3. The Classical Spherical-Harmonics Method in Transport Theory, *R. D. M. Garcia (CTA–Brazil), C. E. Siewert (NCSU), J. R. Thomas, Jr. (VPI&SU), invited*

INTRODUCTION

The spherical-harmonics method (also known as the P_N method) was first suggested by Jeans[1] in 1917 as a solution technique in the field of radiative transfer. In neutron-transport theory, the method was first applied by Marshak[2] and was extensively developed by Mark.[3,4]

The essence of the method is the approximation of the angular dependence of the particle-distribution function by a finite set of spherical harmonics (or Legendre polynomials, for cases where a single variable suffices to describe the angular dependence). Thus in plane geometry, we write[5,6]

$$\Psi(x,\mu) = \sum_{n=0}^{N} \left(\frac{2n+1}{2}\right) \psi_n(x) P_n(\mu) , \qquad (1)$$

where $P_n(\mu)$ denotes the Legendre polynomial of order n and $\psi_n(x)$ the n'th Legendre moment of the particle-distribution function at position x. We note that the various formulations of the spherical-harmonics method reported in the literature differ basically in the way the Legendre moments $\{\psi_n(x)\}$ are determined.

In what we call the numerical approach, Eq. (1) is substituted into the integrodifferential form of the transport equation, and, after projection of the equation against the Legendre polynomials, the problem is reduced to a system of $N+1$ coupled, linear, first-order differential equations for the Legendre moments. The differential equations are subsequently discretized and solved numerically.[6-8] A variant of this approach converts the first-order system to a second-order diffusionlike system before discretization.[6,9]

In the analytical approach, the system of first-order differential equations for the moments is solved by analytical methods. Two variants of this approach can be identified: in the *matrix exponential* approach,[6,10] the vector of moments is expressed in terms of a matrix exponential that is evaluated using methods of linear algebra; in the approach that we call *classical*,[3-5,11,12] due to several points in common with other established methods in transport theory (e.g., the discrete ordinates method of Wick[13] and Chandrasekhar[14]), each mode of the solution is developed explicitly. We note that some aspects of the P_N method that are difficult to treat in the matrix exponential variant, e.g., the associated eigenvalue problem and the scaling of the solution, used to avoid loss of accuracy in the computational implementation of the method for thick layers, are easily dealt with in the classical variant.[12] Theoretically, both analytical variants are equivalent and, when implemented with sufficient care, should give essentially the same results. Nevertheless, it is our opinion that the classical variant is simpler and, consequently, easier to understand, particularly by the nonspecialist.

It is clear that the analytical approach has the potential advantages, in regard to the numerical implementation, of yielding better accuracy and faster computational speed. However, spatial variations in the properties of the medium can be readily accommodated only in the numerical approach. It is also important to mention that, for years, various difficulties encountered in the implementation of the analytical approach have led users of the spherical-harmonics method to conclude that the numerical approach is the only computationally viable way of implementing the method.[6] In our opinion, some recent developments in the context of the analytical approach justify a change in this point of view.

THE CLASSICAL SPHERICAL-HARMONICS METHOD

In this section, we summarize the use of the classical spherical-harmonics method for one-speed problems in plane geometry with anisotropic scattering. We consider here that the order of approximation N is odd; a review of the status of even-order P_N approximations can be found in a recent work by Rulko and Larsen.[15]

An Explicit Expression for the Moments

For a single layer $[0,a]$ without internal sources, it can be shown[12] that the Legendre moments of the particle-distribution function in the P_N approximation with N odd can be expressed, for $n = 0,1,\ldots,N$, as

$$\psi_n(x) = \sum_{j=1}^{J} [A_j e^{-x/\xi_j} + (-1)^n B_j e^{-(a-x)/\xi_j}] g_n(\xi_j) , \qquad (2)$$

where $J = (N+1)/2$, $\{A_j\}$ and $\{B_j\}$ are coefficients to be determined from the boundary conditions of the problem, $g_n(\xi)$ is the Chandrasekhar polynomial of order n, and ξ_j is the j'th positive zero of $g_{N+1}(\xi)$. The calculation of the required ξ_j, $j = 1,2,\ldots,J$, can be reduced to the computation of the eigenvalues of a tridiagonal matrix of order J (Ref. 12).

