NPRE 555
Computer Project 3

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1 Introduction

2 MOOSE

3 Simplified P_3: Mathematical Basis

One dimensional P_3 equations [1]

$$\frac{d}{dx}\phi_{1,g} + \Sigma_{t,g}\phi_{0,g} = \sum_{g'=1}^{G}\Sigma_{s0,g'\to g}\phi_{0,g'} + \frac{\chi_g}{k_{eff}}\sum_{g'=1}^{G}\nu\Sigma_{f,g'}\phi_{0,g'} + Q_{0,g} \tag{1}$$

$$\frac{1}{3}\frac{d}{dx}\phi_{0,g} + \frac{2}{3}\frac{d}{dx}\phi_{2,g} + \Sigma_{t,g}\phi_{1,g} = \sum_{g'=1}^{G}\Sigma_{s1,g'\to g}\phi_{1,g'} + Q_{1,g} \tag{2}$$

$$\frac{2}{5}\frac{d}{dx}\phi_{1,g} + \frac{3}{5}\frac{d}{dx}\phi_{3,g} + \Sigma_{t,g}\phi_{2,g} = \sum_{g'=1}^{G}\Sigma_{s2,g'\to g}\phi_{2,g'} + Q_{2,g} \tag{3}$$

$$\frac{3}{7}\frac{d}{dx}\phi_{2,g} + \Sigma_{t,g}\phi_{3,g} = \sum_{g'=1}^{G}\Sigma_{s3,g'\to g}\phi_{3,g'} + Q_{3,g} \tag{4}$$

where

$\phi_{n,g} = n^{th}$ moment of the group g neutron flux $[n \cdot cm^{-2} \cdot s^{-1}]$
$\Sigma_{t,g} =$ group g macroscopic total cross-section $[cm^{-1}]$
$\Sigma_{sn,g'\to g} = n^{th}$ moment of the group g' to group g macroscopic scattering cross-section $[cm^{-1}]$
$\nu\Sigma_{f,g} =$ group g macroscopic production cross-section $[cm^{-1}]$
$\chi_g =$ group g fission spectrum $[cm^{-1}]$
$k_{eff} =$ multiplication factor $[-]$
$Q_{n,g} = n^{th}$ group g external neutron source $[n \cdot cm^{-3} \cdot s^{-1}]$
$G =$ number of energy groups $[-]$.

Defining the group g "removal" cross-section $\Sigma_{n,g}$, and assuming an isotropic external source and a negligible anisotropic group-to-group scattering [1]

$$\begin{aligned}
&\Sigma_{n,g} = \Sigma_{t,g} - \Sigma_{sn,g'\to g}\\
&Q_{n,g} = 0, \quad n > 0\\
&\Sigma_{sn,g'\to g} = 0, \quad g' \neq g, \quad n > 0
\end{aligned}$$

the P_3 equations become

$$\frac{d}{dx}\phi_{1,g} + \Sigma_{0,g}\phi_{0,g} = \sum_{g'\neq g}^{G}\Sigma_{s0,g'\to g}\phi_{0,g'} + \frac{\chi_g}{k_{eff}}\sum_{g'=1}^{G}\nu\Sigma_{f,g'}\phi_{0,g'} + Q_{0,g} \tag{5}$$

$$\frac{1}{3}\frac{d}{dx}\phi_{0,g} + \frac{2}{3}\frac{d}{dx}\phi_{2,g} + \Sigma_{1,g}\phi_{1,g} = 0 \tag{6}$$

$$\frac{2}{5}\frac{d}{dx}\phi_{1,g} + \frac{3}{5}\frac{d}{dx}\phi_{3,g} + \Sigma_{2,g}\phi_{2,g} = 0 \tag{7}$$

$$\frac{3}{7}\frac{d}{dx}\phi_{2,g} + \Sigma_{3,g}\phi_{3,g} = 0. \tag{8}$$

Reorganizing equations 6 and 8 allows for obtaining a expression for odd moments of the flux $\phi_{1,g}$ and $\phi_{3,g}$

$$\phi_{1,g} = -\frac{1}{3\Sigma_{1,g}}\frac{d}{dx}\left[\phi_{0,g} + 2\phi_{2,g}\right] \tag{9}$$

$$\phi_{3,g} = -\frac{3}{7\Sigma_{3,g}}\frac{d}{dx}\phi_{2,g}. \tag{10}$$

With equations 9 and 10, equations 5 and 7 become

$$-D_{0,g}\frac{d^2}{dx^2}\left(\phi_{0,g} + 2\phi_{2,g}\right) + \Sigma_{0,g}\phi_{0,g} = \sum_{g'\neq g}^{G}\Sigma_{s0,g'\to g}\phi_{0,g'} + \frac{\chi_g}{k_{eff}}\sum_{g'=1}^{G}\nu\Sigma_{f,g'}\phi_{0,g'} + Q_{0,g} \tag{11}$$

