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The Even-Parity Simplified S_N Equations Applied to a MOX Fuel Assembly Benchmark Problem on Distributed Memory Environments

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Criticality calculations for nuclear reactors design are usually performed using the diffusion equation with homogenized cross-sections. The diffusion approximation yields accurate results for problems where the particles flux present a weak angular dependency. However, reactor cores loaded with Mixed Oxide (MOX) fuel assemblies are characterized by strong absorption in the thermal range due to Pu-239 and the interface between fuel and moderator introduces strong angular dependencies in the flux. Because of these aspects, the diffusion equation presents low accuracy. To address this problem, we have investigated the accuracy of the Even-Parity Simplified S_N (EP-SS_N) equations. The EP-SS_N equations allow for higher order angular dependencies, therefore it is expected that the methodology will be more accurate compared to the diffusion model for problems characterized by strong transport effects such as MOX loaded reactor cores.

This paper discusses a new general 3-D parallel code, PENSS_N (Parallel Environment Neutral-particle Simplified S_N), based on the multigroup even-parity form of the SS_N equations. Further, it will present the results obtained for a MOX benchmark problem proposed by OECD/NEA and estimate the accuracy of the EP-SS_N equations compared with the reference Monte Carlo predictions.

KEYWORDS: Reactor Physics, MOX fuel, High Performance Computing, Simplified S_N Equations

1. Introduction

The power distribution and its associated criticality eigenvalue are fundamental quantities in the design and optimization of nuclear reactor cores. The accuracy of the fuel pin power distribution impacts the safety assessment of a core fuel loading, because it is required in the determination of the peak linear heat generation and the Departure from Nucleate Boiling Ratio (DBNR). Currently, the power distribution is calculated using the diffusion equation with homogenized cross sections, and for problems where the particles flux presents weak angular dependencies. However, nuclear reactor cores loaded with Mixed Oxide (MOX) fuel assemblies present a challenge for the diffusion equation due to the presence of strong neutron absorbers, such as Pu-239. In addition, the solution obtained with the diffusion equation is characterized by low accuracy if homogenization techniques are not employed. The main difficulty posed by heterogeneous core configurations is a higher angular dependency introduced by interfaces between fuel and moderator. Recently the OECD/NEA has proposed a benchmark problem [1] to test the current capabilities of modern transport codes to treat such reactor core problems without spatial homogenization.

We have investigated the accuracy of the Even-Parity Simplified S_N (EP-SS_N) equations using a 2-D configuration of the MOX benchmark problem. The EP-SS_N equations are a higher order approximation of the linear Boltzmann equation; they are characterized by an

elliptic operator and allow for higher order angular dependencies compared to the diffusion equation [2]. We derived the EP-SS_N equations starting from the 1-D discrete ordinates (S_N) equations in Cartesian geometry; the equations are discretized with a finite-volume approach and the resulting system of equations is solved with the Conjugate Gradient (CG) method [3]. We implemented the EP-SS_N equations into a new computer code named $PENSS_N$ (Parallel ENvironment Simplified S_N). The code solves the multigroup formulation of the EP-SS_N equations with anisotropic scattering of arbitrary order for fixed source and criticality eigenvalue problems. $PENSS_N$ is designed for distributed memory architectures; the parallelization is achieved through spatial, angular and hybrid (spatial/angular) domain decomposition strategies.

In this paper we present the results obtained for the MOX benchmark problem using the $PENSS_N$ code. We will compare the accuracy of the criticality eigenvalue and pin-power distribution with the reference Monte Carlo predictions. Further, we will discuss the performance of the code.

The remainder of this paper is organized as follows: Section 2 discusses the derivation of the EP-SS_N equations and their implementation on distributed memory architectures; Section 3 presents the 2-D MOX benchmark problem, the numerical results, computational time and memory required by the $PENSS_N$ code. Section 4 concludes this paper with some considerations for future work.

