Spherical harmonics method for neutron transport equation based on unstructured-meshes

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Abstract Based on a new second-order neutron transport equation, self-adjoint angular flux (SAAF) equation, the spherical harmonics (P_N) method for neutron transport equation on unstructured-meshes is derived. The spherical harmonics function is used to expand the angular flux. A set of differential equations about the spatial variable, which are coupled with each other, can be obtained. They are solved iteratively by using the finite element method on unstructured-meshes. A two-dimension transport calculation program is coded according to the model. The numerical results of some benchmark problems demonstrate that this method can give high precision results and avoid the ray effect very well.

Keywords Neutron transport equation, Spherical harmonics method, Finite element method, Unstructured-meshes

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1 Introduction

Many effective methods to solve the multi-group neutron transport equation have been developed in the recent decades. Two deterministic methods, the discrete ordinate (S_N) method and the spherical harmonics (P_N) method, are very common ones among them. S_N method has been paid much attention and proved to have some intrinsic disadvantages.[1] Firstly, the ray effect will lead to serious distortion in non- multiplication media. Secondly, the dimension of the mesh should be very small as N becomes large to get high precision result. This will induce the calculation cost increase greatly. Compared with S_N method, the P_N method has its special merits. Firstly, the method can be used in strong anisotropy scatter area easily. Secondly, the spherical harmonics method is immune from the ray effect. In theory, P_N method can give exact result as long as N is large enough.

Many researchers have paid attention to P_N method recently. Fletcher[2] derived the P_N equations from the traditional first-order transport equation and gave an approximate method to deal with the vacuum boundary condition. Inanc[3] raised a modular approach P_N method, in which various order of spherical harmonics can be used in different regions of the problem. Many researchers[4-6] focused their attention on the even- and odd-parity second-order transport equations. Recently, Morel[7] introduced a so-called self-adjoint angular flux (SAAF) equation, which is a second-order form of the transport equation. He proved that the SAAF equation is very suitable for S_N and P_N method. But all of them haven't derived the general P_N equation which is suitable for unstructured-meshes.

This paper is organized as follows. In Sec. 2, we introduce the SAAF equation. In Sec. 3, the spherical harmonics method is applied into SAAF and the coupled differential equation are educed. In Sec. 4, the finite element method is used to solve the spatial equations. In Sec. 5, a transport code is developed and the numerical results of some benchmark problems are given.

2 SAAF equation

The traditional first order transport equation is:

$$\vec{\Omega} \bullet \vec{\nabla}\phi + \Sigma_t \phi = S\phi + q \qquad (1)$$

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in which the symbols are common ones as in nuclear physics.

We can use Eq.(1) to solve for ϕ as:

$$\phi = -(\Sigma_t - S)^{-1}\vec{\Omega}\bullet\vec{\nabla}\phi + (\Sigma_t - S)^{-1}q \quad (2)$$

and then substitute Eq.(2) into the first term in Eq.(1):

$$-\vec{\Omega}\bullet\vec{\nabla}(\Sigma_t - S)^{-1}\vec{\Omega}\bullet\vec{\nabla}\phi + (\Sigma_t - S)\phi = q - \vec{\Omega}\bullet\vec{\nabla}(\Sigma_t - S)^{-1}q \quad (3)$$

In order to use finite element method, every operator of the equation should be self-adjoint. So Eq.(3) should be written as follows:

$$-\vec{\Omega}\bullet\vec{\nabla}(\Sigma_t - S_d)^{-1}\vec{\Omega}\bullet\vec{\nabla}\phi + (\Sigma_t - S_d)\phi = S_o\phi + q - \vec{\Omega}\bullet\vec{\nabla}(\Sigma_t - S_d)^{-1}(S_o\phi + q) \quad (4)$$

where S_d denotes the within-group block of the multi-group scattering matrix and S_o denotes the between-group block of the multi-group scattering matrix. Eq.(4) is the SAAF equation, which inherits the advantages of the traditional second-order even- and odd-parity transport equation, including (a) the P_N equation educed from them can be solved on finite element meshes using standard continuous finite element discretization techniques; and (b) the resulted matrix is always symmetric positive-definite (SPD), and overcomes some disadvantages of traditional even- and odd-parity transport equation, including (a) the full angular flux is obtained when the SAAF equation is numerically solved rather than either the even-parity or the odd-parity component alone; (b) the reflective boundary conditions are much easier to implement than in traditional equations; and (c) the SAAF equation can be solved in a void.

