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Stable perturbation-based susbtep method for coupled Monte Carlo Codes

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Abstract - *Coupled Monte Carlo (MC) methods are widely used in reactor physics design and different research groups therefore, developed their own coupled MC depletion codes. The coupling scheme refers to the procedure according to which information is exchanged between the MC transport and depletion solvers. The reaction rates obtained from the transport solution, for a predetermined fuel inventory, are provided to the depletion module. The reaction rates are used to solve the depletion problem and obtain the change in isotopic concentrations. It must be pointed out that the reaction rates are obtained by solving a static neutron transport problem at a specific time point. In reality however, reaction rates 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.*

I. INTRODUCTION

Multiple codes that integrate Monte Carlo (MC) neutron transport with burnup calculations have been developed. Various research teams have coupled burnup routines with MC codes, such as Serpent [1], BGCore [2, 3] and MCNPX [4] to name a few. There are however, many notable differences between these codes.

An important aspect that differs among the codes is the coupling scheme used to integrate the MC transport solution with burnup calculations. Recent studies [5] presented the effect of such coupling scheme choice on numerical stability and accuracy of the results. Furthermore, new coupling methods have been developed for MC-burnup applications which also account for the dependence of reaction cross sections on thermal hydraulic conditions [6]. Although these methods resolve the issue of numerical stability, further studies [7, 8] indicate that computational efficiency of these methods may be questionable. In other words, the time discretization needs to be extremely fine to obtain accurate results and this increases the overall calculation time. The same study [7] extends the method by incorporating a substep approach [9]. The results indicated that introduction of substeps leads to substantial performance improvement compared to the previously suggested methods [6]. However, the new method requires an iterative procedure to update cross sections and fluxes. The iterations are needed to improve the quality of correlation between cross sections or reactions rates and nuclide densities. These correlations are then used in the substep procedure to evaluate the reaction rates during each substep. Moreover, each nuclide reaction cross section is correlated only with its own corresponding nuclide density. Although this approach correctly accounts for the self shielding effects, cross-effects between one-group cross sections and atomic densities of different isotopes are disregarded.

Recently, a collision history-based approach to sensitivity calculations has been implemented [10] in an extended Serpent version. The equivalence of this approach to the Generalized Perturbation Theory (GPT) is shown in [10]. 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 is 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. Further studies would be needed to demonstrate the practicality and the computational efficiency of this method.

In this study, 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.

The proposed method is implemented in a script that couples Serpent with a stand-alone burnup solver. The methods are then used to perform 2D burnup calculations of a 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.

II. THEORY

The proposed integration approach that relies on the GPT method is implemented in a linkage code. Serpent [1], which is a continuous energy MC neutron transport code, is used to provide the neutronic solution. In addition, the recent capability implemeted in Serpent to obtain sensitivty coefficients is also used here. The practical implementation and description of the GPT method in Serpent is described in [10] and will not be repeated here. The proposed method was compared against the predictor-corrector method which is also described in this section.

1. Predictor corrector

This method is an extension to the classical explicit Euler method [11], in which the neutron transport solution is obtained only once at the beginning-of-step (BOS). The space and energy dependent microscopic reaction rates are assumed to be constant during the depleted time step. These reaction rates are then used in solving the Bateman equations to obtain nuclide concentrations at the end-of-step (EOS). However, the predicted EOS concentrations are only estimated values and, thus, additional EOS transport solution is performed using the predicted EOS concentrations. Implementation of the subsequent (corrector) stage varies in different existing codes. For example, MCODE [12] re-depletes the problem from t_0 until t_1 with the EOS reaction rates to obtain the corrected concentrations N_1. Then, the final EOS nuclide densities are obtained as a simple average between the predicted and corrected values. Recent studies [13] however, suggested that a more accurate approach would be to average the BOS and EOS reaction rates first and then perform the corrector depletion step. Moreover, the corrector step could be performed more than once to obtain better results. In this study, the predictor-corrector method used averaging of the reaction rates and only one corrector step was applied.

