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Advances in the Pennsylvania State University NEM code

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ABSTRACT

The Pennsylvania State University NEM code has been updated in an attempt to enable the code to model more neutronically complex reactor cores, such as those containing mixed-oxide fuel, low leakage cores, and cores that contain multiple burnable poison types. Current nodal methods, which are primarily focused on solving the diffusion equation using a nodal expansion method with the transverse leakage term solved using the quadratic leakage approximation, are known to be inaccurate in such environments. The NEM code is updated with a transport capability based upon the SP_3 approximation, a semi-analytical solution, and an advanced transverse leakage method based upon the use of analytic basis functions. Each of these new features is described followed by the results of benchmarks to test their effectiveness.

1. Introduction

Modern reactor cores, such as those using mixed-oxide (MOX) fuel, cores with extended operation in a deeply rodded condition, low leakage cores, and those with multiple sub-batches with multiple burnable poison types, require more advanced analysis methodologies due to the neutronic heterogeneity of such cores. These advanced methodologies should address the inadequacies of the methods used in most nodal codes currently in use: namely, the inadequacy of the diffusion approximation in highly heterogeneous cores and near material boundaries and strong absorbers such as control rods and burnable poisons, the limitations of the polynomial nodal expansion method (NEM) in larger spatial nodes with more complicated flux shapes and in areas where steep flux gradients occur, as well as the inadequacy of the quadratic leakage approximation (QLA) to be able to model complex leakage shapes.

Recent advances in the Pennsylvania State University (PSU) Nodal Expansion Method (NEM) code have sought to address these deficiencies by introducing a transport capability based on the SP_3 approximation, a semi-analytical nodal expansion method (SANEM) solution, and an advanced transverse leakage capability (Thompson and Ivanov, 2014) based upon the use of analytic basis functions (ABFs). This paper describes each of these new features and provides the results of benchmarks to test their effectiveness. Each of these improvements are generic enough to be applicable to all geometries, including hexagonal, as well for the transient option in NEM, which is being implemented and will be presented in future work.

2. SP_3 approximation

The Simplified P_N (SP_N) equations were first proposed in an attempt to introduce additional transport effects into the standard P_1 equations without introducing the complexities and undesired increase in runtime that a full transport theory solution would entail. The P_N equations in slab geometry, in an optically thick medium dominated by scattering, may be written as a system of planar diffusion problems in each direction, which can be solved by Fick's Law as is done in the diffusion theory approximation.

The spherical harmonic approximation (P_N) to the neutron transport equation is developed by expanding the angular dependence of the neutron flux and the differential scattering cross section in orthogonal Legendre polynomials up to order *N*. The simplification from spherical harmonics to Legendre polynomials comes from assuming azimuthal symmetry and material isotropy of the scattering medium. More specifically, it is assumed that the scattering medium is invariant under rotation in the phase space R^3, and therefore only depends on the cosine of the scattering angle. This amounts to assuming that the problem under consideration can be approximated as planar transport with a highly forward-peaked scattering kernel. This allows the P_N equations to be written in one dimension as:

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$$\frac{l}{2l+1}\frac{d}{dr}\phi_{l-1,g}(r)+\frac{l+1}{2l+1}\frac{d}{dr}\phi_{l+1,g}(r)+\Sigma_{t,g}\phi_{l,g}(r)=\sum_{g'=1}^{G}\sum_{s,lg'\to g}\phi_{l,g'}(r)+S_{l,g}(r) \quad (1)$$

with ϕ_l being the flux moments, l = 0, 1, …, N, r is an arbitrary spatial coordinate {r: $r = x, y, z$ and $r \in V_{node}$} and G = energy group. As is typically assumed in the P_N equations, for $l = 0$ and $l = N$, ϕ_{n-1} and ϕ_{N+1} are assumed to be 0, $\Sigma_{t,g}$ is the group g total macroscopic cross section, $\Sigma_{s,l,g'\to g}$ is the lth moment of the macroscopic scattering cross section from group g' into group g.

The isotropic source is defined as follows:

$$S_{0,g}(r)=\frac{1}{k_{eff}}\chi_g\sum_{g'=1}^{G}\nu\Sigma_{f,g'}\phi_{0,g'}(r) \quad (2)$$

where χ_g is the isotropic fission spectrum for group g, k_{eff} is the neutron multiplication factor, and $\Sigma_{f,g'}$ is the macroscopic fission cross section for group g'.

The P_3 equations are obtained from the P_N equations above by inputting $l = 0, 1, 2, 3$ into Eq. (1), which produces four linear differential equations for the four flux moments. Using the same assumption as Brantley and Larsen (2000), that there is no anisotropic group-to-group scattering, eliminates all group-to-group scattering terms higher than $l = 0$. However, Beckert and Grundmann (2007) have reported fairly large errors in pin-by-pin SP_3 calculations in which anisotropic group-to-group scattering was completely neglected. Due to these conclusions from Beckert and Grundmann (2007), in which first-order anisotropic group-to-group scattering was considered in the DYN3D code and found to provide significantly better results, only scattering orders higher than $l = 1$ were eliminated from the P_3 equations (for group-to-group scattering). Therefore, linearly anisotropic group-to-group scattering is considered in NEM. This is shown in Eq. (3) below.