3 Derivation of P_N equation

In the P_N method, we can expand the angular flux as (take two dimension *x*-*y* geometry as example):

$$\phi(x,y,\theta,\varphi) = \sum_{n=0}^{N}\sum_{m=0}^{n} P_n^m(\cos\theta)\times \left[\psi_{nm}(x,y)\cos m\varphi + \gamma_{nm}(x,y)\sin m\varphi\right] \quad (5)$$

where $P_n^m(\cos\theta)$ is the associated Legendre function. The items with $n>N+1$ are assumed to be zero. And the source item can be expanded as follows:

$$S_o\phi + q = \sum_{n=0}^{N}\sum_{m=0}^{n}[\overline{\psi}_{n,m}(x,y)\cos m\varphi + \overline{\gamma}_{n,m}(x,y)\sin m\varphi]P_n^m(\cos\theta) \quad (6)$$

Substitute Eq.(5) and Eq.(6) in Eq.(4) and use the recursive relation of the associated Legendre function:

$$\sin\theta P_n^m = \frac{1}{2n+1}[(n+m)(n+m-1)P_{n-1}^{m-1} - (n-m+1)(n-m+2)P_{n+1}^{m-1}] \quad (7)$$

$$\sin\theta P_n^m = \frac{1}{2n+1}(P_{n+1}^{m+1} - P_{n-1}^{m+1}) \quad (8)$$

and the orthogonality of the associated Legendre function:

$$\int_{-1}^{1} P_n^m(\cos\theta)P_{n'}^{m'}(\cos\theta)\mathrm{d}x = \frac{2(n+m)!}{(2n+1)(n-m)!}\delta_{n,n'}\delta_{m,m'} \quad (9)$$

we can obtain the general spatial dependent P_N equations after a serial of lengthy and complex manipulation as follows:

$$a_1\nabla^2\psi_{n-2,m} + a_2\nabla^2\psi_{n,m} + a_3\nabla^2\psi_{n+2,m} + a_4\left(\frac{\partial^2\psi_{n-2,m-2}}{\partial x^2} - 2\frac{\partial^2\gamma_{n-2,m-2}}{\partial x\partial y} - \frac{\partial^2\psi_{n-2,m-2}}{\partial y^2}\right) + a_5\left(\frac{\partial^2\psi_{n,m-2}}{\partial x^2} - 2\frac{\partial^2\gamma_{n,m-2}}{\partial x\partial y} - \frac{\partial^2\psi_{n,m-2}}{\partial y^2}\right) + a_6\left(\frac{\partial^2\psi_{n+2,m-2}}{\partial x^2} - 2\frac{\partial^2\gamma_{n+2,m-2}}{\partial x\partial y} - \frac{\partial^2\psi_{n+2,m-2}}{\partial y^2}\right) + a_7\left(\frac{\partial^2\psi_{n+2,m+2}}{\partial x^2} + 2\frac{\partial^2\gamma_{n+2,m+2}}{\partial x\partial y} - \frac{\partial^2\psi_{n+2,m+2}}{\partial y^2}\right) + a_8\left(\frac{\partial^2\psi_{n,m+2}}{\partial x^2} + 2\frac{\partial^2\gamma_{n,m+2}}{\partial x\partial y} - \frac{\partial^2\psi_{n,m+2}}{\partial y^2}\right) + a_9\left(\frac{\partial^2\psi_{n-2,m+2}}{\partial x^2} + 2\frac{\partial^2\gamma_{n-2,m+2}}{\partial x\partial y} - \frac{\partial^2\psi_{n-2,m+2}}{\partial y^2}\right) + (\Sigma_t - \Sigma_{d,n})\psi_{n,m} = \overline{\psi}_{n,m} - a_{10}\left(\frac{\partial\overline{\psi}_{n-1,m-1}}{\partial x} - \frac{\partial\overline{\gamma}_{n-1,m-1}}{\partial y}\right) + a_{11}\left(\frac{\partial\overline{\psi}_{n+1,m-1}}{\partial x} - \frac{\partial\overline{\gamma}_{n+1,m-1}}{\partial y}\right) + a_{12}\left(\frac{\partial\overline{\psi}_{n+1,m+1}}{\partial x} + \frac{\partial\overline{\gamma}_{n+1,m+1}}{\partial y}\right) + a_{13}\left(\frac{\partial\overline{\psi}_{n-1,m+1}}{\partial x} + \frac{\partial\overline{\gamma}_{n-1,m+1}}{\partial y}\right)$$

