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Nuclide depletion capabilities in the Shift Monte Carlo code ☆

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ABSTRACT

A new depletion capability has been developed in the Exnihilo radiation transport code suite. This capability enables massively parallel domain-decomposed coupling between the Shift continuous-energy Monte Carlo solver and the nuclide depletion solvers in ORIGEN to perform high-performance Monte Carlo depletion calculations. This paper describes this new depletion capability and discusses its various features, including a multi-level parallel decomposition, high-order transport-depletion coupling, and energy-integrated power renormalization. Several test problems are presented to validate the new capability against other Monte Carlo depletion codes, and the parallel performance of the new capability is analyzed.

1. Introduction

Early Monte Carlo depletion codes have typically coupled a stand-alone Monte Carlo transport code (such as MCNP (X-5 Monte Carlo Team, 2008)) to a stand-alone depletion code (such as ORIGEN (Gauld et al., 2011) or CINDER (Wilson et al., 1998)). The coupling module operated by creating the input files necessary to run the Monte Carlo code, extracting the various tallies from the output, and then creating the input file for the depletion code. The updated nuclide number densities were then extracted from the depletion output, a new transport input file was created, and the process would begin again for the next depletion step. Codes using this type of file-based transport-depletion coupling system include VESTA (VESTA, 2008) and Monteburns (Trellue and Poston, 1999).

There are numerous drawbacks to this type of Monte Carlo depletion coupling. The most significant is that requiring each module to write its input and output to disk for each depletion step can be a significant performance bottleneck and, especially, limits the parallel scaling of the Monte Carlo depletion algorithm. Scaling such a system to $O(100k)$ cores would be difficult given typical disk throughput.

More recently, nuclide depletion capabilities have been directly integrated into Monte Carlo simulation codes. Examples include MC21 (Griesheimer et al., 2013), MCNP6 (Goorley et al., 2013), and Serpent (Leppanen, 2015). By coupling a depletion calculation inline to the Monte Carlo solver, expensive writes to disk can be avoided. Moreover, the depletion package can easily exploit any multilevel parallel decomposition present in the Monte Carlo package.

This paper discusses a new nuclide depletion capability that has been implemented into the Exnihilo radiation transport suite. Exnihilo includes the Shift Monte Carlo solver (Pandya et al., 2016) (containing both continuous-energy and multigroup physics), as well as the Denovo deterministic solver (Evans et al., 2010) (containing S_N, SP_N, and method of characteristics (MOC)-based deterministic transport). Currently, the depletion package has only been coupled to the continuous-energy Monte Carlo transport solver in Shift. However, the depletion package was designed to make coupling to a multigroup physics package (either Denovo or multigroup Shift) straightforward. The depletion package in Exnihilo was built to scale well for large problems on high-performance supercomputers.

Two applications have provided most of the motivation behind the development of the continuous-energy Monte Carlo depletion capability in Exnihilo. The first, as part of the Consortium for

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Advanced Simulation of Light Water Reactors (CASL) energy innovation hub (Turinsky and Kothe, 2016), is to provide verification calculations for lattice depletion simulations performed using MPACT (Zhu et al., 2014). Examples of these calculations are provided in Sections 7.2 and 7.3. The other primary motivating application for this capability is faster fuel-cycle depletion analysis for the High Flux Isotope Reactor (HFIR) facility at the Oak Ridge National Laboratory (ORNL) (Ilas et al., 2015). Therefore, most of the methods and results contained in this paper are directed toward these applications.

The nuclide depletion module couples the transport solvers in Exnihilo to ORIGEN (Gauld et al., 2011). ORIGEN is a general purpose nuclide depletion solver supporting fuel depletion, target activation, and decay calculations. Therefore, while development efforts have been directed towards problems of interest for CASL and HFIR, this capability is expected to be used for a wide variety of applications in the future.

