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

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INTRODUCTION

This work presents the implementation of the Simplified P_3 (SP_3) equations [1] in the Multi-physics Object-Oriented Simulation Environment (MOOSE)-based application Cerberus. MOOSE [2] is a computational framework that supports engineering analysis applications. In a nuclear reactor, several partial differential equations describe its physical behavior. These equations are typically nonlinear, and they are often coupled to each other. MOOSE is an open-source Finite Element Method (FEM) framework that supports the development of applications for solving such systems.

All the software built on the MOOSE framework shares the same Application Programming Interface (API), facilitating relatively easy coupling between different phenomena. While Cerberus solves the neutronics in a nuclear reactor using the multi-group steady-state SP_3 equations, other applications may solve the thermal-fluids, and given they share the same API; their integration is straightforward.

The P_N method [3] discretizes the transport equation by expanding the angular dependence of the neutron flux in spherical harmonics, considering up to order N polynomials. If $N \to \infty$, the solution of the P_N equations tends to the exact transport solution. In three-dimensional(3D) geometries, the number of P_N equations is proportional to $(N+1)^2$, whereas, in one-dimensional(1D) planar geometries, the number of P_N equations is $(N+1)$. Gelbard [1] proposed the SP_N approximation by replacing the second derivatives in the 1D planar P_N equations with 3D Laplacian operators. This approximation considerably reduces the number of equations conserving a reasonable accuracy [4].

The SP_N approximation has the disadvantage that the solution does not usually converge to the true transport solution as $N \to \infty$. Additionally, the theoretical basis of Gelbard's formulation of SP_N approximation was weak. For these reasons, the method did not gain widespread use until the 2000s, when thanks to Brantley and Larsen's [5] contribution, the method gained a stronger theoretical basis.

In practice, the SP_N equations are most accurate for diffusive problems or for problems in which the solution behaves nearly one-dimensionally and has weak tangential derivatives at material interfaces. Several results show that the SP_N approximation yields more accurate solutions than the diffusion approximation [6] [7] [8] with considerably less computational expense than the discrete ordinates (S_N) method [5]. For example, the SP_3 approximation is preferable over the diffusion approximation for modeling reactors using MOX/UO_2 fuel assemblies. MOX fuel assemblies have higher thermal absorption and fission cross-sections than UO_2 fuel assemblies, and consequently, their thermal flux is lower while their power production higher. Modeling these characteristics using the diffusion approximation may be challenging [5] [4].

The SP_3 approximation gained usage throughout the last couple of decades, and currently, different software uses it to solve the neutron transport equation. Some examples are PARCS [9] and DYN3D [7].

METHODOLOGY

This section describes the methodology followed for solving the equations. Davidson [3] defined the 1D multi-group P_N equations. In the steady-state, for $N = 3$ and a negligible fixed source, the equations become

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

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

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

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

where

$\phi_{n,g} = n^{th}$ moment of group g neutron flux
$\Sigma_{t,g}$ = group g macroscopic total cross-section
$\Sigma_{sn,g'\to g} = n^{th}$ moment of the group g' to group g macroscopic scattering cross-section
$\nu\Sigma_{f,g}$ = group g macroscopic production cross-section
χ_g = group g fission spectrum
k_{eff} = eigenvalue
G = number of energy groups.

Assuming a negligible anisotropic group-to-group scattering [5]

$$\Sigma_{sn,g'\to g} = 0, \quad g' \neq g, \quad n > 0$$

simplifies equations 2 and 4, allowing to express the odd moments of the flux $\phi_{1,g}$ and $\phi_{3,g}$ as functions of the even moments $\phi_{0,g}$ and $\phi_{2,g}$. Replacing $\phi_{1,g}$ and $\phi_{3,g}$ into equations 1 and 3 reduces the system from four to two equations. Introducing the variables $\Phi_{0,g}$ and $\Phi_{2,g}$, reorganizing the equations, and replacing the second derivatives by Laplacian operators [1] yields the SP_3 equations [7]

$$-D_{0,g}\Delta\Phi_{0,g} + \Sigma_{0,g}\Phi_{0,g} - 2\Sigma_{0,g}\Phi_{2,g} = S_{0,g} \tag{5}$$

$$-D_{2,g}\Delta\Phi_{2,g} + \left(\Sigma_{2,g} + \frac{4}{5}\Sigma_{0,g}\right)\Phi_{2,g} - \frac{2}{5}\Sigma_{0,g}\Phi_{0,g} = -\frac{2}{5}S_{0,g} \tag{6}$$

where

$$\begin{aligned}
\Sigma_{n,g} &= \Sigma_{t,g} - \Sigma_{sn,g'\to g} \\
\Phi_{0,g} &= \phi_{0,g} + 2\phi_{2,g} \\
\Phi_{2,g} &= \phi_{2,g} \\
D_{0,g} &= \frac{1}{3\Sigma_{1,g}} \\
D_{2,g} &= \frac{9}{35\Sigma_{3,g}} \\
S_{0,g} &= \sum_{g'\neq g}^{G} \Sigma_{s0,g'\to g}\left(\Phi_{0,g'} - 2\Phi_{2,g'}\right) \\
&\quad + \frac{\chi_g}{k_{eff}} \sum_{g'=1}^{G} \nu\Sigma_{f,g'}\left(\Phi_{0,g'} - 2\Phi_{2,g'}\right).
\end{aligned} \tag{7}$$

