right) + \cos\delta\sin\left(\delta - \frac{\pi}{2}\right)\right]\sin\beta = 1, \text{ or } \beta = \frac{3\pi}{2}. \tag{17}$$

This has $x''$ point out of the paper, and a final (optional) rotation of $\gamma = \pi/2$ rotates $x'''$ into the desired local $\bar{x}$-direction.

It can be shown that, for a given rotation, the spherical harmonics of order $n$ are transformed into a linear combination of spherical harmonics of the same order $n$. Such operation can be represented in the form of a rotation matrix, where each element of this matrix is a function of Euler angles,

$$Y_n^{m'}(\theta,\psi) = \sum_{m=-n}^{n} \Delta_{mm'}^{n}(\alpha,\beta,\gamma)\bar{Y}_n^{m}(\bar{\theta},\bar{\psi}), \tag{18}$$

where $\Delta^n_{mm'}(\alpha,\beta,\gamma)$ is the representation matrix of the rotation operation for the real spherical harmonics $Y^m_n$ of order $n$. Blanco[2] *et al.* [12] developed a closed-form expression to specify all the elements based on so-called Wigner-$D$ functions, from which the $\Delta^n$ matrices can be obtained in terms of the Euler angles as

$$\begin{aligned}\Delta^n_{mm'} &= \mathrm{sign}(m')\Psi_m(\alpha)\Psi_{m'}(\gamma)[d^n_{|m|,|m'|}(\beta) + (-1)^{m'} d^n_{|m|,-|m'|}(\beta)] \\ &\quad - \mathrm{sign}(m)\Psi_{-m}(\alpha)\Psi_{-m'}(\gamma)[d^n_{|m|,|m'|}(\beta) - (-1)^{m'} d^n_{|m|,-|m'|}(\beta)]\end{aligned} \tag{19}$$

where $\mathrm{sign}(0) = 1$ and the function $\Psi_m$ is defined as

$$\Psi_m(\xi) = \begin{cases} \cos m\xi, & \text{for} \quad m \geq 0, \\ \sin |m|\xi, & \text{for} \quad m < 0. \end{cases} \tag{20}$$

To determine the $\Delta^n$ matrices by Eq. (19) the $d^n$ matrices are needed, which are modified versions of the real parts of the Wigner-$D^n_{mm'}$ functions, and may be calculated from

$$d^n_{mm'}(\beta) = \frac{(-1)^{m+m'}(n-|m|)!(n+|m'|)!}{1+\delta_{m,0}} \sum_{k=\max(0,m'-m)}^{\min(n-m,n+m')} \frac{(-1)^k \left(\cos\frac{\beta}{2}\right)^{2n-2k-m+m'} \left(\sin\frac{\beta}{2}\right)^{2k+m-m'}}{k!(n-m-k)!(n+m'-k)!(m-m'+k)!}. \tag{21}$$

With the rotation of spherical harmonics between local and global coordinates as indicated by Eq. (18), relationships between $I^m_n$ and $\bar{I}^m_n$ can be revealed accordingly by expressing intensity in terms of, both, local and global coordinates, as given by Eq. (9). This leads to [8]

$$I^m_n = \sum_{m'=-n}^{n} \Delta^n_{mm'}(\alpha,\beta,\gamma)\bar{I}^{m'}_n, \text{ and } \bar{I}^m_n = \sum_{m'=-n}^{n} \bar{\Delta}^n_{mm'}(-\gamma,-\beta,-\alpha)I^{m'}_n, \tag{22}$$

where the bar on the $\bar{\Delta}^n_{mm'}$ implies backward rotation from local to global coordinates, as indicated by the arguments. Substitution of Eq. (9) into (10), and assuming the surface intensity $I_w$ to be diffuse, reduces the boundary conditions to

$$\begin{aligned}\sum_{n=0}^{N}\left[\int_0^1 P^m_n(\bar{\mu})P^m_{2i-1}(\bar{\mu})d\bar{\mu}\right]\bar{I}^m_n(\tau_w) &= \left[\int_0^1 P_{2i-1}(\bar{\mu})d\bar{\mu}\right]\delta_{m,0}\, I_w, \\ & i = 1,2,...,\tfrac{1}{2}(N+1), \text{all relevant}\, m.\end{aligned} \tag{23}$$

Before these boundary conditions can be applied to Eqs. (8) the $\bar{I}^m_n$ with odd $n$ must be eliminated. Boundary

[2]In Blanco's derivation, a normalization factor is employed. In order to be consistent with the real spherical harmonics used in the current study, a modification coefficient was included in the transformation.

conditions are usually formulated in terms of local normal and tangential gradients, and this leads to

$$\bar{Y}_{2i-1}^{0}: \quad \sum_{l=0}^{\frac{N-1}{2}} p_{2l,2i-1}^{0} \bar{I}_{2l}^{0} + \frac{\partial}{\partial \tau_{\bar{x}}} \left[ \sum_{l=1}^{\frac{N-1}{2}} v_{li}^{0} \bar{I}_{2l}^{1} \right] + \frac{\partial}{\partial \tau_{\bar{y}}} \left[ \sum_{l=1}^{\frac{N-1}{2}} v_{li}^{0} \bar{I}_{2l}^{-1} \right] - \frac{\partial}{\partial \tau_{\bar{z}}} \left[ \sum_{l=0}^{\frac{N-1}{2}} w_{li}^{0} \bar{I}_{2l}^{0} \right] = I_w p_{0,2i-1}^{0}, \qquad m = 0, \tag{24a}$$

$$\bar{Y}_{2i-1}^{m}: \quad \sum_{l=1}^{\frac{N-1}{2}} p_{2l,2i-1}^{m} \bar{I}_{2l}^{m} - \frac{\partial}{\partial \tau_{\bar{x}}} \left[ \sum_{l=0}^{\frac{N-1}{2}} (1+\delta_{m,1}) u_{li}^{m} \bar{I}_{2l}^{m-1} - \sum_{l=1}^{\frac{N-1}{2}} v_{li}^{m} \bar{I}_{2l}^{m+1} \right] + \frac{\partial}{\partial \tau_{\bar{y}}} \left[ \sum_{l=1}^{\frac{N-1}{2}} (1-\delta_{m,1}) u_{li}^{m} \bar{I}_{2l}^{-(m-1)} + \sum_{l=1}^{\frac{N-1}{2}} v_{li}^{m} \bar{I}_{2l}^{-(m+1)} \right] - \frac{\partial}{\partial \tau_{\bar{z}}} \left[ \sum_{l=1}^{\frac{N-1}{2}} w_{li}^{m} \bar{I}_{2l}^{m} \right] = 0, \qquad m > 0, \tag{24b}$$

