SAUDI INTERNATIONAL CONFERENCE ON NUCLEAR POWER ENGINEERING

Proceedings of SCOPE
13-15 Nov. 2023 – KFUPM
Paper XXXXX

An Exposition of the Discrete Ordinates Method For Complex Irregular Geometries Utilizing A Structured Mesh

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Abstract – *The discrete-ordinates-method (DOM) is one of the primary numerical techniques for the solution of the Boltzmann Transport Equation (BTE) as well as other transport equations that have been derived from the BTE. These transport equations are used for the study of various phenomenon such as the radiation heat transfer in a participating media, heat conduction via phonon transport at the micro/nanometre scales, neutron transport theory, etc. DOM has traditionally been used in rectangular coordinates, however, relatively recently, the DOM technique has been fully extended to be applicable in structured, general, orthogonal as well as non-orthogonal coordinate systems. Orthogonal and non-orthogonal coordinate systems can be successfully used to cover complex, irregular geometrical domains with a structured mesh and hence an efficient solution procedure based on the DOM can be developed.*

Keywords: discrete-ordinates-method, Boltzmann, Neutron transport, curvilinear

I. Introduction

The discrete-ordinates-method (DOM) is one of the primary numerical methods for the solution of the Boltzmann Transport Equation (BTE) as well as for various other equations that have been derived from the BTE. Some of these equations are: the radiative transfer equation (RTE), which is used to model the phenomenon of radiation heat transfer through a participating medium (absorbing, emitting, scattering); the equation of phonon radiative transfer (EPRT) is used to describe sub-continuum heat conduction phenomenon that manifests itself at micro/nanometer scales; in neutron transport theory, the determination of the neutron distribution requires the solution of a BTE type equation. In this paper, the DOM is discussed in the context of the radiative transfer equation (RTE). It is believed that similar analysis applies to other BTE type equations.

The RTE is an integro-differential equation with one dependent variable, the radiation intensity I_ω and seven independent variables; three space variables, (x, y, z) in Cartesian coordinates or (ξ, η, ζ) in general curvilinear coordinates, two direction variables, the polar and the azimuthal angles (φ, ψ), the frequency (energy) variable ω and finally the time variable t. For the exposition of the DOM method in this paper, it is quite adequate to work with an abridged version of the RTE, which is obtained by assuming a steady-state, frequency independent, two-dimensional problem. This implies that,

$$I = I(x, z, \varphi, \psi)$$

It is important to note that no problem is two-dimensional in reality and therefore the approximation to two-dimensionality has to be performed carefully. Here, the 2D approximation means that the radiation intensity gradient $\partial I/\partial y$ is negligible or zero. However, the thermal radiations still travel in a 3D space and therefore, the direction of propagation is described by two angles instead of one. The coordinate independent form of the radiative transfer equation is then written as,

$$\hat{\mathbf{\Omega}} \cdot \nabla I = -\beta_o I + \kappa_a I_b + \frac{\sigma_s}{4\pi} \int_0^{2\pi} \int_0^{\pi} I \Phi \sin\varphi d\varphi d\psi \quad (1)$$

where, $\hat{\mathbf{\Omega}} = \cos\varphi \,\hat{\mathbf{i}} + \sin\varphi\cos\psi \,\hat{\mathbf{j}} + \sin\varphi\sin\psi \,\hat{\mathbf{k}}$ (2)

In the above equation, β_o is the extinction coefficient, κ_a is the absorption coefficient, σ_s is the scattering coefficient and Φ is the scattering phase function. Here we assume isotropic scattering and therefore $\Phi = 1$. Moreover, we will take $\beta_o = k_a + \sigma_s$ and will also assume that radiative equilibrium prevails, which entails,

$$I_b = \frac{1}{4\pi} \int_0^{2\pi} \int_0^{\pi} I \sin\varphi d\varphi d\psi \quad (3)$$

In the preceding equation, I_b is the black-body radiation intensity and is given as,

$$I_b = \frac{\sigma T^4}{\pi} \quad (4)$$

where, σ is the Stefan-Boltzmann constant and $T(x, y)$ (or $T(\xi, \eta)$ in general) is the absolute temperature of the participating medium. Here we will remark that the analysis in this paper focusses on the left-hand-side of equation (1) and none of the many previous, simplifying assumptions have a fundamental effect on this analysis. On the contrary, these assumptions help us to focus on the analysis at hand.