The purpose of this paper is to provide a complete description of the current capabilities of the nuclide depletion package implemented into Exnihilo, to demonstrate and compare the accuracy, efficiency, and performance of these capabilities within a common code framework on several test problems, and to collect into one place a pedagogical description of Monte Carlo-depletion coupling. The numerical methods described herein have been previously published elsewhere (Pandya et al., 2016; Isotalo and Aarnio, 2011; Isotalo and Aarnio, 2011; Isotalo, 2016; Isotalo et al., 2016; Davidson et al., 2016), as have some of the numerical results (Davidson et al., 2016; Gentry et al., 2017). Results not previously published include fuel cycle simulations using Exnihilo for a detailed HFIR model, as described in Sections 7.3.2 and 7.3.3, as well as the parallel scaling study in Section 7.4.

The remainder of this document is organized as follows: in Section 2 the coupled radiation transport and nuclide depletion equations are derived; in Section 3 the multilevel parallelism used in the depletion package within Exnihilo is discussed; in Section 4 the various transport-depletion coupling methods implemented in Exnihilo are presented; Section 5 described the calculation of reaction rates, and Section 6 discusses the various power normalization methods that have been implemented; Section 7 presents simulation results demonstrating the accuracy of the Exnihilo depletion capability and parallel scaling; and Section 8 concludes and discusses future work.

2. Theory and background

Monte Carlo nuclear reactor depletion calculations solve a coupled quasi-static system of equations involving the k-eigenvalue radiation transport equation:

$$\begin{aligned}\hat{\boldsymbol{\Omega}}\cdot\nabla\psi(\boldsymbol{x},\hat{\boldsymbol{\Omega}},E,t)+\Sigma_t(\boldsymbol{x},E,t)\psi(\boldsymbol{x},\hat{\boldsymbol{\Omega}},E,t)\\ =\int_0^\infty\int_{4\pi}\Sigma_s(\boldsymbol{x},\hat{\boldsymbol{\Omega}}'\cdot\hat{\boldsymbol{\Omega}},E'\to E,t)\psi(\boldsymbol{x},\hat{\boldsymbol{\Omega}}',E',t)\,\mathrm{d}\Omega'\mathrm{d}E'\\ +\frac{1}{k_{\mathrm{eff}}(t)}\frac{\chi(\boldsymbol{x},E,t)}{4\pi}\int_0^\infty\nu\Sigma_f(\boldsymbol{x},E',t)\phi(\boldsymbol{x},E',t)\,\mathrm{d}E',\end{aligned}\tag{1a}$$

and the Bateman equations:

$$\begin{aligned}\frac{\partial}{\partial t}N_j(\boldsymbol{x},t)=\sum_{\substack{k\in J\\k\neq j}}\left[\sum_r\gamma_{r,kj}\sigma_{r,k}(\boldsymbol{x},t)\phi(\boldsymbol{x},t)+b_{kj}\lambda_k\right]N_k(\boldsymbol{x},t)\\ -\left[\sum_r\sigma_{r,j}(\boldsymbol{x},t)\phi(\boldsymbol{x},t)+\lambda_j\right]N_j(\boldsymbol{x},t),\quad j\in J.\end{aligned}\tag{1b}$$

Eq. (1a) is an eigenvalue equation describing the population of neutrons in a multiplying medium such as a nuclear reactor. The fundamental unknowns in Eq. (1a) are $\psi(\boldsymbol{x},\hat{\boldsymbol{\Omega}},E,t)$, the eigenfunction, which represents the angular neutron flux at position $\boldsymbol{x}$ traveling in direction $\hat{\boldsymbol{\Omega}}$ in energy E at time t; and $k_{\mathrm{eff}}(t)$, the eigenvalue, which physically represents the factor by which the neutron population is multiplied each generation. A k_{eff} of unity represents a constant population. $\Sigma_t(\boldsymbol{x},E,t)$ is the total macroscopic cross section at position $\boldsymbol{x}$ and energy E at time t, while $\Sigma_s(\boldsymbol{x},\hat{\boldsymbol{\Omega}}'\cdot\hat{\boldsymbol{\Omega}},E'\to E,t)$ is the macroscopic scattering cross section for neutrons scattering through angle $\hat{\boldsymbol{\Omega}}'\cdot\hat{\boldsymbol{\Omega}}$ from energy E' to E at position $\boldsymbol{x}$ and time t. $\chi(\boldsymbol{x},E,t)$ is the probability of a fission neutron being emitted at energy E at position $\boldsymbol{x}$ at time t, ν is the number of neutrons emitted per fission, and $\Sigma_f(\boldsymbol{x},E',t)$ is the macroscopic fission cross section. Finally, $\phi(\boldsymbol{x},E,t)$ is the scalar flux, defined as

$$\phi(\boldsymbol{x},E,t)=\int_{4\pi}\psi(\boldsymbol{x},\hat{\boldsymbol{\Omega}},E,t)\,\mathrm{d}\Omega.\tag{2}$$