$$\bar{Y}_{2i-1}^{-m}: \quad \sum_{l=1}^{\frac{N-1}{2}} p_{2l,2i-1}^{m} \bar{I}_{2l}^{-m} - \frac{\partial}{\partial \tau_{\bar{x}}} \left[ \sum_{l=1}^{\frac{N-1}{2}} (1-\delta_{m,1}) u_{li}^{m} \bar{I}_{2l}^{-(m-1)} - \sum_{l=1}^{\frac{N-1}{2}} v_{li}^{m} \bar{I}_{2l}^{-(m+1)} \right] - \frac{\partial}{\partial \tau_{\bar{y}}} \left[ \sum_{l=0}^{\frac{N-1}{2}} (1+\delta_{m,1}) u_{li}^{m} \bar{I}_{2l}^{m-1} + \sum_{l=1}^{\frac{N-1}{2}} v_{li}^{m} \bar{I}_{2l}^{m+1} \right] - \frac{\partial}{\partial \tau_{\bar{z}}} \left[ \sum_{l=1}^{\frac{N-1}{2}} w_{li}^{m} \bar{I}_{2l}^{-m} \right] = 0, \qquad m > 0, \tag{24c}$$

where the $p_{n,j}^{m}$ are defined as

$$p_{n,j}^{m} = p_{j,n}^{m} = \int_{0}^{1} P_n^m(\bar{\mu}) P_j^m(\bar{\mu}) d\bar{\mu}, \tag{25}$$

and, limiting ourselves to isotropic scattering, the coefficients $u_{li}^{m}, v_{li}^{m}, w_{li}^{m}$ are related to them by

$$u_{li}^{m} = \frac{p_{2l-1,2i-1}^{m} - p_{2l+1,2i-1}^{m}}{2(4l+1)}, \tag{26a}$$

$$v_{li}^{m} = \frac{\pi_2(2l+m) p_{2l-1,2i-1}^{m} - \pi_2(2l-m) p_{2l+1,2i-1}^{m}}{2(4l+1)}, \tag{26b}$$

$$w_{li}^{m} = \frac{(2l+m) p_{2l-1,2i-1}^{m} + (2l-m+1) p_{2l+1,2i-1}^{m}}{(4l+1)}. \tag{26c}$$

In Eqs. (24) and (26) it is implied that coefficients in front of nonsensical $\bar{I}_n^m$ (i.e., $|m| > n$) and $p_{nj}^m$ with nonsensical subscripts ($n < m$) are zero. The $p_{n,j}^{m}$ may be determined through recursion relationships. Employing the standard relations

$$(n+1) x P_n^m(x) = (n-m+1) P_{n+1}^m - (1-x^2) \frac{dP_n^m}{dx}, \tag{27a}$$

$$(2n+1) x P_n^m(x) = (n-m+1) P_{n+1}^m + (n+m) P_{n-1}^m, \tag{27b}$$

we can find

$$(n+j)\int_0^1 xP_n^m(x)P_j^m(x)dx = \frac{n+j}{2n+1}\left[(n-m+1)p_{n+1,j}^m + (n+m)p_{n-1,j}^m\right]$$
$$= (n-m+1)p_{n+1,j}^m + (j-m+1)p_{n,j+1}^m - P_n^m(0)P_j^m(0). \tag{28}$$

The first one of these relationships follows directly from Eq. (27a); the second requires using Eq. (27b) for both $P_n^m$ and $P_j^m$ in the integral, adding the two results, and eliminating an integral through partial integration. Combining the two expressions yields an important recursion formula for the $p_{n,j}^m$:

$$p_{n,j}^m = \frac{(2n-1)\left[P_{n-1}^m(0)P_j^m(0) - (j-m+1)p_{n-1,j+1}^m\right] + (n+j-1)(n+m-1)p_{n-2,j}^m}{(n-j)(n-m)}, \tag{29}$$

where the $P_n^m(0)$ are given by

$$P_n^m(0) = \begin{cases} 0, & n+m \text{ odd}, \\ \dfrac{(-1)^{(n+m)/2}(n+m-1)!}{(\frac{n+m}{2}-1)!2^{n-1}(\frac{n-m}{2})!}, & n+m \text{ even}. \end{cases} \tag{30}$$

Equation (29) is valid for $n > j \geq m$. For the case of $n = j$ the $p_{n,n}^m$ can be calculated directly from

$$p_{n,n}^m = \int_0^1 P_n^m(x)P_n^m(x)dx = \frac{1}{2}\int_{-1}^1 [P_n^m(x)]^2 dx = \frac{(n+m)!}{(2n+1)(n-m)!}. \tag{31}$$

The calculation of all $p_{n,j}^m$ then proceeds as follows, making use of the facts that

$$p_{n,j}^m = p_{j,n}^m \quad \text{and} \quad p_{n,j}^m = 0 \text{ if } n < m \text{ or } j < m. \tag{32}$$

For a given $m$ all $p_{n,n}^m$ are calculated from Eq. (31), and for $n > j$ are obtained from Eq. (29). Values necessary for up to the $P_5$-approximation obtained from these relations are listed in Table 2 (scaled by a factor of $10^{-m}$).

Equations (35) are a set of $(N+2)(N+1)/2$ boundary conditions for $N(N+1)/2$ variables $I_{2l}^m$ $[l = 0, 1, ..., (N-1)/2;\ m = -2l, ..., +2l]$, containing normal as well as tangential derivatives, or $N+1$ too many. Inspecting the boundary conditions (24) we make two important observations:

1. For a given value of $m$ the normal derivatives contain only the spatial coefficients $I_{2l}^m$, for $2l \geq m$, and all carrying the same value of superscript $m$. For even $m$ there are $\frac{1}{2}(N+1-m)$ different $I_{2l}^m$ $(2l = m, m+2, \ldots, N-1)$, while for odd $m$ there are $\frac{1}{2}(N-m)$ different $I_{2l}^m$ $(2l = m+1, m+3, \ldots, N-1)$.

2. For a given value of $m$ the parameter $i$ has a limited range of allowed values, as we must have $2i-1 \geq$

$m$. Thus, for even $m$: $2i-1 = m+1, m+3, \ldots, N$, or $\frac{1}{2}(N+1-m)$ different boundary conditions, or the same number as there are $I_{2l}^m$. However, for odd $m$ there are $2i-1 = m, m+2, \ldots, N$, or $\frac{1}{2}(N-m)+1$ boundary conditions, i.e., one more than there are $I_{2l}^m$ of rank $m$.

Commercial (and other) PDE solvers generally allow for boundary conditions containing normal derivatives. In principle, i.e., if the coefficients in front of the $I_{2l}^m$ inside the normal derivatives form a nonsingular matrix, linear combination of the boundary conditions leads to a set of "natural" boundary conditions for each variable, or

$$\frac{\partial I_{2l}^m}{\partial \tau_{\bar{z}}} = f\left(I_{2l'}^{m'}, \frac{\partial I_{2l'}^{m'}}{\partial \tau_{\bar{x}}}, \frac{\partial I_{2l'}^{m'}}{\partial \tau_{\bar{y}}}; l' = 0, \ldots \tfrac{1}{2}(N-1); m' = -2l', \ldots, +2l'\right),$$
$$l = 0, \ldots, \tfrac{1}{2}(N-1), m = -2l, \ldots, +2l, \tag{33}$$

which can be used with FlexPDE [13] and other commercial programs. Such a nonsingular matrix can be found only if, for the largest value of $i = \frac{1}{2}(N+1)$, only the even values of $m$ are employed (omitting the $N+1$ odd values). Therefore, the qualifier "all relevant $m$" in Eqs. (23), (24) and (35) may be restated precisely as

$$\text{All relevant } m = \begin{cases} i = 1, 2, \ldots, \frac{1}{2}(N-1), & \text{all } m, \\ i = \frac{1}{2}(N+1), & \text{all even } m, \end{cases} \tag{34}$$

which supplies a consistent set of $N(N+1)/2$ boundary conditions for an equal number of variables.

