Implementation of the SP3 equations in a MOOSE-based application

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December 16, 2020

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Outline

Objectives

- Implement and solve SP_3 equations with a MOOSE-based application for the following cases:
- one-dimensonal models:
  - fixed source problem with one energy group,
  - eigenvalue problem with one energy group,
  - fixed source problem with multiple energy groups,
  - eigenvalue source problem with multiple energy groups,
  - compare results to diffusion solver,
- two-dimensonal model: C5 MOX Benchmark [3].

Outline

MOOSE

- Computational framework
- Solves coupled equation systems
- MOOSE defines weak forms
- MOOSE and LibMesh translate them into residual and Jacobian functions
- PetSc solution routines solve the equations

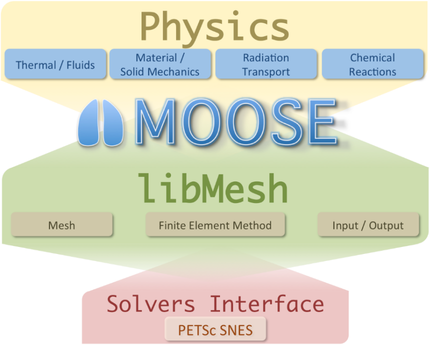

Figure: MOOSE framework. Image reproduced from [4].

P_3 equations

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

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

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

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

Assumptions [2]:

- isotropic external source
- negligible anisotropic group-to-group scattering

P_3 equations (2)

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

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

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

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

Defines:

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

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

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

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

P_3 equations (3)

$$-D_{0,g}\frac{d^2}{dx^2}\Phi_{0,g}+\Sigma_{0,g}\Phi_{0,g}-2\Sigma_{0,g}\Phi_{2,g}=S_{0,g} \tag{9}$$

$$-D_{2,g}\frac{d^2}{dx^2}\Phi_{2,g}+\left(\Sigma_{2,g}+\frac{4}{5}\Sigma_{0,g}\right)\Phi_{2,g}-\frac{2}{5}\Sigma_{0,g}\Phi_{0,g}=-\frac{2}{5}S_{0,g} \tag{10}$$

where

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

SP_3 approximation

- P_N: yields the exact transport solution as $N \to \infty$.
- 3D: $(N+1)^2$ equations.
- 1D: $(N+1)$ equations yield $(N+1)/2$.
- SP_N approximation replaces $\frac{d^2}{dx^2}$ by Δ.

SP_3 equations

$$-D_{0,g}\Delta\Phi_{0,g} + \Sigma_{0,g}\Phi_{0,g} - 2\Sigma_{0,g}\Phi_{2,g} = S_{0,g} \tag{11}$$

$$-D_{2,g}\Delta\Phi_{2,g} + \left(\Sigma_{2,g} + \frac{4}{5}\Sigma_{0,g}\right)\Phi_{2,g} - \frac{2}{5}\Sigma_{0,g}\Phi_{0,g} = -\frac{2}{5}S_{0,g}. \tag{12}$$

With the Marshak vacuum BCs [1]

$$\frac{1}{4}\Phi_{0,g} \pm \frac{1}{2}\hat{n}\cdot J_{0,g} - \frac{3}{16}\Phi_{2,g} = 0 \tag{13}$$

$$-\frac{3}{80}\Phi_{0,g} \pm \frac{1}{2}\hat{n}\cdot J_{2,g} + \frac{21}{80}\Phi_{2,g} = 0 \tag{14}$$

where

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

Weak form

Example Code

Strong Form

$$\rho Cp \frac{\partial T}{\partial t} - \nabla \cdot k(T,B)\nabla T = f$$

Weak Form

$$\underbrace{\int_{\Omega} \rho Cp \frac{\partial T}{\partial t}\psi_i}_{\text{Kernel}} + \underbrace{\int_{\Omega} k\nabla T \cdot \nabla\psi_i}_{\text{Kernel}} - \underbrace{\int_{\partial\Omega} k\nabla T \cdot \mathbf{n}\psi_i}_{\text{BoundaryCondition}} - \underbrace{\int_{\Omega} f\psi_i}_{\text{Kernel}} = 0$$

Actual Code

```
return _k[_qp]*_grad_u[_qp]*_grad_test[_i][_qp];
```

Figure: Translation into MOOSE kernels procedure [4].

Weak form: Equation 1

$$\begin{aligned}
&\langle D_{0,g}\nabla\Phi_{0,g},\nabla\Psi\rangle - \langle D_{0,g}\nabla\Phi_{0,g},\Psi\rangle_{BC} + \langle\Sigma_{0,g}\Phi_{0,g},\Psi\rangle + \langle -2\Sigma_{0,g}\Phi_{2,g},\Psi\rangle \\
&+ \left\langle -\sum_{g'\neq g}^{G}\Sigma_{s0,g'\to g}\left(\Phi_{0,g'} - 2\Phi_{2,g'}\right),\Psi\right\rangle \\
&+ \left\langle -\frac{\chi_g}{k_{eff}}\sum_{g'=1}^{G}\nu\Sigma_{f,g'}\left(\Phi_{0,g'} - 2\Phi_{2,g'}\right),\Psi\right\rangle + \langle -Q_{0,g},\Psi\rangle = 0
\end{aligned} \tag{15}$$

with the boundary condition

$$\langle D_{0,g}\nabla\Phi_{0,g},\Psi\rangle_{BC} = \left\langle \frac{1}{2}\Phi_{0,g} - \frac{3}{4}\Phi_{2,g},\Psi\right\rangle_{BC}. \tag{16}$$