$$\frac{d}{dr}\phi^n_{1,g}(r)+\Sigma^n_{t,g}\phi^n_{0,g}(r)=\sum_{g'=1}^{G}\Sigma^n_{s,0,g'\to g}\phi^n_{0,g'}(r)+S^n_{0,g}(r) \quad (3a)$$

$$\frac{1}{3}\frac{d}{dr}\phi^n_{0,g}(r)+\frac{2}{3}\frac{d}{dr}\phi^n_{2g}(r)+\Sigma^n_{t,g}\phi^n_{1,g}(r)=\sum_{g'=1}^{G}\Sigma^n_{s,1,g'\to g}\phi^n_{1,g'}(r) \quad (3b)$$

$$\frac{2}{5}\frac{d}{dr}\phi^n_{1,g}(r)+\frac{3}{5}\frac{d}{dr}\phi^n_{3g}(r)+\Sigma^n_{t,g}\phi^n_{2,g}(r)=\sum_{g'=1}^{G}\Sigma^n_{s,2,g'\to g}\phi^n_{2,g'}(r) \quad (3c)$$

$$\frac{3}{7}\frac{d}{dr}\phi^n_{2g}(r)+\Sigma^n_{t,g}\phi^n_{3,g}(r)=\sum_{g'=1}^{G}\Sigma^n_{s,3,g'\to g}\phi^n_{3,g'}(r) \quad (3d)$$

where, $\Sigma^n_{s,l,g'\to g}=0$ *for* $g'\neq g, \quad l=2,3$.

To arrive at the simplified P_3 equations (SP_3) from Eqs. (3a)–(3d) above, a few simplifying assumptions/substitutions are made:

(1) The total macroscopic cross section minus the first scattering moment is replaced with the transport cross section in the first equation above:

$$\Sigma_{tr,g}(r)=\Sigma_{t,g}(r)-\sum_{g=1}^{G}\Sigma_{s,1,g\to g'}=\Sigma_{t,g}(r)-\mu_{0,g}(r)\Sigma_{s,0,g}(r) \quad (4)$$

where $\mu_{0,g}(r)$ is the average cosine of the scattering angle.

This assumption is equivalent to the transport correction of the diffusion theory and is based upon the assumption:

$$\sum_{g'=1}^{G}\Sigma^n_{s,1,g\to g'}\Phi^n_{1,g}(r)\approx\sum_{g'=1}^{G}\Sigma^n_{s,1,g'\to g}\Phi^n_{1,g'}(r)$$

This approximation has been shown to be fairly accurate in diffusive environments with weak absorption.

(2) The even flux moments are assumed to be scalars, while the odd flux moments are assumed to be vectors. Pomraning discusses this in more detail is his paper (Pomraning, 1993), and this assumption was utilized by Brantley and Larsen (2000) as well. From a more mathematically rigorous standpoint, the higher order flux moments are in fact higher order tensors, but we nonetheless retain the convention.

(3) The removal cross section is introduced, which is equal to the total cross section minus the within group scattering cross section as follows:

$$\Sigma_{rem,l,g}=\Sigma_{t,g}-\Sigma_{s,l,g\to g} \text{ for } l=0,2,3 \quad (5)$$

(4) The synthesized flux approximation is implemented for the scalar flux and second flux moments as follows:

$$\Phi_{0,g}(r)=\phi_{0,g}(r)+2\phi_{2,g}(r) \quad (6)$$

Using the aforementioned approximations and Eqs. (3a)–(3d), the next step in the derivation is to solve for the odd flux moments in terms of the spatial derivatives of the even flux moments. The following is then obtained:

$$\phi_{1,g}(r)=-\frac{1}{3\Sigma_{tr,1,g}}\frac{d}{dr}\Phi_{0,g}(r) \quad (7)$$

$$\phi_{3,g}(r)=-\frac{3}{7\Sigma_{r,3,g}}\frac{d}{dr}\phi_{2,g}(r)$$

These two equations are then inserted into Eqs. (3a) and (3c) above. The approximation made by Brantley and Larsen (2000) to extend the utility of the SP_3 equations to three dimensions was then applied. Brantley and Larsen replaced the second derivatives in the P_N equations with the Laplacian operator. After doing this, and performing some simplifications, the SP_3 equations as they are implemented in NEM can be obtained:

$$-D_{0,g}\nabla^2\Phi_{0,g}(r)+\Sigma_{rem,0,g}\Phi_{0,g}(r)-2\Sigma_{rem,0,g}\phi_{2,g}(r)=S_{0,g}(r) \quad (8)$$

$$-D_{2,g}\nabla^2\phi_{2,g}(r)+\left[\Sigma_{rem,2,g}+\frac{4}{5}\Sigma_{rem,0,g}\right]\phi_{2,g}(r)-\frac{2}{5}\Sigma_{rem,0,g}\Phi_{0,g}(r)=\frac{-2}{5}S_{0,g}(r)$$

with,

$$S_{0,g}(r)=\sum_{g'=1,g'\neq g}^{G}\Sigma_{s,0,g'\to g}\left[\Phi_{0,g}(r)-2\phi_{2,g}(r)\right]+\frac{\chi_g}{k_{eff}}\sum_{g'=1}^{G}\nu\Sigma_{f,g'}[\Phi_{0,g}(r)-2\phi_{2,g}(r)]$$

$$D_{0,g}=\frac{1}{3\Sigma_{tr,1,g}} \text{ and } D_{2,g}=\frac{9}{35\Sigma_{rem,3,g}}$$

2.1. Marshak boundary conditions

The only remaining parameter to be determined is the boundary condition. The exact boundary condition (using the x dimension as an example), as described by Marchuk and Lebedev (1986), is:

$$\phi(x_{right},\mu)=0 \text{ for } \mu<0 \quad (9)$$

$$\phi(x_{left},\mu)=0 \text{ for } \mu>0$$

Since this exact boundary condition cannot be completely satisfied based on the angular flux approximation afforded by the Legendre polynomials, Marshak (1947) proposed to use the same Legendre polynomial expansion for the angular flux as in the P_N