It remains to rotate the $\bar{I}_n^m$ in Eqs. (24) to global values $I_n^m$, which results in [8]

$$\bar{Y}_{2i-1}^0: \sum_{l=0}^{\frac{N-1}{2}} \sum_{m'=-2l}^{2l} p_{2l,2i-1}^0 \bar{\Delta}_{0,m'}^{2l} I_{2l}^{m'} + \frac{\partial}{\partial \tau_{\bar{x}}} \left\{ \sum_{l=1}^{\frac{N-1}{2}} \sum_{m'=-2l}^{2l} v_{li}^0 \bar{\Delta}_{1,m'}^{2l} I_{2l}^{m'} \right\}$$
$$+ \frac{\partial}{\partial \tau_{\bar{y}}} \left\{ \sum_{l=1}^{\frac{N-1}{2}} \sum_{m'=-2l}^{2l} v_{li}^0 \bar{\Delta}_{-1,m'}^{2l} I_{2l}^{m'} \right\} - \frac{\partial}{\partial \tau_{\bar{z}}} \left\{ \sum_{l=0}^{\frac{N-1}{2}} \sum_{m'=-2l}^{2l} w_{li}^0 \bar{\Delta}_{0,m'}^{2l} I_{2l}^{m'} \right\} = I_w p_{0,2i-1}^0,$$
$$m = 0, \tag{35a}$$

$$\bar{Y}_{2i-1}^m: \sum_{l=1}^{\frac{N-1}{2}} \sum_{m'=-2l}^{2l} p_{2l,2i-1}^m \bar{\Delta}_{m,m'}^{2l} I_{2l}^{m'} - \frac{\partial}{\partial \tau_{\bar{x}}} \left\{ \sum_{l=0}^{\frac{N-1}{2}} \sum_{m'=-2l}^{2l} \left[ (1+\delta_{m,1}) u_{li}^m \bar{\Delta}_{m-1,m'}^{2l} - v_{li}^m \bar{\Delta}_{m+1,m'}^{2l} \right] I_{2l}^{m'} \right\}$$
$$+ \frac{\partial}{\partial \tau_{\bar{y}}} \left\{ \sum_{l=1}^{\frac{N-1}{2}} \sum_{m'=-2l}^{2l} \left[ (1-\delta_{m,1}) u_{li}^m \bar{\Delta}_{-(m-1),m'}^{2l} + v_{li}^m \bar{\Delta}_{-(m+1),m'}^{2l} \right] I_{2l}^{m'} \right\} - \frac{\partial}{\partial \tau_{\bar{z}}} \left\{ \sum_{l=1}^{\frac{N-1}{2}} \sum_{m'=-2l}^{2l} w_{li}^m \bar{\Delta}_{m,m'}^{2l} I_{2l}^{m'} \right\} = 0,$$
$$m > 0, \tag{35b}$$

$$\bar{Y}_{2i-1}^{-m}: \sum_{l=1}^{\frac{N-1}{2}} \sum_{m'=-2l}^{2l} p_{2l,2i-1}^{m} \bar{\Delta}_{-m,m'}^{2l} I_{2l}^{m'} - \frac{\partial}{\partial \tau_{\bar{x}}} \left\{ \sum_{l=1}^{\frac{N-1}{2}} \sum_{m'=-2l}^{2l} \left[ (1-\delta_{m,1}) u_{li}^{m} \bar{\Delta}_{-(m-1),m'}^{2l} - v_{li}^{m} \bar{\Delta}_{-(m+1),m'}^{2l} \right] I_{2l}^{m'} \right\}$$

$$- \frac{\partial}{\partial \tau_{\bar{y}}} \left\{ \sum_{l=0}^{\frac{N-1}{2}} \sum_{m'=-2l}^{2l} \left[ (1+\delta_{m,1}) u_{li}^{m} \bar{\Delta}_{m-1,m'}^{2l} + v_{li}^{m} \bar{\Delta}_{m+1,m'}^{2l} \right] I_{2l}^{m'} \right\} - \frac{\partial}{\partial \tau_{\bar{z}}} \left\{ \sum_{l=1}^{\frac{N-1}{2}} \sum_{m'=-2l}^{2l} w_{li}^{m} \bar{\Delta}_{-m,m'}^{2l} I_{2l}^{m'} \right\} = 0,$$

$$m > 0. \tag{35c}$$

Other codes, such as PDE2D [14] or FDEM [15], use derivatives in global coordinates in the boundary conditions. In that case, the transformation to global $I_n^m$ using Eq. (22) is carried out first, followed by elimination of odd orders. The resulting boundary conditions are given in [8].

Once all $I_n^m$ for even $n$ have been determined, the remaining $I_n^m$ (odd $n$) may be determined from relations given in Modest and Yang [8]. Normally, only incident radiation $G = 4\pi I_0$ and radiative flux are of interest, the latter being related to the $I_1^m$: multiplying Eq. (1) by $Y_1^m$ (or $\hat{\mathbf{s}}$), integrating over $4\pi$, and noting that higher order terms drop out because of the orthogonality of spherical harmonics [16], leads to

$$\mathbf{q}(\mathbf{r}) = \int_{4\pi} I(\mathbf{r}, \hat{\mathbf{s}})\, \hat{\mathbf{s}}\, d\Omega = \frac{4\pi}{3} \begin{pmatrix} -I_1^1 \\ -I_1^{-1} \\ I_1^0 \end{pmatrix}, \tag{36}$$

where the $I_1^m$ are given by [8]

$$I_1^0 = -\frac{\partial I_0}{\partial \tau_z} - \frac{2}{5}\frac{\partial I_2^0}{\partial \tau_z} + \frac{3}{5}\frac{\partial I_2^1}{\partial \tau_x} + \frac{3}{5}\frac{\partial I_2^{-1}}{\partial \tau_y}, \tag{37a}$$

$$I_1^1 = +\frac{\partial I_0}{\partial \tau_x} - \frac{1}{5}\frac{\partial I_2^0}{\partial \tau_x} - \frac{3}{5}\frac{\partial I_2^1}{\partial \tau_z} + \frac{6}{5}\frac{\partial I_2^2}{\partial \tau_x} + \frac{6}{5}\frac{\partial I_2^{-2}}{\partial \tau_y}, \tag{37b}$$

$$I_1^{-1} = +\frac{\partial I_0}{\partial \tau_y} - \frac{1}{5}\frac{\partial I_2^0}{\partial \tau_y} - \frac{3}{5}\frac{\partial I_2^{-1}}{\partial \tau_z} - \frac{6}{5}\frac{\partial I_2^2}{\partial \tau_y} + \frac{6}{5}\frac{\partial I_2^{-2}}{\partial \tau_x}. \tag{37c}$$

Since Eq. (1) is valid for any coordinate system orientation, Eqs. (36) and (37) are valid for both the global coordinate system ($x$-$y$-$z$, $I_n^m$) as well as a local coordinate system at a boundary ($\bar{x}$-$\bar{y}$-$\bar{z}$, $\bar{I}_n^m$).

