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A perturbation-based susbtep method for coupled depletion Monte-Carlo codes

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ABSTRACT

Coupled Monte Carlo (MC) methods are becoming widely used in reactor physics analysis and design. Many research groups therefore, developed their own coupled MC depletion codes. Typically, in such coupled code systems, neutron fluxes and cross sections are provided to the depletion module by solving a static neutron transport problem. These fluxes and cross sections are representative only of a specific time-point. In reality however, both quantities would change through the depletion time interval. Recently, Generalized Perturbation Theory (GPT) equivalent method that relies on collision history approach was implemented in Serpent MC code. This method was used here to calculate the sensitivity of each nuclide and reaction cross section due to the change in concentration of every isotope in the system. The coupling method proposed in this study also uses the substep approach, which incorporates these sensitivity coefficients to account for temporal changes in cross sections. As a result, a notable improvement in time dependent cross section behavior was obtained. The method was implemented in a wrapper script that couples Serpent with an external depletion solver. The performance of this method was compared with other existing methods. The results indicate that the proposed method requires substantially less MC transport solutions to achieve the same accuracy.

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1. Introduction

Multiple codes that integrate Monte Carlo (MC) neutron transport with burnup calculations have been developed. Accurate evaluation of fuel isotopic changes as a function of time is the key to reliable prediction of all other results expected from such codes. Due to steadily growing computing power, such MC codes are gradually becoming a standard calculation tool of choice in reactor analyses. As a result, many research teams have developed their own coupled MC codes, with Serpent (Leppänen et al., 2015), BGCore (Fridman et al., 2008; Kotlyar et al., 2011) and MCNPX (Fensin et al., 2006) to name a few. There are however, many notable differences between these codes, such as the implementation of neutron transport procedure, adopted depletion solver and the method of generating 1-group cross sections required for the solution of the depletion problem.

Additional important aspect that differ among the codes is the coupling scheme used to integrate the MC transport solution with burnup calculations. Recent studies by Kotlyar and Shwageraus (2013) presented the effect of such coupling scheme choice on numerical stability and accuracy of the results. Therefore, new coupling methods have been developed for MC-burnup applications which also account for the dependence of reaction rates on thermal hydraulic conditions (Kotlyar and Shwageraus, 2014). Although these methods resolved the issue of numerical stability, further studies (Kotlyar and Shwageraus, 2015; Kotlyar and Shwageraus, 2016) indicated that computational efficiency of these methods may be questionable. In other words, the time discretization needs to be extremely fine to obtain accurate results. This, in turn, increases the overall calculation time. The same study (Kotlyar and Shwageraus, 2015) extends the method by incorporating a substep approach (Isotalo and Aarnio, 2011). The results indicated that introduction of substeps leads to substantial performance improvement compared to the previously suggested methods (Kotlyar and Shwageraus, 2014). However, the new method required an iterative procedure to update the cross sections and fluxes. The iterations are needed to improve the quality of correlation between the reactions rates and the nuclide densities. These correlations were then used in the substep procedure to evaluate the reaction rates during each substep. Moreover, each nuclide's reaction rate was correlated only with its own corresponding

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nuclide density. While this approach correctly accounts for the self shielding effects, the cross-effects between one-group reaction rates and atomic densities of different isotopes were disregarded.

Recently, a collision history-based approach to sensitivity calculations was implemented (Aufiero et al., 2015) in an extended Serpent version. The equivalence of this approach to the Generalized Perturbation Theory (GPT) was shown by Aufiero et al. (2015). This method allows computing the perturbation effects on virtually any quantity that can be estimated with standard direct Monte Carlo criticality source simulations.

In the current study, this feature was exploited to obtain the relative change in every reaction cross section i (e.g. the one-group capture cross section of Gd^{157}) due to the relative change in the nuclide density of every isotope j in the system (e.g. $Gd^{157}, U^{235}, Pu^{239}$, etc.). This ratio will be referred to here as the sensitivity coefficient for each reaction i to the nuclide j. The GPT-enabled Serpent version allows computing all the sensitivity coefficients in a single run.

This work combines these sensitivity coefficients together with the substep approach to achieve more accurate representation of the time-dependent cross sections. The advantage of this method is that it requires no iterations and, thus, no additional transport calculations. This report should be viewed only as an initial proof of principle and further studies would be needed to demonstrate the practicality and the computational efficiency of this method.

