AUG 25 1965

85024

LA-DC-7320
CONF-651101-29
(~~PTS. I & II~~)

MASTER

Moments Equations and Equivalent Discrete Ordinates Equations*

Part I: Generalized Moments Equations

B. G. Carlson and K. D. Lathrop

University of California

Los Alamos Scientific Laboratory

Los Alamos, New Mexico

LEGAL NOTICE

This report was prepared as an account of Government sponsored work. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission:

A. Makes any warranty or representation, expressed or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately owned rights; or

B. Assumes any liabilities with respect to the use of, or for damages resulting from the use of any information, apparatus, method, or process disclosed in this report.

As used in the above, "person acting on behalf of the Commission" includes any employee or contractor of the Commission, or employee of such contractor, to the extent that such employee or contractor of the Commission, or employee of such contractor prepares, disseminates, or provides access to, any information pursuant to his employment or contract with the Commission, or his employment with such contractor.

RELEASED FOR ANNOUNCEMENT

IN NUCLEAR SCIENCE ABSTRACTS

*Work performed under the auspices of the United States Atomic Energy Commission.

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

Moments Equations and Equivalent Discrete Ordinates Equations

Part I: Generalized Moments Equations

There are two common means of approximating the analytic Boltzmann transport equation: 1) by a finite set of coupled equations among angular moments of the distribution function, and 2) by a discrete ordinates representation of the angular dependence. In Part I of this summary we illustrate the derivation of moments equations in which the assumed form of the angular representation may be freely chosen. Such moments equations have the advantage that the angular dependence assumed may be tailored to suit the requirements of a specific problem without altering the form of the moments equations themselves. In Part II we establish discrete ordinates equations that are equivalent to the moments equations that are derived in Part I; and, conversely, demonstrate that a given discrete ordinates system implies a corresponding moments system. The equivalent discrete ordinates system may usefully be solved instead of the moments system; in addition, the requirements of equivalence provide guidelines for the selection of quadrature coefficients in discrete ordinates systems.

In what follows we illustrate the methods for one-dimensional spherical geometry. The techniques can be extended to geometries in which the angular distribution depends on two angular variables¹. The Boltzmann equation is written, for, say, one group of a multigroup formulation, as

$$\frac{\mu}{r^2} \frac{\partial(r^2 \psi)}{\partial r} + \frac{1}{r} \frac{\partial[1-\mu^2]\psi}{\partial \mu} + \sigma \psi(r, \mu) = S_0 + 3\mu S_1 \quad (1)$$

where, for convenience, the source has been restricted to isotropic (S_0) and linearly anisotropic (S_1) components. A moment operator is defined by

$$\tilde{M}_m = \frac{1}{2} \int_{-1}^1 \mu^m \cdot d\mu \quad (2)$$

and applied to Eq. (1) giving

$$\begin{aligned} \frac{1}{r^2} \frac{d(r^2 \psi_{m+1})}{dr} + \frac{m}{r} (\psi_{m+1} - \psi_{m-1}) + \sigma \psi_m &= S_0/(m+1) \quad m \text{ even} \\ &= 3S_1/(m+2) \quad m \text{ odd} \end{aligned} \quad (3)$$

Above, $\psi_m(r) = \tilde{M}_m \psi(r, \mu)$. Notice that Eq. (3) is simpler than the customary spherical harmonics moment equations in that only one spatial derivative appears in each equation. Notice also that the form of the operator $\tilde{M}_m$ does not fix the form of the angular flux representation. Because of the orthogonality properties of the spherical harmonics functions, use of the spherical harmonics operator fixes the angular representation of $\psi(r, \mu)$ as an orthogonal polynomial expansion. The operator of Eq. (2) thus permits the functional dependence of the angular flux to be chosen freely. At the same time the $m = 0$ equation remains the equation of neutron balance.

