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

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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. ... However, the practical impact of ... is less understood. This paper investigates the ... 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.

This paper seeks to identify the bias between continuous energy and multi-group transport methods for MGXS libraries which account for spatial self-shielding effects[1] to varying degrees. In particular, this paper quantifies the difference in the approximation error between simulations in which the same MGXS are used in each unique fuel pin (*e.g.*, each fuel enrichment) and those in which unique MGXS are used in each and every pin. The former case does little if anything to model spatial self-shielding effects, whereas the latter case "fully" resolves these effects, albeit at the expense of very large MGXS libraries.

The content in this paper is organized as follows. Two different schemes for spatial homogenization of pin-wise MGXS are introduced in Sec. 2. The need for a new, more flexible and specialized approach to spatial homogenization which appropriately captures spatial self-shielding effects with minimal computational expense is discussed in Sec. 5.

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

[1] The effects of neighboring pins, burnable poisons, reflectors and the core baffle are each of interest in the context of spatial self-shielding.

2. Methodology

2.1. Continuous 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 hardware

2.3. Pin-wise Spatial Homogenization Schemes

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

This paper employs two different spatial homogenization schemes to model spatial self-shielding effects in MGXS. Although all spatial zones may experience spatial self-shielding, this chapter only models the impact of spatial self-shielding on MGXS in fissile regions. The null and degenerate spatial homogenization schemes are introduced in Sec. 2.3.1 and Sec. 2.3.2, respectively. These schemes model spatial self-shielding for each fuel pin with increasing granularity and complexity. A fuel assembly and 2×2 colorset with reflector model are color-coded by material and illustrated in Fig. 1 for each homogenization scheme.

The `openmc.mgxs` module was used to compute 70-group MGXS with OpenMC for both the assembly and colorset benchmarks. The tallied MGXS data was condensed to coarse 2-group and 8-group structures with downstream data processing as necessary. The OpenMC simulations were performed with 1000 batches with 10^6 particle histories per batch for each benchmark. Stationarity of the fission source was obtained with 100 inactive batches for each benchmark. OpenMC's "iso-in-lab" feature was employed to enable consistent comparisons between OpenMC's reference results and OpenMOC's calculations with an isotropic in lab scattering source.

