Implementation of the SP3 equations in a MOOSE-based application

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Objectives

- Implement the SP_3 equations in a MOOSE-based application.
- Verify the implementation by conducting the following exercises:
  - One-group, two-dimensional eigenvalue problem.
  - C5 MOX Benchmark.

Motivation

Why a neutronics solver?

- Neutronics provide information on the power distribution.
- Crucial role in the thermal-fluids behavior of a reactor.
- Multi-physics simulations for safety assessment.

Why the SP_3 equations?

- Fewer equations than P_3.
- Reduces the computational expense.
- Conserves a reasonable accuracy.
- More accurate solution than diffusion approximation.

Why MOOSE?

- Partial differential equations describe the reactor physics.
- Computational framework for solving coupled equation systems.
- Open-source.
- Facilitates coupling between various applications targeting different phenomena.

Outline

P_3 equations

- P_N expands the angular dependence in spherical harmonics.
- For N=3, steady-state, and one-dimension [5]:

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

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

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

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

P_3 equations (2)

Assumptions [2]:

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

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

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

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

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

P_3 equations (3)

With the following definitions:

$$D_{0,g} = \frac{1}{3\Sigma_{1,g}}, \quad D_{2,g} = \frac{9}{35\Sigma_{3,g}}$$
$$\Phi_{0,g} = \phi_{0,g} + 2\phi_{2,g}, \quad \Phi_{2,g} = \phi_{2,g}$$

the equations become:

$$-D_{0,g}\frac{d^2}{dx^2}\Phi_{0,g} + \Sigma_{0,g}\Phi_{0,g} - 2\Sigma_{0,g}\Phi_{2,g} = S_{0,g} \tag{9}$$
$$-D_{2,g}\frac{d^2}{dx^2}\Phi_{2,g} + \left(\Sigma_{2,g} + \frac{4}{5}\Sigma_{0,g}\right)\Phi_{2,g} - \frac{2}{5}\Sigma_{0,g}\Phi_{0,g} = -\frac{2}{5}S_{0,g} \tag{10}$$

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

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

MOOSE

- Computational framework for solving coupled equation systems.
- Input are the equation weak forms.
- MOOSE and LibMesh translate them into residual and Jacobian functions.
- PetSc solution routines solve the equations.

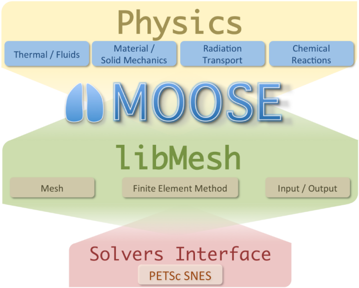

Figure: MOOSE framework. Image reproduced from [6].

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 [6].

Weak form: Equation 1

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

with the boundary condition

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

Weak form: Equation 2

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

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 name	Equation 1
SP3Diffusion	$\langle D_{0,g} \nabla \Phi_{0,g}, \nabla \Psi \rangle$
SP3SigmaR	$\langle \Sigma_{0,g} \Phi_{0,g}, \Psi \rangle$
SP3SigmaCoupled	$\langle -2\Sigma_{0,g} \Phi_{2,g}, \Psi \rangle$
SP3InScatter	$\left\langle -\sum_{g' \neq g}^{G} \Sigma_{s0,g' \to g} \left(\Phi_{0,g'} - 2\Phi_{2,g'} \right), \Psi \right\rangle$
SP3FissionEigenKernel	$\left\langle -\frac{\chi_g}{k_{eff}} \sum_{g'=1}^{G} \nu \Sigma_{f,g'} \left(\Phi_{0,g'} - 2\Phi_{2,g'} \right), \Psi \right\rangle$
BodyForce (MOOSE)	$\langle -Q_{0,g}, \Psi \rangle$
BC Kernel name	
SP3Vacuum	$\left\langle \frac{1}{2}\Phi_{0,g} - \frac{3}{4}\Phi_{2,g}, \Psi \right\rangle_{BC}$

SP3 Kernels: Equation 2

Table: SP_3 kernels.