$$-\frac{2}{5}D_{0,g}\frac{d^2}{dx^2}\left(\phi_{0,g} + 2\phi_{2,g}\right) - D_{2,g}\frac{d^2}{dx^2}\phi_{2,g} + \Sigma_{2,g}\phi_{2,g} = 0 \tag{12}$$

where

$$D_{0,g} = \frac{1}{3\Sigma_{1,g}}$$

$$D_{2,g} = \frac{9}{35\Sigma_{3,g}}$$

Introducing the variables $\Phi_{0,g}$ and $\Phi_{2,g}$ and reorganizing equations 11 and 12 yields

$$-D_{0,g}\frac{d^2}{dx^2}\Phi_{0,g} + \Sigma_{0,g}\Phi_{0,g} - 2\Sigma_{0,g}\Phi_{2,g} = S_{0,g} \tag{13}$$

$$-D_{2,g}\frac{d^2}{dx^2}\Phi_{2,g} + \left(\Sigma_{2,g} + \frac{4}{5}\Sigma_{0,g}\right)\Phi_{2,g} - \frac{2}{5}\Sigma_{0,g}\Phi_{0,g} = -\frac{2}{5}S_{0,g} \tag{14}$$

where

$$\Phi_{0,g} = \phi_{0,g} + 2\phi_{2,g}$$

$$\Phi_{2,g} = \phi_{2,g}$$

$$S_{0,g} = \sum_{g'\neq g}^{G}\Sigma_{s0,g'\to g}\left(\Phi_{0,g'} - 2\Phi_{2,g'}\right) + \frac{\chi_g}{k_{eff}}\sum_{g'=1}^{G}\nu\Sigma_{f,g'}\left(\Phi_{0,g'} - 2\Phi_{2,g'}\right) + Q_{0,g}.$$

The three-dimensional SP3 equations [2] replace the second-derivatives in equations 13 and 14 by the Laplace operator Δ (See PARCS manual)

$$-D_{0,g}\Delta\Phi_{0,g} + \Sigma_{0,g}\Phi_{0,g} - 2\Sigma_{0,g}\Phi_{2,g} = S_{0,g} \tag{15}$$

$$-D_{2,g}\Delta\Phi_{2,g} + \left(\Sigma_{2,g} + \frac{4}{5}\Sigma_{0,g}\right)\Phi_{2,g} - \frac{2}{5}\Sigma_{0,g}\Phi_{0,g} = -\frac{2}{5}S_{0,g}. \tag{16}$$

The Marshak vacuum boundary conditions complete the system of equations

$$\frac{1}{4}\Phi_{0,g} \pm \frac{1}{2}\hat{n}\cdot J_{0,g} - \frac{3}{16}\Phi_{2,g} = 0 \tag{17}$$

$$-\frac{3}{80}\Phi_{0,g} \pm \frac{1}{2}\hat{n}\cdot J_{2,g} + \frac{21}{80}\Phi_{2,g} = 0 \tag{18}$$

where

$$J_{n,g} = -D_{n,g} \nabla \Phi_{n,g}.$$

Variational formulation

$$\langle \Phi, \Psi \rangle = \int_V \Phi \Psi dV \tag{19}$$
$$\langle \Phi, \Psi \rangle_{BC} = \int_S \Phi \Psi dS \tag{20}$$

where

$$\Psi = \text{test function}$$
$$S = \text{boundary surface.}$$

$$\langle -D_{0,g} \Delta \Phi_{0,g}, \Psi \rangle + \langle \Sigma_{0,g} \Phi_{0,g}, \Psi \rangle + \langle -2\Sigma_{0,g} \Phi_{2,g}, \Psi \rangle + \langle -S_{0,g}, \Psi \rangle = 0 \tag{21}$$
$$\langle -D_{2,g} \Delta \Phi_{2,g}, \Psi \rangle + \left\langle \left(\Sigma_{2,g} + \frac{4}{5} \Sigma_{0,g} \right) \Phi_{2,g}, \Psi \right\rangle + \left\langle -\frac{2}{5} \Sigma_{0,g} \Phi_{0,g} D_{2,g}, \Psi \right\rangle + \left\langle \frac{2}{5} S_{0,g}, \Psi \right\rangle = 0. \tag{22}$$