The RTE in the Cartesian coordinates can then be written as,

$$\cos\varphi \frac{\partial I}{\partial x} + \sin\varphi\sin\psi \frac{\partial I}{\partial z} = \beta_o (I_b - I) \quad (5)$$

To solve equation (5), the DOM can be used, a basic outline of which is now given. The 2D region is first discretized by covering it with a mesh with spacing Δx and Δz. The 4π solid angle is also discretized by choosing a set number of directions. This entails equally dividing the range of the polar and azimuthal angles θ and ϕ in to a number of values. The angular spacings are $\Delta\varphi$ and $\Delta\psi$. The derivatives are approximated by their finite-difference counterparts and the integration is performed by means of either the Simpsons rule if $\Delta\varphi$ and $\Delta\psi$ have constant values or by other quadrature algorithms with non-uniform $\Delta\varphi$ and $\Delta\psi$. The resulting system of linear, simultaneous equations can then be solved to determine the radiation intensity I. There is more detail in the numerical solution procedure but the previous discussion will suffice for our purposes.

II. Complex, Irregular Geometries

Real life problems often involve regions that cannot be identified by standard shapes such as the rectangle, circle, ellipse, etc. and hence such regions are termed as irregular. Within the scope of the DOM, the solution of these problems can be approached in two ways. We may either use a structured mesh (finite-difference method) or an unstructured mesh (finite-volume method with say triangular cells). Algorithms based on structured meshes are more efficient than those based on unstructured meshed and this is especially true in the case of the finite-volume method. This is because, in the finite-volume method, a full database has to be constructed that keeps track of the various relations between the nodes, edges and cells. Moreover, connectivity information has also to be obtained from this database. If an iterative procedure is being used for the solution of the simultaneous equations, then this database is used repeatedly. None of this overhead occurs when a structured mesh is used, and this is because relations between the nodes, edges and cells as well as the connectivity information is built into the mesh. However, until relatively recently, the only structured meshes that were available for the solution of the RTE were those associated with the Cartesian, Cylindrical and Spherical coordinate systems. So, for example, the RTE can be solved approximately by means of the DOM in a complex, irregular region by covering that region with a Cartesian mesh, the curved boundaries being approximated by a "staircase". The RTE is then discretized in the usual manner resulting in a system of simultaneous linear equations which can then be solved. As is apparent, this is not a satisfactory approach to the solution of such problems.

When it is said that a structured mesh, such as the Cartesian/Cylindrical/Spherical, is available for the solution of RTE, this implies that the specific form of the RTE, that is applicable in these coordinate systems is known. The RTE in any coordinate system is of course written in terms of the space coordinates in those systems. So, for example, the RTE in the cylindrical coordinate system is given as,

$$\frac{\cos\varphi}{\rho}\frac{\partial\rho I}{\partial\rho}+\frac{\sin\varphi\cos\psi}{\rho}\frac{\partial I}{\partial\theta}+\frac{\sin\varphi\sin\psi}{\rho}\frac{\partial I}{\partial z}-\frac{\cos^2\psi}{\rho}\frac{\partial\sin\varphi I}{\partial\varphi}+\frac{\cos\varphi\sin\psi}{\rho}\frac{\partial\cos\psi I}{\partial\psi}=\beta_o(I_b-I) \tag{6}$$

In equation (6) above, it is observed that derivatives of the intensity variable I with respect to the polar and azimuthal angles also now appear on the left-hand-side. And this is true in general for all curvilinear coordinate systems. The origin of these derivatives lies in the fact that the basis vectors in a general curvilinear coordinate system change from one point to another, unlike in the Cartesian system, in which they are the same. The polar and azimuthal angles are measured from a fixed direction and these usually correspond to directions associated to any two of the basis vectors. It is required that the range of the polar angle is always $0\le\varphi\le\pi$ and that of the azimuthal angle to be $0\le\psi\le 2\pi$, hence when the basis vectors change as we move from one point to another neighboring point, the same numerical value of the polar and azimuthal angles do not correspond to the same direction in space. And this is the source of the derivatives of the radiation intensity with respect to the polar and azimuthal angles.