Finally, for nonblack surfaces the boundary radiosity $J_w = \pi I_w$ must be related to the wall's emissive power and/or net radiative flux. From Eq. (36) we have

$$q_n = \frac{\epsilon\pi}{1-\epsilon}\left[I_{bw} - I_w\right] = \frac{4\pi}{3}\bar{I}_1^0, \tag{38}$$

where $\epsilon$ is the surface's emittance, and with $\bar{I}_1^0$ transformed to global $I_1^m$ through Eq. (22). If the temperature of the surface, $T_w$, is specified, $I_w$ is determined from

$$I_w = I_{bw} - \frac{4}{3}\left(\frac{1}{\epsilon} - 1\right)\bar{I}_1^0. \tag{39}$$

To demonstrate how the equations and boundary conditions are used, we will extract the $P_3$-approximation and its boundary conditions for a medium at temperature $T(x, y)$, confined inside a two-dimensional enclosure as shown in Fig. 1. The medium is gray and absorbs and emits, but does not scatter.

For a two-dimensional problem with polar angle $\theta$ measured from the $z$-axis we must have $I(\theta, \psi) = I(\pi - \theta, \psi)$, i.e., all $I_n^m$, for which the accompanying associated Legendre polynomials $P_n^m(\cos\theta)$ have an odd-power dependence on $\cos\theta$, must vanish. This is the case whenever $n + m$ is odd. Therefore, $I_n^m = 0$ for $n + m =$ odd and, since the governing equations are cast in terms of even $n$, terms with odd $m$ in Eqs. (8) vanish. Using this, and eliminating all terms with $z$-derivatives, we get from Eqs. (8)

$$\begin{aligned}
Y_0^0:&\quad (\mathscr{L}_{xx} - \mathscr{L}_{yy})e_1^{00}I_2^2 + (\mathscr{L}_{xy} + \mathscr{L}_{yx})e_1^{00}I_2^{-2} + (\mathscr{L}_{xx} + \mathscr{L}_{yy})c_1^{00}I_2^0 + (\mathscr{L}_{xx} + \mathscr{L}_{yy})c_2^{00}I_0^0 - I_0^0 = -I_b,\\
Y_2^0:&\quad (\mathscr{L}_{xx} - \mathscr{L}_{yy})e_2^{20}I_2^2 + (\mathscr{L}_{xy} + \mathscr{L}_{yx})e_2^{20}I_2^{-2} + (\mathscr{L}_{xx} + \mathscr{L}_{yy})c_2^{20}I_2^0 + (\mathscr{L}_{xx} + \mathscr{L}_{yy})c_3^{20}I_0^0 - I_2^0 = 0,\\
Y_2^2:&\quad (\mathscr{L}_{xx} - \mathscr{L}_{yy})2a_2^{22}I_2^0 + (\mathscr{L}_{xx} + \mathscr{L}_{yy})c_2^{22}I_2^2 + (\mathscr{L}_{xx} - \mathscr{L}_{yy})2a_3^{22}I_0^0 - I_2^2 = 0,\\
Y_2^{-2}:&\quad (\mathscr{L}_{xy} + \mathscr{L}_{yx})2a_2^{22}I_2^0 + (\mathscr{L}_{xx} + \mathscr{L}_{yy})c_2^{22}I_2^{-2} + (\mathscr{L}_{xy} + \mathscr{L}_{yx})2a_3^{22}I_0^0 - I_0^{-2} = 0.
\end{aligned}$$

For $n = 0$ the case of $k = 3$ is not needed, since this leads to nonexistent $I_{-2}^m$, and, similarly, for $n = 2$ the case of $k = 1$, producing $I_4^m$, i.e., terms omitted in the $P_3$-approximation. In addition, all $I_n^m$ with odd $m$ and with $m > n$ are dropped. Equations (8) are also valid for $n = 2, m = \pm 1$, but every term in these equations vanishes. Thus the above set constitutes the needed four equations for the four unknowns. The coefficients are evaluated from Table 1 and substituting them into the four governing equations, we find

$$Y_0^0:\quad \frac{2}{5}(\mathscr{L}_{xx} - \mathscr{L}_{yy})I_2^2 + \frac{2}{5}(\mathscr{L}_{xy} + \mathscr{L}_{yx})I_2^{-2} - (\mathscr{L}_{xx} + \mathscr{L}_{yy})\left(\frac{1}{15}I_2^0 - \frac{1}{3}I_0^0\right) - I_0^0 = -I_b, \tag{40a}$$

$$Y_2^0:\quad -\frac{4}{7}(\mathscr{L}_{xx} - \mathscr{L}_{yy})I_2^2 - \frac{4}{7}(\mathscr{L}_{xy} + \mathscr{L}_{yx})I_2^{-2} + (\mathscr{L}_{xx} + \mathscr{L}_{yy})\left(\frac{5}{21}I_2^0 - \frac{1}{3}I_0^0\right) - I_2^0 = 0, \tag{40b}$$

$$Y_2^2:\quad \frac{3}{7}(\mathscr{L}_{xx} + \mathscr{L}_{yy})I_2^2 - (\mathscr{L}_{xx} - \mathscr{L}_{yy})\left(\frac{1}{21}I_2^0 - \frac{1}{6}I_0^0\right) - I_2^2 = 0, \tag{40c}$$

$$Y_2^{-2}:\quad \frac{3}{7}(\mathscr{L}_{xx} + \mathscr{L}_{yy})I_2^{-2} - (\mathscr{L}_{xy} + \mathscr{L}_{yx})\left(\frac{1}{21}I_2^0 - \frac{1}{6}I_0^0\right) - I_2^{-2} = 0. \tag{40d}$$

The boundary conditions are usually expressed in terms of local coordinates (i.e., in terms of gradients into the surface normal and tangential directions); either using local spherical harmonics $\bar{I}_n^m$, Eq. (24), followed by rotation to global spherical harmonics $I_n^m$, or by directly applying Eq. (35). In general, it would be advantageous to calculate all coefficients in Eq. (35) with a small computer program. For illustrative purposes we will carry out the individual calculations by following the first track. With local azimuthal angle $\bar{\psi}$ defined from the $\bar{x}$-axis in the $\bar{x}$–$\bar{y}$–plane, for this two-dimensional problem independent of $\bar{y}$ we must have $I(\bar{\theta},\bar{\psi}) = I(\bar{\theta},-\bar{\psi})$ and, therefore, all $\bar{I}_n^m$ with negative $m$ vanish. Thus, from Eq. (24), eliminating all terms with negative $m$ and $\bar{y}$-gradients, we obtain

