Finite-Volume Formulation and Solution of the $P_3$ Equations of Radiative Transfer on Unstructured Meshes

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Abstract

The method of spherical harmonics (or $P_N$) is a popular method for approximate solution of the radiative transfer equation (RTE) in participating media. A rigorous conservative finite-volume (FV) procedure is presented for discretization of the $P_3$ equations of radiative transfer in two-dimensional geometry—a set of four coupled, second-order partial differential equations. The FV procedure presented here is applicable to any arbitrary unstructured mesh topology. The resulting coupled set of discrete algebraic equations are solved implicitly using a coupled solver that involves decomposition of the computational domain into groups of geometrically contiguous cells using the binary spatial partitioning algorithm, followed by fully implicit coupled solution within each cell group using a preconditioned generalized minimum residual solver. The RTE solver is first verified by comparing predicted results with published Monte Carlo (MC) results for two benchmark problems. For completeness, results using the $P_1$ approximation are also presented. As expected, results agree well with MC results for large/intermediate optical thicknesses, and the discrepancy between MC and $P_3$ results increase as the optical thickness is decreased. The $P_3$ approximation is found to be more accurate than the $P_1$ approximation for optically thick cases. Finally, the new RTE solver is coupled to a reacting flow code and demonstrated for a laminar flame calculation using an unstructured mesh. It is found that the solution of the four $P_3$ equations requires 14.5% additional CPU time, while the solution of the single $P_1$ equation requires 9.3% additional CPU time over the case without radiation. [DOI: 10.1115/1.4000184]

Keywords: radiation, participating media, $P_3$, RTE solver, finite-volume, unstructured

1 Introduction

Radiation is the dominant mode of heat transfer in many high-temperature applications, such as combustion and rapid thermal chemical vapor deposition. With growing concerns over global warming, solar radiation transport through the atmosphere is rapidly becoming a subject of intense interest and research. Radiation is also a critical mode of energy transfer in modern laser-based manufacturing processes, and in biological applications—both for laser-induced remediation and cure of tissues, and for detection using optical tomography based techniques.

The problem of radiation transport entails solution of the radiative transfer equation (RTE) for the radiative intensity. The RTE is an integro-differential equation in seven independent variables—time, three space coordinates, two angular coordinates, and wave number. Therefore, it is difficult to solve exactly even for simple one-dimensional (1D) problems [1,2]. Hence, approximate solution methods are necessary to solve the RTE for more practical situations. A survey of the literature over the past four decades reveals that the four most popular methods to solve the RTE are as follows: (i) the spherical harmonics method and its variations [3–5], (ii) the discrete ordinates method and its variations, including its finite-volume variant (the so-called control angle discrete ordinates method) [6,7], (iii) the zonal method [8–10], and (iv) the Monte Carlo (MC) method [1,2].

Broadly, these four methods to solve the RTE can be categorized into two types, as follows: (1) photon-based methods, and (2) photon-free methods. The methods that belong to the former category are the discrete ordinates ($S_N$), zonal, and the MC methods, while the spherical harmonics ($P_N$) method is a photon-free method. In photon-based methods, photons are essentially tracked along a line of sight, and directional radiative intensities along various lines of sight are finally summed over solid angle $4\pi$ to obtain the net radiation intensity at any point. In the popular $S_N$ method, the lines of sight are predetermined, resulting in a deterministic RTE solver. In the MC method, on the other hand, the lines of sight are stochastically determined. In the photon-free $P_N$ method, integration over all lines of sight (or solid angles) is performed analytically using orthogonal basis functions: Legendre polynomials in spherical coordinates. The $P_N$ method, as opposed to photon-based methods, is, thus, a spectral method. Each of these methods has its relative advantages and disadvantages.

To date, the $S_N$ method has been arguably the most popular method for solving the RTE. In essence, the $S_N$ method is a straightforward extension of the finite-difference method for spatial discretization, with additional discretization in the angular direction as well. The $S_N$ method, however, suffers from a few well-known shortcomings. It produces inaccurate results in geometries with large aspect ratios, or geometries with sharp corners (e.g., a wedge) because of its inability to resolve acute solid angles using a finite number of predetermined directions. Inaccuracies resulting from this inability to properly resolve acute solid angles are often referred to in literature as “ray effects.” [11] The minimum number of partial differential equations (PDEs) that need to be solved in this method even for a gray gas is equal to the number of
directions (NDIR). If, for example, the Sn method is used, NDIR=12 in two-dimensional (2D) and NDIR=24 in three-dimensional (3D) geometries. The convergence of the Sn method deteriorates rapidly with increase in the optical thickness of the medium. This is because the boundary-to-boundary information (intensity) propagation is almost nonexistent in an optically thick medium. Numerically, this results in a poorly conditioned system of equations. In the presence of scattering, the Sn equations are strongly coupled. In such a scenario, segregated solution of the directional equations (i.e., one direction at a time) results in poor convergence [12]. While coupled solution of the Sn equations is conceivable [12], it is difficult both from algorithmic as well as memory standpoints.

The Pn method, as discussed above, is a spectral method in which no angular discretization is necessary, and thus, it does not suffer from any of the aforementioned problems encountered in the Sn method. In addition, the number of PDEs that ultimately need to be solved in the Pn method is substantially less compared with the Sn method. For example, the lowest order Pn method, namely, the P1 method, results in a single Helmholtz equation with Robin-type boundary conditions [1]. Despite these advantages, the Pn method has its own set of shortcomings. The P1 method is invalid for nonparticipating media. In other words, one cannot use this method in a scenario where the medium may be participating in some regions and nonparticipating in some others. The P1 method is known to yield poor results in cases where emission from boundaries is dominant (i.e., cold medium bounded by hot walls) [1]. The convergence of the P1 method is poor if the medium is optically thin—a scenario which renders the governing equations stiff [13]. Extension of the spherical harmonics method from P1 to higher orders of accuracy (P3, P5, etc.) is quite cumbersome because the resulting partial differential equations have cross-derivatives, and because of the difficulty in implementing the boundary conditions [14,15].

The above discussion clearly points to the fact that both Sn and Pn methods are incapable of treating arbitrary optical thicknesses, especially when the extinction coefficient of the medium may vary by orders of magnitude within the computational domain. The accuracy of Sn method is particularly poor for optically thick situations, while Pn is invalid for transparent media. The MC method is capable of remedying most of the drawbacks with the Sn and Pn methods with relative ease. The MC method has long been known as the method of choice for obtaining benchmark solutions to the RTE. Unfortunately, the MC method can be prohibitively slow, especially in optically thick media and in complex 3D geometries. Even with modern computing technology and parallel architectures, the MC method is not deemed practical for engineering calculations. In recent years, in view of the shortcomings of both Sn and Pn methods, researchers have begun to explore a new class of methods. In this new class of methods, strengths of the stochastic MC method are selectively combined with the computational efficiency of Sn and Pn deterministic approaches to yield more accurate results at reasonable computational costs. This class of methods is referred to as the hybrid approach. For example, the Sn method has been combined with MC to eliminate problems associated with “ray effects.” Similarly, the P1 method has been modified to yield the so-called modified differential approximation (MDA) [3,4] and improved differential approximation (IDA) [5] methods—both of which can better handle large variations in optical thickness of the medium. While the idea of hybrid methods has existed for quite some time, to the best of our knowledge, they have not been used often, and have not yet been demonstrated for practical engineering applications.