Let us suppose that an orthogonal/non-orthogonal coordinate system is available and its transformation equations from the Cartesian coordinates are known as given below,

$$x=x(\xi,\eta,\zeta)\quad y=y(\xi,\eta,\zeta)\quad z=z(\xi,\eta,\zeta) \tag{7}$$

then, it is not so unwieldy to derive expressions for $\partial I/\partial x, \partial I/\partial y, \partial I/\partial z$ in terms of the derivatives $\partial I/\partial \xi, \partial I/\partial \eta, \partial I/\partial \zeta$. These can then be substituted in to the left-hand-side of the RTE. What is missing are terms involving the derivatives $\partial I/\partial \varphi, \partial I/\partial \psi$. To write these derivatives, it is first required to determine the expressions for the following derivatives,

$$\frac{\partial \theta}{\partial \xi}, \frac{\partial \theta}{\partial \eta}, \frac{\partial \theta}{\partial \zeta} \quad \text{and} \quad \frac{\partial \psi}{\partial \xi}, \frac{\partial \psi}{\partial \eta}, \frac{\partial \psi}{\partial \zeta} \tag{8}$$

Until relatively recently, the expressions for these derivatives were undetermined and hence the RTE in a general curvilinear coordinate system could not be written. This scenario changed with the publication of his paper [1] in 2011 by Freimanis, in which he derived the RTE in a general, curvilinear coordinate system. The explicit expressions for the derivatives of the polar and azimuthal angles were more clearly presented by Yilbas et al. in [2]. They presented the expressions for the above derivatives, both for the orthogonal as well as for the non-orthogonal coordinate systems. For the orthogonal coordinates, these expressions are [2],

$$\begin{aligned}
\frac{\partial \varphi}{\partial \xi} &= \frac{\cos\psi}{h_2}\frac{\partial h_1}{\partial \eta} + \frac{\sin\psi}{h_3}\frac{\partial h_1}{\partial \zeta} \\
\frac{\partial \varphi}{\partial \eta} &= -\frac{\cos\psi}{h_1}\frac{\partial h_2}{\partial \xi} \\
\frac{\partial \varphi}{\partial \zeta} &= -\frac{\sin\psi}{h_1}\frac{\partial h_3}{\partial \xi} \\
\frac{\partial \psi}{\partial \xi} &= \cot\varphi\left[-\frac{\sin\psi}{h_2}\frac{\partial h_1}{\partial \eta} + \frac{\cos\psi}{h_3}\frac{\partial h_1}{\partial \zeta}\right] \\
\frac{\partial \psi}{\partial \eta} &= \frac{\cot\varphi\sin\psi}{h_1}\frac{\partial h_2}{\partial \xi} + \frac{1}{h_3}\frac{\partial h_2}{\partial \zeta} \\
\frac{\partial \psi}{\partial \zeta} &= -\frac{\cot\varphi\cos\psi}{h_1}\frac{\partial h_3}{\partial \xi} - \frac{1}{h_2}\frac{\partial h_3}{\partial \eta}
\end{aligned} \tag{9}$$

The above expressions are based on selecting the ξ-direction as the polar axis (the polar angle is measured from the basis vector in the ξ-direction). The azimuthal angle is measured from the basis vector in the η-direction. h_1, h_2, h_3 are the scale factors (diagonal entries of the metric tensor) of the orthogonal coordinate system. The RTE in an orthogonal coordinate system can then be written as [2],