If the moments equations are to be solved after truncation at the $m = n-1$ (n even) equation, ψ_n must be eliminated from the last equation to reduce the number of unknown moments to the number of equations. This

OCT 4 1963

reduction is accomplished by using the properties of the assumed angular representation. Suppose, for example, that a separate polynomial expansion is chosen for each μ half range, letting

$$\begin{aligned}\psi(r, \mu) &= \sum_{i=0}^{n/2-1} [a_{2i+1}(r) + a_{2i}(r)] \mu^i \quad \mu > 0 \\ &= \sum_{i=0}^{n/2-1} [a_{2i+1}(r) - a_{2i}(r)] (-\mu)^i \quad \mu < 0\end{aligned}\tag{4}$$

with n undetermined constants a_i . Applying $\tilde{M}_m$ to this representation gives

$$\begin{aligned}\psi_m(r) &= \sum_{i=0}^{n/2-1} a_{2i}(r)/(i+m+1) \quad \text{even } m \\ &= \sum_{i=0}^{n/2-1} a_{2i+1}(r)/(i+m+1) \quad \text{odd } m\end{aligned}\tag{5}$$

Hence, Eq. (5) for $m = 0, 1, \dots, n-1$, allows the a_i to be expressed in terms of the ψ_m . Therefore ψ_n , as given by Eq. (5) can be expressed in terms of the ψ_m , $m < n$, and thus can be eliminated from the finite set of moments equations to be solved. Pomraning² has used a similar type of terminating condition (within the framework of spherical harmonics) to achieve desirable properties of the moments equations, e.g., the correct asymptotic eigenvalue in all orders of truncation. Here, the entire angular representation can be adjusted. For a single polynomial over the whole μ range, a step function representation in subranges of μ , and

Eq. (4), the terminating condition can be simply expressed as

$$\sum_{m=0}^{n/2} \psi_{2m}(r) C_{2m} = 0 \quad (6)$$

where the constants C_m depend only on the choice of angular representation. The single polynomial representation reduces the moments equations of Eq. (3) to the spherical harmonics moments equations.

For the three representations described above, the Marshak boundary conditions of no incoming flux at a boundary, say $r = b$,

$$\int_{-1}^0 \mu^m \psi(b, \mu) d\mu = 0 \quad m = 1, 3, \dots, n-1 \quad (7)$$

can also be expressed as a condition among the ψ_m . Hence the same set of moments equations can be solved for at least three, and undoubtedly for many, different angular representations with only the terminating and boundary conditions changing.

References

1. B. G. Carlson, "A Method of Moments for Solving the Neutron Transport Equation," Los Alamos Scientific Laboratory Report LA-3060 (Feb., 1965).
2. G. C. Pomraning, Nucl. Sci. and Engr. 22, 328 (1965).

Moments Equations and Equivalent Discrete Ordinates Equations*

Part II: Equivalent Discrete Ordinates Equations

B. G. Carlson and K. D. Lathrop

University of California

Los Alamos Scientific Laboratory

Los Alamos, New Mexico

*Work performed under the auspices of the United States Atomic Energy Commission.

OCT 4 1955

Moments Equations and Equivalent Discrete Ordinates Equations

Part II: Equivalent Discrete Ordinates Equations

Suppose that, as in Part I, a set of moments equations for one dimensional spherical geometry is given by

$$\frac{1}{r^2} \frac{d(r^2 \psi_{m+1})}{dr} + \frac{m}{r} (\psi_{m+1} - \psi_{m-1}) + \sigma \psi_m = S_0 / (m+1) \quad m \text{ even}$$

$$= S_1 / (m+2) \quad m \text{ odd}$$

(1)

$$m = 0, 1, \dots, n-1$$

Suppose also that a discrete ordinates approximation for the same transport equation from which Eq. (1) was derived is

$$\frac{\mu_k}{r^2} \frac{d}{dr} (r^2 \phi_k) + \frac{1}{r} \sum_{\ell=1}^n \beta_{k\ell} \phi_{\ell} + \sigma \phi_k = S_0 + \beta_{k1} S_1$$

(2)

$$k = 1, 2, \dots, n$$

in which $\phi_k = \psi(r, \mu_k)$ and the number of discrete directions, n , corresponds to the number of moments equations in Eq. (1). The $\beta_{k\ell}$ are coefficients representing the angular derivative. A reasonable requirement for equivalence of Eq. (1) and Eq. (2) is that the result of applying the discrete moment operator

$$M_m = \sum_{k=1}^n w_k \mu_k^m$$

(3)