The Marshak-like vacuum boundary conditions (BCs) complete the system of equations [7]

$$\frac{1}{4}\Phi_{0,g} \pm \frac{1}{2}\hat{n}\cdot J_{0,g} - \frac{3}{16}\Phi_{2,g} = 0 \tag{8}$$

$$-\frac{3}{80}\Phi_{0,g} \pm \frac{1}{2}\hat{n}\cdot J_{2,g} + \frac{21}{80}\Phi_{2,g} = 0 \tag{9}$$

where

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

Finally, multiplying equations 5 and 6 by a test function and integrating over the domain yields the weak form of the equations modularized into kernels by Cerberus. For brevity, we will not display the derivation of the kernels here. Such procedure is standard in weighted residual methods and can be found in [8] or any finite elements book [10].

RESULTS

This section presents several numerical results that validate Cerberus' calculation scheme. The following sections discuss the results of a one group exercise and describe the results of a two-dimensional(2D) and a 3D configuration of the C5 MOX Benchmark [11].

One group 2D problem

This section describes a one group, isotropic-scattering eigenvalue problem introduced by Brantley and Larsen [5]. This section also presents the eigenvalue obtained with Cerberus and compares it against the reference value. Figure 1 shows the problem's geometry, in which the fuel plates have a 1 cm-thickness, the distance between them being 2 cm. Due to the problem's symmetry, the model included only a quarter of the core. Using the *Gmsh* [12] meshing tool, we created the mesh, which had 6×10^3 elements. The problem cross-sections can be found in [5]. The simulation convergence criterion was 10^{-8} for the neutron flux. Table I compares the eigenvalue obtained with Cerberus and the reference value from Brantley and Larsen [5].

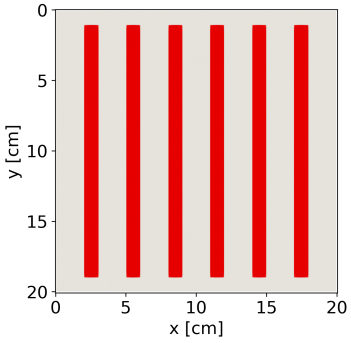

Fig. 1: Geometry of the one group eigenvalue problem. Fuel in red. Moderator in gray.

k_{Ref}	k_{SP_3}	Δ_ρ [pcm]
0.79862	0.79854	12

TABLE I: Comparison between the result obtained with Cerberus and the reference result for the one group eigenvalue problem.

C5G2 2D Benchmark

The open literature describes different versions and extensions of the C5 MOX benchmark, originally introduced by Cavarec et al. in 1994 [11]. The Organisation for Economic Co-operation and Development (OECD)/Nuclear Energy Agency (NEA) developed this benchmark to validate methods and identify their strengths, limitations, and accuracy, and suggest needs for method development. This section describes the benchmark exercise and presents Cerberus results.

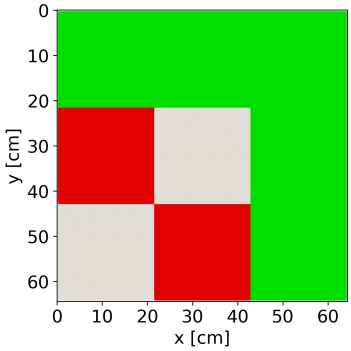

Fig. 2: C5 MOX Benchmark configuration. UO_2 assembly in gray. MOX assembly in red. Reflector in green.

Two types of fuel assembly (MOX and UO_2) and a reflector comprise the core, shown in Figure 2. Due to the problem's symmetry, the model included only a quarter of the core. Each fuel assembly consists of a 17×17 array of squared pin cells, as displayed in Figure 3. The dimensions of each pin cell are 1.26×1.26 cm, being 21.42×21.42 cm the dimensions of each assembly. The benchmark [11] specifies the cross-sections, which have a two-energy group structure.

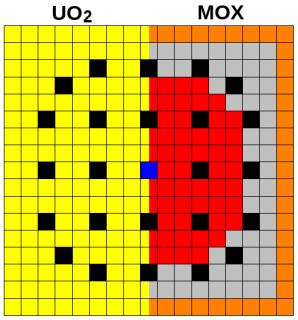

Fig. 3: Structure of the UO_2 and MOX assemblies. UO_2 in yellow, 8.7% MOX in red, 7% MOX in gray, 4.3% in orange, guide tubes in black, and fission chamber in blue.

When no anisotropic component of the scattering cross-section is available, the benchmark recommends applying the diagonal transport correction

$$D_{0,g} = \frac{1}{3\Sigma_{tr,g}} \tag{10}$$
$$\Sigma_{tr} = \Sigma_{t,g} - \bar{\mu}_g \Sigma_{s0,g}$$

where

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

$\bar{\mu}_g$ = group g average cosine deviation angle.

