U.S. Department of Energy

Multi-group Transport Cross Section and Diffusion Coefficient Generation for Deterministic Reactor Models Using Monte Carlo Calculations

PI: **Kord Smith (MIT)** **Collaborators**: **Benoit Forget (MIT) and Javi Ortensi (INL)**

Program: **NEAMS**

ABSTRACT:

This project will overcome current accuracy limitations of full-core deterministic transport methods by developing solid theoretical methods for **computing multi-group anisotropic diffusion coefficients and transport cross sections directly from Monte Carlo** for four distinct core modeling approaches: 1) homogenized fuel elements, 2) homogenized pin-cells or plates, 3) explicit heterogeneous pin and coolant models, and 4) fully heterogeneous models with intra-pellet radial and azimuthal regions, as needed for true high-fidelity core models. The project will develop equivalence parameters needed in downstream deterministic diffusion and transport models in order to exactly reproduce reference Monte Carlo results.

The new methods will build upon the new "Cumulative Migration Area Method" that project authors have recently published at PHYSOR 2016. The new methods will be capable of rigorously preserving neutron transport (migration) within heterogeneous reference geometries, and they will eliminate reliance on inaccurate methods (e.g., classic out-scatter approximations or Monte Carlo-tallied mean cosine scattering angles) that are often used for generating approximate transport cross sections. Data generation and testing will utilize recently added tally capabilities of OpenMC that permit generation and processing of multi-group cross sections directly in full-core geometries. Machine-learning algorithms will be used to explore terabyte cross section tallies in order to identify and coalesce "clusters" of multi-group isotropic cross sections that yield accurate core predictions in full-core deterministic transport calculations, while minimizing the required number of energy groups and data storage requirements.

The methods developed will satisfy the goal of supporting 95/95 reliability factors < 5.0% on total power peaking factors – as currently required by commercial LWR vendors. These improvements represent important developments needed to convince industry that the move from current two-group homogenized nodal diffusion models to full-core heterogeneous transport models can fully deliver on the promise of improved local predictions of core physics phenomenon – at the pin and intra-pin level. Validation of methods for application to operational reactors will be made by comparing computational results with measured power distributions for the BEAVRS PWR and TREAT test reactor.

A stretch goal of the project will determine if it is practical to perform full-core deterministic core simulations with partially-converged, full-core, Monte Carlo calculations being used as the on-the-fly deterministic cross section data generator. If this approach is successful, the standard technique of generating cross section data using "spectral geometries" and resonance self-shielded data tables will be eliminated. While this approach may be most attractive for supporting High Performance Computing (HPC) applications on Petascale or Exascale machines, advantages of machine learning applications will be applied even when utilizing traditional spectral geometries for generating data used in full-core deterministic diffusion or transport reactor computations.