Flexible cross section generation in OpenMC with TOGA (Tool for Optimization and Group-structure Analysis)

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INTRODUCTION

The roll-out of advanced reactors has taken a large leap forward in recent years. Many of the designs being proposed rely on novel feedback mechanisms to deliver negative reactivity in accident scenarios. We need computational tools to model these transient mechanisms. While Monte Carlo has long been the gold standard for reactor modeling, it is often times still very limiting in time-dependent problems. In practice, reactor developers turn to deterministic methods which require multigroup cross sections.

Traditionally, lattice calculations are conducted on pincell models to generate multigroup cross sections. Then, equivalence methods are used to extrapolate those cross sections for full-core models. While this process has been well refined for light water reactors, it is a cumbersome workflow for new reactors, especially during the reactor design phase. Instead, running a Monte Carlo simulation for a portion of a reactor geometry is a much more flexible process. For microreactors, it may even be feasible to generate cross sections for the entire core.

In this work, a tool named TOGA has been developed: Tool for Optimization and Group-structure Analysis. TOGA is a wrapper which runs OpenMC to easily, flexibly, and optimally generate multigroup cross sections in a reactor-agnostic way for fine-mesh multigroup transport applications [1]. In a number of post-processing steps, TOGA identifies the best group structures and Legendre scattering expansion orders on behalf of the user and outputs the final, optimized results in a format readable by the MOOSE software Griffin (formerly Rattlesnake) [2].

METHODS

OpenMC Cross Section Generation Tools

OpenMC is an open-source Monte Carlo neutron and photon transport simulation code [3]. The code supports both continuous-energy and multigroup transport. OpenMC has a very flexible and user-friendly multigroup cross section module which calculates multigroup cross sections during a continuous-energy calculation. Once the multigroup library is populated, it can easily be condensed to coarser energy group structures. Furthermore, the creation of a multi-group input file is automated so that the problem can be re-run with the newly generated multigroup cross sections as a means of determining the difference induced by the new data structure. The final cross sections are output in an HDF5 format [4]. The flexibility of OpenMC's multigroup library makes it ideal for experimental cross section generation.

TOGA users need to install OpenMC and create an input deck for their geometry. A few extra variables are needed in the input file such as the domain over which to generate cross sections. Currently, materials, geometry cells, and rectilinear mesh cells are supported domains. Other settings in TOGA include group structures, Legendre scattering expansion orders, cross section types, optimization choices, plotting options, and parallel computation settings.

During the run, OpenMC creates a multigroup cross section library and all necessary tallies. First, a continuous energy calculation is run to populate the library. This is the most expensive part, especially considering the number of tallies needed to characterize all the cross sections. The OpenMC mgxs module merges tallies as appropriate to reduce the memory burden. Depending on the optimization choices set by the user, a multigroup input file is created, and the simulation is re-run in multigroup mode. Multigroup Monte Carlo is much less costly and can be performed several times in the same time as a single continuous energy run.

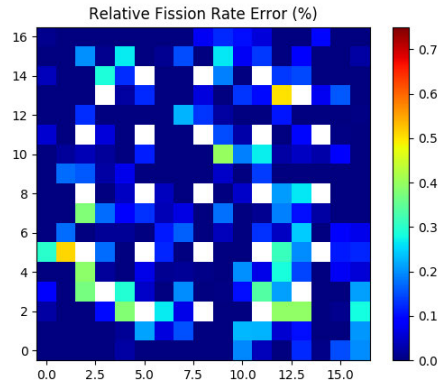

Fig. 1. Fission rate error of a multigroup run in OpenMC for a PWR assembly geometry.

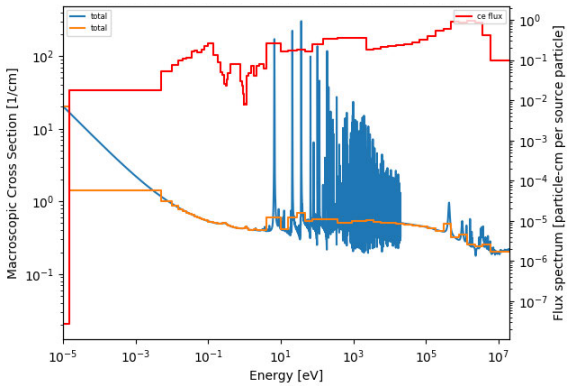

Fig. 2. Continuous energy and multigroup total cross sections in the fuel using a CASMO 70-group structure. In red, the flux tallied in each energy bin.