In this study, a number of simplifying assumptions were made. Firstly, the flux was assumed to be constant and only cross sections were allowed to vary with time. This is in order to separate the effects of changing flux amplitude, due to power normalization, and spectrum. Temporal change in the amplitude of the flux at each substep is easier to account for through re-normalization than for changes in the flux spectrum (reaction cross sections). Secondly, the method was applied to a single burnable region. In a multi-region problem, reaction cross sections in one region could be sensitive not only to nuclide densities in that region but also to nuclide densities in all or some other regions.

Low-order and higher-order (quadratic) methods, denoted here as GPT/LI and GPT/QI respectively, were developed in this work. The methods were implemented in a script that couples Serpent with a stand-alone burnup solver. The methods were then used to perform 2D burnup calculations of a typical PWR fuel pin containing Gd burnable absorber since it is typically very challenging for depletion methods to handle accurately. The performance of the proposed methods was compared to that of other existing methods.

2. Codes and methods

2.1. Computer codes

Serpent (Leppänen et al., 2015) is a continuous energy MC neutron transport code. It was developed as an alternative to deterministic lattice physics codes for generation of homogenized multi-group constants for reactor analyses using nodal diffusion codes. Serpent allows modelling of complicated three-dimensional geometries. The code has a number of features that considerably reduce computational effort requirements, such as the unified energy grid (Leppänen, 2009) and the use of Woodcock delta-tracking (Leppänen, 2010) of particles. Serpent also has a built-in fuel depletion solver (Pusa and Leppänen, 2010) however this capability was not used for the most part of this work.

2.2. Collision history and weight perturbation

Practical implementation of the GPT method in Serpent is described in Aufiero et al. (2015). The details of the implementation are beyond the scope of the present paper. Nonetheless, a brief introduction to the collision–history approach is presented in the following.

The main step of the method is propagating the collision information through the neutron generations. The history of a particle and its ancestors is followed over multiple generations. If accepted and rejected collisions are scored, the effect of nuclear data perturbations on the particle can be adjusted by modifying the particle's weight. Instead of sampling a new particle path in a perturbed system, the neutron is allowed to follow the same sequence of events as in the reference history but its statistical weight is adjusted to maintain fair game.

In this study, we only considered first order perturbations, meaning that the effect of a perturbation in parameter x on the response R is expressed in terms of relative changes (Williams, 1986):

$$S_x^R = \frac{dR/R}{dx/x} \tag{1}$$

S_x^R is the sensitivity coefficient of R to a perturbation of x. As mentioned above, the current method is limited to first order perturbation of particle weights. This perturbation of particle weights can be used to calculate the effects of perturbations on generic response functions via standard Monte Carlo estimators (Aufiero et al., 2015).

This capability was used here to obtain the relative change in every reaction cross-section, $R \equiv \sigma$, with respect to the change in concentration of every nuclide j in the system, $x \equiv N_j$, i.e. $S_{N_j}^{\sigma} = \frac{\partial\sigma/\sigma}{\partial N_j/N_j}$.

In case of criticality source simulations, the Generalized Perturbation Theory (GPT) formulation requires the response function R to be in the form or a ratio of linear functions of the forward flux of bilinear functions of the forward and adjoint flux. In case of R being a one-group transmutation cross section, it is defined in the following form:

$$R \equiv \sigma = \frac{\int \phi(E) \cdot \sigma(E) dE}{\int \phi(E) dE} \tag{2}$$

the integration being performed over the fuel material volume.

Standard Monte Carlo track-length or collisional estimators are adopted to derive the numerator and denominator of Eq. (2). If we define the expected value of the estimators for the numerator and denominator of R as $E[e_1]$ and $E[e_1], S_{N_j}^{\sigma}$ can be estimated from the correlation in the particle population between the collisions on the nuclide j and the scores for e_1 and e_2 (Aufiero et al., 2015):

$$S_{N_j}^{\sigma} = \frac{COV\left[e_1, \sum^{history} (ACC_j - REJ_j)\right]}{E[e_1]} - \frac{COV\left[e_2, \sum^{history} (ACC_j - REJ_j)\right]}{E[e_2]} \tag{3}$$

$\sum^{history} (ACC_j - REJ_j)$ represents the net sum of collisions events in the particle buffer involving the nuclide j. Multi-generation effects are implicitly taken into account by following the particle histories over multiple generations.

3. Calculation methodology

Serpent code was used here to provide the transport solution and compute the sensitivity coefficients. An external wrapper script was written to couple Serpent with a stand-alone depletion