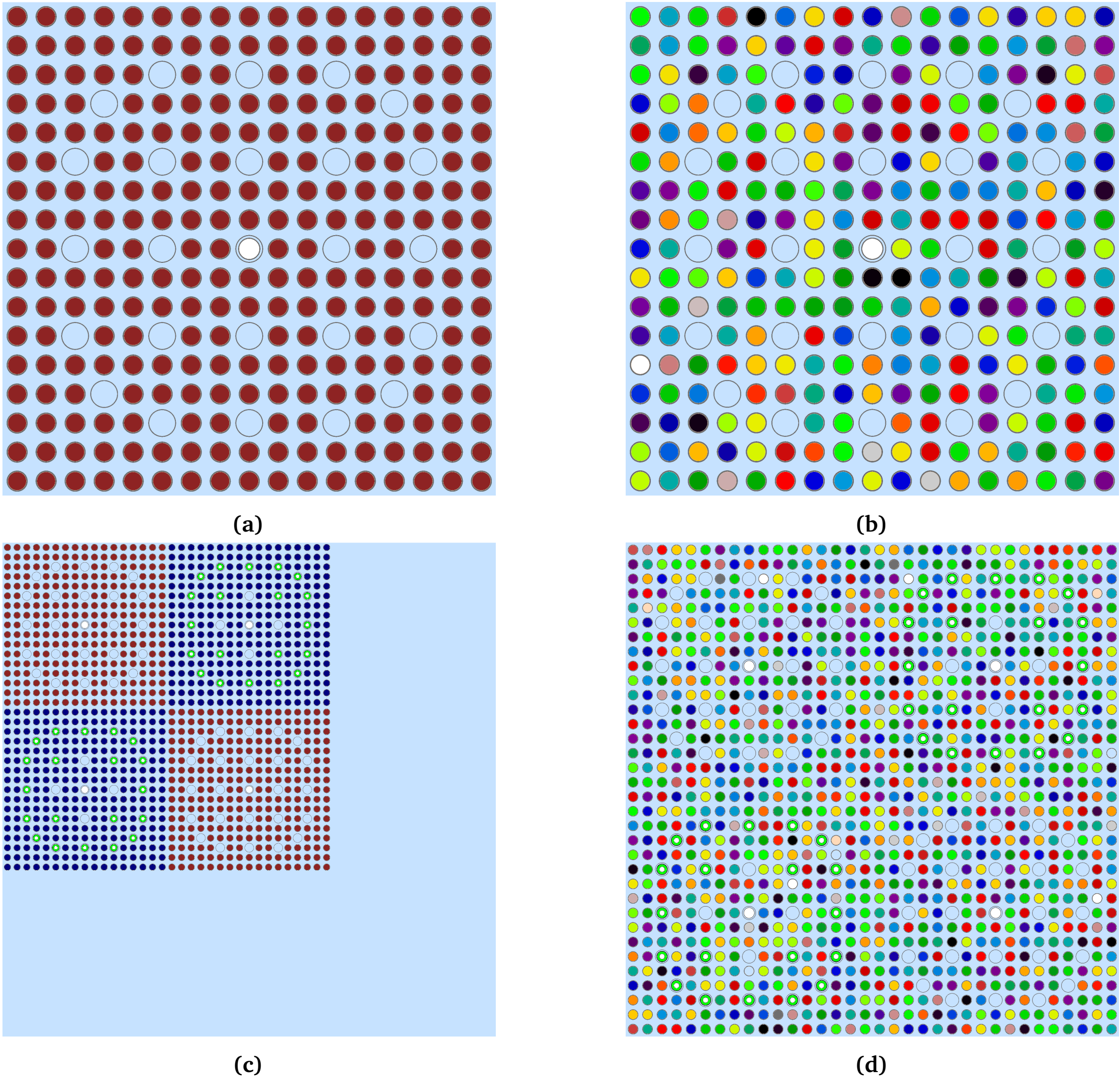


Figure 1. OpenMOC materials for the (a)-(b) assembly and (c)-(d) 2×2 colorset models with null and degenerate homogenization, respectively.

2.3.1. Null Homogenization

The *null* spatial homogenization scheme uses a single Monte Carlo calculation of the complete heterogeneous geometry to generate MGXS for each material. In this way, the null scheme fully abandons the multi-level approach used by most traditional approaches to generate MGXS. The spatially self-shielded flux is used to collapse the cross sections in each material with a unique isotopic composition. The null scheme does not account for spatial self-shielding effects experienced by different fuel pins filled by the same type of fuel, and instead averages these effects across the entire geometry. A single MGXS is employed in each instance of a material zone, such as a fuel pin replicated many times throughout a benchmark geometry.

2.3.2. Degenerate Homogenization

Unlike the null spatial homogenization scheme, the *degenerate* scheme accounts for the different spatial self-shielding effects experienced by each instance of each fuel pin throughout a heterogeneous geometry. Like the null scheme, a single MC calculation of the complete heterogeneous geometry is used to generate MGXS for all materials. Unlike the null scheme, the MGXS are tallied separately for each instance of fissile material zones. For example, if a heterogeneous benchmark includes N fuel pins, then N collections of MGXS are separately tabulated for each fuel pin instance. The degenerate scheme tallies different MGXS even if the isotopic compositions in the fuel pin instances are identical (*e.g.*, fresh fuel at the beginning of life) since each instance may experience different spatial self-shielding effects and hence have different MGXS.

The degenerate scheme generates MGXS for each fuel pin instance using OpenMC's distributed cell tallies (Lax et al., 2014). The OpenCG region differentiation algorithm (Boyd et al., 2015) is used to build a new OpenMOC geometry with unique cells and materials for each fuel pin. The MGXS are appropriately selected from OpenMC's distributed cell tallies to populate the MGXS in the OpenMOC materials. Multi-group transport calculations with MGXS generated using null and degenerate schemes may be compared to quantify the impact of modeling spatial self-shielding effects in MGXS for fissile zones in heterogeneous geometries.