Kernel name	Equation 2
SP3Diffusion	$\langle D_{2,g} \nabla \Phi_{2,g}, \nabla \Psi \rangle$
SP3SigmaR	$\left\langle \left(\Sigma_{2,g} + \frac{4}{5} \Sigma_{0,g} \right) \Phi_{2,g}, \Psi \right\rangle$
SP3SigmaCoupled	$\left\langle -\frac{2}{5} \Sigma_{0,g} \Phi_{0,g}, \Psi \right\rangle$
SP3InScatter	$\left\langle \frac{2}{5} \sum_{g' \neq g}^{G} \Sigma_{s0,g' \to g} \left(\Phi_{0,g'} - 2\Phi_{2,g'} \right), \Psi \right\rangle$
SP3FissionEigenKernel	$\left\langle \frac{2}{5} \frac{\chi_g}{k_{eff}} \sum_{g'=1}^{G} \nu \Sigma_{f,g'} \left(\Phi_{0,g'} - 2\Phi_{2,g'} \right), \Psi \right\rangle$
BodyForce (MOOSE)	$\left\langle \frac{2}{5} Q_{0,g}, \Psi \right\rangle$
BC Kernel name	
SP3Vacuum	$\left\langle -\frac{3}{40} \Phi_{0,g} + \frac{21}{40} \Phi_{2,g}, \Psi \right\rangle_{BC}$

Outline

One-group, two-dimensional eigenvalue problem

- Problem presented in Brantley and Larsen, 2000 [2].
- One-energy group.
- Two-dimensional problem.
- Two materials: fuel and moderator.

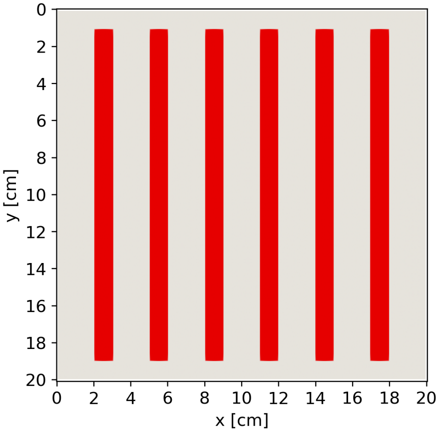

Figure: Problem's geometry.

One-group, two-dimensional eigenvalue problem (2)

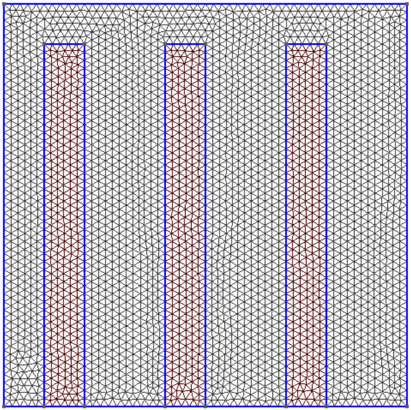

Figure: Gmsh 2D mesh.

One-group, two-dimensional eigenvalue problem (3)

Table: Eigenvalue comparison.

k_{Ref}	k_{SP_3}	Δ_ρ
0.79862	0.79854	12

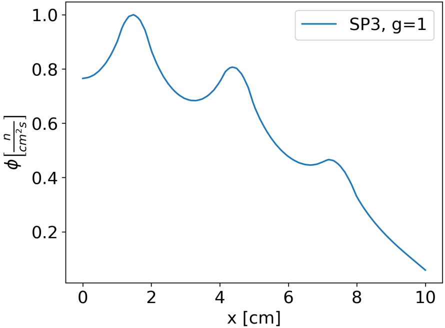

Figure: Scalar flux over line at y=4.5 cm.

C5 MOX Benchmark

- Exercise defined in 1994 by OECD/NEA [4].
- Two-energy groups.
- Two-dimensional problem.
- Two types of fuel: UO_2, MOX.

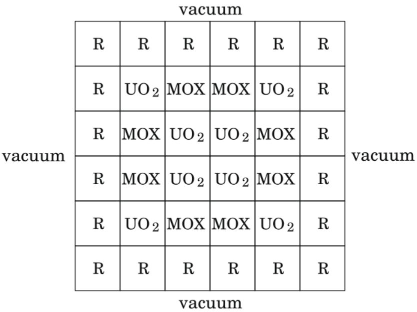

Figure: 2-D C5 MOX benchmark configuration. *R* represents the reflectors. Image reproduced from [3].

C5 MOX Benchmark (2)

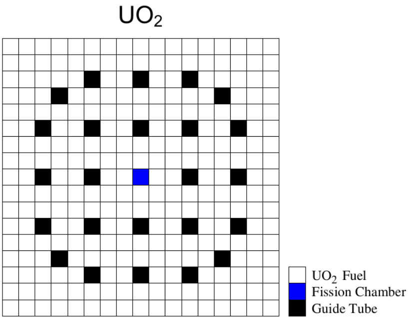

Figure: UO_2 assembly. Image reproduced from [3].

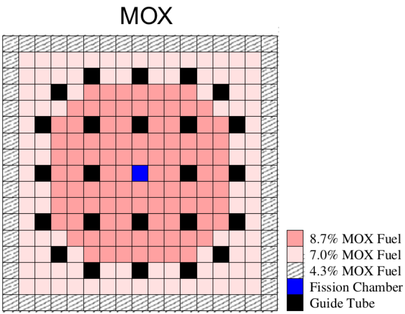

Figure: MOX assembly. Image reproduced from [3].