$$n = 0,1\cdots\cdots N; m = 0,1\cdots\cdots n \quad (10)$$

where a_i (i =1~13) is coefficient varying with m and n.

4 Finite element discretization

The P_N equations are coupled with each other and can't be solved simultaneously, so an iterate strategy should be used to solve them. Taking the $\psi_{n,m}$ for unknown and the other items for constant (in fact, they can be initial guess or the value of the last iteration), we can find Eq.(10) can be written as:

$$a_2(n,m)\left(\frac{\partial^2\psi_{n,m}}{\partial x^2}+\frac{\partial^2\psi_{n,m}}{\partial y^2}\right)+(\Sigma_t-\Sigma_{d,n})\psi_{n,m}=F \tag{11}$$

Assume the boundary condition to be:

a) reflective boundary

$$\phi(\vec{r},\vec{\Omega})=\phi(\vec{r},-\vec{\Omega}) \quad \vec{r}\in\Gamma_1 \tag{12}$$

b) vacuum boundary

$$\phi(\vec{r},\vec{\Omega})=0 \quad (\vec{\Omega}\bullet\vec{n})<0 \quad \vec{r}\in\Gamma_2 \tag{13}$$

Eq.(11) is a standard elliptic equation and can be solved by using the continuous finite element spatial discretization techniques on unstructured-meshes. Multiplied by an arbitrary function $\psi^0\in H^1(\Omega)$, and integral in space, Eq.(11) becomes:

$$\iint a_2\left(\frac{\partial^2\psi_{n,m}}{\partial x^2}+\frac{\partial^2\psi_{n,m}}{\partial y^2}\right)\psi^0\mathrm{d}x\mathrm{d}y+\iint(\Sigma_t-\Sigma_{d,n})\psi_{n,m}\psi^0\mathrm{d}x\mathrm{d}y=\iint F\psi^0\mathrm{d}x\mathrm{d}y \tag{14}$$

Use the Gauss theorem, the first item of Eq.(14) can be written as:

$$\iint a_2\left(\frac{\partial\psi_{n,m}}{\partial x}\times\frac{\partial\psi^0}{\partial x}+\frac{\partial\psi_{n,m}}{\partial y}\times\frac{\partial\psi^0}{\partial y}\right)\mathrm{d}x\mathrm{d}y+\oint_{\Gamma_1+\Gamma_2}\frac{\partial\psi_{n,m}}{\partial n}\psi^0\mathrm{d}s \tag{15}$$

From Eq.(12) we can get

$$\left[\frac{\partial\psi_{n,m}}{\partial n}\right]_{\Gamma_1}=0 \tag{16}$$

in reflective boundary and from Eq.(13) we can get

$$\left[\frac{\partial\psi_{n,m}}{\partial n}\delta_{0n}\delta_{0m}+\frac{3}{2}\Sigma_{tr}\psi_{n,m}\right]_{\Gamma_2}=0 \tag{17}$$

in vacuum boundary approximatively.