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

Table 1. Reference OpenMC eigenvalues for each test case.

Assembly	Colorset
0.99326 ± 0.00001	0.94574 ± 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:

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

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

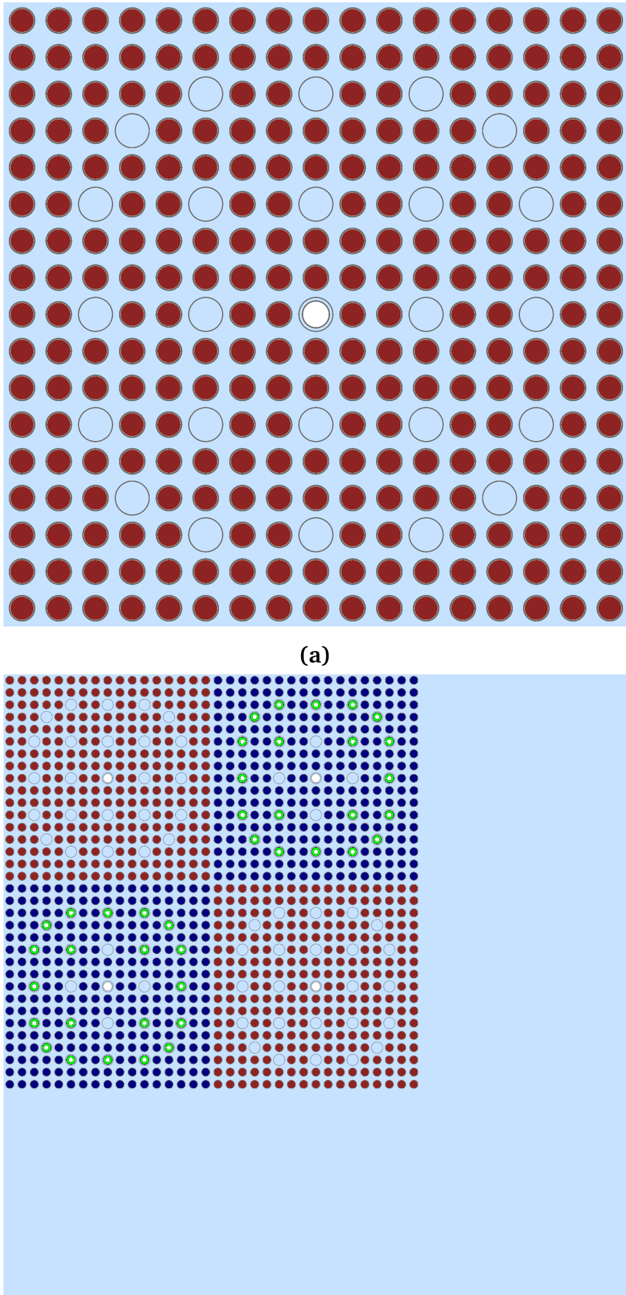
Benchmark	Null	Degenerate
Assembly	-161	-161
Colorset	-142	-132

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

4.3. Capture Rates

-add figures of spatial distribution of errors



(a)

(b)

Figure 2. A (a) fuel assembly and (b) 2×2 assembly colorset with reflector.

