Cerberus: A MOOSE-based application for solving the SP_3 equations

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Outline

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   - Objectives
   - Motivation
2. Methodology
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   - Implementation
   - Kernels
3. Results
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   - Conclusions
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Objectives

- Describe the implementation of 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 (2D)
  - C5 MOX Benchmark (3D mini-core variation)

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, enabling wider collaboration.
- API that 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]:

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

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

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

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

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. If N $=$ 3, 16 equations.
- 1D: $(N+1)$ equations yield $(N+1)/2$. If N $=$3, 2 equations.
- 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 weak form of the equations.
- MOOSE and LibMesh translate them into residual and Jacobian functions.
- PetSc solution routines solve the equations.

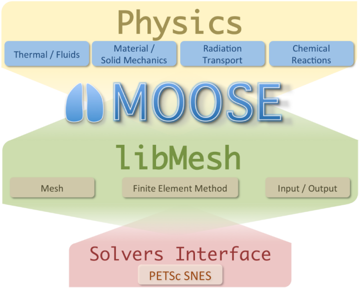

Figure: MOOSE framework. Image reproduced from [6].

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

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

Cerberus 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	$\left\langle \frac{1}{2}\Phi_{0,g} - \frac{3}{4}\Phi_{2,g} , \Psi \right\rangle_{BC}$

Cerberus 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	$\left\langle -\frac{3}{40} \Phi_{0,g} + \frac{21}{40} \Phi_{2,g}, \Psi \right\rangle_{BC}$

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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.

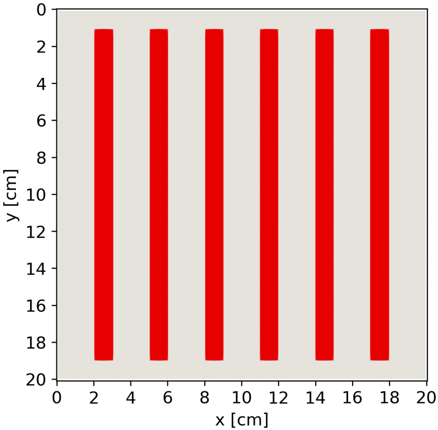

Figure: Problem's geometry.

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

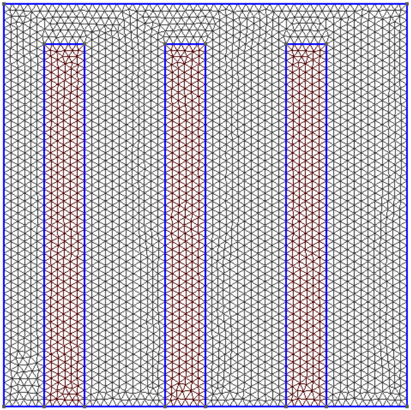

Figure: Gmsh 2D mesh.

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

Table: Eigenvalue comparison.

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

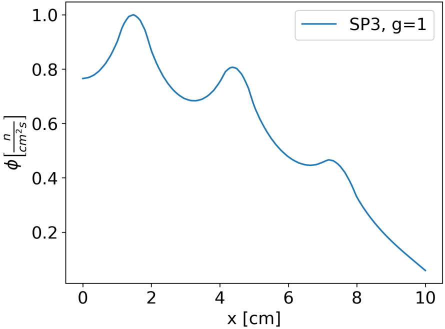

Figure: Scalar flux over line at y=4.5 cm.

C5 MOX Benchmark

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

C5 MOX Benchmark (2)

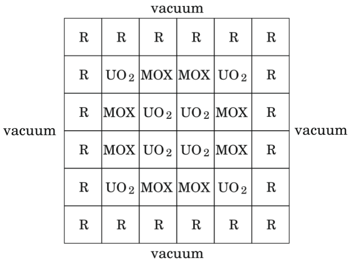

Figure: 2-D C5 MOX benchmark configuration. *R* represents the reflectors. Image reproduced from [3].

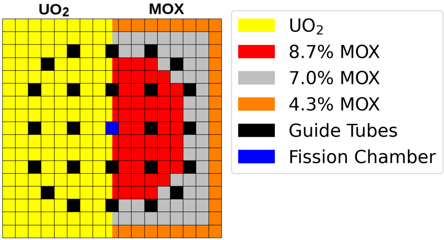

Figure: Structure of the UO2 and MOX assemblies.