The P1 method continues to be a popular method for solution of the RTE because it is easy to implement in a general-purpose computational fluid dynamics (CFD) code, and is, therefore, amenable for practical engineering calculations. However, as documented above and elsewhere [1], it often produces inaccurate results. Since the P1 method is a spectral method, it is conceivable that the gain in accuracy will be significant if one were to use the next higher order, namely, P3. The P3 method has witnessed limited use [14–19] on account of its complexity—both from a mathematical as well as a computational algorithm development standpoint. In recent years, Yang and Modest [14,15] generalized the Pn equations to make them amenable for solution using canned PDE solvers, such as FLEXPDE and PDE2D. Solution to the P3 equations has been obtained for two different benchmark problems by Yang and Modest [14,15] using relatively coarse orthogonal meshes in 2D. Comparison of their P1/P3 results with MC results indicates that the accuracy of P3 is superior to that of P1, as expected, at least for optically thick situations. Other notable work in this area includes the work done by McClaren et al. [20], who solved the time-dependent one-dimensional P3 equations using both finite-volume (FV) and finite-element techniques [20,21].

In order to make the P1 method attractive for practical engineering calculations, it is necessary to develop a solution procedure that is compatible to the mesh topology and discretization procedures used in modern-day CFD codes. Most modern CFD codes use unstructured (or nonconformal) mesh topology and the finite-volume method. In such a framework, structured body-fitted meshes, which continue to be used in many codes within the government and academia, can be thought of simply as an unstructured mesh with skewed quadrilateral (in 2D) or hexahedral (in 3D) control volumes (or cells). In other words, an unstructured mesh formulation is all-encompassing, and can be used for any mesh topology. In this article, we present a conservative unstructured finite-volume formulation for solution of the P3 equations of radiative transfer in two-dimensional geometry. The P3 equations represent a set of four coupled, second-order elliptic PDEs. A new solver for coupled implicit solution of the four PDEs, after finite-volume discretization, is also developed and demonstrated. Finally, the new RTE solver is coupled to an unstructured CFD code, and demonstrated for a laminar flame calculation. While the method is demonstrated here only for 2D geometries, the finite-volume formulation presented here is also valid for 3D, and may be used as a starting point for future development in this area.

2 Mathematical Formulation and Solution

2.1 Governing Equations. In nondimensional optical coordinates, the RTE is written as [1]

\[
\hat{s} \cdot \nabla I(\tau, \mathbf{s}) + I(\tau, \mathbf{s}) = (1 - \omega) I_{b} + \omega \int_{4 \pi} I(\tau, \mathbf{s}') \varphi(\mathbf{s}, \mathbf{s}') d\Omega',
\]

(1)

where \(I(\tau, \mathbf{s})\) is the intensity at an optical position \(\tau\) and along a light of sight \(\mathbf{s}\), \(\omega\) is the scattering albedo, \(I_{b}\) is the Planck function, and \(\varphi(\mathbf{s}, \mathbf{s}')\) is the scattering phase function. In the method of spherical harmonics, the intensity is expressed as an infinite series of orthogonal basis functions [14,15]

\[
I(\tau, \mathbf{s}) = \frac{1}{4 \pi} \sum_{n} (2n + 1) J_{n}(\tau, \mathbf{s})
\]

(2)

where

\[
J_{n}(\tau, \mathbf{s}) = \frac{1}{2n + 1} \sum_{m=-n}^{n} I_{n}^{m}(\tau) Y_{n}^{m}(\mathbf{s})
\]

(3)

In Eq. (3), the function \(J_{n}(\tau, \mathbf{s})\) has been expressed as the sum of the product of two functions—a location-dependent coefficient function \(I_{n}^{m}(\tau)\), and a spherical harmonic function \(Y_{n}^{m}(\mathbf{s})\). The spherical harmonic functions can be expressed in terms of Legendre polynomials [14,15]. Yang and Modest [14,15] recently formalized the \(P_{3}\) equations and boundary conditions of radiative transfer for 3D geometries. The result is a set of coupled, second-order, elliptic PDEs. In this section, rather than start from the
general \( P_y \) equations, we start from the \( P_3 \) equations in 2D geometries, as presented by Yang and Modest [14,15]

\[
\frac{\partial}{\partial x} \left[ 2 \gamma_s \frac{1}{\beta} \frac{\partial I_y}{\partial x} - \frac{1}{\beta} \frac{\partial \varphi_0}{\partial x} + 2 \gamma_s \frac{1}{\beta} \frac{1}{\alpha} \frac{\partial I_y}{\partial \beta} + 5 \frac{1}{\alpha} \frac{\partial \varphi_0}{\partial \beta} \right] + \frac{\partial}{\partial y} \left[ 2 \gamma_s \frac{1}{\beta} \frac{1}{\alpha} \frac{\partial I_y}{\partial y} - \frac{1}{\beta} \frac{\partial \varphi_0}{\partial y} + 2 \gamma_s \frac{1}{\beta} \frac{1}{\alpha} \frac{\partial I_y}{\partial \beta} + 5 \frac{1}{\alpha} \frac{\partial \varphi_0}{\partial \beta} \right] = -2 \beta \alpha I_y^2 = 0
\]  
\[
(4a)
\]

\[
\frac{\partial}{\partial x} \left[ \gamma_s \frac{1}{\beta} \frac{1}{\alpha} \frac{\partial I_y}{\partial x} - \frac{1}{\beta} \frac{\partial \varphi_0}{\partial x} + \gamma_s \frac{1}{\beta} \frac{1}{\alpha} \frac{1}{\alpha} \frac{\partial I_y}{\partial \beta} + 5 \frac{1}{\alpha} \frac{\partial \varphi_0}{\partial \beta} \right] + \frac{\partial}{\partial y} \left[ \gamma_s \frac{1}{\beta} \frac{1}{\alpha} \frac{\partial I_y}{\partial y} + \gamma_s \frac{1}{\beta} \frac{1}{\alpha} \frac{1}{\alpha} \frac{\partial I_y}{\partial \beta} - \gamma_s \frac{1}{\beta} \frac{1}{\alpha} \frac{1}{\alpha} \frac{\partial I_y}{\partial \beta} + 5 \frac{1}{\alpha} \frac{\partial \varphi_0}{\partial \beta} \right] = -2 \beta \alpha I_y^2 = 0
\]
\[
(4b)
\]