Denoting the BOS time by t_0, the EOS time by t_1, the predictor-corrector method, therefore, was implemented as follows:

1. Obtain $\sigma(t_0)$ at t_0 from transport solution
2. Use $\sigma(t_0)$ to deplete the materials N_0 from t_0 until t_1 and obtain the predicted EOS concentrations N_1^p
3. Obtain transport solution $\sigma(t_1)$ for the EOS $\mathrm{N}_1^{\mathrm{p}}$ at t_1
4. Calculate average reaction rates $\bar{\sigma} = \frac{\sigma(t_0)+\sigma(t_1)}{2}$
5. Perform additional depletion calculation from t_0 until t_1 with $\bar{\sigma}$ and obtain the EOS N_1
6. The EOS N_1 is set to be the initial composition for the next step

2. Sub-step algorithm

As mentioned in the previous section, a new feature developed and implemented in Serpent allows computing sensitivity coefficients for practically any response to any perturbed input parameter. In this study, the parameter of interest is the relative change in one-group cross-section σ_j of type j (e.g. radiative capture), due to the change in concentration N_i of nuclide i. Knowing these sensitivity coefficients $S_i^j \equiv \frac{\partial\sigma_j/\sigma_j}{\partial N_i/N_i}$ provides a valuable information to predict the time dependent behavior of the cross section as shown in eq. 1

$$\sigma_j(t) = \sigma_j(t_0) \cdot \left(1 + \sum_i^M S_i^j(t_0) \cdot \frac{N_i(t) - N(t_0)}{N_i(t_0)}\right) \quad (1)$$

Changing concentration of nuclides, most notably depletion of burnable poisons and fissile material, may lead to significant changes in neutron spectrum, even within relatively short timestep. The spectrum averaged reaction cross sections of the nuclides in the system would change correspondingly. Equation 1 serves to capture this effect. It should also be noted that t_0 in eq. 1 is just a reference point at which the transport solution is obtained. The sensitivity coefficients are also calculated at this point. This equation shows that a first-order estimate for any cross section can be evaluated as long as the change in nuclide density $N_i(t)$ is known for all the M nuclides defined in the problem.

Three algorithms are implemented in this work. The first one (GPT/BOS) uses the beginning-of-step (BOS) at t_0 cross sections and their corresponding derivatives. The second one uses linear interpolation (LI) between BOS at t_0 cross sections and their corresponding derivatives and those at end-of-step (EOS) (t_1). This method is denoted as GPT/LI. The third algorithm is a second order Quadratic Interpolation (QI) method that incorporates the cross section values and derivatives also from the previous time-point t_{-1}. It is denoted as GPT/QI. The first method is equivalent (single MC solution per time interval) to the explicit Euler method while the second and third methods are equivalent to the predictor-corrector method (i.e. require 2 MC solutions per timestep).

Linear Lagrange interpolation scheme is adopted for GPT/LI. In general, any function $\sigma(t)$ can be approximated using the following relation:

$$\sigma(t) = \hat{\sigma}(t) + E(t) \quad (2)$$

where $E(t)$ denotes the approximation error. The interpolation of function $\hat{\sigma}$ can then be performed using eq.(3).

$$\hat{\sigma}(t) = \sum_{j=0}^{n} l_j^{(n)} \sigma\left(t_j\right) \quad (3)$$

where $l_j^{(n)}$ is a polynomial of degree (n), and $\sigma\left(t_j\right)$ are known values of the function at tabulated points t_j. The polynomials $l_j^{(n)}$ are constructed using eq.(4)

$$l_j^{(n)} = \prod_{\substack{i=0 \\ i\neq j}}^{n} \frac{t - t_i}{t_j - t_i} \quad (4)$$

Eq. 1 can then be extended by linearly interpolating between t_0 and t_1 time points by applying eqs. 3–4 as follows:

$$\sigma_j(t) = \frac{t-t_1}{t_0-t_1}\sigma_j(t_0)\cdot\left(1+\sum_i^M S_i^j(t_0)\cdot\frac{N_i(t)-N(t_0)}{N_i(t_0)}\right)+ \frac{t-t_0}{t_1-t_0}\sigma_j(t_1)\cdot\left(1+\sum_i^M S_i^j(t_1)\cdot\frac{N_i(t)-N(t_1)}{N_i(t_1)}\right) \quad (5)$$

Based on the above interpolation schemes, the following method is developed. For simplification, the superscript j in S_i^j will be omitted in the algorithm description presented below. However, the practical implementation evaluates the sensitivity coefficients for every reaction j as a function of every perturbed nuclide density i. Following are the main steps of the algorithm.