2. The Even-Parity Simplified S_N (EP-SS_N) Equations

2.1 Derivation of the EP-SS_N equations with anisotropic scattering

In a previous paper, we addressed the derivation of the EP-SS_N equations for the isotropic scattering case. In this section, we derive the multigroup EP-SS_N equations considering an anisotropic scattering kernel and isotropic external source, starting from the 1-D S_N equations in Cartesian geometry given by

$$\mu_m \frac{\partial \psi(x,\mu_m)}{\partial x} + \sigma_t(x)\psi(x,\mu_m) = Q(x,\mu_m) \quad \text{for m=1, N/2} \tag{1}$$

where,

$$Q(x,\mu_m) = \sum_{l=0}^{L} \frac{2l+1}{2}\sigma_{sl}(x)\phi_l(x)P_l(\mu_m) + \frac{S_0(x)}{2} + q_f(x) \tag{2}$$

and,

$$q_f(x) = \frac{1}{k}\nu\sigma_f(x)\phi_0(x) \qquad \phi_l(x) = \sum_{m=1}^{N/2} w_m P_l(\mu_m)\psi(x,\mu_m) \tag{3}$$

The 1-D S_N quadrature set is selected as roots and weights of the P_N Gauss-Legendre quadrature formula; the weights are normalized to unity. In Eqs. 4 and 5, we define the even- and odd-parity angular fluxes, respectively.

$$\psi_m^E = \frac{1}{2}\left[\psi(x,\mu_m) + \psi(x,-\mu_m)\right] \tag{4}$$

$$\psi_m^O = \frac{1}{2}\left[\psi(x,\mu_m) - \psi(x,-\mu_m)\right] \tag{5}$$

Using Eqs. 4 and 5 in Eq. 1, we obtain coupled equations for even and odd angular fluxes given by

$$\mu \frac{\partial}{\partial x}\psi_m^O(x) + \sigma_t(x)\psi_m^E(x) = \sum_{l=0,2,\ldots}^{L-1}(2l+1)\sigma_{sl}(x)P_l(\mu_m)\phi_l(x) + q_f(x) + S_0(x) \tag{6}$$

$$\mu \frac{\partial}{\partial x}\psi_m^E(x) + \sigma_t(x)\psi_m^O(x) = \sum_{l=1,3,\ldots}^{L}(2l+1)\sigma_{sl}(x)P_l(\mu_m)\phi_l(x) \tag{7}$$

Solving for the odd-parity angular fluxes from Eq. 7.

$$\psi_m^O(x) = \frac{1}{\sigma_t(x)}\left[-\mu \frac{\partial}{\partial x}\psi_m^E(x) + \sum_{l=1,3,\ldots}^{L}(2l+1)\sigma_{sl}(x)P_l(\mu_m)\phi_l(x)\right] \tag{8}$$

And eliminating the odd-parity angular fluxes in Eq. 6 leads to

$$-\frac{\partial}{\partial x}\frac{\mu_m^2}{\sigma_t(x)}\frac{\partial}{\partial x}\psi_m^E(x) + \sigma_t(x)\psi_m^E(x) = \sum_{l=0,2,\ldots}^{L-1}(2l+1)\sigma_{sl}(x)P_l(\mu_m)\phi_l(x) \tag{9}$$

$$-\frac{\mu_m}{\sigma_t(x)}\frac{\partial}{\partial x}\left[\sum_{l=1,3,\ldots}^{L}(2l+1)\sigma_{sl}(x)P_l(\mu_m)\phi_l(x)\right] + q_f(x) + S_0(x) \qquad \text{for m=1,N/2}$$

Finally, we substitute the partial derivative in Eq. 9 with the gradient operator, and we obtain the even-parity simplified Sn (EP-SS_N) equations for the 3-D Cartesian geometry given by

$$-\vec{\nabla}\cdot\frac{\mu_m^2}{\sigma_t(x)}\vec{\nabla}\psi_m^E(\vec{r}) + \sigma_t(\vec{r})\psi_m^E(\vec{r}) = \sum_{l=0,2,\ldots}^{L-1}(2l+1)\sigma_{sl}(\vec{r})P_l(\mu_m)\phi_l(\vec{r}) \tag{10}$$

$$-\frac{\mu_m}{\sigma_t(\vec{r})}\vec{\nabla}\cdot\left[\sum_{l=1,3,\ldots}^{L}(2l+1)\sigma_{sl}(\vec{r})P_l(\mu_m)\phi_l(\vec{r})\right] + q_f(\vec{r}) + S_0(\vec{r}) \qquad \text{for m=1,N/2}$$