\[
\frac{\delta}{\delta x} \left[ \frac{2 \gamma_s}{\beta} \frac{1}{\alpha} \frac{1}{\alpha} \frac{\partial I_y}{\partial x} + \frac{1}{\beta} \frac{\partial \varphi_0}{\partial x} + \frac{1}{\beta} \frac{1}{\alpha} \frac{1}{\alpha} \frac{\partial I_y}{\partial \beta} + \frac{61 \frac{1}{\alpha} \frac{\partial \varphi_0}{\partial \beta} \right] + \frac{\partial}{\partial y} \left[ \frac{1}{\beta} \frac{1}{\alpha} \frac{1}{\alpha} \frac{\partial I_y}{\partial y} + \frac{61 \frac{1}{\alpha} \frac{\partial \varphi_0}{\partial \beta} \right] = -5 \beta \alpha (I_y - 4 \pi I_0) = 0
\]
\[
(4d)
\]

where \( \beta \) is the extinction coefficient, and \( \gamma_{ij} \) are coefficients written as [14,15]

\[
\gamma_{ij} = \left( \frac{i}{\alpha} + \frac{j}{\alpha} \right)
\]
\[
(5)
\]

where

\[
\alpha_a = (2n + 1) - \omega A_n
\]
\[
(6)
\]

where \( A_n \) are the coefficients associated with expansion of the scattering phase function [15]. Equations (4a)–(4d) represent a set of four coupled, linear, second-order, elliptic PDEs for the four unknowns, namely, \( I_0, I_y, I_z, \) and \( I_y^2 \). For nongray media, Eqs. (4a)–(4d) must be considered in a spectral sense.

Solution of Eqs. (4a)–(4d) requires four boundary conditions. Following Modest and Yang [15], who applied Marshak’s procedure to derive the boundary conditions, the boundary conditions are written as [15]

\[
\begin{align*}
I_0 + 3 \sin 2 \delta t^2_0 - \frac{1}{2} I_y^2 + 3 \cos 2 \delta t^2_0 &= \frac{48}{5 \alpha_\beta} \frac{\partial}{\partial \alpha} \left[ \cos 2 \delta t^2_0 \\
- \sin 2 \delta t^2_0 - \frac{1}{2} \frac{\partial}{\partial \alpha} \left[ 3 \sin 2 \delta t^2_0 + \frac{1}{2} I_y^2 + 3 \cos 2 \delta t^2_0 \right] \right] = 4 \pi I_0
\end{align*}
\]
\[
(7a)
\]

\[
\begin{align*}
- \frac{3}{2} \cos 2 \delta t^2_0 + 2 \sin 2 \delta t^2_0 + \frac{1}{2} \frac{\partial}{\partial \alpha} \left[ 3 \sin 2 \delta t^2_0 - \sin 2 \delta t^2_0 \right] = 0
\end{align*}
\]
\[
(7b)
\]

where \( I_0 \) is the intensity at the surface, and is written as [15]

\[
I_0 = I_{00} - \left( \frac{1}{3} \frac{1}{\pi} \right) \left( M \right)
\]
\[
(8)
\]

where \( I_{00} \) is the Planck function at the surface. The quantity \( M \) is one of the space-dependent coefficients of the intensity function written in the local (at the boundary surface) coordinate system, and can be expressed in terms of the dependent variables (namely, \( I_0, I_y, I_z, \) and \( I_y^2 \)) after tedious algebra using transformation relations from local \((\tilde{x}, \tilde{y}, \tilde{z})\) to global \((x, y, z)\) coordinate systems [15]. Following this transformation, Eqs. (7a) and (7c) can be written solely in terms of the four dependent variables. Similarly, the derivatives appearing in Eqs. (7a)–(7d) with respect to local space variables can be transformed to derivatives with respect to global space variables. In Eqs. (7a)–(7d), \( \delta \) is an angle associated with the Euler angles of transformation from local to global coordinate systems, and can also be obtained using relations provided by Modest and Yang [15].

### 2.2 Finite-Volume Formulation and Block-Implicit Equations

In this subsection, the finite-volume formulation of the governing equations is presented. As a starting point, we introduce the following notations to make Eqs. (4a)–(4d) more general and compact

\[
\begin{align*}
\Phi_1 &= \Gamma_1^2, \quad \Phi_2 = \Gamma_2, \quad \Phi_3 = \Gamma_3, \quad \Phi_4 = \Gamma_4 \\
\Gamma_1 &= \frac{2 \gamma_s}{\beta}, \quad \Gamma_2 = \frac{\gamma_{zz}}{\beta}, \quad \Gamma_3 = \frac{2 \gamma_{zz}}{\beta}, \quad \Gamma_4 = \frac{5}{\beta \alpha}, \quad \Gamma_5 = \frac{2 \alpha_5}{\beta}
\end{align*}
\]
\[
(9)
\]

Using these notations, Eq. (4a) may be written as

\[
\frac{\partial}{\partial x} \left[ \Gamma_1 \frac{\partial \Phi_1}{\partial x} - \Gamma_2 \frac{\partial \Phi_1}{\partial y} + \Gamma_3 \frac{\partial \Phi_3}{\partial y} + \Gamma_4 \frac{\partial \Phi_4}{\partial y} \right] + \frac{\partial}{\partial y} \left[ \Gamma_1 \frac{\partial \Phi_1}{\partial y} - \Gamma_2 \frac{\partial \Phi_1}{\partial x} \right] = -\Gamma_5 \frac{\partial \Phi_1}{\partial x} = 0
\]
\[
(10)
\]

Rearranging, we get

\[
\nabla \cdot \mathbf{U}_1 - \nabla \cdot \mathbf{U}_2 + \nabla \cdot \mathbf{U}_3 + \nabla \cdot \mathbf{U}_4 - \Gamma_5 \frac{\partial \Phi_1}{\partial x} = 0
\]
\[
(11)
\]

where

\[
\begin{align*}
\mathbf{U}_1 &= \Gamma_1 \nabla \Phi_1 \\
\mathbf{U}_2 &= \Gamma_2 \left[ \frac{\partial \Phi_2}{\partial y} + \frac{\partial \Phi_3}{\partial y} \right] \\
\mathbf{U}_3 &= \Gamma_3 \left[ \frac{\partial \Phi_3}{\partial y} - \frac{\partial \Phi_4}{\partial y} \right] \\
\mathbf{U}_4 &= \Gamma_4 \left[ \frac{\partial \Phi_4}{\partial y} - \frac{\partial \Phi_1}{\partial x} \right]
\end{align*}
\]
\[
(12)
\]

Equations (4b)–(4d) may also be written in a similar manner, and thus, the finite-volume procedure to be presented next is also applicable to Eqs. (4b)–(4d) without any major modifications.
four divergence terms in Eq. (11) can be categorized into two types of terms. The first term represents the divergence of a gradient operator, while the other three terms represent divergence of vectors that cannot be written as the gradient of a scalar. The treatment of these two types of terms is discussed next.

