# The Impact of Spatial Self-Shielding on Pin-wise Reaction Rates

William Boyd, Benoit Forget, Kord Smith

Massachusetts Institute of Technology, Department of Nuclear Science and Engineering, 77 Massachusetts Avenue, Building 24, Cambridge, MA 02139, United States

#### **Abstract**

Keywords: Multi-group cross-sections, spatial homogenization, spatia self-shielding

#### 1. Introduction

The nuclear reactor physics community has long strived for deterministic neutron transport-based tools for whole-core reactor analysis. A key challenge for whole-core multi-group transport methods is accurate reactor agnostic multi-group cross section (MGXS) generation. The MGXS generation process applies a series of approximations to produce spatially homogenized and energy condensed MGXS in each spatial zone and energy group. Many approximations related to multi-group theory, including the selection of discretized energy group structures and the truncation of the Legendre expansion of the multi-group scattering kernel, are widely studied in the literature. However, the practical impact of the flux separability approximation, which permits the use of the scalar rather than the angular neutron flux to weight the continuous energy cross sections, is less understood. This paper investigates the flux separability approximation and quantifies its significance for heterogeneous PWR problems.

This work employs Monte Carlo (MC) neutron transport simulations to generate MGXS. Monte Carlo methods have increasingly been used to generate few group constants for coarse mesh diffusion, most notably by the Serpent MC code (Leppänen, 2013), and to a much lesser extent, for high-fidelity neutron transport methods (Redmond, 1997; Nelson, 2014; Cai, 2014; Boyd, 2016). The advantage of a MC-based approach is that all of the relevant physics are directly embedded into MGXS by weighting the continuous energy cross sections with a statistical proxy to the "true" neutron flux. However, this paper shows that even when the "true" scalar flux is used to generate MGXS, the flux separability approximation results in a non-negligible eigenvalue bias between continuous energy and multi-group calculations due to underprediction of U-238 capture in resonance energy groups.

The content in this paper is organized as follows.

# 2. Methodology

### 2.1. Continous Energy Calculations with OpenMC

-OpenMC Romano and Forget (2013) -Python API Boyd et al. (2016a) -NNDC data National Nuclear Data Center,

Brookhaven National Laboratory (2016) -distribcell tallies Lax et al. (2014) -openmc.mgxs -tallied in CASMO's seventy energy group structure Rhodes et al. (2006) -iso-in-lab -runtime parameters: -num. particles, batches -computer hardware

# 2.2. Multi-Group Calculations with OpenMOC

-OpenMOC Boyd et al. (2014) -multi-core parallelism Boyd et al. (2016b) -runtime parameters: -azim angles, spacing -num. FSRs -CMFD energy and spatial mesh -computer hard-ware

### 2.3. Pin-wise Spatial Homogenization Schemes

-from Sec. 8.2 -focus less on introducing these as "schemes" per se -rather two spatial self-shielding models to quantify approx. error

# 2.3.1. Null Homogenization

-from Sec. 8.2.2

### 2.3.2. Degenerate Homogenization

-from Sec. 8.2.3

-OpenCG region differentiation Boyd et al. (2015)

#### 3. Test Cases

-Benchmarks for Evaluation and Validation of Reactor Simulations (BEAVRS) Horelik et al. (2013)

-need to describe both pinwise fissoin rates and U-238 capture rates -latter papers can cite this one as reason to only analyze capture rates?

- 3.1. Benchmark Configurations
- 3.2. Single Fuel Assembly
- 3.3. Reflected Assembly Colorset
- 3.4. Verification Metrics

-reference results generated with OpenMC simulations (Sec. 7.3) -eigenvalues -pin-wise fission rates -pin-wise U-238 capture rates -iso-in-lab in OpenMC

Email addresses: wboyd@mit.edu (William Boyd), bforget@mit.edu (Benoit Forget), kord@mit.edu (Kord Smith)

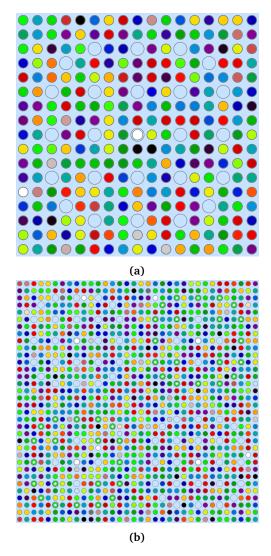


Figure 1. OpenMOC materials for the (a) assembly and (b)  $2\times 2$  colorset models with degenerate homogenization.

