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The Multi-P_N approximation to neutron transport equation

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ABSTRACT

The Multi-P_N (MP_N) approximation to the first-order neutron transport equation in one- and two-dimensional geometries is presented using a variational approach. The directional variations of the angular flux have been modeled by separate spherical harmonics expansions in M subdomains, while finite elements have been utilized to represent the spatial dependence. A straightforward procedure has been proposed to handle any order of discretized polynomial expansions in both isotropic and anisotropic scattering medium. A key problem with much of the literature regarding the full-range spherical harmonic method is that it cannot exactly describe the discontinuous nature of the angular flux. Thus, the use of customary expansions leads to substantial defect at boundary and interface of two distinct media (e.g. interface of fuel elements and moderators). The major contribution of the MP_N discretization is a theory that overcomes these difficulties. The work represents the generalization of the Double-P_N (DP_N) approximation previously applied to the neutron transport equation. Numerical results in one- and two-dimensional problems compare MP_N and customary P_N calculations to the reference transport calculations.

1. Introduction

Accurate analysis of the neutron transport equation has been historically a challenging problem, as its variables are required to be independently determined via numerical methods. For this purpose, considerable attention has been given to the well-known flexibility of finite element method that has been used to obtain variational methods of extremum kinds (Ackroyd, 1997). The basic concept in the physical interpretation of problems in finite element method is the breakdown of a complex problem into simpler components or elements, using a variational principle. This method has been used to treat steady state and time-dependent problems. It is also particularly advantageous because various methods for representing the angular dependence can be handled by using it. These features of finite element method provide a good guide in many practical designs.

The finite element method has also been used to generate variational principles for both first- and second-order neutron transport equations (Ackroyd, 1995; De Oliveira, 1986; Ackroyd, 1986; Ackroyd, 1997; Abbassi et al., 2011). The potential advantages of the variational formulations led Ackroyd to propose several schemes based on the generalized least squares method. These schemes treat both the first- and second-order forms of the transport equation, while the Euler-Lagrange derivation is less direct than that of the generalized least-squares method. In addition, the weighted residual approach was adopted with a combination of the application of finite elements to one or more of the variables.

The finite element framework is also compatible with several available methods to represent the angular dependence of the neutron transport equation. A great amount of literature is available on each of those algorithms. The most popular can be carried out by representing the angular flux as a truncated series expansion or identifying the directions by a finite set of director cosines (Duderstadt and Martin, 1979; Lewis and Miller, 1984; Laboure et al., 2017; Varin and Samba, 2005; Buchan et al., 2010). In some other studies of the transport equation, phase-space finite elements have been used to represent both spatial and directional dependencies of the angular flux (Miller et al., 1973; Mordant, 1986).

One of the well-known ways in general use for expressing the directional dependence of the angular flux is the method of spherical harmonics or P_N approximation, which has been successfully applied to the neutron transport calculations by various authors (Bell and Glasstone, 1970; Williams, 1971). This approximation can be treated by expanding the angular dependence of the flux in a set of spherical harmonic functions which can be combined naturally with the Legendre functions to handle the anisotropic scattering laws. The exact solution of transport equation can be obtained when $N \to \infty$, however usually only a few orders of the spherical harmonics are manageable for many analysis. The number of unknowns of P_N equations in multidimensional

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geometries grows and it is relatively complicated to be dealt with. But P_N equations for these cases can be formulated as second-order equations by defining even and odd parity fluxes (Yousefi et al., 2017).

The most important mathematical difficulty in approximating the angular flux distribution is probably the exact incorporation of discontinuous boundary conditions of the angular flux. The sharp changes of directional density at interfaces and boundaries give rise to the discontinuities. This difficulty impedes the diffusion theory and spherical harmonic expansions of the accurate description of the flux near boundaries. In problems in which a large number of neutrons are emerging near specific direction, the use of continuous polynomials over the angular domain results in a poor representation of the angular flux (Bell and Glasstone, 1970). Although the higher orders of spherical harmonics are able to produce accurate solutions, the convergence of these approximations in described situations may be achieved inconveniently. Considering a problem with multi regions in which the angular flux should satisfy boundary conditions for each adjacent region, the above difficulties will be multiplied. But in problems with a larger dimension in comparison to the mean-free path, suitable results can be obtained using lower approximations and there is no significant improvement in accuracy when higher approximations are utilized.

These realizations led Yvon (1957) to propose the DP_N approximation. In the double spherical harmonics method, which has been employed for one-dimensional problems, the angular flux distribution is represented as two separate series on the Legendre functions in forward and backward hemispheres. Insertion of these expansions into the proper equations and use of the orthogonality relations over each spherical range, lead to a set of equations for the unknown coefficients (Williams, 1971). Yvon's method accounts for its ability in dealing with discontinuities of the angular flux and such expansions converge rapidly to exact solutions in prescribed regions.