The "bias" is determined as the difference in k-eff between the continuous energy and multigroup runs. Additional plots can be generated to quantify the error. Figure 1 is an example of spatially distributed error. Figure 2 is a comparison of the cross sections, including a flux profile. Both of these figures are generated automatically for the user in TOGA.

Optimization Routines

Multigroup cross section parameters can be optimized for accuracy as well as efficiency. For instance, a 2-group model will allow for very fast deterministic calculations, but at low-accuracy. TOGA performs a "least-cost" optimization on the group structure and the Legendre scattering expansion order to obtain the best accuracy and efficiency trade-off.

Group Structure

The optimization over energy groups takes as input any number of group structures, as long as they are each subsets of the largest group structure. For example, the CASMO group structures are ideal: there are a large number of group structures between 2 and 70 groups, and the 70-group structure contains all the smaller structures [5]. Other useful sets include the Argonne National Laboratory group structures [6], or the WIMS-69 and APOLLO-99 structures which are each subsets of the XMAS-172 [9]. The WIMS-69 is catered toward thermal reactors [7] and APOLLO-99 is catered toward fast reactors [8]. TOGA includes some of these group structures in the user options and also allows for custom group structures.

The optimization process iteratively condenses the multigroup cross section library and runs OpenMC in multigroup mode to evaluate the difference in k-eff with respect to the continuous-energy run. Figure 3 is an example of this optimization process. In Figure 3, we first notice that even at the largest group structure (70 groups), the bias between the continuous-energy and multigroup OpenMC runs is still over 1000 pcm. This suggests that this reactor is not suited for CASMO groups which work best for light water reactors. Instead, a different group structure should be explored.

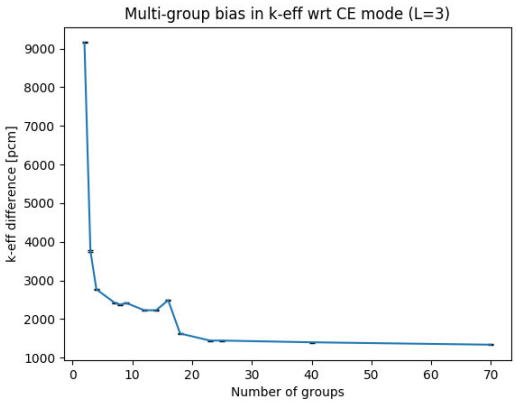

Fig. 3. Bias induced by CASMO groups on a fictitious microreactor geometry, with error bars. The Legendre scattering expansion order is set to 3.

Secondly, we notice that the increase in accuracy is almost asymptotic, but there is an exception at 16 groups. In fact, the 16-group structure appears to perform worse than the 7-, 8-, 9-, 12-, and 14-group structures. An analysis of the group structure boundaries provides a possible explanation. Table I highlights the differences in energy group boundaries in the range of the first several resonances of U-238. Notice that while the 14- and 18-group structures each isolate one of the resonances, the 16-group structure lumps them in with the bulk resonance region. This difference and the performance drop observed are evidence that those resonances are an important source of absorption in this reactor design.

TABLE I. Selected Group Structure Boundaries

Grp. Struc.	Energy group boundaries (eV)				
14 groups	1.15	1.3	4.0	4.8052e1	5.53e3
16 groups	1.15	1.3	4.0		5.53e3
18 groups	1.15	1.3	4.0	9.877	5.53e3

In this example, we illustrate the analysis tools that TOGA provides. In the automated decision-making, the bias of each multigroup calculation is weighted by the number of groups. The least-cost group structure is chosen that delivers the best accuracy within a user-defined tolerance of the largest group structure. In the example of Figure 3, the 70-group structure has an error of 1,200 pcm. With a tolerance of 5%, the

smallest group structure that delivers at most 1,260 pcm error is selected. Here, that is 40 groups.

Scattering Expansion

Griffin only accepts Legendre scattering representation. However, OpenMC also offers histogram scattering representation. Therefore, only Legendre scattering order is accounted for during the optimization, but an isotropic and angle-dependent histogram tally can be produced for error quantification. Figure 4 provides an illustration.