1. Obtain transport solution $\sigma(t_0)$ and $S_i(t_0)$ at t_0
2. Divide the timestep into S substeps, each with an increment of $\triangle t = \frac{t_1-t_0}{S}$, i.e. $t_0 < t_0+\triangle t < t_0+2\triangle t < ... < t_0+s\triangle t = t_1$. For each $s = 1...S$:
   (a) perform depletion with $\sigma(t_0+(s-1)\triangle t)$ and obtain $N(t_0+s\triangle t)$.
   (b) update the cross section by substituting $N(t_0+s\triangle t)$ into eq. 1
   (c) continue until the timestep is completed and the predicted EOS N_1^p at t_1 is known.
3. Obtain transport solution $\sigma(t_1)$ and $S_i(t_1)$ for the EOS N_1^p at t_1
4. For each substep $s = 1...S$:
   (a) perform depletion with $\sigma(t_0+(s-1)\triangle t)$ and obtain $N(t_0+s\triangle t)$.
   (b) update the cross section by substituting $t = t_0+s\triangle t$ and $N(t_0+s\triangle t)$ into eq. 5.
   (c) continue until the timestep is completed and the EOS N_1 at t_1 is known.
5. The EOS compositions are then set to be the initial ones for the next step

Stage 4 is omitted for the GPT/BOS method.

III. RESULTS AND ANALYSIS

A typical PWR unit cell with UO_2 fuel and water coolant was adopted. The outer radius of the fuel is 0.4095 cm and the outer radius of the clad is 0.475 cm (no gap was included here). The initial enrichment is assumed to be 3.5 ^{w}%. The fuel also contained 0.5 ^{w}% of Gd_2O_3. The pin is not subdivided into radial zones and therefore the differential spatial burnup of Gd isotopes and its effect on criticality is not realistically tracked.

In order to obtain relatively small statistical uncertainties, 400 active fission source iteration cycles with 25,000 histories per cycle are used in the neutron transport calculations with Serpent.

The problem includes Gd absorber that strongly affects the neutron spectrum. Many nuclides, such as Gd^{157}, are very sensitive to such spectral changes. In order to accurately capture the real time-dependent behavior of various cross sections, the analyzed burnup problem should be solved using very short timesteps, during which the cross sections can be assumed constant and then would be frequently updated. The examined test case presents a significant modeling challenge to depletion codes because of the rapid variation of cross sections with time.

The reference solution was obtained using the PC/LI method with very fine timesteps of 0.5 days. Then, the performance of the two proposed methods (i.e. GPT/LI and GPT/QI) was investigated. The solutions with the GPT/LI, GPT/QI and PC/LI were also performed with longer timesteps of 20 days.

Fig. 1 shows the relative difference (%) between the reference and the three studied coupling schemes in concentration of Gd^{157}. This figure shows that the PC/LI method considerably over-predicts the concentration of Gd. The proposed GPT/LI allows achieving better results relative to the PC/LI solution but the relative difference in Gd concentration is still high. A very good agreement with the reference solution is observed when the higher order GPT/QI method is used. The maximum differences in Gd^{157} are 8.4%, 5.1% and -0.4% when the PC/LI, GPT/LI and GPT/QI methods are used respectively.

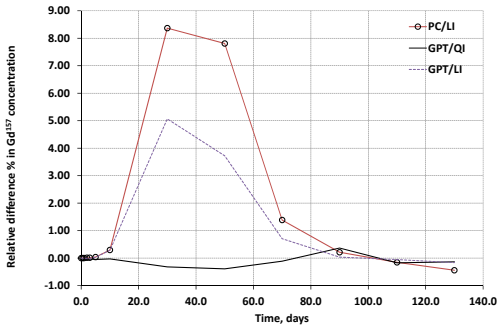

Fig. 1. Relative difference (%) in Gd^{157} concentration.

The substep method is capable of accurately predicting the change in isotopic composition and various cross sections for each substep. The results show that the GPT/QI method has notably better performance over all other methods. This is due to much better capability of predicting the behavior of the cross sections within the timestep, as illustrated in Fig. 6.

To understand the convergence of the proposed method as a function of the timestep size, the results are repeated here for different timestep values, i.e. 0.5, 1, 2.5, 5, 10 and 20 days. Figures 2 through 5 present the maximum errors (over the examined cycle) in reactivity and concentration of Gd^{157}.

The most important conclusion drawn here is that the GPT/BOS and GPT/QI approaches converge much faster than the Explicit Euler and PC/LI methods, respectively.

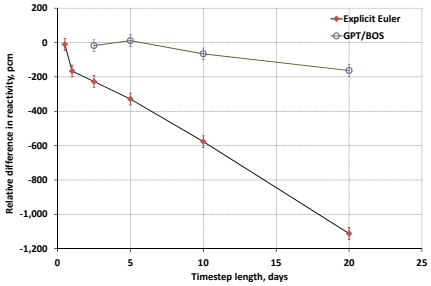

Fig. 2. Difference in reactivity (pcm), 1× MC per step.