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

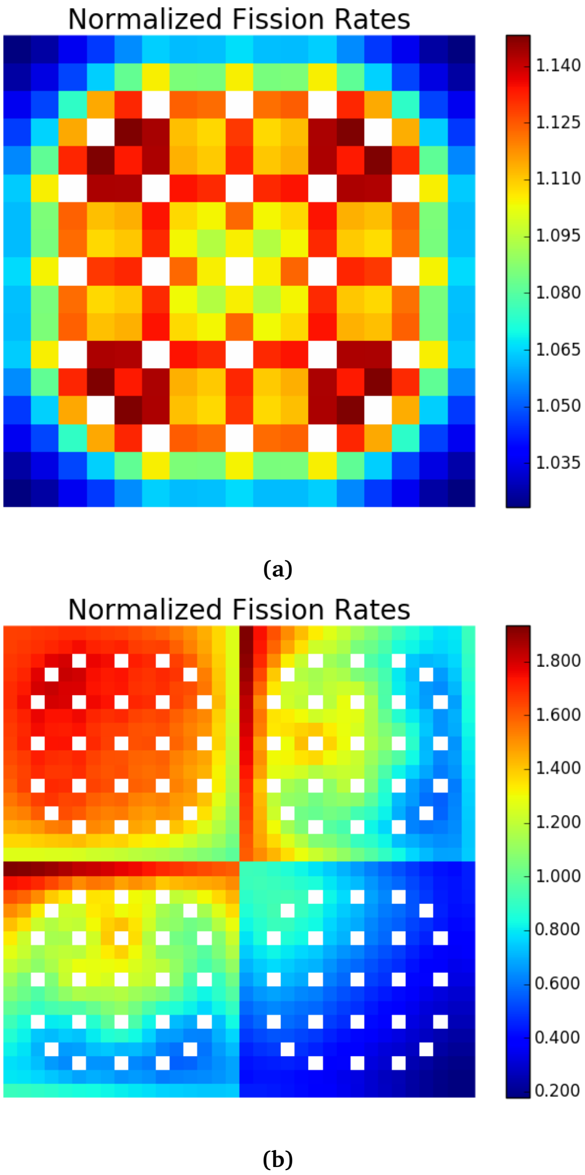


Figure 3. Fission rates for the (a) assembly and (b) 2×2 colorset.

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

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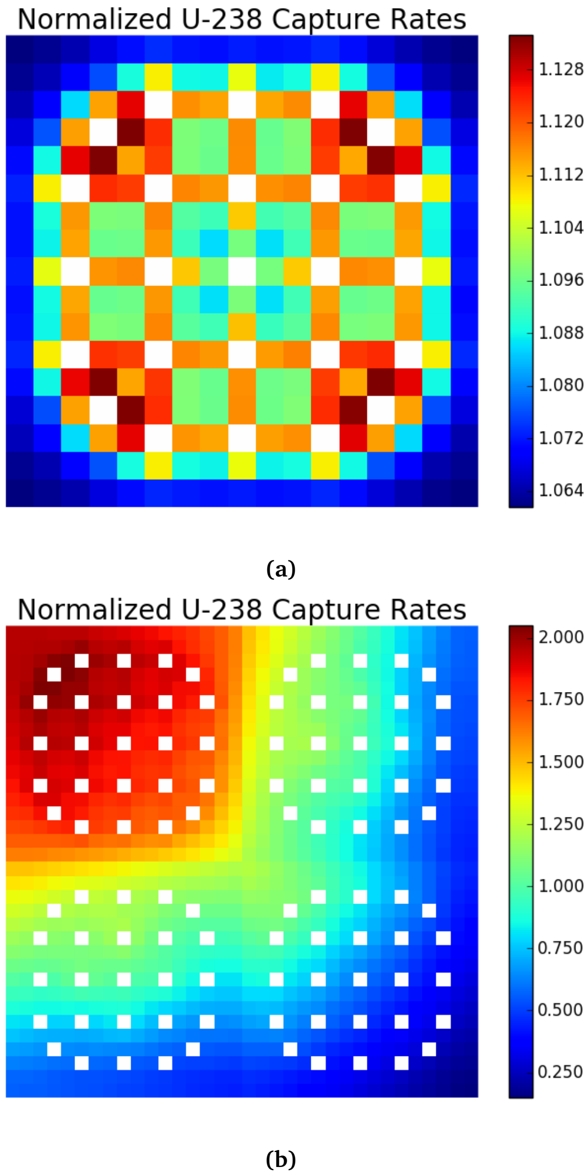

Figure 4. U-238 capture rates for the (a) assembly and (b) 2×2 colorset.