Table 1. Reference OpenMC eigenvalues for each test case.

Assembly	Colorset
$0.99326 \pm 0.00001$	$0.94574 \pm 0.00001$

# 4. Results

# 4.1. Eigenvalues

In the results that follow, the bias  $\Delta \rho$  compares the eigenvalue  $k_{eff}^{MOC}$  computed by OpenMOC to that of the reference eigenvalue  $k_{eff}^{MC}$  computed by OpenMC in units of pcm:

$$\Delta \rho = \left(k_{eff}^{MOC} - k_{eff}^{MC}\right) \times 10^5 \tag{1}$$

# 4.2. Fission Rates

-add figures of spatial distribution of errors -can I reproduce these plots? Do I have the batchwise.h5 results stored on my external hard drive??? If so, I should customize them for only 70 groups

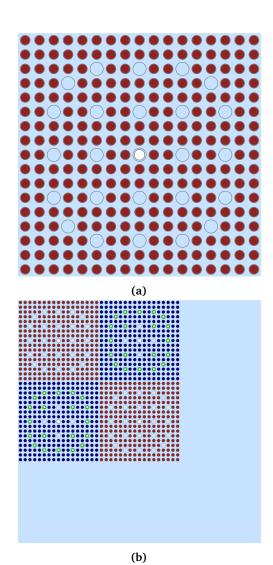


Figure 2. A (a) fuel assembly and (b)  $2{\times}2$  assembly colorset with reflector.

**Table 2.** OpenMOC eigenvalue bias  $\Delta \rho$ .

Benchmark	Null	Degenerate
Assembly	-161	-161
Colorset	-142	-132

Table 3. OpenMOC fission rate percent relative errors.

Benchmark	Metric	Null	Degenerate
Assembly	Max	0.380	0.315
	Mean	0.074	0.079
Colorset	Max	0.764	0.602
	Mean	0.178	0.138

# 4.3. Capture Rates

-add figures of spatial distribution of errors

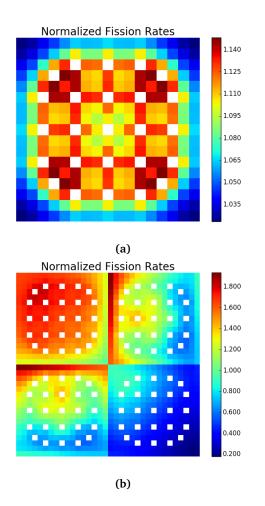


Figure 3. Fission rates for the (a) assembly and (b)  $2\times 2$  colorset.

Table 4. OpenMOC U-238 capture rate percent relative errors.

Benchmark	Metric	Null	Degenerate
Assembly	Max	-1.101	0.386
	Mean	0.479	0.086
Colorset	Max	-1.969	-0.783
	Mean	0.478	0.165

#### 5. Conclusions

# Acknowledgments

This work was supported by the Idaho National Laboratory and the National Science Foundation Graduate Research Fellowship Grant No. 1122374. This research made use of the resources of the High Performance Computing Center at Idaho National Laboratory, which is supported by the Office of Nuclear Energy of the U.S. Department of Energy and the Nuclear Science User Facilities under Contract No. DE-AC07-05ID14517.

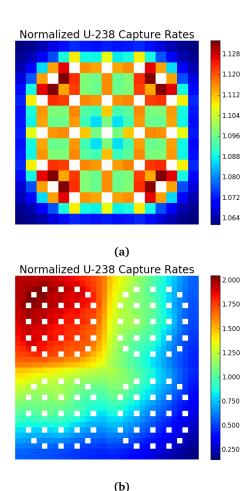


Figure 4. U-238 capture rates for the (a) assembly and (b)  $2\times2$  colorset.

# References

Boyd, W., Forget, B., Smith, K., 2015. OpenCG: A Combinatorial Geometry Modeling Tool for Data Processing and Code Verification. In: Int'l Conf. on Mathematics and Computational Methods Applied to Nuclear Science & Engineering. Nashville, TN, USA.