Substitute Eq.(16) and Eq.(17) in Eq.(15), and substitute Eq.(15) to Eq.(14), we can obtain:

$$B(\psi_{n,m},\psi^0)=F(\psi^0) \tag{18}$$

where

$$B(\psi_{n,m},\psi^0)=\iint\left[a_2\left(\frac{\partial\psi_{n,m}}{\partial x}\times\frac{\partial\psi^0}{\partial x}+\frac{\partial\psi_{n,m}}{\partial y}\times\frac{\partial\psi^0}{\partial y}\right)+(\Sigma_t-\Sigma_{d,n})\psi_{n,m}\psi^0\right]\mathrm{d}x\mathrm{d}y-\frac{3}{2}\oint_{\Gamma_2}\Sigma_{tr}\psi_{n,m}\psi^0\mathrm{d}s \tag{19}$$

$$F(\psi^0)=\iint F\psi^0\mathrm{d}x\mathrm{d}y \tag{20}$$

Eq.(18) is the variational form of P_N equation.

5 Numerical result

A two-dimension multi-group transport calculation computer code, TEPFEM, was developed according to the method described above. It can solve fixed source problems and eigenvalue problems in arbitrary geometry without constraint to the anisotropy of source and scattering. The element can be triangle meshes or rectangle meshes. Two typical boundary conditions, reflective boundary condition and vacuum boundary condition, are taken into account by using approximation method given by Fletcher.[2] Several benchmark problems are calculated using this code. Three of them are given below.

5.1 Problem 1: Natelson benchmark

This benchmark is the one-group two-region system given by Natelson[8], where the system is a 3 cm square, and there is a neutron source of strength Q=1 $\mathrm{cm}^{-2}\cdot\mathrm{s}^{-1}$ in a 1 cm square, as shown in Fig.1. The cross section of regions are Σ_t=1.0cm^{-1}, Σ_s=0.5 cm^{-1}, and Σ_t=1.0cm^{-1}, Σ_s=0.25cm^{-1}, respectively. The reflective boundary condition is used for all outer boundaries. The comparison of the calculation and reference results are given in Fig.2. The flux along

y=0 calculated by S_N code TWOTRAN exhibit the oscillations attributed to ray effects. But the P_3 result of TEPFEM is in good agreement with the reference value and avoids the ray effect. The P_5 result is in excellent agreement with SK_5. It demonstrates that spherical harmonics can avoid ray effect and give high precision.

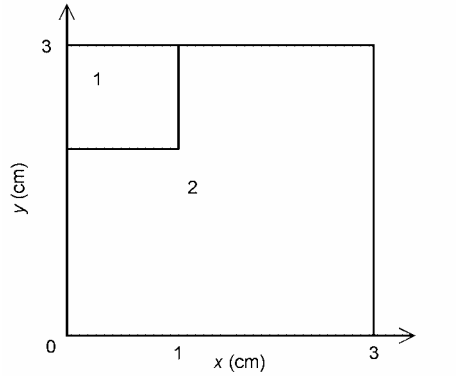

Fig.1 Geometry of Natelson benchmark.

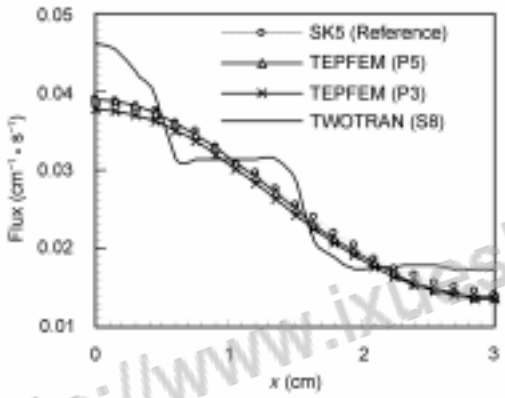

Fig.2 The flux along y=0.

5.2 Problem 2: IAEA light water reactor

This problem was defined by Stepanek[4] to simulate a light water reactor. It's a one energy group, 5-region problem with vacuum boundary condition at all the outer surfaces. The geometry is shown in Fig.3 and the cross section of each region is given in Table 1. Table 2 gives the result calculated by TEPFEM and the result from Ref.[9] and Ref.[5]. It shows that the result calculated by TEPFEM is in good agreement with the other two codes except in Region 3 because the flux is very low.