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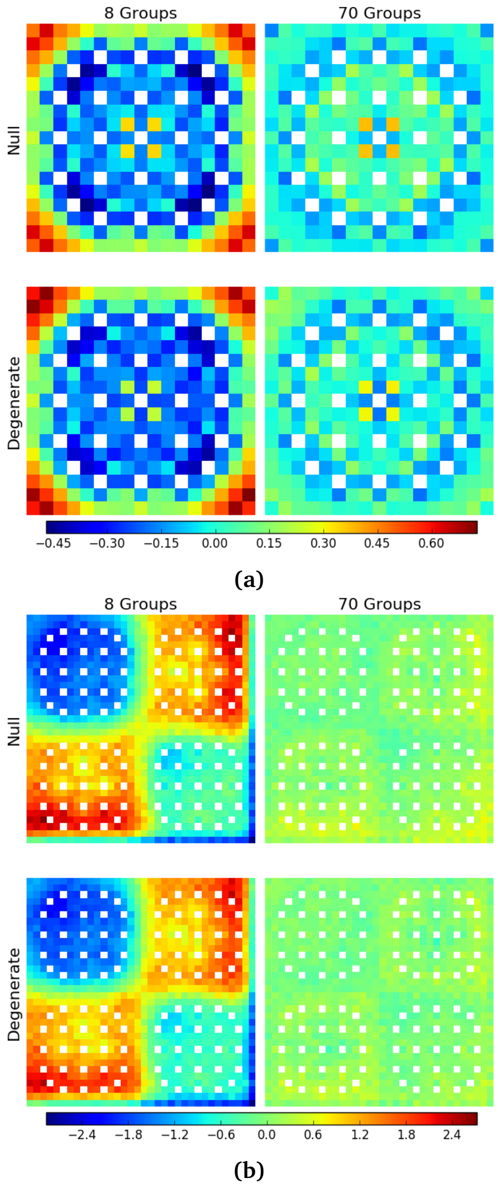

Figure 5. OpenMOC fission rate percent relative errors for the (a) assembly and (b) 2×2 colorset models.

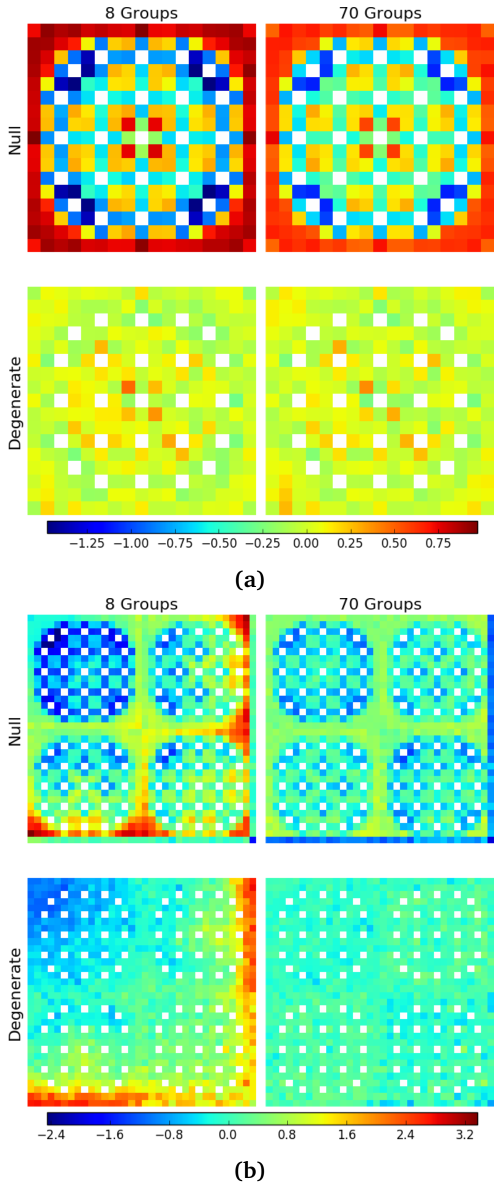

Figure 6. OpenMOC U-238 capture rate percent relative errors for the (a) assembly and (b) 2×2 colorset models.

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