$$
\begin{aligned}
\bar{Y}_1^0: &\quad p_{01}^0\bar{I}_0^0 + p_{21}^0\bar{I}_2^0 + \frac{\partial}{\partial\tau_{\bar{x}}}\left[v_{11}^0\bar{I}_2^1\right] - \frac{\partial}{\partial\tau_{\bar{z}}}\left[w_{01}^0\bar{I}_0^0 + w_{11}^0\bar{I}_2^0\right] = I_{bw}p_{01}^0,\\
\bar{Y}_1^1: &\quad p_{21}^1\bar{I}_2^1 - \frac{\partial}{\partial\tau_{\bar{x}}}\left[2u_{01}^1\bar{I}_0^0 + 2u_{11}^1\bar{I}_2^0 - v_{11}^1\bar{I}_2^2\right] - \frac{\partial}{\partial\tau_{\bar{z}}}\left[w_{11}^1\bar{I}_2^1\right] = 0,\\
\bar{Y}_3^0: &\quad p_{03}^0\bar{I}_0^0 + p_{23}^0\bar{I}_2^0 + \frac{\partial}{\partial\tau_{\bar{x}}}\left[v_{12}^0\bar{I}_2^1\right] - \frac{\partial}{\partial\tau_{\bar{z}}}\left[w_{02}^0\bar{I}_0^0 + w_{12}^0\bar{I}_2^0\right] = I_{bw}p_{03}^0,\\
\bar{Y}_3^2: &\quad p_{23}^2\bar{I}_2^2 - \frac{\partial}{\partial\tau_{\bar{x}}}\left[u_{12}^2\bar{I}_2^1\right] - \frac{\partial}{\partial\tau_{\bar{z}}}\left[w_{12}^2\bar{I}_2^2\right] = 0.
\end{aligned}
$$

The equations for $\bar{Y}_1^{-1}$ and $\bar{Y}_3^{-2}$ contain only $\bar{I}_n^m$ with negative $m$ and, thus, vanish identically, leaving us with the proper 4 boundary conditions for the 4 unknown $\bar{I}_n^m$. The coefficients $p_{nj}^m$, $u_{li}^m$, $v_{li}^m$ and $w_{li}^m$ are found from Table 2 and, after normalization with the leading term,

$$
\begin{aligned}
\bar{Y}_1^0: &\quad \bar{I}_0^0 + \frac{1}{4}\bar{I}_2^0 + \frac{2}{5}\frac{\partial\bar{I}_2^1}{\partial\tau_{\bar{x}}} - \frac{2}{3}\frac{\partial\bar{I}_0^0}{\partial\tau_{\bar{z}}} - \frac{4}{15}\frac{\partial\bar{I}_2^0}{\partial\tau_{\bar{z}}} = I_{bw}, && \text{(41a)}\\
\bar{Y}_1^1: &\quad \bar{I}_2^1 + \frac{\partial}{\partial\tau_{\bar{x}}}\left[\frac{8}{9}\bar{I}_0^0 - \frac{8}{45}\bar{I}_2^0 + \frac{16}{15}\bar{I}_2^2\right] - \frac{8}{15}\frac{\partial\bar{I}_2^1}{\partial\tau_{\bar{z}}} = 0, && \text{(41b)}\\
\bar{Y}_3^0: &\quad \bar{I}_0^0 - \bar{I}_2^0 + \frac{24}{35}\frac{\partial\bar{I}_2^1}{\partial\tau_{\bar{x}}} + \frac{24}{35}\frac{\partial\bar{I}_2^0}{\partial\tau_{\bar{z}}} = I_{bw}, && \text{(41c)}\\
\bar{Y}_3^2: &\quad \bar{I}_2^2 + \frac{8}{35}\frac{\partial\bar{I}_2^1}{\partial\tau_{\bar{x}}} - \frac{16}{35}\frac{\partial\bar{I}_2^2}{\partial\tau_{\bar{z}}} = 0. && \text{(41d)}\\
& && \text{(41e)}
\end{aligned}
$$

Next, the local $\bar{I}_n^m$ must be converted to global $I_n^m$ with Eq. (22). For $n = 0$ this simply gives $\bar{I}_0^0 = I_0^0$, i.e., $I_0^0$ is nondirectional and does not vary with rotation, and we will drop the unnecessary superscript from $I_0$. Remembering that, in global coordinates, $I_n^m$ with odd $m$ vanish (as opposed to negative $m$ in local coordinates), for $n = 2$ this leads to

$$\bar{I}_2^0 = \bar{\Delta}^2_{0,-2} I_2^{-2} + \bar{\Delta}^2_{0,0} I_2^0 + \bar{\Delta}^2_{0,2} I_2^2,$$
$$\bar{I}_2^1 = \bar{\Delta}^2_{1,-2} I_2^{-2} + \bar{\Delta}^2_{1,0} I_2^0 + \bar{\Delta}^2_{1,2} I_2^2,$$
$$\bar{I}_2^2 = \bar{\Delta}^2_{2,-2} I_2^{-2} + \bar{\Delta}^2_{2,0} I_2^0 + \bar{\Delta}^2_{2,2} I_2^2.$$

The necessary $\bar{\Delta}^2_{m,m'}(-\gamma = -\frac{\pi}{2}, -\beta = -\frac{3\pi}{2}, -\alpha = \frac{\pi}{2} - \delta)$ are determined via backward rotation from Eq. (19) with

$$\Psi_m\left(-\frac{\pi}{2}\right) = \begin{cases} -1, & m = 2 \\ 0, & 1 \\ 1, & 0 \\ -1, & -1 \\ 0, & -2 \end{cases}, \quad \Psi_{m'}\left(\frac{\pi}{2} - \delta\right) = \begin{cases} -\cos 2\delta, & m' = 2 \\ \sin\delta, & 1 \\ 1, & 0 \\ \cos\delta, & -1 \\ \sin 2\delta, & -2 \end{cases},$$

and $\cos(\frac{\beta}{2}) = \sin(\frac{\beta}{2}) = \cos(-\frac{3\pi}{4}) = -\frac{1}{\sqrt{2}}$. The $d^2_{mm'}$ follow from Eq. (21) after some painful algebra. Finally,

$$\bar{I}_2^0 = -3\sin 2\delta\, I_2^{-2} - \frac{1}{2} I_2^0 - 3\cos 2\delta\, I_2^2,$$
$$\bar{I}_2^1 = -2\cos 2\delta\, I_2^{-2} + 2\sin 2\delta\, I_2^2,$$
$$\bar{I}_2^2 = \frac{1}{2}\sin 2\delta\, I_2^{-2} - \frac{1}{4} I_2^0 + \frac{1}{2}\cos 2\delta\, I_2^2.$$