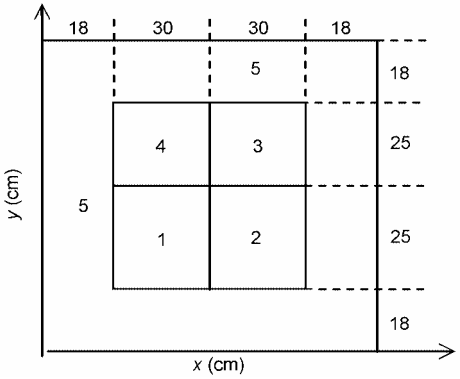

Fig.3 Geometry of IAEA benchmark.

Table 1 Cross-section of IAEA benchmark

Region	Σ_t	Σ_s	$\nu\Sigma_f$
1	0.60	0.53	0.079
2	0.48	0.20	0
3	0.70	0.66	0.043
4	0.65	0.50	0
5	0.90	0.89	0

Table 2 Average fluxes in various regions of IAEA benchmark*

	Region 1	Region 2	Region 3	Region 4	Region 5	K_{eff}
SURCU[9]	0.01686	0.000125	0.000041	0.000295	0.000791	1.0083
FELICIT[5]	0.01685	0.000127	0.000042	0.000300	0.000797	1.0069
TEPFEM	0.01686	0.000126	0.000032	0.000296	0.000786	1.0079

*The fluxes are normalized so that $\int \nu\Sigma_f \Phi \mathrm{d}V = 1$.

5.3 Problem with unstructured-meshes

A problem with non-regular geometry is designed to show the adaptability of the code to unstructured-meshes. It contains a fuel rod surrounded by light water. Triangle element is used to mesh the system as shown in Fig.4. The calculated flux distribution is shown in Fig.5.

6 Conclusion

This paper derived the general equations for any

order of spherical harmonics on unstructured-meshes based on the SAAF equation. A two-dimension transport calculation code is programmed by using finite element method to discretize the space variable. According to the numerical results in Sec. 5, we can draw some conclusions: (a) Compared with S_N method, P_N method avoids ray effect well as already known. (b) The code TEPFEM can give high precision. (c) This method can be applied to unstructured-meshes.

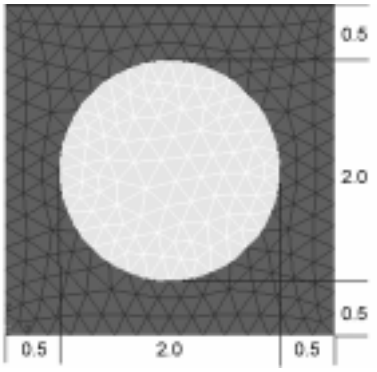

Fig.4 Unstructured mech (cm).

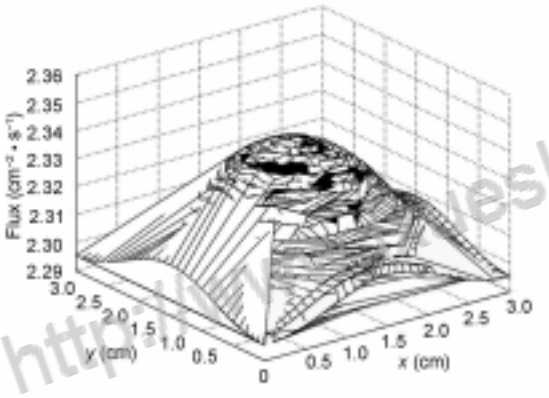

Fig.5 The flux distribution of Problem 3.

As the vacuum boundary condition was treated in an approximation way, the calculation result of the small dimension (~10 cm) problem with vacuum boundary condition is not very good. The flux near the vacuum boundary is not in good agreement. This problem is a hot focus in international nuclear physics field and there isn't a method accepted commonly by now. This project plans to do some research work on it in the near future.

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