Weak form: Equation 2

$$
\begin{aligned}
&\langle D_{2,g}\nabla\Phi_{2,g},\nabla\Psi\rangle-\langle D_{2,g}\nabla\Phi_{2,g},\Psi\rangle_{BC}+\left\langle\left(\Sigma_{2,g}+\frac{4}{5}\Sigma_{0,g}\right)\Phi_{2,g},\Psi\right\rangle\\
&+\left\langle-\frac{2}{5}\Sigma_{0,g}\Phi_{0,g},\Psi\right\rangle+\left\langle\frac{2}{5}\sum_{g'\neq g}^{G}\Sigma_{s0,g'\to g}\left(\Phi_{0,g'}-2\Phi_{2,g'}\right),\Psi\right\rangle\\
&+\left\langle\frac{2}{5}\frac{\chi_g}{k_{eff}}\sum_{g'=1}^{G}\nu\Sigma_{f,g'}\left(\Phi_{0,g'}-2\Phi_{2,g'}\right),\Psi\right\rangle+\left\langle\frac{2}{5}Q_{0,g},\Psi\right\rangle=0.
\end{aligned}
\tag{17}
$$

with the boundary condition

$$
\langle D_{2,g}\nabla\Phi_{2,g},\Psi\rangle_{BC}=\left\langle-\frac{3}{40}\Phi_{0,g}+\frac{21}{40}\Phi_{2,g},\Psi\right\rangle_{BC}.
\tag{18}
$$

SP3 Kernels: Equation 1

Table: SP_3 kernels.

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

SP3 Kernels: Equation 2

Table: SP_3 kernels.

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

Moltres

$$\nabla \cdot D_g \nabla \phi_g - \Sigma_g^r \phi_g + \sum_{g' \neq g}^{G} \Sigma_{g' \to g}^s \phi_{g'} + \chi_g^t \sum_{g'=1}^{G} \frac{1}{k_{eff}} \nu \Sigma_{g'}^f \phi_{g'} + Q_g = 0. \quad (19)$$

Benchmark definition

- 7-group cross-sections: C5G7 [5].
- Capilla et al [3]: C5G2.

vacuum

	R	R	R	R	R	R	
	R	UO_2	MOX	MOX	UO_2	R	
	R	MOX	UO_2	UO_2	MOX	R	
vacuum	R	MOX	UO_2	UO_2	MOX	R	vacuum
	R	UO_2	MOX	MOX	UO_2	R	
	R	R	R	R	R	R	

vacuum

Figure: 2-D C5 MOX benchmark configuration. Image reproduced from [3]. *R* represents the reflectors.

Benchmark definition (2)

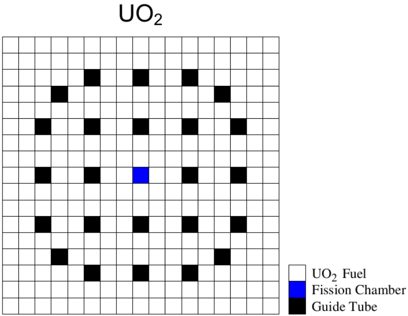

Figure: UO_2 assembly. Image reproduced from [3].

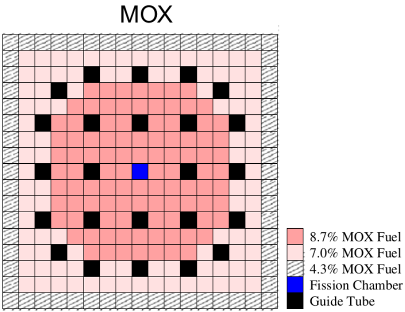

Figure: MOX assembly. Image reproduced from [3].

Benchmark geometry

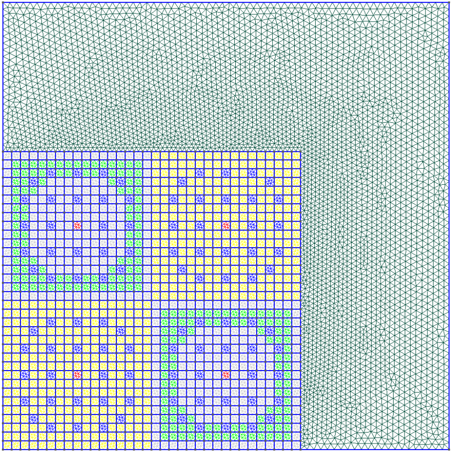

Figure: Gmsh 2D geometry.

Outline

Fixed source

Comparison between SP_3 and Diffusion solutions of the scalar flux.