Although the DP_N approximation has been examined by many authors, the P_N method has found favor for a variety of reasons. This may be because a general variational formulation for DP_N equations in multi-dimensional geometry has not previously been presented due to the difficulties engendered by complex treatments of these equations. Ziering and Schiff (1958) reported significant improvements in accuracy over full-range Legendre expansions and several discrete ordinate methods by applying the half-range expansions to neutron transport theory for both finite and semi-finite slabs, which consist of isotropically scattering media. These researchers subsequently extended the DP_N approximation to two-dimensional geometries (Schiff and Ziering, 1960). Due to the computational difficulties, they carried out the fourfold P_0 and P_1 calculations only and compared the results with diffusion theory. The method referred to has been successfully applied to the slab geometries by various authors (Gelbard et al., 1959; Stepanek, 1981; Brantley, 2005).

The first attempt has been made by Drawbaugh and Noderer (1959) for solving the $\mathrm{DP_N}$ approximation in cylindrical and spherical geometries. Some features of the DPN approximation were shown in that study. A variational spherical harmonics method was developed by Khouaja et al. (1997) in conjunction with the finite element method to solve DP1 and DP3 equations in finite axisymmetric cylindrical geometry. Numerical results indicated that the DP3 expansion could yield more accurate solutions without excessive computational time. Stepanek (1983) has developed the general surface flux method to solve the integral neutron transport equation. He used multiple-P_N method in angle and discontinuous finite elements in space for first-order transport equation.

In this paper, we show that the MP_N approximation can be derived for second-order form of the transport equation which not only provides improved solutions in comparison to customary spherical harmonics methods but also represents a general formulation in one- and two-dimensional planar geometries. Our primary goal is to extend the ordinary half-range spherical harmonics method by choosing multiple directions for angular flux distribution in the hopes that it will find wider application. Our variational method yields the unrestricted one- and two-dimensional equations which can be used to break the angular flux domain into sub-domains with arbitrary order of spherical harmonics. Our secondary goal is to use continuous finite element method in space which helps us to use unstructured mesh in complicated 2D geometries. Our final goal is to compare the solutions of various approximations of the presented method with full-range expansions.

As a final introductory remark, it is beneficial to note that the use of extended double spherical harmonics method improves the accuracy of full-range P_N approximation with lower computational cost, as reported in our recent paper (Ghazaie et al., 2017). For example, the calculation of the eigenvalue and disadvantage factor show the excellence of the DP_N method with fewer unknowns, compared to the full-range expansion. This is due to the capability of detached expansions in approximating the discontinuous behavior of angular flux.

The remainder of this paper is organized as follows. In Sec. 2, we outline some features of the first- and second-order forms of transport calculations. Also, we outline a maximum principle for the first-order form of the transport equation and corresponding boundary conditions. In Sec. 3, we outline some aspects of our method for slabs. A set of orthogonal Legendre polynomials in various subdomains of the angular variable is introduced in Sec. 3.1 and subsequent angular flux expansions for each discretized direction are given. In Sec. 3.2, we present a general formulation of the maximum principle for one-dimensional geometry based on the MP_N discretization. Considering physically meaningful interpretations, we define the integral operators of maximum principle and formulate the two-dimensional MP_N approximation in Sec. 4. We present numerical results in Sec. 5 to verify our theoretical claim that the MP_N approximation is more accurate than the customary expansion. Finally, a brief concluding discussion is given in Sec. 6.

2. Variational principle for the first order Boltzmann equation

The first-order form of the transport equation has advantages and disadvantages relative to the second-order equation. However, the equivalence of the maximum principles for these two kinds of equations can be shown using the properties of the transport operators (Ackroyd, 1983a). In finite element method for neutron transport calculations, the use of second-order equation is mostly preferred to the utilization of the first-order equation. By eliminating the even (odd) spherical harmonics from the coupled first-order equations, a set of coupled second order equations can be obtained which is of key importance.

Generally, the Euler-Lagrange equation is of order 2 m and the functional includes derivatives of order up to m. Thus, the classical Euler-Lagrange method can be used to generate variational principles for the second-order form of the Boltzmann equation. For the first-order transport equation, extremum principles can be obtained from a generalized least-squares approach, while the classical Euler-Lagrange method cannot directly construct variational principles.[1] The full angular flux is obtained by solving the first-order equation rather than either the even or odd components. The angular flux need not be even or odd function of the angular variable in the first-order equation. Both the first- and second-order forms of the transport equations can be solved on multi-dimensional finite element meshes using continuous and discontinuous finite element techniques. The application of these methods results in matrix equations which are symmetric positive-definite. Solution techniques for such matrices are generally more efficient than those for non-symmetric positive-definite matrix equations.

There are several ways to express the first-order form of the monoenergetic transport equation. In order to use some significant features of the integral operator in the Boltzmann equation, it can be written as

$$\mathbf{\Omega}\cdot\nabla\phi_0(\mathbf{r},\,\mathbf{\Omega}) + \Sigma\phi_0(\mathbf{r},\,\mathbf{\Omega}) = s(\mathbf{r},\,\mathbf{\Omega}) \tag{1}$$

where$\phi_0(\mathbf{r},\,\mathbf{\Omega})$= angular flux which depends on the position $\mathbf{r}$ for the direction $\mathbf{\Omega}s(\mathbf{r},\,\mathbf{\Omega})$= volume source and the integral operator Σ is