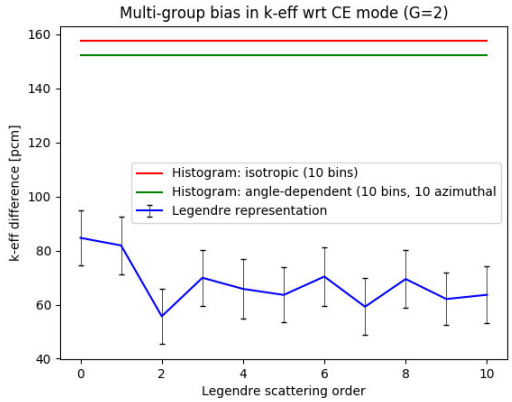

Fig. 4. Bias induced on a PWR assembly model by using Legendre scattering expansion orders between 0 and 10, along with isotropic and angle-dependent histogram representations.

Figure 4 showcases how Legendre scattering expansion orders affect the accuracy of multigroup simulations and contrasts that with the histogram approaches. The histogram approach is considered the ideal scattering representation, especially when the number of energy bins and azimuthal angle bins are high (100-200). Note that this figure shows better results with Legendre representations than with histograms. This indicates that the number of histogram bins is insufficient. Nonetheless, we also observe that the Legendre representation is very robust for a PWR assembly and that there is little difference between L=2 and L=10.

Similar to the energy-group decision making, the bias of each expansion is weighted by the order to determine the least-cost expansion that delivers the best accuracy. In this case, L=2 is chosen.

Combined Schemes

Since TOGA optimizes over two parameters, there are several approaches for combining the decision.

The first optimization scheme begins by selecting the best energy group structure with L=0. Then, that best energy group structure is used to select the best Legendre scattering expansion order. Finally, that scattering expansion is used to re-select the best energy group structure. This scheme could be expanded to operate in a loop until the decision no longer changes.

The second optimization scheme selects the best energy group structure for every value of L, and the best combination is selected. This scheme is potentially more costly, but it is more thorough.

Output to ISOXML for MOOSE

TOGA outputs the cross sections in a format directly readable by Griffin by translating the HDF5 data to xml [10]. Griffin input files support cross sections for multiple reactor states, called tabulation. TOGA allows for tabulation by repeating the optimization process for multiple OpenMC input files representing new states of the same reactor. For example, temperature changes are ideal for tabulation. TOGA's optimization accommodates tabulation by storing the best multigroup parameters from each state and uses a Python ranked-choice voting library to determine the best overall parameters. Griffin then uses tabulation to interpolate cross sections between reactor states. Other output structures could easily be added to expand TOGA's applicability.

In addition to cross sections, basic information needed for super-homogenization factors is also included. It is unclear in the literature what the best practice is for handling equivalence during a transient, so we advise caution to users who wish to generate equivalence factors.

RESULTS

For new reactor designs, experimentation is needed to determine the best group structures. In some cases, the ideal group structures haven't been formulated yet. The fictional microreactor from the analysis in Figure 3 illustrates that problem firsthand. This reactor design was created for illustrative purposes only and is not expected to be a viable design. The reactor is comprised of fuel pins, moderator pins, and heat pipes arranged in a hexagonal lattice and contained in a graphite monolith. The fuel is UZrH at 20% enrichment, the moderator is ZrH_2, and the heat pipes carry sodium vapor. It is purposefully unclear what energy regime best describes the reactor. Figure 5 shows the tallied flux in the fuel material in a 70-group CASMO structure. It is observed that the absorption in the U-238 early resonances has an outsized effect in this reactor concept which compromises the thermal region of the neutron spectrum.

Although the OpenMC runs were converged to 5 pcm error, in Figure 3, the CASMO groups bottom out

around 1000 pcm bias. The same reactor was also run with the ANL group structures which have shown promise for other advanced reactor designs [11]. The ANL groups, as with the CASMO groups, fail to properly capture the energy regime of this reactor with an error around 1200 pcm. In this case, the user will either proceed with flawed cross-sections, knowing the value of the error induced or will conduct further work to determine better group structures using custom group structure definitions.

This example underscores the need for efficient techniques for generating results under a large number of potential energy group structures. TOGA helps such efforts by providing easy comparisons between multigroup and continuous energy Monte Carlo.