RELEASED FOR ANNOUNCEMENT
IN NUCLEAR SCIENCE ABSTRACTS

to Eq. (2) reproduce Eq. (1) in terms of $\psi_m = M_m \phi$. In Eq. (3) the ω_k are quadrature weights associated with the directions μ_k . Applying M_m to the right side of Eq. (2) gives the right side of Eq. (1) if

$$\sum_{k=1}^n \omega_k \mu_k^{2m} = 1/(2m+1) \quad (4)$$

$$m = 0, 1, \dots, n/2$$

Thus, for equivalence, the quadrature set should correctly integrate the first $n/2$ even powers of μ . Applying M_m to the left of Eq. (2) reproduces Eq. (1) if

$$\begin{aligned} \sum_{k=1}^n \omega_k \mu_k^m \sum_{\ell=1}^n \beta_{k\ell} \phi_{\ell} &= m(\psi_{m+1} - \psi_{m-1}) \\ &= m \sum_{k=1}^n \omega_k \mu_k^{m-1} (\mu_k^2 - 1) \phi_k \end{aligned} \quad (5)$$

that is, if for each ℓ ,

$$\sum_{k=1}^n \omega_k \mu_k^m \beta_{k\ell} = -m \mu_{\ell}^{m-1} (1 - \mu_{\ell}^2) \quad (6)$$

$$m = 0, 1, \dots, n-1$$

Equation (6) thus defines the $\beta_{k\ell}$ in terms of the quadrature coefficients. Now if the terminating condition for the moments equations is of the form, as in Part I

$$0 = \sum_{m=0}^{n/2} C_{2m} \psi_{2m}(r) = \sum_{m=0}^{n/2} C_{2m} \sum_{k=1}^n w_k \mu_k^{2m} \phi_k(r) \quad (7)$$

this condition can be satisfied independently of the values of $\phi_k(r)$ by requiring

$$\sum_{m=0}^{n/2} C_{2m} \mu_k^{2m} = 0 \quad (8)$$

This condition selects n values ($\pm$ paired) of μ_k . If it is assumed that the symmetric directions ($\pm$ paired) are assigned equal weights, then Eqs. (8), (6) and (4) define all the coefficients of a discrete ordinates quadrature that makes the discrete ordinates equations, Eq. (2), equivalent to the moments equations, Eq. (1). Equation (8) defines n directions, Eq. (4) defines $n/2$ weights, and Eq. (6) defines the curvature coefficients. Indeed, if a single polynomial is used in the angular representation of the moments equations, the coefficients C_{2m} are such that Eq. (8) is $P_n(\mu) = 0$ and the resulting discrete ordinates equations use the Gauss-Legendre quadrature coefficients. In this case the β matrix is full. This fact illustrates that the S_n discrete ordinates method, as commonly used,¹ is not equivalent to a spherical harmonics solution even if Gauss-Legendre quadrature coefficients are used in the S_n solution since the S_n method uses a simplified treatment of the curvature term.

Under the conditions established above, Eq. (1) and Eq. (2) are equivalent and should yield the same solution provided boundary conditions

are applied in the same manner to both equations. For the discrete ordinates equation, Mark boundary conditions are the easiest to apply, but the Marshak conditions can also be applied.

Equivalence can also be established starting from the discrete ordinates equations. That is, suppose a set of quadrature coefficients w_k and μ_k is given. It is then possible to establish a terminating condition to apply to the set of moments equations, Eq. (1). Since

$$\psi_m = \sum_{k=1}^n w_k \mu_k^m \phi_k \quad (9)$$

the ϕ_k can be expressed in terms of ψ_m , $m = 0, 1, \dots, n-1$. Then ψ_n can be expressed in terms of ψ_m , $m < n$ to form the terminating condition used to eliminate ψ_n from the moments equations. In this situation, if Eq. (4) is satisfied, if the β_{kl} are defined by Eq. (6), and if boundary conditions are applied in the same manner, the resulting moments equations are equivalent to the discrete ordinates equations. The question of whether a given discrete quadrature set also implies a functional angular representation is much more difficult. Certainly, in the formulation illustrated here, a single polynomial representation (equivalent to a Legendre polynomial expansion) implies the use of Gauss-Legendre quadrature, but, it has not been found possible to establish the representation implied by an arbitrary quadrature.

References

1. B. G. Carlson, "Numerical Formulation and Solution of Neutron Transport Problems," Los Alamos Scientific Laboratory Report LA-2996 (April, 1964).
2. G. Goertzel, Nucl. Sci. and Engr. 4, 581 (1958).