Finite-volume integration of the first term in Eq. (11) over a volume \( \Omega_f \) and control surface area \( S \), followed by application of the Gauss divergence theorem, results in

\[
\int_{\Omega_f} \nabla \cdot \mathbf{U}_f \, dV = \int_S \mathbf{U}_f \cdot \mathbf{n} dA = \sum_f (\mathbf{U}_{f,j} \cdot \mathbf{n}_j) A_f
\]

(13)

where the surface integral in Eq. (13) has been replaced by a summation over the discrete faces \( f \) of the control volume in question. \( \Gamma_{1,f} \) is the value of \( \Gamma_1 \) at any face \( f \), and can be computed using distance-weighted interpolation of the two cell center values of \( \Gamma_1 \). The area \( A_f \) and surface normal \( \mathbf{n}_j \) are known from the geometric description of the mesh. The objective of the finite-volume formulation is to ultimately derive a set of algebraic equations, linking the cell center values of the unknowns, namely, \( \phi_1, \phi_2, \phi_3, \) and \( \phi_4 \). In order to do so, the gradient at the cell face \( \nabla \phi_{i,f} \) must be expressed in terms of the cell center values of \( \phi_1 \). We start with the vector identity

\[
\nabla \phi_{i,f} = (\nabla \phi_{i,f}) \mathbf{n}_i + (\mathbf{n}_i \times \nabla \phi_{i,j}) \times \mathbf{n}_j
\]

(14)

For two-dimensional geometry, Eq. (14) can be written in simplified form as

\[
\nabla \phi_{i,f} = (\nabla \phi_{i,f}) \mathbf{n}_i + (\mathbf{n}_i \cdot \mathbf{l}_j) \mathbf{l}_j
\]

(15)

where \( \mathbf{l}_j \) is the unit tangent of the face \( f \) (Fig. 1), and is also known from the geometric description of the mesh. Performing a dot product with the vector \( \mathbf{l}_j \) (Fig. 1), we get

\[
\nabla \phi_{i,f} \cdot \mathbf{l}_j = (\nabla \phi_{i,f} \cdot \mathbf{n}_i) \mathbf{l}_j + (\mathbf{n}_i \cdot \mathbf{l}_j) \mathbf{l}_j \cdot \mathbf{l}_j
\]

(16)

which upon further simplification, yields

\[
\phi_{i,N,f} - \phi_{i,O} = (\nabla \phi_{i,f} \cdot \mathbf{n}_i) \delta_j + (\nabla \phi_{i,f} \cdot \mathbf{l}_j) \mathbf{l}_j \cdot \mathbf{l}_j
\]

(17)

where \( \phi_{i,N,f} \) is the value of \( \phi_i \) at the center of the neighboring cell to face \( f \), which is different from \( O \), and \( \delta_j \) is the distance in the direction of the surface normal between the two cells straddling the face \( f \) (Fig. 1). It is computed from the geometric description of the mesh, and is stored for each face. Equation (17) can be further rearranged as

\[
(\nabla \phi_{i,f} \cdot \mathbf{n}_j) = \frac{\phi_{i,N,f} - \phi_{i,O}}{\delta_j} - \frac{(\nabla \phi_{i,f} \cdot \mathbf{l}_j) \mathbf{l}_j \cdot \mathbf{l}_j}{\delta_j}
\]

(18)

Essentially, in the above derivation, the flux normal to a cell face has been expressed in terms of the cell center values straddling the face, and a separate tangential flux term, which will, henceforth, be denoted by \( \mathcal{J}_j \), and is written as

\[
\mathcal{J}_j = \frac{(\phi_{1,b} - \phi_{1,a}) \mathbf{l}_j \cdot \mathbf{l}_j}{|ab|} \mathbf{l}_j \cdot \mathbf{l}_j
\]

(19)

where \( \phi_{1,a} \) and \( \phi_{1,b} \) are vertex values of \( \phi_i \) at vertices \( a \) and \( b \) (Fig. 1). If the vectors \( \mathbf{n}_j \) and \( \mathbf{l}_j \) are aligned, this term vanishes since \( \mathbf{l}_j \cdot \mathbf{l}_j = 0 \). Substitution of Eq. (18) into Eq. (13) yields

\[
\int_{\Omega_f} \nabla \cdot \mathbf{U}_f dV = \sum_f \Gamma_{1,f} (\nabla \phi_{i,f} \cdot \mathbf{n}_j) A_f
\]

(20)

In our scheme, the first term of the right hand side of Eq. (20) is treated implicitly, while the second term is treated explicitly, i.e., it is computed from previous iteration values. This computation of the second term requires determination of vertex values. While, in principle, the vertex values can be expressed in terms of the cell center values using interpolation functions, and the whole term can be treated implicitly, such a scheme becomes quite tedious, especially in 3D. Thus, the second term is treated explicitly.

Next, we consider the finite-volume integration of the second type of term, i.e., term that cannot be expressed as a divergence of a gradient. Finite-volume integration of the second term in Eq. (11) over a volume \( \Omega_f \) and control surface area \( S \), followed by application of the Gauss divergence theorem, results in

\[
\int_{\Omega_f} \nabla \cdot \mathbf{U}_f dV = \int_S \mathbf{U}_f \cdot \mathbf{n} dA = \sum_f (\mathbf{U}_{f,j} \cdot \mathbf{n}_j) A_f
\]

(21)

From Eq. (12), we get

\[
\mathbf{U}_2 = \Gamma_2 \left[ \frac{\partial \phi_2}{\partial x} \mathbf{i} + \frac{\partial \phi_2}{\partial y} \mathbf{j} \right] + \Gamma_3 \left[ (\nabla \phi_2 \cdot \mathbf{j}) \mathbf{j} + (\nabla \phi_2 \cdot \mathbf{i}) \mathbf{i} \right]
\]

(22)

Therefore,

\[
\mathbf{U}_{f,j} = \Gamma_{2,f} \left[ (\nabla \phi_{2,f}) \mathbf{j} \right] n_j + (\nabla \phi_{2,f} \cdot \mathbf{i}) n_i
\]

(23)

Using the same vector identity as before (Eq. (15)), we get

\[
\nabla \phi_{2,f} \cdot \mathbf{i} = (\nabla \phi_{2,f} \cdot \mathbf{n}_i) n_i + (\nabla \phi_{2,f} \cdot \mathbf{l}_j) l_j \cdot l_j \cdot \mathbf{l}_j \cdot \mathbf{l}_j
\]