C5 MOX Benchmark (3)

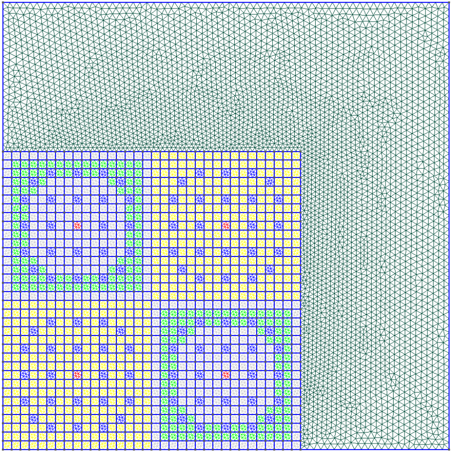

Figure: Gmsh 2D mesh.

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	Cerberus	
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)

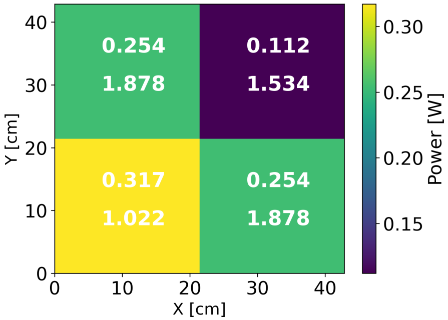

Figure: Assembly power distribution. Top: Assembly power. Bottom: Pin power relative difference expressed in %.

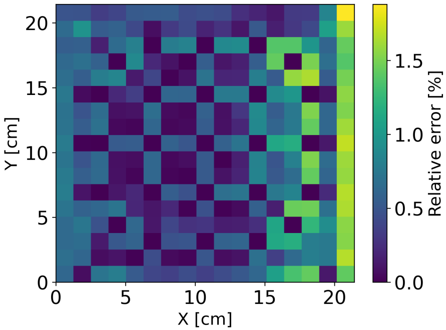

Figure: MOX assembly pin power relative difference expressed in %.

C5 MOX Benchmark (7)

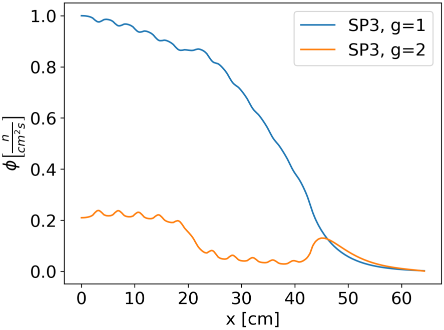

Figure: Scalar flux at y=10.71cm.

C5 MOX 3D

- 3D mini-core variation of the C5 MOX benchmark introduced by Ryu et al., 2013 [7].
- Two-energy group.
- Three-dimensional problem.
- Three materials: UO_2, MOX, and reflector.

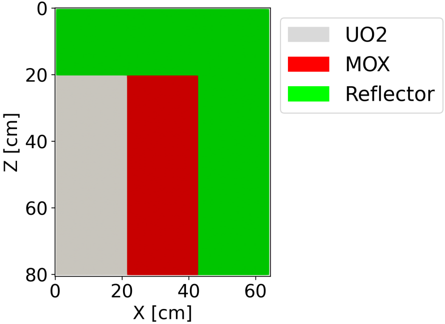

Figure: Axial layout of the C5G2 3D Benchmark.

C5 MOX 3D (2)

Table: Eigenvalue comparison.

k_{Ref}	k_{SP_3}	Δ_ρ
0.91974	0.91979	6

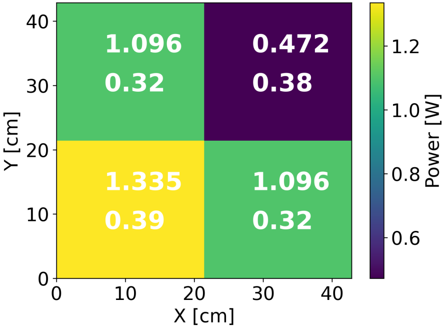

Figure: Power distribution in the C5G2 3D Benchmark. Top: power distribution. Bottom: relative difference expressed in %.

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Conclusions

- Implemented the kernels to solve the steady-state SP_3 equations in the MOOSE-based application Cerberus.
- Conducted three exercises whose reference results were known:
  - First exercise: Eigenvalue difference of 12 pcm.
  - Second exercise:
    - Eigenvalue difference of 145 pcm.
    - Pin power distribution within 2% difference.
  - Third exercise:
    - Eigenvalue difference of 6 pcm.
    - Assembly power distribution within 1% difference.
- Transport correction is necessary when the scattering higher moments are unknown.
- 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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