Sticking this into Eq. (41) delivers the desired local boundary conditions as

$$\bar{Y}_1^0 : \quad I_0 - \frac{3}{4}\sin 2\delta\, I_2^{-2} - \frac{1}{8} I_2^0 - \frac{3}{4}\cos 2\delta\, I_2^2 - \frac{4}{5}\frac{\partial}{\partial\tau_{\bar{x}}}\left[\cos 2\delta\, I_2^{-2} - \sin 2\delta\, I_2^2\right]$$
$$-\frac{2}{15}\frac{\partial}{\partial\tau_{\bar{z}}}\left[5I_0 - 6\sin 2\delta\, I_2^{-2} - I_2^0 - 6\cos 2\delta\, I_2^2\right] = I_w,$$
$$\bar{Y}_1^1 : \quad -2\cos 2\delta\, I_2^{-2} + 2\sin 2\delta\, I_2^2 + \frac{8}{45}\frac{\partial}{\partial\tau_{\bar{x}}}\left[5I_0 - I_2 + 6\sin 2\delta\, I_2^{-2} + 6\cos 2\delta\, I_2^2\right]$$
$$+\frac{48}{45}\frac{\partial}{\partial\tau_{\bar{z}}}\left[\cos 2\delta\, I_2^{-2} - \sin 2\delta\, I_2^2\right] = 0,$$
$$\bar{Y}_3^0 : \quad I_0 + 3\sin 2\delta\, I_2^{-2} + \frac{1}{2} I_2^0 + 3\cos 2\delta\, I_2^2 - \frac{48}{35}\frac{\partial}{\partial\tau_{\bar{x}}}\left[\cos 2\delta\, I_2^{-2} - \sin 2\delta\, I_2^2\right]$$
$$-\frac{24}{35}\frac{\partial}{\partial\tau_{\bar{z}}}\left[3\sin 2\delta\, I_2^{-2} + \frac{1}{2} I_2^0 + 3\cos 2\delta\, I_2^2\right] = I_w,$$
$$\bar{Y}_3^2 : \quad \frac{1}{2}\sin 2\delta\, I_2^{-2} - \frac{1}{4} I_2^0 + \frac{1}{2}\cos 2\delta\, I_2^2 - \frac{16}{35}\frac{\partial}{\partial\tau_{\bar{x}}}\left[\cos 2\delta\, I_2^{-2} - \sin 2\delta\, I_2^2\right]$$
$$-\frac{4}{35}\frac{\partial}{\partial\tau_{\bar{z}}}\left[2\sin 2\delta\, I_2^{-2} - I_2^0 + 2\cos 2\delta\, I_2^2\right] = 0.$$

## 3 Sample Calculations

Several one- and two-dimensional radiative heat transfer problems have been reported in [7, 8], in particular a nonabsorbing, isotropically scattering medium confined in a rectangular enclosure with a heated strip was studied, as well as a triangular enclosure with benignly varying absorption coefficient; the results were compared with those obtained from DOM/FVM and the Monte Carlo method. We will provide here one more example, exploring the accuracy of the $P_N$-approximation (up to $P_5$) for fields with strongly varying temperatures and absorption coefficients. We will consider two-dimensional heat transfer in a square enclosure with variable, but gray, absorption coefficient. Although scattering poses no additional difficulty for the spherical harmonics method (as opposed to the DOM or FVM), we will limit ourselves to a nonscattering medium, in order to reduce the number of variables. The following nondimensional field will be studied for a square enclosure [17]:

$$I_b = 1 + 5r^2(2 - r^2), \tag{42a}$$

$$\kappa = C_k \left[1 + 5(2 - r^2)^2\right], \tag{42b}$$

with

$$r^2 = x^2 + y^2; \qquad -1 \le x \le +1, \quad -1 \le y \le +1, \tag{42c}$$

i.e., the blackbody intensity (Planck function) is normalized with its minimum value (obtained at the center and the 4 corners), with a maximum value of $I_b = 6$ at a distance of $r = 1$ from the centerline. The absorption coefficient, normalized in terms of length units, has a maximum value of $\kappa = 16C_k$ at $x = y = 0$, and rapidly diminishes away from the center to a minimum value of $\kappa = C_k$ at the four corners. Thus the problem is radially one-dimensional, except for the conditions at the four perpendicular walls, which are assumed cold and black. The optical thickness of the square enclosure is $\tau_D = 18\sqrt{2}C_k$ along a diagonal, and $\tau_D = 23.5C_k$ along an $x = 0$ or $y = 0$ line, respectively. Here we investigate values of $C_k = 1$ (optically thick), $C_k = 0.1$ (optically intermediate), and $C_k = 0.01$ (optically thin conditions).

Results for incident radiation $G = 4\pi I_0$ and divergence of the radiative flux $\nabla \cdot \mathbf{q}$ are shown in Figs. 3 through 5, comparing results from the $P_1$, $P_3$ and $P_5$ methods with those of a Monte Carlo simulation. All calculations were performed with a relatively fine $41 \times 41$ cell system to ensure adequate resolution of sharp gradients [especially in the case of the a zeroth-order photon Monte Carlo (PMC) method]. For the optically thick case, Fig. 3, all 3 $P_N$-methods do very well, although $P_1$ has difficulty following the sharp peaks in both $G$ and $\nabla \cdot \mathbf{q}$, with $P_3$ being almost exact, and $P_5$ even closer to the PMC results. In the optically intermediate case, Fig. 4, both $P_1$ and $P_3$ have difficulties following the peaks and valleys of the incident radiation $G$, doing better with $\nabla \cdot \mathbf{q}$. Only $P_5$ follows the variations in $G$ well, and is essentially exact in the prediction of $\nabla \cdot \mathbf{q}$. For the optically thin case, Fig. 5, $P_3$ and $P_5$ perform better than $P_1$, but it is clear that neither can follow the true variation in incident radiation; gratifyingly, all three $P_N$-methods predict $\nabla \cdot \mathbf{q}$ relatively well (i.e., the quantity of greatest importance, providing the radiative source term in the overall energy equation), but higher order methods perform only marginally better than $P_1$.

Figure 6 depicts radiative fluxes along a wall for the same 3 cases. It is seen that, for the optically thick case, $P_1$ incurs serious errors (6% at the center, 40% in the corners). This is not surprising, since it is well known that the $P_1$-approximation performs poorly for optically thick situations in the vicinity of temperature discontinuities [1]. $P_3$ and $P_5$, on the other hand, perform rather well. Similar observations can be made for the optically intermediate case: while $P_1$ does well near $x = 0$ (where the problem is close to 1D), it fails miserably toward the corners. Again, both $P_3$ and $P_5$ perform extremely well. Finally, in the optically thin case, $P_1$ essentially predicts a constant value, while $P_3$ and $P_5$ perform better, but incur maximum errors of 10–15%.

Judging from the results given here, it appears that the $P_3$-method constitutes a distinct improvement over $P_1$, but requiring 4 (2D) or 6 (3D) simultaneous PDEs as opposed to the single PDE for $P_1$. While $P_5$ is clearly more accurate still, the increase in accuracy is relatively small, perhaps not justifying the additional numerical effort (9 simultaneous PDEs for 2D, 15 for 3D).

## 4 Summary and Conclusions

A new compact formulation of the $P_N$-approximation for isotropically scattering media, based on the development given by Modest and Yang [7, 8], has been presented in this paper. By carefully developing the applicable Marshak boundary conditions the age-old ambiguity of too many boundary conditions was removed and a self-consistent set of $N(N + 1)/$ simultaneous second-order elliptic PDEs and boundary conditions was formulated for three-dimensional geometries, reducing to $(N + 1)^2/4$ PDEs and boundary conditions for two-dimensional fields. As an example, the two-dimensional $P_3$-approximation was extracted from the set (resulting in 4 PDEs and boundary conditions). New 2D example calculations were carried out for a square enclosure with strongly varying temperatures and absorption coefficients, employing the $P_1$, $P_3$ and $P_5$ approximations, and were compared against exact Monte Carlo. It was found that $P_1$ results cannot predict radiative fluxes and radiative sources satisfactorily in general multi-dimensional geometries, while $P_3$ gives answers of very respectably accuracy for all but most extreme optically-thin situations. While the most accurate, the improvements observed with the $P_5$ method were relatively small, perhaps making it uncompetitive considering the higher computational costs.