(24)

Substitution of Eq. (18) into Eq. (24) yields

\[
\nabla \phi_{2,f} \cdot \mathbf{i} = \left[ \frac{\phi_{2,N,f} - \phi_{2,O}}{\delta_j} - \frac{(\nabla \phi_{2,f} \cdot \mathbf{l}_j) \mathbf{l}_j \cdot \mathbf{l}_j}{\delta_j} \right] n_j + (\nabla \phi_{2,f} \cdot \mathbf{l}_j) l_j \cdot l_j \cdot \mathbf{l}_j \cdot \mathbf{l}_j
\]

(25)

Using \( \mathbf{n}_j \cdot n_i = n_c \) and \( \mathbf{l}_j \cdot l_i = l_c \), Eq. (25) may be simplified as

\[
\nabla \phi_{2,f} \cdot \mathbf{i} = \left[ \frac{\phi_{2,N,f} - \phi_{2,O}}{\delta_j} n_c + (\nabla \phi_{2,f} \cdot \mathbf{l}_j) l_c \right] n_i + (\nabla \phi_{2,f} \cdot \mathbf{l}_j) l_j \cdot l_j \cdot \mathbf{l}_j \cdot \mathbf{l}_j
\]

(26)
\[ \nabla \cdot \mathbf{U}_{2} dV = \sum_{j} \left( \mathbf{U}_{2,j} \cdot \hat{n}_{j} \right) A_{j} = \sum_{j} \Gamma_{2,j} n_{j} \Delta_{j} \left[ \phi_{2,j} - \phi_{1} \right] \delta_{j} + \sum_{j} \left( \frac{\phi_{2,j} - \phi_{1}}{ab} \right) t_{j} - \left( \mathbf{f} \cdot \mathbf{l} \right) n_{j} \delta_{j} \]

Substitution of Eqs. (26) and (27) into Eq. (23), followed by substitution of the resulting equation into Eq. (21) yields

\[ \int_{\Omega_{v}} \Gamma_{2} \phi_{2} dV = \Gamma_{5,0} \phi_{1} \Omega_{v,0} \]

where \( \Omega_{v,0} \) is the volume of the control volume with its centroid at \( O \). The five terms in Eq. (11), after finite-volume integration, can be arranged to write a single algebraic equation for the cell center values of \( \phi \), namely, \( \phi_{1,0} \), \( \phi_{2,0} \), \( \phi_{3,0} \), and \( \phi_{4,0} \), and the cell center values of the neighboring cells. For cells adjacent to boundaries, the flux at the boundary face must be replaced by the appropriate boundary condition given by Eqs. (7a)–(7d). The treatment of such Robin-type boundary conditions in a finite-volume formulation is relatively straightforward, and is omitted here for the sake of brevity.

Thus far, only finite-volume integration of Eq. (4a) has been discussed. The same procedure can also be used to integrate Eqs. (4b)–(4d), resulting in three additional algebraic equations relating the cell center values of \( \phi \). Overall, these four sets of equations represent a total of \( 4 \times N_{c} \) algebraic equations (i.e., for each cell there are four algebraic equations resulting from the finite-volume integration of Eqs. (4a)–(4d)). These equations actually have a block-implicit structure, as follows:

\[ \begin{bmatrix} A_{1,1,0} & A_{1,2,0} & A_{1,3,0} & A_{1,4,0} \\ A_{2,1,0} & A_{2,2,0} & A_{2,3,0} & A_{2,4,0} \\ A_{3,1,0} & A_{3,2,0} & A_{3,3,0} & A_{3,4,0} \\ A_{4,1,0} & A_{4,2,0} & A_{4,3,0} & A_{4,4,0} \end{bmatrix} \begin{bmatrix} \phi_{1,0} \\ \phi_{2,0} \\ \phi_{3,0} \\ \phi_{4,0} \end{bmatrix} = \begin{bmatrix} S_{1} \\ S_{2} \\ S_{3} \\ S_{4} \end{bmatrix} \]

where \( A_{1,1,0} \) for example, denotes the coefficient premultiplying \( \phi_{1,0} \) that arises out of finite-volume integration of Eq. (4a). Similarly, \( A_{2,1,0} \) denotes the coefficient premultiplying \( \phi_{1,0} \) that arises out of finite-volume integration of Eq. (4b). The second term denotes summation over all the neighboring cells, where \( nb \) is the total number of neighbors of node \( O \). The right hand side denotes generic source terms that may arise due to the fact that the tangential flux terms are treated explicitly, as discussed earlier. There may also be additional sources due to the treatment of boundary conditions.

Equation (30) addresses both variable-to-variable (i.e., \( \phi_{1} \) through \( \phi_{4} \)) as well as node-to-node (spatial) coupling implicitly. When written for all nodes \( (=N_{c}) \) in the computational domain, i.e., \( O \in 1,2,\ldots,N_{c} \), Eq. (30) represents a block matrix system of equations, where each element of the block matrix is a \( 4 \times 4 \) matrix itself. These element matrices are shown explicitly in Eq. (30) for a representative node \( O \).

### 2.3 Solution of Discrete Algebraic Equations

The discrete equations presented in Sec. 2.2 can be solved using several different techniques. One approach is to solve the system of equations directly using full lower-upper (LU) decomposition, followed by backward substitution, i.e., Gaussian elimination. Such a direct solution approach will provide the solution to the system of equations without any iteration since the governing equations are linear. Unfortunately, direct solution is prohibitive for two reasons, as follows: (1) the entire coefficient matrix of size \( 4N_{c} \times 4N_{c} \) need to be stored, and (2) the number of major floating point operations scales as \( O(M^{3}) \) [22], where \( M \) is the total number of unknowns \( (=4N_{c}) \) in this case. For sufficiently large \( N_{c} \), direct Gaussian elimination is prohibitive both from a memory as well as efficiency standpoint. The alternative is to adopt an iterative solution procedure. The simplest iterative procedure would entail sequential iterative solution of the discrete versions of Eqs. (4a) and (4b), i.e., first solve Eq. (4a) iteratively while holding \( \phi_{2} \), \( \phi_{3} \), and \( \phi_{4} \) constant, followed by solving Eq. (4b) while holding \( \phi_{1} \), \( \phi_{2} \), and \( \phi_{3} \) constant, and so on. During this study, it was found that this segregated method is inherently unstable because of the strong coupling between the four governing equations, and coupled (as opposed to segregated) solution of the governing equations is warranted.