$$\begin{aligned}
&\frac{\cos\varphi}{h_1}\frac{\partial I}{\partial \xi} + \frac{\sin\varphi\cos\psi}{h_2}\frac{\partial I}{\partial \eta} + \frac{\sin\varphi\sin\psi}{h_3}\frac{\partial I}{\partial \zeta} + \\
&\left[\begin{array}{l}\frac{\cos\varphi}{h_1}\left(\frac{\cos\psi}{h_2}\frac{\partial h_1}{\partial \eta} + \frac{\sin\psi}{h_3}\frac{\partial h_1}{\partial \zeta}\right) - \\ \frac{\sin\varphi}{h_1}\left(\frac{\cos^2\psi}{h_2}\frac{\partial h_2}{\partial \xi} + \frac{\sin^2\psi}{h_3}\frac{\partial h_3}{\partial \xi}\right)\end{array}\right]\frac{\partial I}{\partial \varphi} + \\
&\left[\begin{array}{l}h_3\frac{\cos\psi\sin\psi\cos\varphi}{h_1 h_2}\frac{\partial}{\partial \xi}\left(\frac{h_2}{h_3}\right) - \\ \frac{\sin\psi\cos\varphi}{h_2}\left(\frac{\tan\varphi}{h_3}\frac{\partial h_3}{\partial \eta} + \frac{\cot\varphi}{h_1}\frac{\partial h_1}{\partial \eta}\right) + \\ \frac{\cos\psi\cos\varphi}{h_3}\left(\frac{\cot\varphi}{h_1}\frac{\partial h_1}{\partial \zeta} + \frac{\tan\varphi}{h_2}\frac{\partial h_2}{\partial \zeta}\right)\end{array}\right]\frac{\partial I}{\partial \psi} \\
&= \beta_o(I_b - I)
\end{aligned} \tag{10}$$

Similar, but much more involved analysis can be carried out for the case of a non-orthogonal system. The details are presented in [2].

III. Numerical Examples

Equation (10) and the related equation in a non-orthogonal coordinate system can be solved by any of the three methods: finite-difference method, finite volume method, finite element method. Out of these three, the finite-difference method is the most straightforward approach. The orthogonal/non-orthogonal mesh can be generated by means of the methods of Numerical Grid Generation as described in [3]. In particular, Elliptic Grid Generation system can be used to obtain equations (7). Once equations (7) are available (in array form in computer memory), the metric tensor and the connection coefficients of the curvilinear coordinate system can be determined. In the next step, the coefficients of the various derivatives in the relevant RTE are calculated. The RTE is then solved by means of the discrete-ordinates-method. The details of the numerical solution procedure for the DOM for an orthogonal coordinate system are provided in [4, 5, 6, 7]. The details of the numerical solution procedure for a non-orthogonal coordinate system are provided in [8, 9].

For the present paper, two illustrative problems are solved by means of the non-orthogonal meshes. The results obtained are compared with those published earlier [10]. It is observed that the two solutions are reasonably close.

III.A. Absorbing, emitting and isotropically scattering medium in a quadrilateral enclosure

The problem is concerned with a medium that absorbs, emits and isotropically scatters thermal radiation. The medium temperature is maintained at a constant temperature of T_g whereas the enclosure walls are considered black and are maintained at a constant temperature of $0\,K$. In this problem, the radiative equilibrium is not maintained and therefore equation (3) is not applicable. However, equation (4) is still applicable and equation (1), the RTE, is modified by replacing β_o by κ_a. The geometry and the non-orthogonal mesh are shown in figure 1. The dimensionless heat flux distribution along the dimensionless distance at the bottom wall for three different values of κ_a are presented in figure 2.

III.B. Isotopically scattering medium in a quadrilateral enclosure under radiative equilibrium

The problem is concerned with a participating medium that isotropically scatters thermal radiation and is under radiative equilibrium. The medium temperature is to be determined whereas the enclosure walls are maintained at a constant temperature of $0\,K$ except the bottom wall, which is maintained at $300\,K$. The extinction coefficient is $\beta_o = 1 m^{-1}$. In this problem equations (1), (3) and (4) are all applicable. The geometry and the non-orthogonal mesh are the same as in figure 1. The dimensionless heat flux distribution along the dimensionless distance at the top wall is presented in figure 3.