## Acknowledgment

The majority of the work presented here was carried out by the author while at the University of Karlsruhe, Germany, in the framework of a Humboldt Research Award. The author acknowledges the support provided by both the University of Karlsruhe and the Alexander von Humboldt Foundation. In addition, Dr. S. Lei is acknowledged for providing the Monte Carlo results.

## References

[1] M. F. Modest, *Radiative Heat Transfer*, 2nd ed., Academic Press, New York, 2003.

[2] J. C. Chai, H. S. Lee, and S. V. Patankar, "Ray effect and false scattering in the discrete ordinates method", *Numer. Heat Transfer B*, vol. 24, pp. 373–389, 1993.

[3] D. B. Olfe, "A Modification of the Differential Approximation for Radiative Transfer", *A.I.A.A. Jl*, vol. 5, no. 4, pp. 638–643, 1967.

[4] M. F. Modest, "The Modified Differential Approximation for Radiative Transfer in General Three-Dimensional Media", *J. Thermoph. Heat Transfer*, vol. 3, no. 3, pp. 283–288, 1989.

[5] B. Davison, *Neutron Transport Theory*, Oxford University Press, London, 1958.

[6] S. C. S. Ou and K. N. Liou, "Generalization of the Spherical Harmonic Method to Radiative Transfer in Multi-Dimensional Space", *J. Quant. Spectrosc. Radiat. Transfer*, vol. 28, no. 4, pp. 271–288, 1982.

[7] J. Yang and M. F. Modest, "High-Order *P-N* Approximation for Radiative Transfer in Arbitrary Geometries", *J. Quant. Spectrosc. Radiat. Transfer*, vol. 104, no. 2, pp. 217–227, 2007.

[8] M. F. Modest and J. Yang, "Elliptic PDE formulation and boundary conditions of the spherical harmonics method of arbitrary order for general three-dimensional geometries", *J. Quant. Spectrosc. Radiat. Transfer*, vol. 109, pp. 1641–1666, 2008.

[9] R. E. Marshak, "Note on the Spherical Harmonics Method as Applied to the Milne Problem for a Sphere", *Phys. Rev.*, vol. 71, pp. 443–446, 1947.

[10] T. M. MacRobert, *Spherical Harmonics*, 3rd ed., Pergamon Press, New York, 1967.

[11] D. A. Varshalovich, A. N. Moskalev, and V. K. Khersonskii, *Quantum Theory of Angular Momentum*, World Scientific, Singapore, 1981.

[12] M. A. Blanco, M. Flórez, and M. Bermejo, "Evaluation of the rotation matrices in the basis of real spherical harmonics", *Journal of Molecular Structure (Theochem)*, vol. 49, pp. 19–27, 1997.

[13] *FlexPDE software*, PDE Solutions Inc., Antioch.

[14] G. Sewell, "PDE2D 9.0", http://www.pde2d.com/.

[15] W. Schönauer, "FDEM", 2005, see the "Fuel Cell Report" at http://www.rz.uni-karlsruhe.de/produkte/5336.php.

[16] M. Abramowitz and I. A. Stegun (eds.), *Handbook of Mathematical Functions*, Dover Publications, New York, 1965.

[17] K. V. Deshmukh, M. F. Modest, and D. C. Haworth, "Higher-Order Spherical Harmonics to model radiation in Direct Numerical Simulation of Turbulent Reacting Flows", *Computational Thermal Sciences*, vol. 1, pp. 207–230, 2009.

Table 1: Elliptic $P_N$-approximation coefficients for isotropic scattering

| | $k=1$ | $k=2$ | $k=3$ |
|---|---|---|---|
| $a_k^{nm\ (a)}$ | $\frac{1}{4(2n+5)(2n+3)}$ | $-\frac{1}{2(2n+3)(2n-1)}$ | $\frac{1}{4(2n-1)(2n-3)}$ |
| $b_k^{nm\ (a)}$ | $\frac{n+m+1}{2(2n+5)(2n+3)}$ | $-\frac{2m-1}{2(2n+3)(2n-1)}$ | $-\frac{n-m}{2(2n-1)(2n-3)}$ |
| $c_k^{nm}$ | $-\frac{\pi_2(n+m+1)}{2(2n+5)(2n+3)}$ | $\frac{n^2+n-1+m^2}{(2n+3)(2n-1)}$ | $-\frac{\pi_2(n-m-1)}{2(2n-1)(2n-3)}$ |
| $d_k^{nm}$ | $-\frac{\pi_3(n+m+1)}{2(2n+5)(2n+3)}$ | $-\frac{(2m+1)(n+m+1)(n-m)}{2(2n+3)(2n-1)}$ | $\frac{\pi_3(n-m-2)}{2(2n-1)(2n-3)}$ |
| $e_k^{nm}$ | $\frac{\pi_4(n+m+1)}{4(2n+5)(2n+3)}$ | $-\frac{\pi_2(n+m+1)\pi_2(n-m-1)}{2(2n+3)(2n-1)}$ | $\frac{\pi_4(n-m-3)}{4(2n-1)(2n-3)}$ |

$^{(a)}a_k^{nm} = 0$ for $m \le 1$, $b_k^{nm} = 0$ for $m = 0$;

$$\pi_k(n) = \prod_{j=0}^{k-1}(n+j); \; f_n = \frac{(2n+1)^2}{(2n+3)(2n-1)}$$

Table 2: Half-moments of associated Legendre polynomials, $10^{-m} \times p^m_{n,j}$.

| $m$ | $n \backslash j$ | 0 | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|---|
| 0 | 0 | 1.00000 | . | . | . | . | . |
| | 1 | 0.50000 | 0.33333 | . | . | . | . |
| | 2 | 0.00000 | 0.12500 | 0.20000 | . | . | . |
| | 3 | –0.12500 | 0.00000 | 0.12500 | 0.14286 | . | . |
| | 4 | 0.00000 | –0.02083 | 0.00000 | 0.07031 | 0.11111 | . |
| | 5 | 0.06250 | 0.00000 | –0.03906 | 0.00000 | 0.07031 | 0.09091 |
| 1 | 1 | . | 0.06667 | . | . | . | . |
| | 2 | . | 0.07500 | 0.12000 | . | . | . |
| | 3 | . | 0.00000 | 0.07500 | 0.17143 | . | . |
| | 4 | . | –0.04167 | 0.00000 | 0.14062 | 0.22222 | . |
| | 5 | . | 0.00000 | –0.02344 | 0.00000 | 0.14062 | 0.27273 |
| 2 | 2 | . | . | 0.04800 | . | . | . |
| | 3 | . | . | 0.07500 | 0.17143 | . | . |
| | 4 | . | . | 0.00000 | 0.14062 | 0.40000 | . |
| | 5 | . | . | –0.06563 | 0.00000 | 0.39375 | 0.76364 |
| 3 | 3 | . | . | . | 0.10286 | . | . |
| | 4 | . | . | . | 0.19687 | 0.56000 | . |
| | 5 | . | . | . | 0.00000 | 0.55125 | 1.83273 |
| 4 | 4 | . | . | . | . | 0.44800 | . |
| | 5 | . | . | . | . | 0.99225 | 3.29891 |
| 5 | 5 | . | . | . | . | . | 3.29891 |