The simplest coupled solution approach is to use the block-Gauss-Seidel (BGS) procedure [23]. In this procedure, the dependence of all spatial nodes around a given node is treated explicitly, and the whole computational domain is swept through point-by-point repeatedly until convergence is attained. In this case, at each point, a \( 4 \times 4 \) matrix has to be inverted. Unfortunately, the BGS method becomes very slow as the mesh is refined because the spectral radius of convergence (largest eigenvalue of the iteration matrix) rapidly approaches unity as the mesh is refined [23]. Here, we use a new approach, which was originally developed for coupled implicit solution of the species conservation equations on an unstructured mesh [24,25]. This is described next.

The approach used here subdivides the computational domain into subdomains that are small enough such that for each of these subdomains a fully implicit solution of the governing equations is affordable from a memory standpoint. The rationale is that this approach will enable spatial as well as variable-to-variable implicit coupling, and the extent of spatial coupling is to be dictated by memory constraints. Thus, the performance of this approach is expected to be significantly better than a BGS solver.

The development of the coupled solver entails three major steps, as follows:

1. The computational domain is decomposed into smaller groups of cells that are geometrically contiguous—a process termed internal domain decomposition (IDD). This is a one-time preprocessing step. This step is performed using the binary spatial partitioning algorithm [26,27].

2. For each subdomain, an iterative solver based on Krylov subspace iterations (i.e., the restarted and preconditioned generalized minimum residual (GMRES) solver [28]) are employed to obtain the solution at all nodes within the subdomain and for all variables \( (\phi_{1} \text{ through } \phi_{4}) \) simultaneously. Other subdomains adjacent to the subdomain in question are treated explicitly, and ghost (or virtual) boundary conditions are applied at interfaces between subdomains to transfer information between subdomains.
3. An overall (or outer) iteration is performed within which the preceding step is repeated until convergence. Iterations are necessary to resolve the explicit coupling between subdomains, and also to couple the RTE with the overall energy equation.

The overall algorithm for solution of the RTE, and how it is coupled to the overall energy conservation equation is depicted in Fig. 2. Further details pertaining to this solver, henceforth referred to as the IDD+GMRES solver, may be obtained from Kumar and Mazumder [24,25]. The factor that motivated the choice of GMRES over other iterative solvers is that it has extremely good convergence properties when preconditioned appropriately even for relatively large matrix sizes. In this solver, memory requirement can be limited by specifying the largest Krylov subspace size and the number of internal iterations can be limited by specifying the maximum number of GMRES iterations. In essence, the solver chosen is very flexible and appropriate for use in the current solution strategy.

3 Results and Discussion

In this section, the accuracy and efficiency of the $P_3$-based RTE solver is discussed. The standalone $P_1$-based RTE solver was first verified against MC results available from the literature for two benchmark problems. For comparison, a $P_1$-based RTE solver was also developed. The governing equation and boundary condition solver is discussed. The standalone benchmark problems. For comparison, a $P_3$-based RTE solver was first verified against MC results available from the literature for two cavity problems. The governing equation is an isotropic scattering is considered. Since the gas does not absorb or emit radiation, it is not necessary to couple the RTE to the overall energy equation in this case. The problem is one of radiative equilibrium, in which the radiation energy emitted by the hot wall is directionally redistributed by scattering. The dimension of the cavity is kept fixed, while the scattering coefficient $\sigma_r$ is varied to change the overall optical thickness of the medium, defined as $\tau_a=hr_0$. Three different values of optical thickness are considered for the present study, namely, $\tau_a=0.1$, 1, and 5.

Prior to comparison with MC results, grid independence studies were performed. Four different quadrilateral mesh sizes and four different triangular mesh sizes were considered. For these studies, the second verification problem, to be described shortly, was considered because this particular problem, with a partly heated bottom wall, has a discontinuity in temperature at the bottom wall, and therefore, requires high spatial resolution. The results of these studies are shown in Fig. 4. It is evident from Fig. 4 that grid-independent solution is obtained if the mesh size is increased beyond approximately 6000 cells for quadrilateral cells and beyond 9000 cells for triangular cells. Since the same mesh is used in both verification studies, the mesh that was determined to be appropriate for the second verification case was also deemed appropriate for the first verification case.

Figure 5 shows the nondimensional radiative heat fluxes (normalized by $\sigma T_a^4$) predicted by the various methods for $\tau_a=0.1$. These results were computed with 9492 triangular cells, and the computational mesh is shown in Fig. 3(b). Triangular mesh is chosen for these studies because they represent the worst-case scenario, both in terms of geometrical complexity in 2D and numerical convergence. While $P_3$ calculations have been performed in 2D using orthogonal meshes [14,15], to the best of our knowledge, no such calculations have been performed on unstructured meshes, and this is one of the key contributions of the current...
article. It is worth noting that the calculations were conducted on the full cavity (rather than apply symmetry boundary conditions), and therefore, the mesh is not perfectly symmetric (see Fig. 3(b)) about the midplane. This was done so that we could use as large a mesh size as possible for efficiency studies to be presented in Sec. 3.2. Both $P_1$ and $P_3$ methods perform poorly for this optically thin case. In fact, both methods produce unphysical results, as evident from the fact that the nondimensional heat flux exceeds a value of unity. Similar unphysical results have also been reported by Modest and Yang [15], and are inherent to the $P_N$ approximation for optically thin scenarios. Figure 6 shows the nondimensional radiative heat fluxes predicted by the various methods for $\tau_a = 1$. In this case, the predictions by both $P_1$ and $P_3$ match the MC results better. Also, while the unphysical results are still present, they are confined to smaller regions, and the degree to which the nondimensional heat fluxes overshoot unity is significantly reduced. Figure 7 shows the nondimensional radiative heat fluxes predicted by the various methods for $\tau_a = 5$. In this case, the match between results predicted by the $P_N$ method and the MC method is quite good. In particular, the $P_3$ method is more accurate than the $P_1$ method for heat flux predictions at the bottom.

Fig. 4 Comparison of the nondimensional heat flux computed at the bottom (hot wall) using various mesh sizes and the $P_3$-based RTE solver: (a) various structured grids (quadrilateral cells), and (b) various unstructured grids (triangular cells)

Fig. 5 Comparison of nondimensional heat fluxes predicted using the $P_1$ and $P_3$ methods with benchmark MC results [15] for $\tau_a = 0.1$: (a) bottom, (b) right (side), and (c) top walls. The heat fluxes are normalized by $\sigma T_0^4$. 
Fig. 6 Comparison of nondimensional heat fluxes predicted using the $P_1$ and $P_3$ methods with benchmark MC results [15] for $\gamma_0=1$: (a) bottom, (b) right (side), and (c) top walls. The heat fluxes are normalized by $\sigma T^4_r$.