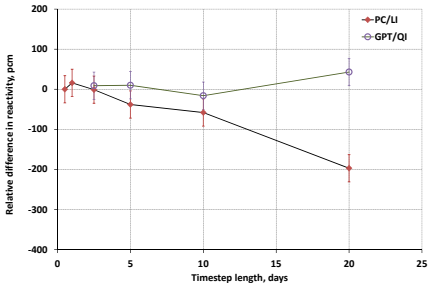

Fig. 3. Difference in reactivity (pcm), 2× MC per step.

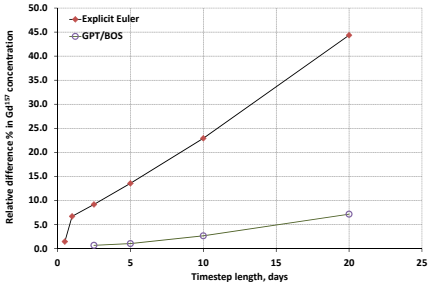

Fig. 4. Relative difference (%) in Gd^{157} concentration as a function of $\triangle$t, 1× MC per step.

In addition, the efficiency of the proposed GPT methods is considerably better. For example, the difference in reactivity is -197 and -163 when Explicit Euler method with $\triangle$t=1 days and GPT/BOS method with $\triangle$t=20 days are used respectively. More specifically, to achieve similar performance Explicit Euler method requires 20 times more MC transport solutions than GPT/BOS for this specific case.

IV. CONCLUSIONS

The importance of coupling procedure to integrate Monte Carlo neutron transport solution with depletion or/and thermal

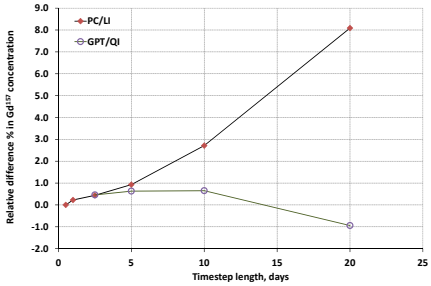

Fig. 5. Relative difference (%) in Gd^{157} concentration as a function of $\triangle$t, 2× MC per step.

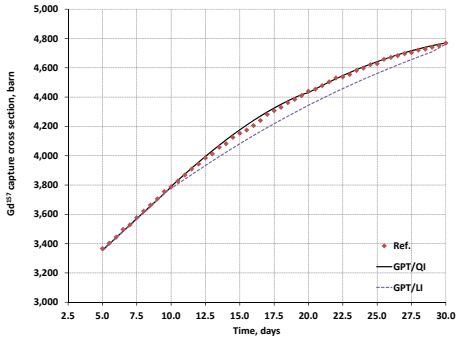

Fig. 6. Comparison of Gd^{157} capture cross section within the timestep.

hydraulic feedbacks has been recognized and has recently become a major topic of research. Coupled MC codes are now routinely used for fuel cycle calculations and assessment of new reactor designs, so that the adopted coupling schemes may have major effect on the numerical stability and accuracy of the results. Previous studies proposed and investigated many coupling methods to evaluate these effects.

This study proposes an iteration-free method which takes advantage of the additional information provided in the form of sensitivity coefficients calculated using Generalized Perturbation Theory in Serpent MC transport code. The GPT-enabled Serpent transport solution provides not only the reaction cross sections but also their derivatives with respect to the change in concentration of every isotope in the system. These derivatives allow obtaining significantly more accurate prediction of temporal variation of cross sections during depletion timestep. In the substep approach, each timestep is divided into smaller steps. The transport solution is performed at the BOS and thus the cross sections and their derivatives are known. Then, the BOS quantities (i.e. initial composition, cross sections and their derivatives with respect to all nuclide concentrations) are used to obtain the end of first substep compositions. These are then used to update the cross sections and the procedure continues until the timestep depletion is completed. Such a procedure allows accounting for the variation in cross sections and reaction rates very accurately. Moreover, in principle, the

method requires only the data obtained from a single time point (i.e. a single transport solution).

It was found that the new method clearly outperforms the alternative ones in terms of accuracy and computational efficiency.

Moreover, the proposed approach is expected to be a useful tool in case of multi-regions burnup simulations in which standard non-iterative techniques give rise to spatial oscillations that lead to instabilities. The GPT-based approach could offer an iteration-free stabilization technique.

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