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Implementation, capabilities, and benchmarking of Shift, a massively parallel Monte Carlo radiation transport code ☆

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A B S T R A C T

This work discusses the implementation, capabilities, and validation of Shift, a massively parallel Monte Carlo radiation transport package authored at Oak Ridge National Laboratory. Shift has been developed to scale well from laptops to small computing clusters to advanced supercomputers and includes features such as support for multiple geometry and physics engines, hybrid capabilities for variance reduction methods such as the Consistent Adjoint-Driven Importance Sampling methodology, advanced parallel decompositions, and tally methods optimized for scalability on supercomputing architectures. The scaling studies presented in this paper demonstrate good weak and strong scaling behavior for the implemented algorithms. Shift has also been validated and verified against various reactor physics benchmarks, including the Consortium for Advanced Simulation of Light Water Reactors' Virtual Environment for Reactor Analysis criticality test suite and several Westinghouse AP1000® problems presented in this paper. These benchmark results compare well to those from other contemporary Monte Carlo codes such as MCNP5 and KENO.

1. Introduction

The reactor physics community increasingly relies on high-fidelity transport simulations for safety analyses, reactor system upgrades, maintenance studies, and other applications. This need drives the demand for shorter solution times, increased accuracy, and more flexible capabilities in the radiation transport codes that power these simulations. Shift is a new Monte Carlo (MC) radiation transport code that has been developed in response to the growing need for flexible, fast, and accurate nuclear engineering analyses.

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This work presents the development, implementation, verification, and validation of Shift. This MC code is developed and maintained at Oak Ridge National Laboratory (ORNL) by the Radiation Transport Group. Shift is the MC package in Exnihilo, a radiation transport code suite that also contains the Denovo deterministic transport code [1,2]. Development of Shift began at ORNL in 2010 to provide a massively parallel MC code for enabling reactor analysis on the Oak Ridge Leadership Computing Facility (OLCF) high-performance computing (HPC) architectures.

Shift is designed and optimized for performing MC radiation transport calculations on current and near-future computing architectures. Shift can also run most radiation transport problems on laptops or small clusters with correspondingly reduced performance. Challenges for developing and running Shift on massively parallel computing architectures include memory management (as with all MC radiation transport codes), scaling of parallel algorithms, and tally optimization.

The implementation and benchmarking of Shift is discussed in the remainder of this paper. We describe Shift's capabilities in §2. In §3 we discuss validation and verification results, and in §4 we summarize the main features of Shift and review its benchmarking results. Several features in Shift make it a unique tool for reactor analysis calculations. These include the parallel domain replication and domain decomposition algorithms discussed in §2.8 and the tally algorithm and its scaling capabilities discussed in §2.5 and §3.4.

2. Background and features of Shift

Shift was designed to provide a massively parallel MC tool for reactor applications. After its initial implementation, Shift became the production MC application in the Consortium for the Advanced Simulation of Light Water Reactors (CASL) energy simulation hub [3]. Although initially developed for pressurized water reactor (PWR) analysis, Shift has been used to model other systems, including ORNL's High Flux Isotope Reactor (HFIR) [4], a very small high-flux reactor.

Shift is a general purpose radiation transport code that performs stochastic modeling of neutral particle physics using the MC method [5,6]. It can perform eigenvalue calculations as well as fixed source calculations in neutron, photon, or coupled neutron–photon mode. The focus of this paper is on eigenvalue problems for reactor analysis for which Shift uses the well-known *k*-eigenvalue algorithm [6–8] described in §2.1. The main modules of Shift include physics, tallies, geometry, source definitions, parallel decomposition, and variance reduction. These features and capabilities are discussed in the following sections.

Shift serves as the MC package of Exnihilo, the massively parallel radiation transport code suite developed and maintained at ORNL. Through this framework, Shift is combined with the deterministic radiation transport solvers in Exnihilo to take advantage of variance reduction and acceleration techniques offered by advanced hybrid methods. These hybrid methods are also discussed in the following sections.

Recently, Exnihilo has been incorporated into the SCALE code system [7], a criticality code suite developed and maintained at ORNL. The SCALE code suite has been used worldwide for over 30 years and currently has over 5600 users in over 55 countries [7]. This incorporation enables Shift to utilize the data, depletion, and sensitivity/uncertainty analysis capabilities in SCALE. In particular, the principal continuous-energy (CE) and multigroup (MG) data used in Shift comes through SCALE.

2.1. The Monte Carlo K-eigenvalue method

Here we give a brief description of the fundamental numerical methods used by Shift to model the steady-state and quasi-static neutronics behavior in operational nuclear power reactors. This material is covered in significant detail in Refs. [5–9]. Accordingly, only a brief discussion is given here.

The steady-state behavior of neutrons in a nuclear reactor core is governed by the eigenvalue form of the linear Boltzmann neutron transport equation. Written in operator notation, this equation is

$$(\hat{\mathrm{T}} - \hat{\mathrm{S}})\psi = \frac{1}{k}\hat{\chi}\hat{\mathrm{F}}\psi\,, \tag{1}$$

where the continuous operators are defined as

$$\hat{\mathrm{T}} \equiv \hat{\mathbf{\Omega}} \cdot \nabla + \sigma_{\mathrm{t}}\,, \tag{2}$$

$$\hat{\mathrm{S}} \equiv \iint \mathrm{d}\mathbf{\Omega}'\mathrm{d}E'\,\sigma_{\mathrm{s}}(\hat{\mathbf{\Omega}} \cdot \hat{\mathbf{\Omega}}', E' \to E)\,, \tag{3}$$

$$\hat{\chi} \equiv \frac{\chi(E)}{4\pi}\,, \tag{4}$$

$$\hat{\mathrm{F}} \equiv \iint \mathrm{d}\mathbf{\Omega}'\mathrm{d}E'\,\nu\sigma_{\mathrm{f}}(E')\,. \tag{5}$$

Here, σ_{t} is the total interaction cross section, σ_{s} is the differential scattering cross section, and σ_{f} is the fission cross section. The energy spectrum resulting from fission is given by $\hat{\chi}$, and ν is the average number of neutrons per fission. The fundamental unknown is the angular flux ψ, which is a function of space, angle, and energy. Rearranging terms in Eq. (1) yields