Fig. 7 Comparison of nondimensional heat fluxes predicted using the $P_1$ and $P_3$ methods with benchmark MC results [15] for $\gamma_0=5$: (a) bottom, (b) right (side), and (c) top walls. The heat fluxes are normalized by $\sigma T^4_r$. 
and right walls. At the top wall, it appears that the $P_1$ method slightly outperforms the $P_3$ method. However, the actual heat flux values are too small for this difference to be of much significance. No unphysical results are produced for the optically thick case with either of the two $P_N$ methods.

The second verification study was performed on a case that is identical to the first case, except that only part of the bottom wall is heated, as shown in Fig. 8. The same computational mesh as the first case was used. The results are shown in Figs. 9–11 for the three different optical thickness values. Once again, it is observed that the predictions of both $P_1$ and $P_3$ do not match the “exact” MC results for $\tau_w=0.1$. In this case also, the nondimensional heat flux at the heated section of the bottom wall attains unphysical values above unity. Once again, though unphysical, these results are consistent with the results shown by Modest and Yang [15]. As the optical thickness is increased, the results start approaching MC results. For $\tau_w=5$, $P_3$ results are more accurate than $P_1$ results.

In the two problems just discussed, there is no emission or absorption by the medium. The energy emitted by the hot surface is simply scattered. Thus, both problems are that of radiative equilibrium, i.e., $\nabla \cdot \mathbf{q}_R=0$, where $\mathbf{q}_R$ is the radiative heat flux. In a conservative finite-volume procedure, as used here, the radiative heat fluxes must balance when summed over all the boundary faces. In order to verify our formulation and code, the aforementioned flux balance test was conducted for both test cases. Table 1 shows the fluxes computed at each wall using the two $P_N$ methods, as well as the overall imbalance in flux. In all cases, it is seen that the imbalance is approximately six orders of magnitude smaller than the flux at the hot surface. This is consistent with the fact that the convergence criterion used to generate these results was six orders of magnitude decrease in the residuals ($L^2$ norm) of the $P_N$ equations. These results indicate that even though for optically thin situations the $P_N$ method produces unphysical results locally, the overall energy conservation (first law) is satisfied in all cases.

The $P_3$ equations arise out of mathematical manipulations of a physical conservation equation (the RTE). As such, they do not have a physical meaning. One of the key steps in the whole FV formulation presented here is to express the original equations proposed by Modest and Yang [15] in divergence form (Eq. (11)). Since the FV method solves the governing PDEs in weak form after integration, if the entire governing equation is in divergence form, as Eq. (11) is, the formulation is fully conservative, and will balance fluxes (not physical fluxes, but the sum of $U_1$ through $U_5$) even on the coarsest of meshes.

Fig. 8 Geometry and boundary conditions for the second benchmark problem

Fig. 9 Comparison of nondimensional heat fluxes predicted using the $P_1$ and $P_3$ methods with benchmark MC results [15] for $\tau_w=0.1$: (a) partly heated bottom, (b) right (side), and (c) top walls. The heat fluxes are normalized by $\sigma T_0^4$.
Fig. 10 Comparison of nondimensional heat fluxes predicted using the $P_1$ and $P_3$ methods with benchmark MC results [15] for $T_{w}=1$: (a) partly heated bottom, (b) right (side), and (c) top walls. The heat fluxes are normalized by $uT_{w}$.

Fig. 11 Comparison of nondimensional heat fluxes predicted using the $P_1$ and $P_3$ methods with benchmark MC results [15] for $T_{w}=5$: (a) partly heated bottom, (b) right (side), and (c) top walls. The heat fluxes are normalized by $uT_{w}$.
3.2 Performance of RTE Solver. The solution of the RTE using the $P_3$ method involves solution of a set of four coupled, second-order, elliptic PDEs. As mentioned earlier, it was found that these equations cannot be brought to convergence using a segregated solution approach, and a coupled solver was used in this study. One of the critical issues in the coupled solver, as described in Sec. 2.3, is how many cells should be included in each internal subdomain. The IDD+GMRES solver was tested for the first verification case with various numbers of cells in each subdomain. The overall computational domain consisted of 22,902 triangular cells. Table 2 shows the CPU time taken and the memory required for various subdomain sizes. All computations were performed on an Intel core 2 duo processor with 2.3 GHz processor speed.

3.3 Coupling With Reacting Flow Solver. As a final step to demonstrate the new $P_3$-based RTE solver, it was coupled with an in-house 2D reacting flow solver [24,25]. Overall outer iterations were performed (Fig. 2) to couple all the conservation equations, and to address nonlinearities in the governing equations, which were all solved in appropriate linearized form.

The test problem considered is that of steady state homogeneous combustion of a methane-air mixture under laminar flow conditions, i.e., a laminar flame. A simple 2D diffusion flame configuration, as shown in Fig. 12(a), is considered. Based on the inlet conditions, the overall equivalence ratio is unity, and the Reynolds number based on the channel width is approximately 150. A two-step reaction mechanism [29] involving six gas-phase species (CH$_4$, CO$_2$, H$_2$O, N$_2$, O$_2$, and CO) was used for gas-phase chemistry calculations. The computational mesh comprised of 19,953 triangular cells, and part of the mesh is shown in Fig. 12(b). Convergence was deemed to have been attained when the $L_2$ norm of all the governing equations decreased by six orders of magnitude. The extinction coefficient was assumed to be constant, and two different values were considered, as follows: 5 m$^{-1}$ and 50 m$^{-1}$ (resulting in optical thickness of 0.25 and 2.5, respectively, based on the channel width), while a constant value of 0.5 was assumed for the scattering albedo.

The temperature distributions predicted by the $P_1$ and $P_3$ methods are shown in Fig. 13 for the optically thick case since the $P_N$ approximation is more accurate in optically thick situations, as found from the results of the preceding verification studies. It is clear that inclusion of radiation lowers the temperature of the...
flame significantly, as expected. The temperature distributions predicted using both $P_N$ methods are almost identical, although a close inspection reveals minor differences especially at the tip of the flame. Both methods resulted in smooth overall convergence, and the residuals for both optical thicknesses are shown in Fig. 14. It is worth noting that although the physical results are error-prone for the optically thin case, this case represents the worst-case scenario in terms of numerical convergence, and has, therefore, been considered in this study. The following discussion focuses on this optically thin case. For the $P_1$ approximation, the RTE converges ahead of the overall energy equation, and the overall convergence is held up by the energy equation. For the $P_3$ approximation, the convergence of the RTE is slowest, and affects the overall convergence of the flow solver adversely. For the optically thick case (not shown), the $P_N$ equations converged very rapidly compared with the other equations, as expected. From a memory standpoint, the $P_1$ solver required an additional 16% memory for the one additional PDE that needed to be solved: 77 Mbytes for overall solver with $P_1$ versus 67 Mbytes for solver without radiation. The memory requirement of the $P_1$ solver (IDD+GMRES solver) depends on the number of subdomains used. As discussed earlier, if no internal domain decomposition is performed, the performance is the best, but the memory requirement is too high. For the present computations, four subdomains were used. The rationale for this choice is that four subdomains resulted in an additional 40 Mbytes memory requirement for the four additional PDEs, which is roughly a linear scale-up from the memory required by the $P_1$ solver. Perhaps, because the most efficient setup (of using no internal domain decomposition) is not utilized in this case, the overall convergence of the flow solver is adversely affected by the slow convergence of the $P_1$ equations to some degree. One of the ways to improve the convergence is to use tighter tolerance criteria within the GMRES solver for the $P_1$ equations, and further research is underway to investigate this issue. The flow solver with $P_3$ requires slightly more number of outer iterations (2553 versus 2361) than the flow solver with $P_1$ for six orders of magnitude convergence (Fig. 14), and the overall CPU time consumed increases from an extra 9.3–14.5%. The total CPU time taken by the flow solver with $P_1$ is 11,242 s while the CPU time taken by the flow solver with $P_3$ is 12,746 s. The number of PDEs solved in the flow solver without radiation is 10, while the number of PDEs solved with $P_3$ radiation is 14. Thus, a 14.5% increase in the CPU time due to the extra four PDEs represents significantly better than linear scale-up, and is, therefore, deemed acceptable.