The multigroup EP-SS_N equations are given by

$$-\vec{\nabla}\cdot\frac{\mu_m^2}{\sigma_{t,g}(x)}\vec{\nabla}\psi_{m,g}^E(\vec{r}) + \sigma_{t,g}(\vec{r})\psi_{m,g}^E(\vec{r}) = \sum_{g'=1}^{G}\sum_{l=0,2,\ldots}^{L-1}(2l+1)\sigma_{sl,g'\to g}(\vec{r})P_l(\mu_m)\phi_{l,g'}(\vec{r}) \tag{11}$$

$$-\frac{\mu_m}{\sigma_{t,g}(\vec{r})}\vec{\nabla}\cdot\left[\sum_{g'=1}^{G}\sum_{l=1,3,\ldots}^{L}(2l+1)\sigma_{sl,g'\to g}(\vec{r})P_l(\mu_m)\phi_{l,g'}(\vec{r})\right] + q_{f,g}(\vec{r}) + S_{0,g}(\vec{r})$$

for m=1,N/2

The vacuum boundary conditions for the EP-SS_N equations are obtained by setting the incoming angular flux on the boundary surface equal to zero, as follows

$$\psi(x_b, -\mu_m) = \psi^E(x_b, \mu_m) - \hat{n}\cdot\psi^O(x_b, \mu_m) = 0 \tag{12}$$

Hence, the boundary even-parity angular flux is given by

$$\psi^E(x_b, \mu_m) = \hat{n}\cdot\psi^O(x_b, \mu_m) \tag{13}$$

The EP-SS_N equations are discretized with a standard finite-volume approach. For brevity, this derivation is omitted, but interested readers should consult Ref. 3 which discusses the use of the Conjugate Gradient method for solving the resulting system of equations.

2.2 Implementation of the EP-SS_N equations on distributed memory architectures

We implemented EP-SS_N equations described above in a new code, PENSS_N (Parallel ENvironment Simplified S_N). The code solves the multigroup EP-SS_N equations with

anisotropic scattering of arbitrary order for fixed source and criticality problems. The code is designed for distributed memory architectures using the Message Passing Interface (MPI) [4]. The parallel algorithms implemented are angular, spatial and hybrid (spatial/angular) domain decompositions.

In order to parallelize the EP-SS_N equations, we partition the spatial domain into a number of coarse meshes and allocate them to different processors. Similarly, the angular domain is partitioned by allocating individual directions or groups to each processor. The hybrid spatial and angular domain decomposition allows for simultaneous processing spatial and angular subdomains. Once the system is partitioned and the parallel vector is specified, the $PENSS_N$ code proceeds to sequentially allocate different sub-domain onto different processors, generating a so-called virtual topology. It is worth noting that the $PENSS_N$ code achieves complete memory parallelization by allocating every array as a local variable.

Figure 1 shows the virtual topology for a hybrid domain decomposition with 4 spatial and 2 angular subdomains.

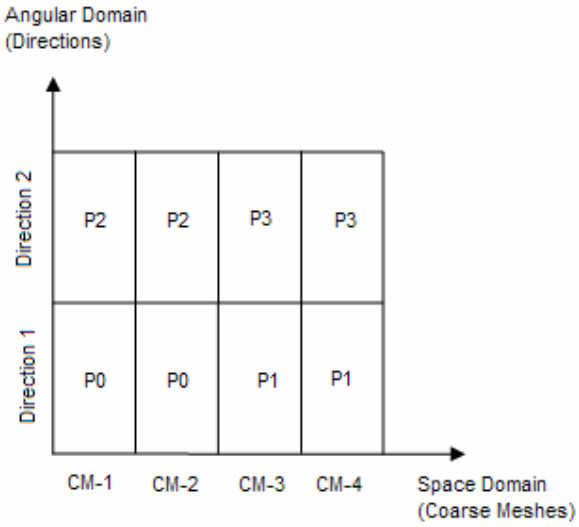

Fig. 1 Virtual topology generated by the $PENSS_N$ code on four processors (P0, P1, P2, P3).

3. The 2-D MOX Fuel Assembly Benchmark Problem

We have considered the 2-D configuration of the MOX fuel assembly benchmark problem proposed by the OECD/NEA [1]. The benchmark was proposed to test the capabilities of modern deterministic transport methods and codes to treat reactor core problems without spatial homogenization.

The benchmark geometry consists of sixteen fuel assembly (quarter core symmetry); the overall dimensions of the problem are 64.26 cm x 64.26 cm, while each assembly measures 21.42 cm x 21.42 cm. Figure 2 shows the geometry configuration and the material distribution; vacuum boundary conditions are prescribed at x=64.26 cm and y=64.26 cm, and reflective at x=0.0 cm and y=0.0 cm. A seven-group, transport corrected cross sections, with isotropic scattering cross-section set is provided for UO_2 fuel, MOX fuel with three different enrichments, guide tubes, fission chambers and moderator.