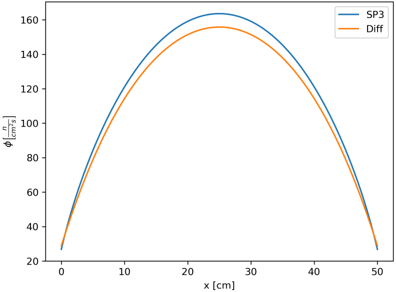

Figure: 1 group.

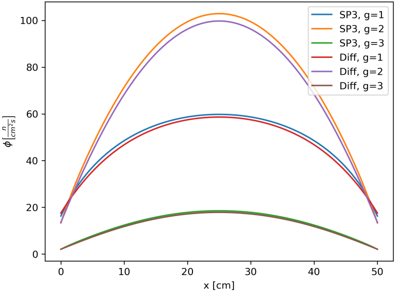

Figure: 3 groups.

Eigenvalue problem

Comparison between SP_3 and Diffusion solutions of the scalar flux. Solutions are normalized to the maximum value of the flux (fast flux for the 3 group case).

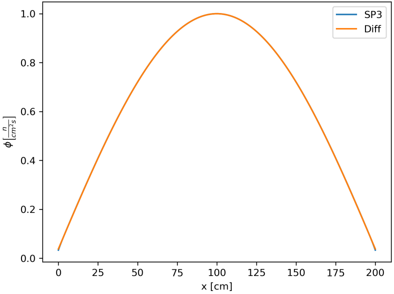

Figure: 1 group.

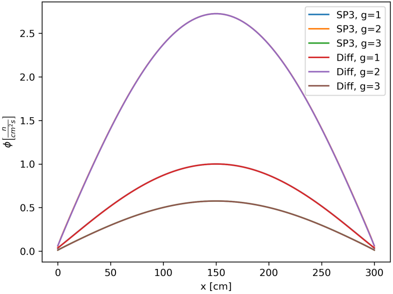

Figure: 3 groups.

C5G2 MOX Benchmark

	C5G2 Benchmark	SP3	
Case	k_{Ref}	k_{SP_3}	Δ_ρ [pcm]
Heterogeneous	0.96969	0.97106	145
Homogeneous	0.96983	0.97061	83

C5G2 MOX Benchmark (2)

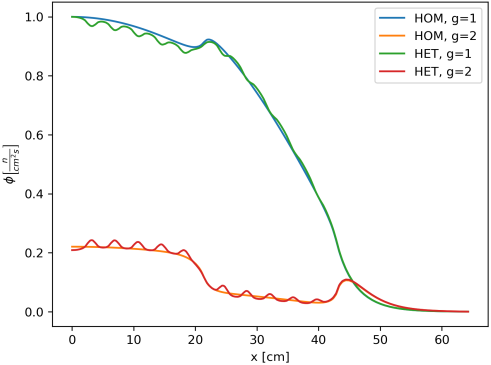

Figure: Comparison of the heterogenous and homogeneous cases scalar flux.

C5G2 MOX Benchmark (3)

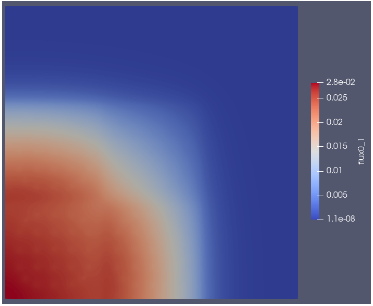

Figure: $\Phi_{0,1}$.

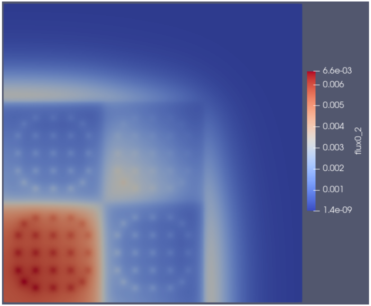

Figure: $\Phi_{0,2}$.

C5G2 MOX Benchmark (4)

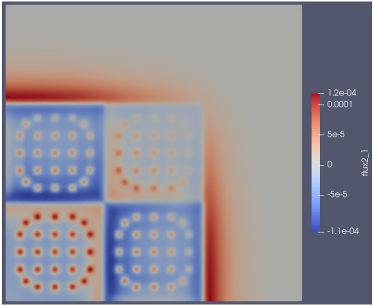

Figure: $\Phi_{2,1}$.

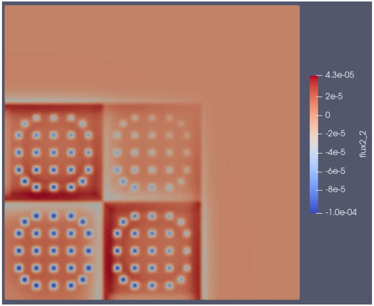

Figure: $\Phi_{2,2}$.

Outline

Conclusions

- 2-D test case: suggest SP_3 equations implementation is correct
- 1-D test cases: solutions are very similar to diffusion solution
- SP_N have a higher computational expense than diffusion
- further studies are necessary to conclude anything on the accuracy
- In general, SP_N are more accurate than diffusion [2]
- Less computational expense than S_N or P_N
- the study cases do not show an increased accuracy over diffusion

References I

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