Also, an effective method for computing the Chandrasekhar polynomials accurately in high order has been made available recently.[16]

A General Particular Solution

In the presence of internal sources, the general solution of the problem can be expressed as a combination of the homogeneous solution and a particular solution. In this respect, an interesting new development in the framework of the classical spherical-harmonics method is a reported particular solution for an angularly and spatially dependent inhomogeneous source term. Following the technique of variation of parameters and a previous work by Siewert and Thomas,[17] McCormick and Siewert[18] were able to develop a particular solution of the form

$$\Psi_p(x,\mu) = \sum_{n=0}^{N} \left(\frac{2n+1}{2}\right)\phi_n(x)P_n(\mu) \quad (3)$$

along with an explicit representation for the Legendre moments $\phi_n(x)$.

Treatment of the Boundary Conditions

As noted, the classical spherical-harmonics method reduces the single-layer problem to the determination of $2J$ constants. Since boundary conditions cannot be satisfied exactly in the spherical-harmonics method,[5,6] J approximate boundary conditions are generally used at each boundary. For example, in the case of a free surface, one can use the Marshak boundary conditions,[2] which are equivalent to imposing that the incident current and higher order odd moments of the incident angular flux at the boundary be zero or the Mark boundary conditions,[4,5] which are equivalent to replacing the vacuum external to the medium by an infinite, purely absorbing medium. Since they are derived by variational methods, the Federighi[19] and Pomraning[20,21] boundary conditions are sometimes regarded as superior to the foregoing two classes of boundary conditions, at least in low order and when the quantity being computed is an integral quantity[22]; however, exceptions to this idea have been observed.[23] In high order, e.g., $N > 100$, there is, to the authors' knowledge, no reported comparison concerning the various types of boundary conditions; it has been our experience that all three types of boundary conditions yield essentially the same results for high-order solutions to one-speed problems in plane geometry. We note that the matter of improved boundary conditions for the spherical-harmonics method is still a subject of current interest.[23-25]

Postprocessing the Solution

Once the unknown constants are determined, the particle-distribution function at any spatial location in the layer could, in principle, be computed with Eqs. (1) and (2) for the case without internal sources and with these same equations plus Eq. (3) for the case with an internal source. However, due to the oscillatory character of the spherical-harmonics solution, it is known that these expressions do not yield good results. Among several proposed postprocessing techniques,[26-29] the *source-function integration* technique[29] emerges as an effective tool for obtaining accurate results. The basic idea behind this technique is the derivation of improved expressions for the particle-distribution function by means of a formal integration of the transport equation with the scattering term expressed in terms of the computed Legendre moments.

CONCLUDING REMARKS

In plane geometry, the classical spherical-harmonics method described in this paper has been successfully used to solve azimuthally dependent problems,[12] radiative-transfer problems with reflective boundary conditions,[30] multiple light-scattering problems with polarization,[31] and fully coupled multigroup problems.[32] As can be seen from the numerical results reported in these works, the postprocessed results for the particle-distribution function are always good, and the results for $|\mu| \to 0$ at the boundaries are the least accurate, as expected.

In regard to other one-dimensional geometries, we note that the spherical-harmonics method has been formally derived for both the spherical[5] and cylindrical[5,33] geometries. Nevertheless, during an implementation of the spherical-harmonics method to solve some problems in spherical geometry, Aronson[34,35] found that P_N calculations in spherical geometry become ill conditioned and ultimately diverge for spheres of sufficiently small radii or, for any radius, for sufficiently large N. Presumably, a similar phenomenon also happens in cylindrical geometry. In any case, this ill-conditioning problem needs to be resolved before the spherical-harmonics method can be considered a reliable tool for solving general problems in spherical and cylindrical geometries.