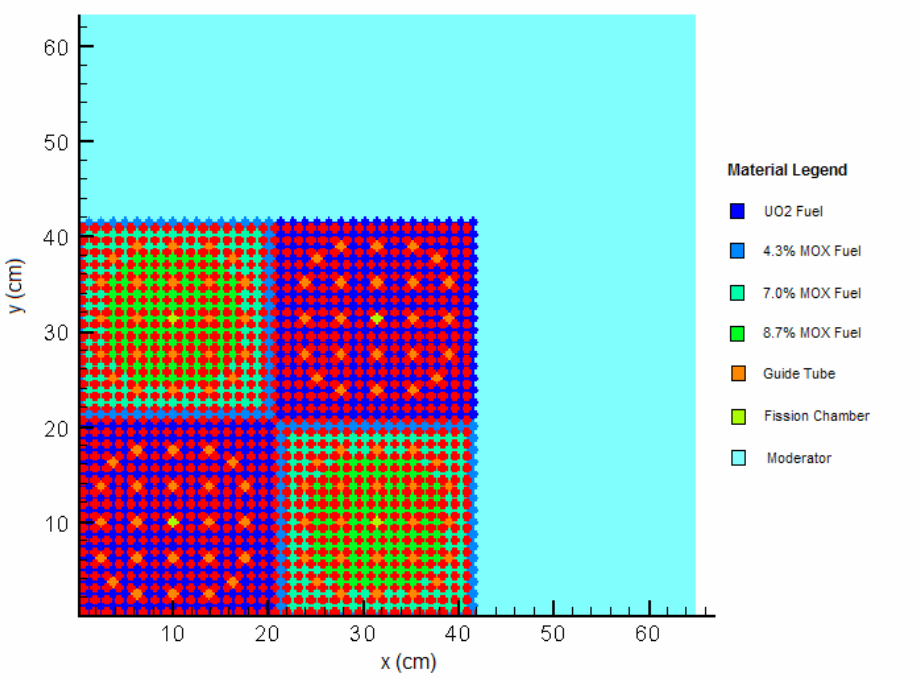

Fig. 2 Geometry and material distribution for the benchmark problem.

The fuel pins have been discretized with 5x5 and 7x7 fine meshes and the problem has been solved with the EP-SS_2 equation (diffusion model) and the EP-SS_4. Table 1 shows the criticality eigenvalues obtained with different EP-SS_N methods.

Table 1 $PENSS_N$ calculated eigenvalues for different Sn orders.

Fine mesh[a]	EP-SS_2	EP-SS_4
5x5	1.20989	1.20498
7x7	1.19549	1.19393

(a) Fuel pin fine mesh discretization.

Table 2 gives the relative difference (PCM) between $PENSS_N$ results and the reference MCNP calculated eigenvalue of 1.18655±0.003.

Table 2 Comparison of $PENSS_N$ eigenvalues to the reference MCNP prediction.

Fine mesh[a]	PCM (S_2)	PCM (S_4)
5x5	1967.05	1553.24
7x7	753.44	621.97

(a) Fuel pin fine mesh discretization.

Table 2 indicates that $PENSS_N$ with higher quadrature order and smaller meshes yields closer agreement with the Monte Carlo results.

In Table 3, we have represented the maximum and minimum normalized pin power obtained with the $PENSS_N$ code, using a 7x7 fine mesh discretization of the fuel pin.

Table 3 Maximum and minimum normalized pin power obtained with PENSS$_N$.

Method	MAX power	MIN power
EP-SS$_2$	2.490	0.240
EP-SS$_4$	2.493	0.238
MCNP Ref.	2.498	0.23

The results in Table 3 confirm that the higher order EP-SS$_4$ equations also yield better accuracy for maximum and minimum pin power. The EP-SS$_2$ equations yield a -0.32% and 4.35% relative differences for maximum and minimum pin-power values, respectively; while the EP-SS$_4$ reduces the relative differences to -0.2% and 3.26%, respectively. For demonstration, in Figure 3, we show the pin-power distribution obtained with the EP-SS$_4$ equations and a 7x7 fuel pin discretization.

