

Implementation of the SP3 equations
in a MOOSE-based application
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1-G, 2-D
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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.



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P_3 equations

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

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

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

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

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

P_3 equations (2)

Assumptions [2]:

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

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

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

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

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

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:

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

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

where

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

SP_3 approximation

- P_N : yields the exact transport solution as $N \rightarrow \infty$.
- 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

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

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

With the Marshak vacuum BCs [1]

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

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

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.

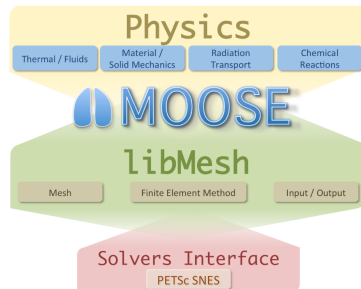


Figure: MOOSE framework. Image reproduced from [6].

Weak form



Example Code

Strong Form

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

Weak Form

$$\int_{\Omega} \rho C_p \frac{\partial T}{\partial t} \psi_i + \int_{\Omega} k \nabla T \cdot \nabla \psi_i - \int_{\partial \Omega} k \nabla T \cdot \mathbf{n} \psi_i - \int_{\Omega} f \psi_i = 0$$

Kernel Kernel BoundaryCondition Kernel

Actual Code

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

Figure: Translation into MOOSE kernels procedure [6].

Weak form: Equation 1

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

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

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

with the boundary condition

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

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



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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.

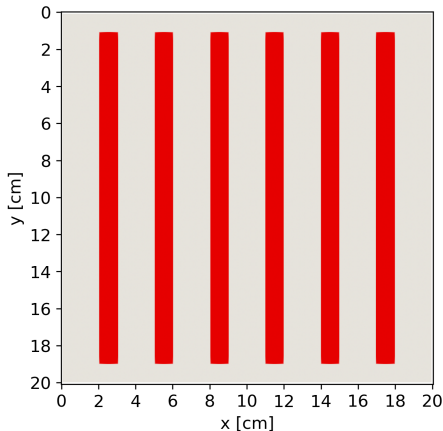


Figure: Problem's geometry.

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

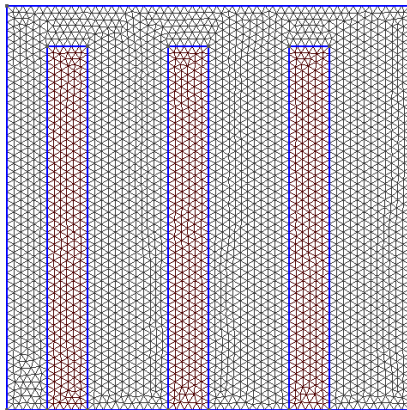
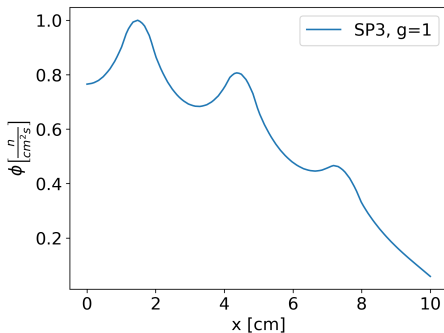


Figure: Gmsh 2D mesh.

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.

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

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

C5 MOX Benchmark (2)

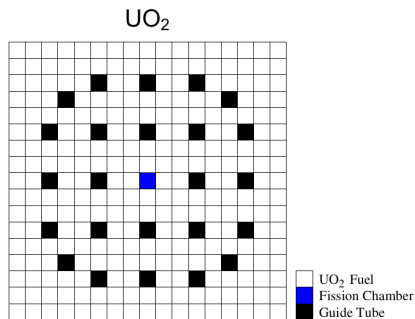


Figure: UO₂ assembly. Image reproduced from [3].

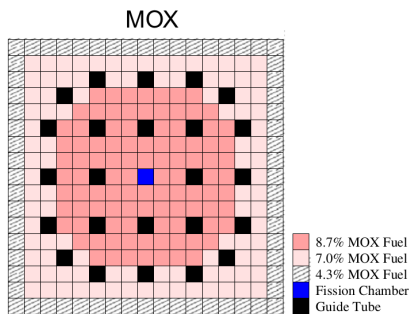


Figure: MOX assembly. Image reproduced from [3].

C5 MOX Benchmark (3)

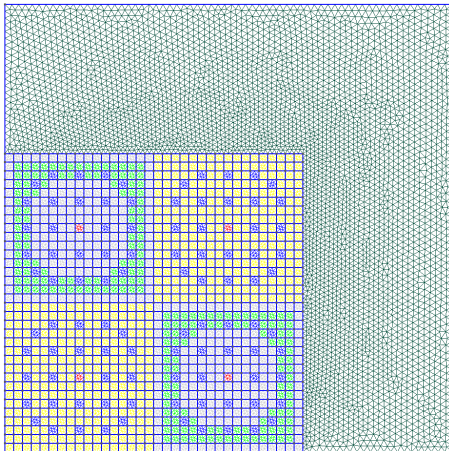


Figure: Gmsh 2D mesh.



C5 MOX Benchmark (4)

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

$$D_{0,g} = \frac{1}{3\Sigma_{1,g}} = \frac{1}{3\Sigma_{t,g}} \quad (19)$$

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

$$D_{0,g} = \frac{1}{3\Sigma_{tr,g}} \quad (20)$$
$$\Sigma_{tr,g} = \Sigma_{t,g} - \bar{\mu}_g \Sigma_{s0,g}$$

where

$\Sigma_{tr,g}$ = group g transport cross-section

$\bar{\mu}_g$ = group g 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)

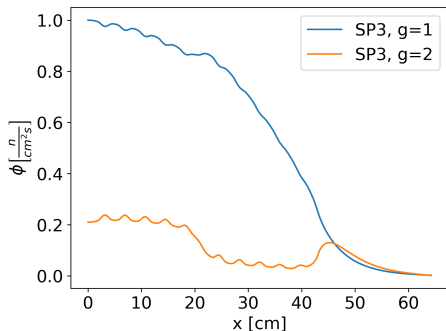


Figure: Scalar flux at $y=10.71\text{cm}$.

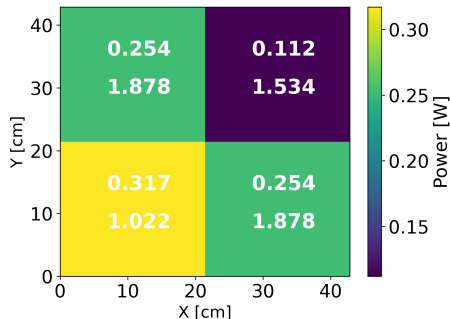


Figure: Assembly power distribution. Top: Assembly power. Bottom: Pin power relative difference expressed in %.



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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?**

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