Fig. 12 (a) Geometry and boundary conditions for the reaction flow test case (2D laminar methane-air flame), and (b) computational mesh: only one-third of the channel is shown for clarity

Fig. 13 Temperature distributions for a laminar methane-air diffusion flame: (a) without including radiation, (b) including radiation calculated using $P_1$, and (c) including radiation calculated using $P_3$
4 Summary and Conclusions

A conservative finite-volume procedure has been presented for discretization of the $P_1$ equations of radiative transfer on an unstructured mesh. The resulting block-implicit equations have been solved using a new solver, referred to as the IDD+GMRES solver. The solver facilitates both variable-to-variable as well as spatial (cell-to-cell) coupling in an implicit manner. The solver is based on the decomposition of the computational domain into subdomains using the binary spatial partitioning algorithm, and subsequent solution of the block-implicit equations within each subdomain using an incomplete LU-preconditioned restarted GMRES solver.

The finite-volume procedure and the coupled solver were tested for two benchmark problems. The two benchmark problems were chosen such that they represent worst-case scenarios for the $P_N$ method, namely, cold medium surrounded by hot walls [1]. It was found that for low to intermediate optical thicknesses, both $P_1$ and $P_3$ methods produce inaccurate results when compared with exact Monte Carlo results. In some cases, the results are also locally unphysical. For optically thick situations, both $P_1$ and $P_3$ produced reasonably accurate results. Overall, the $P_3$ method appears to be superior in accuracy over the $P_1$ method—a finding that is consistent with past findings [14,15], and one that warrants further research on higher-order $P_N$ methods. It is worth emphasizing that the findings reported here are for worst-case scenarios for the $P_N$ method, and by no means, discount either the $P_1$ or $P_3$ approximation as possible methods for solution of the RTE. For cases with cold walls and strongly emitting media, the accuracy of both $P_1$ and $P_3$ methods is expected to be substantially better [1].

Flux conservation property of the method was tested thoroughly, and it was found that the formulation and numerical procedure presented here conserves the radiative heat fluxes (overall energy) exactly, irrespective of the mesh or the optical thickness used. This is an important aspect of any numerical scheme for solution of the RTE since violation of the radiative flux conservation will also lead to violation of the overall energy conservation.

The performance of the new RTE solver was investigated by changing the maximum number of cells within each internal subdomain. The best performance was obtained when no partitioning was used and the RTE was solved using a full-field GMRES solver. Six orders of magnitude convergence was obtained on a 22,902-cell mesh in just 32 s. However, this required 152 Mbytes of memory. In order to keep memory requirements reasonable, it would be necessary to use more than one partition in large-scale computations, and further research is necessary to arrive at a compromise between memory and efficiency.

As a final step, the $P_1/P_3$-based RTE solver was coupled to a standalone flow and energy equation solver, and subsequently demonstrated for a 2D laminar flame case with six species, resulting in a total of ten PDEs for the flow, energy, and species conservation equations. The $P_1$ method (one additional PDE) was found to require approximately 9.3% additional CPU over the core flow solver, while the $P_3$ method (four additional PDEs) required an additional 14.5% CPU. The results presented here clearly demonstrate the feasibility of using the $P_3$ approximation for computation of reacting flows. Future work will focus on extension of the current procedure to three-dimensional geometry.

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Nomenclature

$A_f$ = area of face $f$ (m$^2$)
$A_{i,j,k}$ = link coefficients
$h$ = cavity width (m)
$I$ = intensity (W m$^{-2}$ sr$^{-1}$)
$I_S$ = intensity at surface (W m$^{-2}$ sr$^{-1}$)
$I_b$ = Planck function (W m$^{-2}$ sr$^{-1}$)
$I_{n}^p$ = position dependent coefficients in intensity expansion expression
$I_{n}^p$ = position dependent coefficients expressed in local coordinates
$\hat{n}$ = unit surface normal vector
$N_C$ = total number of cells in computational domain
$N_{C,m}$ = maximum number of cells in subdomain
$q_R$ = radiative heat flux (W m$^{-2}$)
$S$ = surface area of cell (m$^2$)
$\hat{s}$ = direction vector
$T$ = temperature (K)
$x, y, z$ = global coordinates (m)
$x, y, z$ = local coordinates (m)
$\gamma_{m}^n$ = spherical harmonic functions
Greek

\[ \alpha_s = \text{coefficients in } P_3 \text{ equations (see Eq. (6))} \]
\[ \beta = \text{extinction coefficient (m}^{-1}) \]
\[ \delta_f = \text{distance between two cell centers straddling face } f \text{ along normal (m)} \]
\[ \phi_f = \text{unknowns in general form of } P_3 \text{ equation (see Eq. (9))} \]
\[ \Phi = \text{scattering phase function} \]
\[ \gamma_{ij} = \text{coefficients in } P_3 \text{ equations (see Eq. (4))} \]
\[ \Gamma_i = \text{coefficients in general for of } P_3 \text{ equations (see Eq. (9))} \]
\[ \tau = \text{optical coordinates (dimensionless)} \]
\[ \tau_b = \text{optical thickness based on cavity width (dimensionless)} \]
\[ \omega = \text{scattering albedo (dimensionless)} \]
\[ \Omega = \text{solid angle (sr)} \]
\[ \Omega_v = \text{volume of cell (m}^3) \]
\[ \sigma = \text{Stefan–Boltzmann constant (} \approx 5.67 \times 10^{-8} \text{ W m}^{-2} \text{ K}^{-4} \) \]
\[ \sigma_s = \text{scattering coefficient (m}^{-1}) \]

References