## List of figure captions

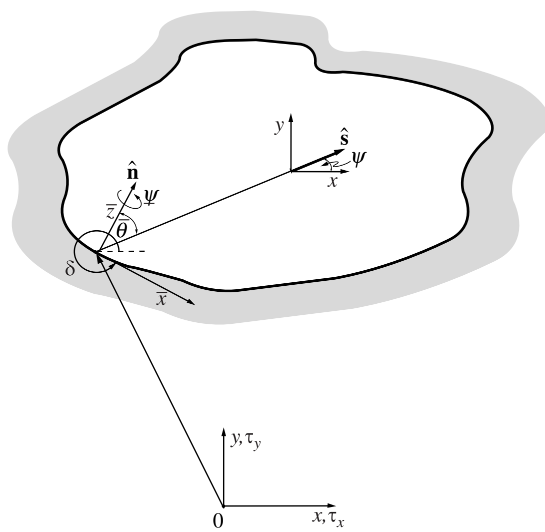


Figure 1: Local and Global Coordinates for a Two-Dimensional Enclosure

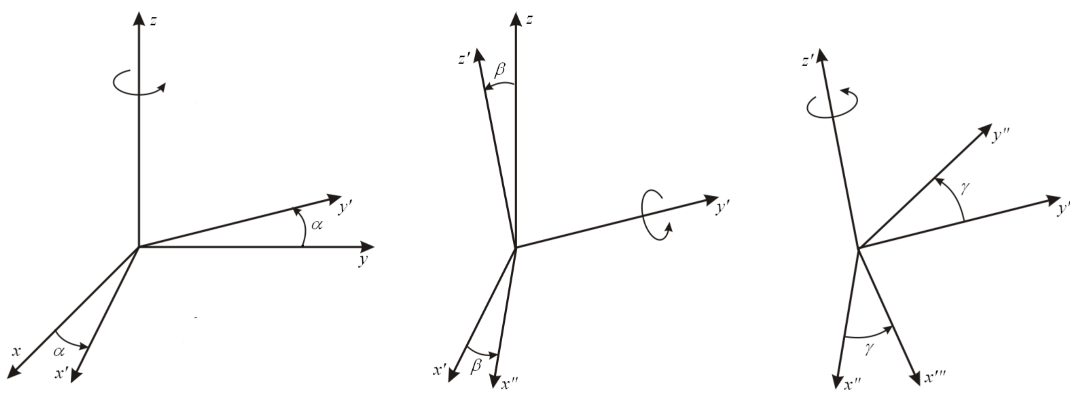


Figure 2: Definition of Euler Angles for an Arbitrary Rotation

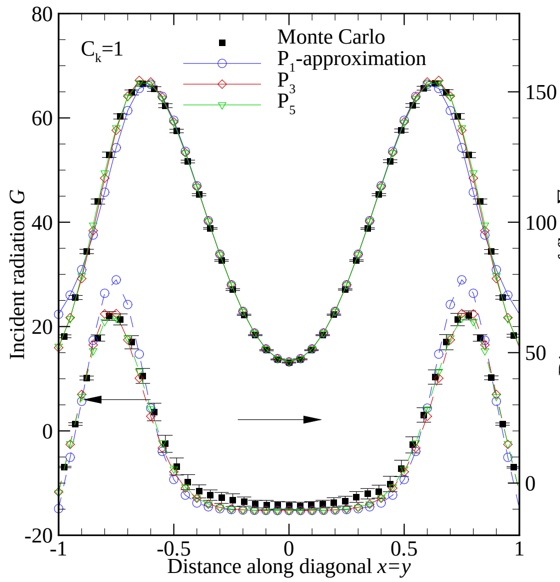


Figure 3: Incident radiation and radiative source for a square enclosure; optically thick case ($C_k = 1$).

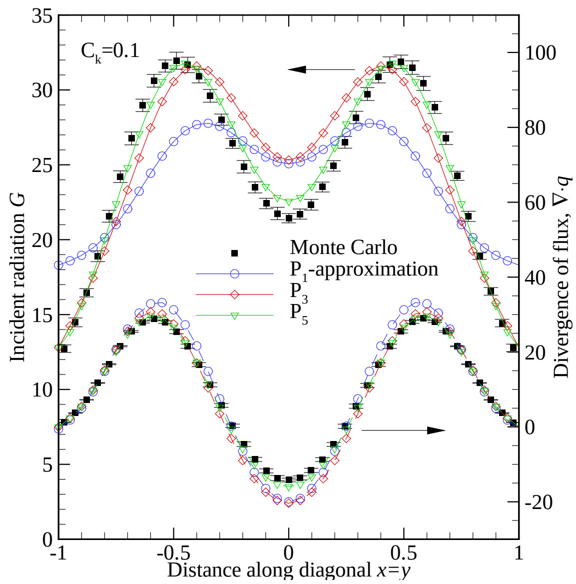


Figure 4: Incident radiation and radiative source for a square enclosure; optically intermediate case ($C_k$ = 0.1).

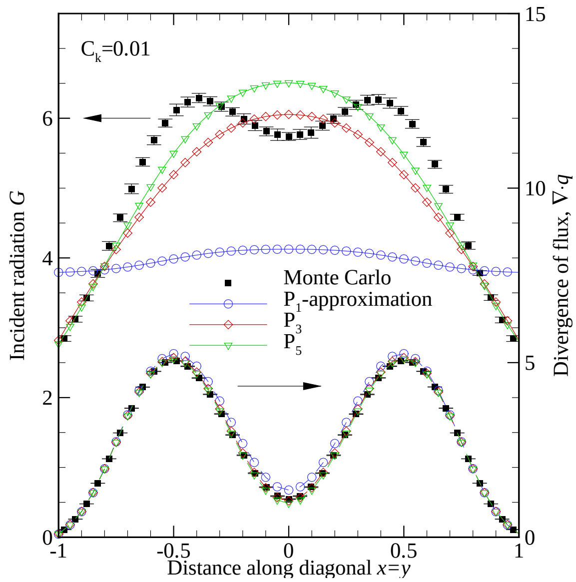


Figure 5: Incident radiation and radiative source for a square enclosure; optically thin case ($C_k = 0.01$).

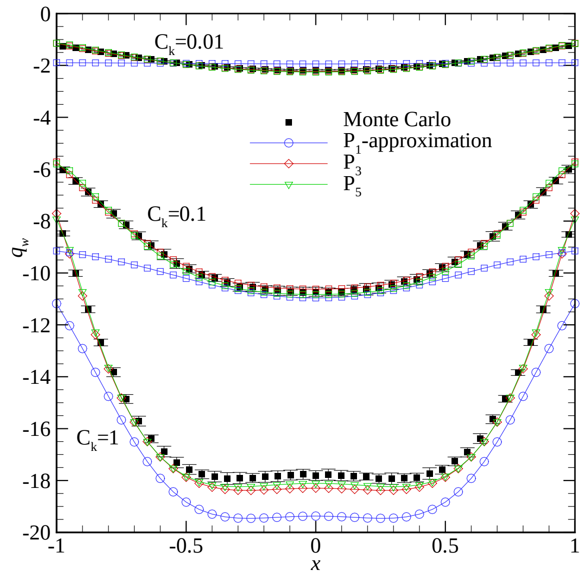


Figure 6: Radiative flux along bottom wall ($y = -1$).