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Deterministically estimated fission source distributions for Monte Carlo k-eigenvalue problems ☆

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ABSTRACT

The standard Monte Carlo (MC) k-eigenvalue algorithm involves iteratively converging the fission source distribution using a series of potentially time-consuming *inactive cycles* before quantities of interest can be tallied. One strategy for reducing the computational time requirements of these inactive cycles is the Sourcerer method, in which a deterministic eigenvalue calculation is performed to obtain an improved initial guess for the fission source distribution. This method has been implemented in the Exnihilo software suite within SCALE using the SP_N or S_N solvers in Denovo and the Shift MC code. The efficacy of this method is assessed with different Denovo solution parameters for a series of typical k-eigenvalue problems including small criticality benchmarks, full-core reactors, and a fuel cask. It is found that, in most cases, when a large number of histories per cycle are required to obtain a detailed flux distribution, the Sourcerer method can be used to reduce the computational time requirements of the inactive cycles.

1. Introduction

The design and operation of nuclear fission reactors requires a detailed solution to the neutron transport k-eigenvalue problem to obtain the neutron multiplication factor (k_{eff}) for criticality safety analyses and pin- and subpin-resolved flux distributions for depletion, thermohydraulic-coupling, and radiation damage analyses. In some cases, the accuracy required for these analyses necessitates the use of Monte Carlo (MC) methods for neutron transport. The traditional MC power iteration algorithm for solving the k-eigenvalue problem involves carrying out a series of *cycles*, in which a collection of neutron histories are simulated and the induced fission sites are recorded. Since the fission source distribution is not known *a priori*, an initial guess must be used for the first cycle. For subsequent cycles, the fission source can be formed from the fission sites from the previous cycle. *Inactive* cycles—in which no events are tallied—are first carried out to obtain a converged fission source. *Active* cycles are then performed, and an estimate of k_{eff} and the flux distribution are recorded for each cycle. The final estimate for k_{eff} and the flux distribution can then be ascertained by averaging together the estimates from the active cycles.

Full-core reactor analysis generally requires a large number of inactive cycles that are computationally expensive. For eigenvalue-only calculations inactive cycles may account for approximately half of the total runtime. For calculations that require more detailed tallies the relative expense of inactive cycles is reduced. Numerous strategies have been proposed to reduce the computational time spent on inactive cycles.

Acceleration techniques such as the fission matrix method (Urbatsch, 1995; Carney et al., 2014) attempt to improve how a new fission source is generated from the previous iteration by using additional information garnered from solving an approximate problem. Preliminary analysis using a deterministic-based fission matrix acceleration method yielded promising results, but further investigation is required before adopting this method for production-level use (Hamilton and Evans, 2015; Hamilton et al., 2016). With the particle ramp-up method (Lund et al., 2017), the number of histories per cycle is gradually increased during inactive cycles so that less computational time is wasted simulating particle histories when the fission source is far from converged. However, it is possible that this method would exacerbate issues with neutron clustering (Nowak et al., 2016). With the MC version of

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Wielandt's method the fission source is formed from a combination of the induced fission sites from the previous cycle and also the current cycle, in order to increase the interaction between decoupled regions of a problem (Yamamoto and Miyoshi, 2004).

Another strategy is to use an improved initial guess for the fission source distribution such that fewer inactive cycles are required to obtain a converged fission source. As opposed to acceleration methods, this technique does not modify the rate of convergence of power iteration. In principle this could be done in concert with the other two strategies, but in this work this third strategy is studied in isolation. The default initial guess for the fission source for k-eigenvalue problems is usually generated from a flux distribution that is uniform throughout all space. The conversion between the flux distribution and the fission source is later described in Eq. (4). For reactor problems, flux distributions that are uniform radially and have a cosine or flattened cosine[2] shape axially can be used. The Watt fission spectrum is typically used for the energy distribution, and isotropic emission is used for the angular distribution. The complexity of the spatial distribution of the fission source is not captured by these typical initial guesses, especially in the presence of inhomogeneities such as control and burnable absorber rods, mixed fuels, and variable burnup states.

The Sourcerer method (Ibrahim et al., 2013) can be used to obtain an improved initial guess for arbitrary configurations, thereby providing an automatic means of reducing the number of inactive cycles. With this method, a deterministic neutron transport calculation is first carried out as a preprocessing step. The resulting approximate mesh-based flux distribution is used to calculate a mesh-based fission source distribution that is used as an initial guess. This method has previously been implemented in the Sourcerer module within the SCALE modeling and simulation suite (Rearden and Jessee, 2016) using Denovo (Evans et al., 2010) as a discrete ordinates (S_N) solver and the KENO MC transport code (Rearden and Jessee, 2016). The method was demonstrated to be effective for a spent fuel canister problem with both transport codes run in serial (Ibrahim et al., 2013). Another method similar to the Sourcerer method has previously been proposed, but does not appear to have ever been implemented (Urbatsch, 1995).