Boyd, W., Romano, P. K., Harper, S., 2016a. Equipping OpenMC for the Big Data Era. In: PHYSOR. Sun Valley, ID, USA.

Boyd, W., Shaner, S., Li, L., Forget, B., Smith, K., 2014. The OpenMOC Method of Characteristics Neutral Particle Transport Code. Annals of Nuclear Energy 68, 43–52.

Boyd, W., Siegel, A., He, S., Forget, B., Smith, K., 2016b. Parallel Performance Results for the OpenMOC Neutron Transport Code on Multicore Platforms. Int'l Journ. of High Performance Computing Applications.

Boyd, W. R. D., 2016. Reactor Agnostic Multi-Group Cross Section Generation for Fine-Mesh Deterministic Neutron Transport Simulations. Ph.D. thesis, Massachusetts Institute of Technology (submitted).

Cai, L., 2014. Condensation and Homogenization of Cross Sections for the Deterministic Transport Codes with Monte Carlo Method: Application to the GEN IV Fast Neutron Reactors. Ph.D. thesis, Université Paris Sud-Paris

Horelik, N., Herman, B., Forget, B., Smith, K., 2013. Benchmark for Evaluation and Validation of Reactor Simulations (BEAVRS), v1.0.1. In: Int. Conf. Math. and Comp. Methods Applied to Nuc. Sci. & Eng. Sun Valley, Idaho, USA.

Lax, D., Boyd, W., Horelik, N., 2014. An Algorithm for Identifying Unique Regions in Constructive Solid Geometries. In: PHYSOR. Kyoto, Japan.

Leppänen, J., 2013. Serpent – A Continuous-Energy Monte Carlo Reactor Physics Burnup Calculation Code. VTT Technical Research Centre of Fin-

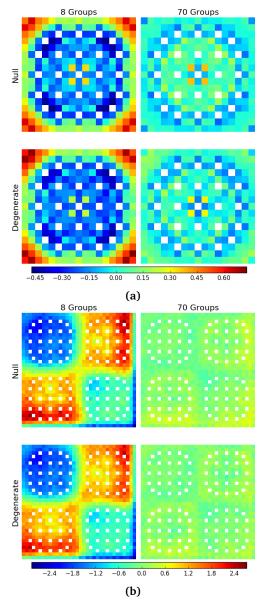


Figure 5. OpenMOC fission rate percent relative errors for the (a) assembly and (b)  $2\times2$  colorset models.

National Nuclear Data Center, Brookhaven National Laboratory, 2016. ENDF/B-VII.1 Evaluated Nuclear Data Library. http://www.nndc.bnl.gov/endf/b7.1/, accessed: 2016-08-09.

Nelson, A., 2014. Improved Convergence Rate of Multi-Group Scattering Moment Tallies for Monte Carlo Neutron Transport Codes. Ph.D. thesis, University of Michigan.

Redmond, E. L., 1997. Multi-Group Cross Section Generation via Monte Carlo Methods. Ph.D. thesis, Massachusetts Institute of Technology.

Rhodes, J., Smith, K., Lee, D., 2006. Casmo-5 development and applications. In: ANS Topical Meeting on Reactor Physics (PHYSOR). pp. 10–14.

Romano, P. K., Forget, B., 2013. The OpenMC Monte Carlo Particle Transport Code. Annals of Nuclear Energy 51, 274–281.

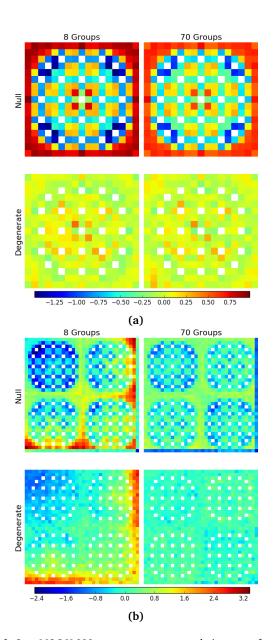


Figure 6. OpenMOC U-238 capture rate percent relative errors for the (a) assembly and (b)  $2\times 2$  colorset models.