For the sake of comparison, we conducted the exercise with and without the transport correction for calculating $D_{0,g}$ with equations 10 and 7, respectively. The mesh had 2.4×10^4 elements. The simulation convergence criterion was 10^{-8} for the neutron flux.

Table II compares the eigenvalues obtained with Cerberus and the references. For the method without correction, we used a reference value from Capilla et al. [4] as they conducted the exercise without correction. For the method with transport correction, we used the reference value from the benchmark [11].

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

TABLE II: Comparison between the results obtained with Cerberus using no correction (equation 7), the transport correction (equation 10), and the reference results for the C5 MOX Benchmark.

The results obtained Cerberus solver are within 145 pcm of the reference values. However, the difference between the reference values of the different schemes is 3535 pcm, suggesting that the use of the transport correction is necessary.

The next step was to calculate the pin power distribution, and for conciseness, we only calculated it using the transport correction. Figure 4 shows the relative difference to the reference of the pin power distribution calculated with Cerberus. We present this result only for the MOX assembly located in the lower right of Figure 2, as it had the largest relative errors. The largest relative error is 1.88%.

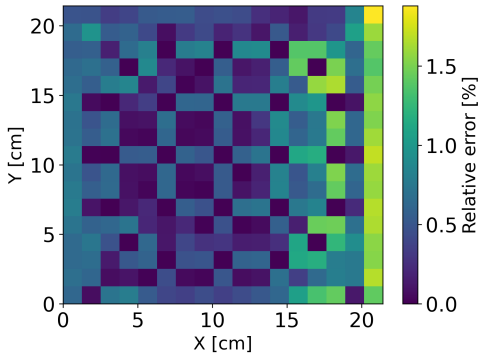

Fig. 4: Relative difference to the reference values in [11] of the power distribution in the lower-right MOX assembly of the C5 MOX Benchmark.

C5G2 3D BENCHMARK

As mentioned earlier, the open literature describes different versions of the C5 MOX benchmark. Ryu et al. [8] defined a 3D mini-core variation of the C5 MOX Benchmark with spatial homogenization of the fuel assemblies. The radial and axial layout of the core are shown in Figures 2 and 5. This section uses the results in Ryu et al. as a reference.

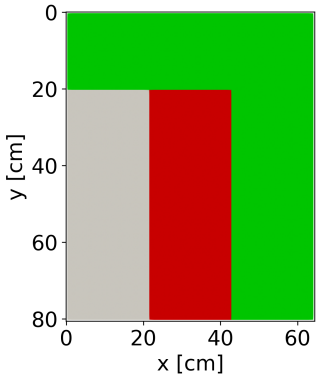

Fig. 5: Axial layout of the C5G2 3D Benchmark. UO_2 assembly in gray. MOX assembly in red. Reflector in green.

Ryu et al. calculated and presented the two-group assembly homogenized cross-sections for this exercise. Because the data was missing the self-scattering cross-sections, we calculated it by volume averaging the cross-sections from the C5G2

2D Benchmark [11]. The mesh had 1.1×10^5 elements. The simulation convergence criterion was 10^{-8} for the neutron flux. Table III compares the eigenvalue obtained with Cerberus to the reference value.

k_{Ref}	k_{SP_3}	Δ_ρ [pcm]
0.91974	0.91979	6

TABLE III: Comparison between the result obtained with Cerberus and the reference result for the C5G2 3D benchmark problem in [8].

Figure 6 displays the power distribution and the relative difference to the reference provided by Ryu et al. [8]. The results of the power distribution are within 1% difference.

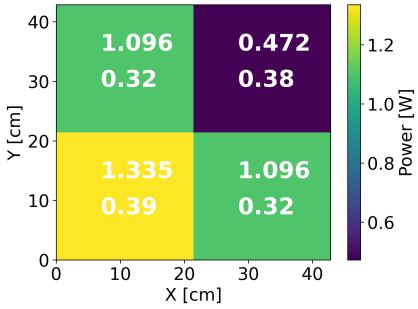

Fig. 6: Power distribution in the C5G2 3D Benchmark. Top: power distribution. Bottom: relative difference to reference values expressed in %.

CONCLUSIONS

MOOSE is a computational framework that solves systems of nonlinear differential equations. As part of this work, we developed the MOOSE-based application Cerberus to solve the steady-state multi-group SP_3 equations. Additionally, we validated Cerberus' calculation scheme by carrying out three exercises whose reference results were known. The first and second exercises solved 2D eigenvalue problems with results within 12 and 145 pcm, respectively. For the second exercise, we calculated the pin-by-pin power distribution and its relative error was within 2% error. The third exercise solved a 3D eigenvalue problem with a result within 6 pcm from the reference. The calculation of the power distribution yielded results within 1% of the reference.

Cerberus is an application with great potential for further development. While the SP_3 equations solve the neutronics in a nuclear reactor, future work may develop other applications to solve the thermal-fluids or integrate Cerberus into existing applications. MOOSE-based applications share the same API making their integration straightforward.

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