C5 MOX Benchmark (3)

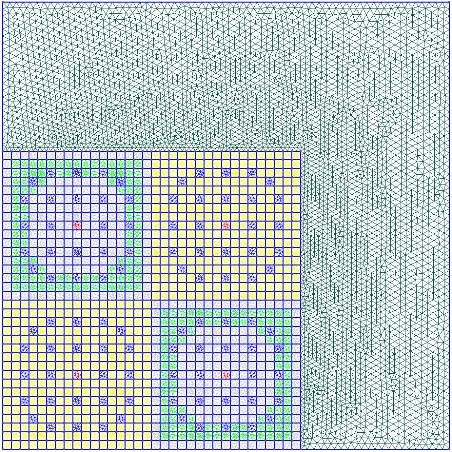

Figure: Gmsh 2D mesh.

C5 MOX Benchmark (4)

If the higher order information of the scattering cross-section is not available (no correction):

$$D_{0,g} = \frac{1}{3\Sigma_{1,g}} = \frac{1}{3\Sigma_{t,g}} \tag{19}$$

The definition of the benchmark [4] recommends applying the diagonal transport correction:

$$\begin{aligned} D_{0,g} &= \frac{1}{3\Sigma_{tr,g}} \\ \Sigma_{tr,g} &= \Sigma_{t,g} - \bar{\mu}_g \Sigma_{s0,g} \end{aligned} \tag{20}$$

where

$$\Sigma_{tr,g} = \text{group } g \text{ transport cross-section}$$
$$\bar{\mu}_g = \text{group } g \text{ average cosine deviation angle.}$$

C5 MOX Benchmark (5)

	C5G2 Benchmark	SP3	
Case	k_{Ref}	k_{SP_3}	Δ_ρ [pcm]
No correction	0.96969	0.97106	145
Transport correction	0.93755	0.93792	43

C5 MOX Benchmark (6)

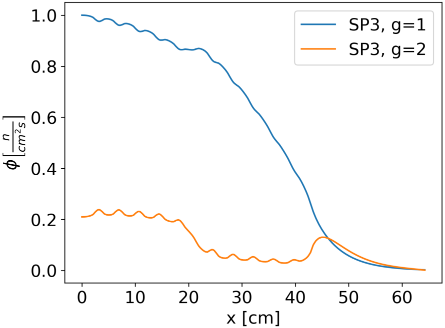

Figure: Scalar flux at y=10.71cm.

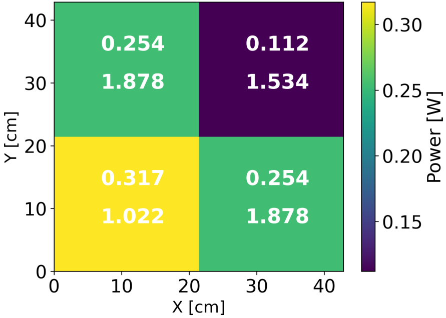

Figure: Assembly power distribution. Top: Assembly power. Bottom: Pin power relative difference expressed in %.

Outline

Conclusions

- Implemented the kernels to solve the steady-state SP_3 equations in a MOOSE-based application.
- Conducted two exercises whose reference results were known.
- Eigenvalue for the first exercise within 12 pcm.
- Eigenvalues for the second exercise within 145 pcm.
- Transport correction is necessary when the scattering higher moments are unknown.
- Calculated pin power values within 2% difference.
- Future work may develop new applications or integrate this application to other physics solvers.

Acknowledgement

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Thank you.
Questions?

References I

[1] C. Beckert and U. Grundmann.
Development and verification of a nodal approach for solving the multigroup P3 equations.
Annals of Nuclear Energy, 2007.

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

[3] M. Capilla, D. Ginestar, and G. Verdú.
Applications of the multidimensional equations to complex fuel assembly problems.
Annals of Nuclear Energy, 36(10):1624–1634, October 2009.

[4] C. Cavarec, J.F. Perron, D. Verwaerde, and J.P. West.
Benchmark Calculations of Power Distributions within Assemblies.
Technical Report HT-12/94006 A, NEA/NSC/DOC (94) 28, Nuclear Energy Agency Committee on Reactor Physics, 1994.

[5] B. Davidson.
Neutron Transport Theory.
Oxford University Press, London, 1957.

References II

[6] INL.
Moose Workshop Slides, December 2020.
https://mooseframework.inl.gov/workshop.