The Sourcerer method is effective only if a deterministic estimate of the flux distribution can be obtained quickly relative to the time required for the MC inactive cycles. As a practical consideration, the computer memory requirements for the deterministic solution should not be so large that an analyst must use additional computer resources solely to employ the Sourcerer method. Though most deterministic techniques are likely to satisfy these criteria for small reactor problems, full-core analysis poses significant challenges. Full-core modeling with the S_N method requires leadership-class computer resources (Jarrell et al., 2013), making the application of the Sourcerer method to full-core analysis impractical in most cases. The Simplified P_N (SP_N) method is a low-order approximation of the transport equation that can provide estimates of the flux distribution for full-core problems in significantly less processor time and with smaller memory requirements than S_N methods (Hamilton and Evans, 2015). When a high degree of accuracy is not required, the SP_N method is preferable to the S_N method provided that the problem does not contain regions with extremely long mean free paths (e.g., air or void regions) that cannot be handled by the former method.

In this work, the performance of the Sourcerer method is assessed using deterministic estimates of the neutron flux with varying degrees of accuracy for a collection of typical k-eigenvalue problems. The Sourcerer method has been implemented using the Denovo SP_N (Hamilton and Evans, 2015) and S_N solvers, so the Sourcerer method can be applied to a wide range of problems, including full-core reactor analysis. This implementation is done in the Exnihilo software suite (Johnson et al., 2017) within SCALE using the Shift MC transport code (Pandya et al., 2016). Shift, like Denovo, was designed to be massively parallel and has demonstrated excellent scaling behavior from laptops to leadership-class supercomputers (Evans et al., 2010; Pandya et al., 2016). Both codes support a variety of geometry and physics packages. Shift and Denovo are easily coupled through the Omnibus front-end (Johnson, 2014), which is common to both codes. This implementation requires the user to choose the solution parameters for the Denovo solver, including the SP_N order or S_N quadrature set, resonance self-shielding treatment for cross section generation, number of energy groups, and solution mesh. The accuracy of the Denovo solution—which is governed by this choice of parameters—could affect the efficiency of the Sourcerer method.

The rest of this paper proceeds as follows. Section 2 provides the theoretical background for the Sourcerer method and the use of Shannon entropy (Ueki and Brown, 2005) to qualitatively assess fission source convergence. Section 3 first details how the Sourcerer method is implemented within Exnihilo and how cross sections are generated with different resonance self-shielding treatments. Criteria are then proposed for quantitatively assessing the cycle in which an MC simulation can be deemed converged, based on Shannon entropy. Using results from these convergence criteria, a quantitative metric $N_{\text{break-even}}$ is then described that can be used to determine when the use of the Sourcerer method is justified. This parameter considers the number of inactive cycles saved using the Sourcerer method and the computational time requirements of the two transport steps.

Section 4 describes the models used for experimentation, which include two small criticality benchmark problems, three full-core reactor problems, and a fuel cask problem:

1. A modified version of the 2003 C5G7 mixed-oxide (MOX) fuel benchmark problem (Smith et al., 2003).
2. Core 17 of the Babcock & Wilcox® (B&W) 1810 benchmark (Newman et al., 1984).
3. Watts Bar Nuclear Power Station, Unit 1 (WBN1) (Gehin et al., 2013).
4. Westinghouse AP1000® reactor (Franceschini et al., 2014).
5. Westinghouse AP1000® reactor, unrodded configuration (Franceschini et al., 2014).
6. NAC International Inc. Universal Multi-Purpose Canister System (NAC UMS®) fuel cask (Peterson et al., 2013).

For each of these problems, the number of inactive cycles saved using the Sourcerer method, as well as $N_{\text{break-even}}$, are determined. The results of these experiments are discussed in Section 5. Section 6 provides concluding remarks.

This work demonstrates that the Sourcerer method might provide performance enhancements in a subset of problems—especially those where a large number of histories per cycle are required—but further advancements in the speed and accuracy of deterministic methods are necessary for Sourcerer to be advantageous for arbitrary use cases.

2. Theory

MC neutron transport can be used to estimate k_{eff} via the power iteration method, which involves successively solving the neutron transport equation to obtain convergent estimates of the fission source. The neutron transport equation can be formulated in operator notation as

[2] The flattened cosine shape is defined as $f(x) = 1 - (1 - cos(x))^2$.