Finally, the practical use of the spherical-harmonics method in two and three dimensions has apparently been restricted to the numerical approach referred to earlier in this work.[9,36]

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1. J. H. JEANS, *Mon. Not. Royal Astron. Soc.*, **78**, 28, (1917).
2. R. E. MARSHAK, *Phys. Rev.*, **71**, 443 (1947).
3. J. C. MARK, *The Spherical Harmonics Method. I*, MT 92, Nuclear Regulatory Commission, Ottawa (1944).
4. J. C. MARK, *The Spherical Harmonics Method. II*, MT 97, Nuclear Regulatory Commission, Ottawa (1945).
5. B. DAVISON, *Neutron Transport Theory*, Oxford University Press, London (1957).
6. E. M. GELBARD, *Computing Methods in Reactor Physics*, H. GREENSPAN, C. N. KELBER, D. OKRENT, Eds., Gordon & Breach, New York (1968).
7. J. CANOSA, H. R. PENAFIEL, *J. Quant. Spectrosc. Radiat. Transfer*, **13**, 21 (1973).
8. J. V. DAVE, *J. Atmos. Sci.*, **32**, 790 (1975).
9. J. K. FLETCHER, *Nucl. Sci. Eng.*, **84**, 33 (1983).
10. A. H. KARP, J. GREENSTADT, J. A. FILLMORE, *J. Quant. Spectrosc. Radiat. Transfer*, **24**, 391 (1980).
11. J. LENOBLE, *C. R. Acad. Sc. Paris*, **252**, 2087 (1961).
12. M. BENASSI, R. D. M. GARCIA, A. H. KARP, C. E. SIEWERT, *Astrophys. J.*, **280**, 853 (1984).
13. G. C. WICK, *Z. Phys.*, **121**, 702 (1943).
14. S. CHANDRASEKHAR, *Radiative Transfer*, Oxford University Press, London (1950).
15. R. P. RULKO, E. W. LARSEN, *Nucl. Sci. Eng.*, **114**, 271 (1993).
16. R. D. M. GARCIA, C. E. SIEWERT, *J. Quant. Spectrosc. Radiat. Transfer*, **43**, 201 (1990).
17. C. E. SIEWERT, J. R. THOMAS, Jr., *J. Quant. Spectrosc. Radiat. Transfer*, **43**, 433 (1990).
18. N. J. McCORMICK, C. E. SIEWERT, *J. Quant. Spectrosc. Radiat. Transfer*, **46**, 519 (1991).
19. F. D. FEDERIGHI, *Nukleonik*, **6**, 277 (1964).
20. G. C. POMRANING, *Nucl. Sci. Eng.*, **18**, 528 (1964).
21. G. C. POMRANING, *Ann. Phys.*, **27**, 193 (1964).
22. J. CANOSA, *Nucl. Sci. Eng.*, **43**, 349 (1971).

23. R. P. RULKO, E. W. LARSEN, G. C. POMRANING, *Nucl. Sci. Eng.*, **109**, 76 (1991).

24. E. W. LARSEN, G. C. POMRANING, *Nucl. Sci. Eng.*, **109**, 49 (1991).

25. B. D. GANAPOL, C. T. KELLEY, G. C. POMRANING, *Nucl. Sci. Eng.*, **114**, 12 (1993).

26. J. V. DAVE, B. H. ARMSTRONG, *J. Atmos. Sci.*, **31**, 1934 (1974).

27. A. H. KARP, *J. Quant. Spectrosc. Radiat. Transfer*, **25**, 403 (1981).

28. C. E. SIEWERT, *J. Quant. Spectrosc. Radiat. Transfer*, **50**, 555 (1993).

29. V. KOURGANOFF, *Basic Methods in Transfer Problems*, Clarendon Press, Oxford (1952).

30. M. BENASSI, R. M. COTTA, C. E. SIEWERT, *J. Quant. Spectrosc. Radiat. Transfer*, **30**, 547 (1983).

31. R. D. M. GARCIA, C. E. SIEWERT, *J. Quant. Spectrosc. Radiat. Transfer*, **36**, 401 (1986).

32. C. E. SIEWERT, *J. Quant. Spectrosc. Radiat. Transfer*, **49**, 95 (1993).

33. W. KOFINK, *Nucl. Sci. Eng.*, **6**, 475 (1959).

34. R. ARONSON, *Nucl. Sci. Eng.*, **86**, 136 (1984).

35. R. ARONSON, *Nucl. Sci. Eng.*, **86**, 150 (1984).

36. J. K. FLETCHER, *Transp. Theory Stat. Phys.*, **15**, 157 (1986).