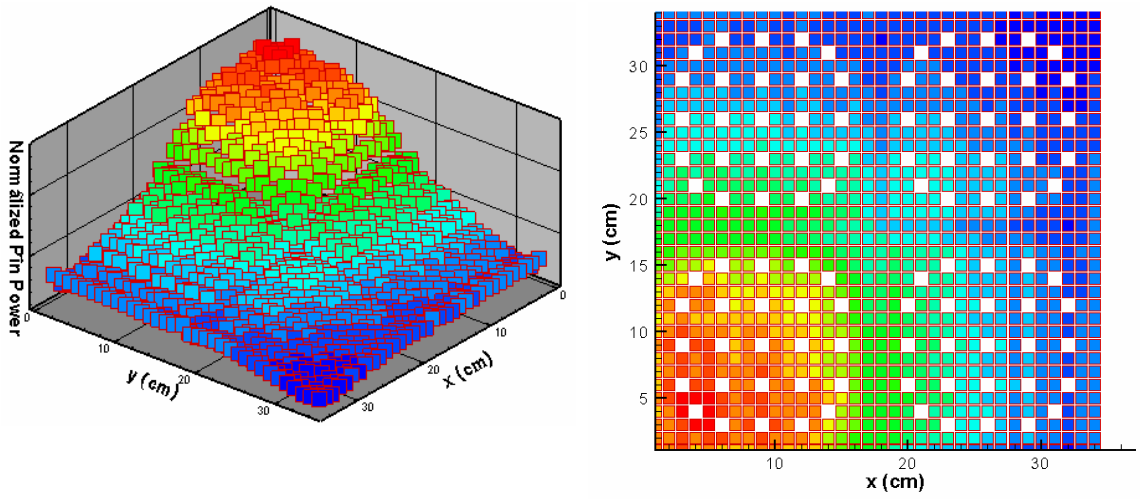

Fig. 3 Pin power distribution for the MOX fuel assemblies obtained with the EP-SS$_4$ equations.

All the PENSS$_N$ calculations were performed on an 8-node PC-Cluster, which uses Dual Intel Pentium Xeon 2.4 GHz processors, 1 GBit/sec CISCO switch and ~4 GBytes of memory per processor. Table 4 givess the computational time and the memory required for this problem using 9 processors

Table 4 Computational time and memory required for the simulation on 9 processors.

	Computational Time (minutes)		Memory required (Mbytes/Processors)	
Fine mesh	**EP-SS$_2$**	**EP-SS$_4$**	**EP-SS$_2$**	**EP-SS$_4$**
5x5	37.7	50.3	11.3	15.6
7x7	68.1	151.5	21.8	30.3

The memory requirement for EP-SS_4 compared to EP-SS_2 increases by only 38% and 39% for the 5x5 and 7x7 fuel pin discretizations, respectively. Note that the computational time shown here has been obtained by running the code on a non-dedicated machine; hence, the effective performance of the code cannot be assessed at this moment.

4. Summary

We have developed a 3-D parallel simplified even-party Sn code with anisotropic scattering capability The $PENSS_N$ code allows for hybrid spatial and angular domain decomposition We have demonstrated that the higher order EP-SS_N methods yields relatively accurate results for the 2-D MOX fuel assembly benchmark problem considered. Because of the heterogeneous configuration of the problem, a fine discretization of the fuel pin is required in order to obtain to improve the accuracy of results. Also, it is concluded that the EP-SS_4 equations yields more accurate solutions compared to the diffusion equation for both criticality eigenvalues and pin-power distribution. Currently, we are examining the performance of the $PENSS_N$ code in a dedicated environment, and examine the limitations of the EP-SS_N formulations.

References

1) Benchmark on Deterministic Transport Calculations Without Spatial Homogenisation, OECD/NEA.
2) G. Longoni, G. Sjoden, and A. Haghighat, "Development and Applications of the SP_L Methodology for a Criticality Eigenvalue Benchmark Problem," Proc. Conf. of the Nuclear Mathematical and Computational Sciences, M&C 2003, Gatlinburg, TN, USA, (2003).
3) J. H. Ferziger and M. Peric, "Computational Methods for Fluid Dynamics," Springer Verlag, Berlin, Germany (1999).
4) W. Gropp, E. Lusk and A. Skjellum, "Using MPI: Portable Parallel Programming with the Message-Passing Interface," The MIT Press, Cambridge Massachussets (1999).