IV. Conclusions

Boltzmann Transport Equation (BTE) is used to describe various sub-continuum transport processes. BTE, in realistic situations, is typically solved numerically and DOM is a commonly used method. DOM has recently been further developed so as to be applicable in structured, orthogonal/non-orthogonal meshes. Complex, irregular regions can be discretized by such meshes through the Numerical Grid Generation procedures. Subsequently, DOM can be used to solve the BTE in such regions. Two numerical examples are finally presented.

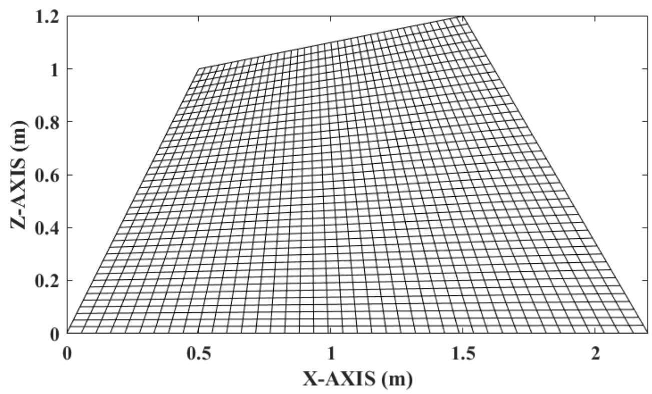

Fig. 1. Geometry and non-orthogonal mesh.

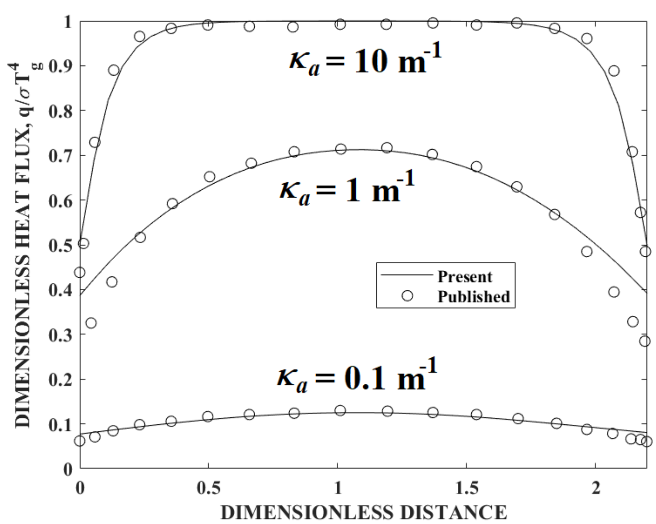

Fig. 2. Dimensionless radiative heat flux at the bottom wall.

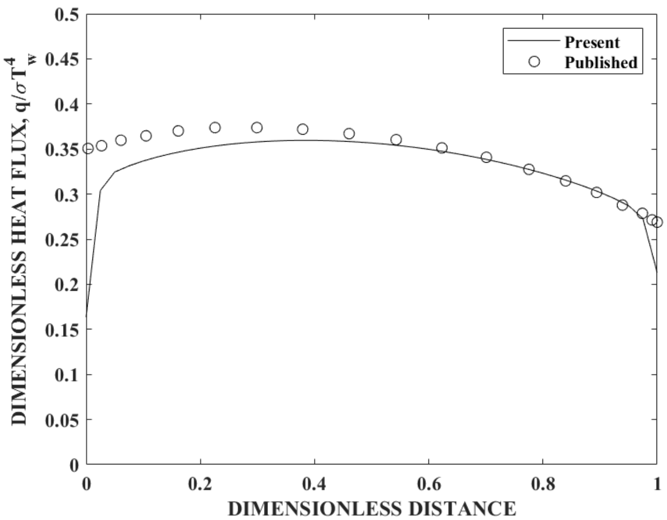

Fig. 3. Dimensionless radiative heat flux at the top wall.

Acknowledgments

The author acknowledges the support of the Mechanical Engineering Department at King Fahd University of Petroleum & Minerals (KFUPM); and acknowledgement is extended to the Interdisciplinary Research Center for Renewable Energy and Power Systems (IRC-REPS)

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