The quasi-static approximation is valid when the change in nuclide concentrations is very slow relative to a neutron lifetime. Eq. (1a) is also accompanied with associated boundary conditions, which for simplicity we have omitted.

Eq. (1b) is the general Bateman equation, representing the evolution of the atomic density of a given nuclide j. $N_j(\boldsymbol{x},t)$ represents the atomic density of nuclide j at position $\boldsymbol{x}$ and time t. The first term in Eq. (1b) represents the production of nuclide j from nuclide k for various reactions r, where the yield $\gamma_{r,kj}$ represents the probability that a reaction r will transform nuclide k into nuclide j, $\phi(\boldsymbol{x},t)$ represents the energy-integrated scalar flux at position $\boldsymbol{x}$ and time t, and $\sigma_{r,k}(\boldsymbol{x},t)$ represents the energy-integrated, flux-weighted cross section for reaction r and nuclide k at position $\boldsymbol{x}$ and time t, i.e.,

$$\sigma_{r,k}(\boldsymbol{x},t)=\frac{\int_0^\infty\sigma_{r,k}(E)\phi(\boldsymbol{x},E,t)\,\mathrm{d}E}{\int_0^\infty\phi(\boldsymbol{x},E,t)\,\mathrm{d}E}.\tag{3}$$

All of the reactions modeled by ORIGEN are given in A. Quantity $b_{k,j}$ represents the branching ratio from nuclide k into nuclide j, i.e., the probability that nuclide j will be produced in the decay of nuclide k, and λ_k is the decay constant for nuclide k. The second term in Eq. (1b) represents losses of nuclide j through various reactions r as well as losses due to decay. Other loss mechanisms are possible, such as loss through chemical separation in the case of molten-salt reactors. However, in this paper we assume a solid-fueled reactor with only the loss mechanisms described above. J represents the set of all nuclides to be simulated. Eq. (1b) also has associated initial conditions which have been omitted for brevity, and the yields $\gamma_{r,kj}$ in Eq. (1b) are represented as energy-independent for simplicity, though ORIGEN supports energy-dependent yields.

Eqs. (1a) and (1b) are coupled through the neutron flux and cross sections. The macroscopic cross sections in Eq. (1a) are defined as:

$$\Sigma_t(\boldsymbol{x},E,t)=\sum_{j\in J}N_j(\boldsymbol{x},t)\left[\sigma_{a,j}(E)+\sigma_{s,j}(E)\right],\tag{4a}$$

$$\Sigma_s(\boldsymbol{x},\hat{\boldsymbol{\Omega}}'\cdot\hat{\boldsymbol{\Omega}},E'\to E,t)=\sum_{j\in J}N_j(\boldsymbol{x},t)\sigma_{s,j}(\hat{\boldsymbol{\Omega}}'\cdot\hat{\boldsymbol{\Omega}},E'\to E),\tag{4b}$$

$$\Sigma_f(\boldsymbol{x},E,t)=\sum_{j\in J}N_j(\boldsymbol{x},t)\sigma_{f,j}(E),\tag{4c}$$

where $\sigma_{a,j}(E)$ and $\sigma_{s,j}(E)$ are the microscopic absorption and scattering cross sections for nuclide j, respectively.

Eqs. (2–4) describe how Eqs. (1a) and (1b) are coupled. The macroscopic cross sections described in Eq. (4) and used in Eq. (1a) are coupled to the nuclide number densities calculated using Eq. (1b). The energy-integrated flux calculated using Eqs. (1a)