By means of the Gauss theorem (?), equations 24 and 26 become

$$\langle D_{0,g} \nabla \Phi_{0,g}, \nabla \Psi \rangle + \langle -D_{0,g} \nabla \Phi_{0,g}, \Psi \rangle_{BC} + \langle \Sigma_{0,g} \Phi_{0,g}, \Psi \rangle + \langle -2\Sigma_{0,g} \Phi_{2,g}, \Psi \rangle \tag{23}$$
$$+ \left\langle -\sum_{g' \neq g}^{G} \Sigma_{s0,g' \to g} \left(\Phi_{0,g'} - 2\Phi_{2,g'} \right), \Psi \right\rangle + \left\langle -\frac{\chi_g}{k_{eff}} \sum_{g'=1}^{G} \nu \Sigma_{f,g'} \left(\Phi_{0,g'} - 2\Phi_{2,g'} \right), \Psi \right\rangle + \langle -Q_{0,g}, \Psi \rangle = 0 \tag{24}$$
$$\langle D_{2,g} \nabla \Phi_{2,g}, \nabla \Psi \rangle + \langle -D_{2,g} \nabla \Phi_{2,g}, \Psi \rangle_{BC} + \left\langle \left(\Sigma_{2,g} + \frac{4}{5} \Sigma_{0,g} \right) \Phi_{2,g}, \Psi \right\rangle + \left\langle -\frac{2}{5} \Sigma_{0,g} \Phi_{0,g}, \Psi \right\rangle \tag{25}$$
$$+ \left\langle \frac{2}{5} \sum_{g' \neq g}^{G} \Sigma_{s0,g' \to g} \left(\Phi_{0,g'} - 2\Phi_{2,g'} \right), \Psi \right\rangle + \left\langle \frac{2}{5} \frac{\chi_g}{k_{eff}} \sum_{g'=1}^{G} \nu \Sigma_{f,g'} \left(\Phi_{0,g'} - 2\Phi_{2,g'} \right), \Psi \right\rangle + \left\langle \frac{2}{5} Q_{0,g}, \Psi \right\rangle = 0. \tag{26}$$

Vacuum BCs kernels?

$$\langle -D_{0,g} \nabla \Phi_{0,g}, \Psi \rangle_{BC} = \left\langle -\frac{1}{2} \Phi_{0,g} + \frac{3}{4} \Phi_{2,g}, \Psi \right\rangle_{BC} \tag{27}$$
$$\langle -D_{2,g} \nabla \Phi_{2,g}, \Psi \rangle_{BC} = \left\langle \frac{3}{40} \Phi_{0,g} - \frac{21}{40} \Phi_{2,g}, \Psi \right\rangle_{BC} \tag{28}$$
$$\tag{29}$$

4 Results

5 Conclusions

Table 1: .

Kernel	Equation A	Equation B
P3Diffusion	$\langle D_{0,g} \nabla \Phi_{0,g}, \nabla \Psi \rangle$	$\langle D_{2,g} \nabla \Phi_{2,g}, \nabla \Psi \rangle$
P3SigmaR	$\langle \Sigma_{0,g} \Phi_{0,g}, \Psi \rangle$	$\left\langle \left(\Sigma_{2,g} + \frac{4}{5} \Sigma_{0,g} \right) \Phi_{2,g}, \Psi \right\rangle$
P3SigmaCoupled	$\langle -2\Sigma_{0,g} \Phi_{2,g}, \Psi \rangle$	$\left\langle -\frac{2}{5} \Sigma_{0,g} \Phi_{0,g}, \Psi \right\rangle$
P3InScatter	$\left\langle -\sum_{g' \neq g}^{G} \Sigma_{s0,g' \to g} \left(\Phi_{0,g'} - 2\Phi_{2,g'} \right), \Psi \right\rangle$	$\left\langle \frac{2}{5} \sum_{g' \neq g}^{G} \Sigma_{s0,g' \to g} \left(\Phi_{0,g'} - 2\Phi_{2,g'} \right), \Psi \right\rangle$
P3FissionEigenKernel	$\left\langle \frac{\chi_g}{k_{eff}} \sum_{g'=1}^{G} \nu \Sigma_{f,g'} \left(\Phi_{0,g'} - 2\Phi_{2,g'} \right), \Psi \right\rangle$	$\left\langle \frac{2}{5} \frac{\chi_g}{k_{eff}} \sum_{g'=1}^{G} \nu \Sigma_{f,g'} \left(\Phi_{0,g'} - 2\Phi_{2,g'} \right), \Psi \right\rangle$
Boundary Condition Kernel	**Equation A**	**Equation B**
Vacuum	$\left\langle -\frac{1}{2} \Phi_{0,g} + \frac{3}{4} \Phi_{2,g}, \Psi \right\rangle_{BC}$	$\left\langle \frac{3}{40} \Phi_{0,g} - \frac{21}{40} \Phi_{2,g}, \Psi \right\rangle_{BC}$

References

[1] P.S. Brantley and E.W. Larsen. The Simplified P3 Approximation. *Nuclear Science and Engineering*, 2000.

[2] E.M. Gelbard. Application of spherical harmonics methods to reactor problems. Technical Report WAPD-BT-20, Bettis Atomic Power Laboratory, 1960.