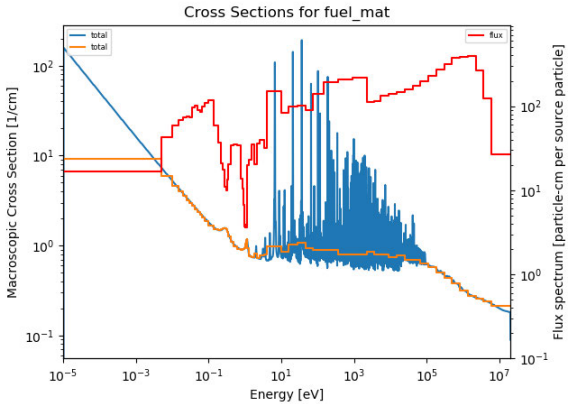

Fig. 5. Fuel cross sections and flux for the fictitious microreactor.

CONCLUSION

The Tool for Optimization and Group-structure Analysis (TOGA) provides a hands-off method for users to generate optimized cross sections for any reactor. Since many new proposed reactor designs are not necessarily thermal reactors, the selection of good group structures is not trivial. This tool allows users to compare a large number of group structures and aids in the choice. Many features in TOGA allow the user to make decisions for themselves, if desired, by looking at helpful analysis plots of the errors, both spatially and globally. These plots help raise a number of questions about the assumptions we commonly make in cross section generation including the effect of the group boundaries on the accuracy of the results.

Overall, the flexible cross section generation in OpenMC, enhanced by TOGA, keeps users from going in blind with multigroup cross sections that are of an unknown accuracy. Instead, the user can now quantify their multigroup cross section error and attempt to improve it through a number of optimization schemes.

ACKNOWLEDGEMENTS

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REFERENCES

[1] W. BOYD, A. NELSON, P. ROMANO, S. SHANER, B. FORGET, K. SMITH, "Multigroup Cross-Section Generation with the OpenMC Monte Carlo Particle Transport Code" *Nucl. Techn*. **205**, 928-944 (2019).
[2] D. GASTON, C. NEWMAN, G. HANSEN, D. LEBRUN-GRANDIÉ, "MOOSE: a Parallel Computational Framework for Coupled Systems of Nonlinear Equations" *Nucl. Eng. and Design*, **239**, 1768 (2009).
[3] P. ROMANO, N. HORELIK, B. HERMAN, A. NELSON, B. FORGET, and K. SMITH, "OpenMC: A State-of-the-Art Monte Carlo Code for Research and Development" *Ann. Nucl. Energy* **82**, 90 (2015).
[4] S. KORANNE, *Handbook of Open Source Tools* p. 191–200, Springer US (2011).
[5] J. RHODES, K. SMITH, D. LEE, "CASMO-5 Development and Applications," *Proc. PHYSOR 2006* Vancouver, British Columbia, September 10–14, 2006, American Nuclear Society (2006).
[6] C. LEE, Y. JUNG, W. YANG, "MC^2-3: Multigroup Cross Section Generation Code for Fast Reactor Analysis," Argonne National Laboratory report ANL/NE-11/41 Rev. 3 (2018).
[7] https://www-nds.iaea.org/wimsd/energy.htm
[8] A. HOFFMANN, F. JEANPIERRE, A. KAVENOKY, M. LIVOLANT, H. LORAIN, "APOLLO: Code Multigroupe de Résolution de l'Equation du Transport pour les Neutrons Thermiques et Rapides," Centre d'Etudes Nucleaires de Saclay report CEA-N-1610 (1973).
[9] E. SARTORI, "OECD/NEA Data Bank: Standard Energy Group Structures of Cross Section Libraries for Reactor Shielding, Reactor Cell and Fusion Neutronics Applications: VITAMIN-J, ECCO-33, ECCO-2000 and XMAS JEF/DOC-315" (1990).
[10] Y. WANG, J. ORTENSI, "The XML Multigroup Cross Section Library," Idaho National Laboratory report (2018).
[11] A. KASAM-GRIFFITH, A. NELSON, F. HEIDET, "OpenMC-based generation of multigroup cross-sections for analysis of the Versatile Test Reactor" *Trans. Am. Nucl. Soc.* **123** 1404 (2020).