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Technical note

New perturbation and sensitivity capabilities in TRIPOLI-4®

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ABSTRACT

Estimating the changes in a nuclear system due to perturbations in the input nuclear data by separate Monte Carlo calculations might be extremely cumbersome for reactor applications. The Iterated Fission Probability (IFP) method has recently paved the way for the application of first-order standard perturbation theory in continuous-energy Monte Carlo codes. In this work, we detail the reactivity perturbation and *k*-eigenvalue sensitivity analysis capabilities of the Monte Carlo code TRIPOLI-4®. Simulation results obtained by using the newly implemented IFP algorithm of TRIPOLI-4® are compared to findings coming from other Monte Carlo methods (such as the differential operator and the correlated sampling) and codes (such as MCNP6 and KENO). For this purpose, we select some benchmark configurations (Godiva, Stacy, Jezebel, Flattop and a fuel lattice) and we test some of the most common perturbation and sensitivity methods currently available in production codes. Their respective advantages and drawbacks are analyzed, and possible future improvements are suggested. Our main finding is that TRIPOLI-4® produces very similar results to MCNP6 when the same techniques are used. Uncertainty propagation based on the obtained sensitivity profiles and on the COMAC nuclear data covariance matrices is finally discussed.

1. Introduction

Monte Carlo simulation has become the golden standard for nuclear reactor safety analysis and design. In principle, a change in reactivity due to a system perturbation could be estimated performing two separate *k*-eigenvalue Monte Carlo calculations for the perturbed and the unperturbed system, and then computing the difference of the inverse of the two eigenvalues. However, if the perturbation is small, performing two separate Monte Carlo runs might be infeasible due to the simulation time required to achieve a sufficiently small statistical uncertainty. Furthermore, modern engineering analyses involve the calculation of a considerable number of sensitivity coefficients, so that it would be extremely cumbersome to compute these quantities by performing separate calculations.

Until recently, the only available perturbation methods for continuous-energy Monte Carlo codes were the differential operator sampling and the correlated sampling (Rief et al., 1986). The rediscovery of the so-called Iterated Fission Probability (IFP) interpretation of the adjoint flux $\varphi^{\dagger}$ has allowed computing adjoint-weighted scores within standard *k*-eigenvalue problems by formally identifying the adjoint neutron flux with the neutron importance, which can be obtained in regular forward Monte Carlo simulations by counting the descendant neutrons coming from a common ancestor (Nauchi and Kameyama, 2010; Kiedrowski et al., 2011). According to standard perturbation theory (SPT) (Gandini, 1981), reactivity perturbations and k_{eff} sensitivity coefficients to nuclear data can be expressed as ratios of bi-linear forms involving the adjoint and forward flux, and can thus be estimated in production Monte Carlo codes by the IFP method (Kiedrowski et al., 2011; Kiedrowski and Brown, 2013; Shim et al., 2011; Perfetti, 2012; Qiu et al., 2016). Other importance-based techniques for sensitivities have later been proposed, such as the collision–history-based GPT equivalent implementation (Aufiero et al., 2015), the adjoint Wielandt method (Choi and Shim, 2016), the CLUTCH [1] method (Perfetti et al., 2016; Peng et al., 2017) and the super-history method (Qiu et al., 2016).

In TRIPOLI-4®, the production Monte Carlo code developed at CEA (Brun et al., 2015), the correlated sampling method has been available for many years to compute reactivity perturbations in criticality calculations (Morillon, 1998; Lee, 2007). The possibility of computing exact adjoint-weighted perturbations has been recently investigated (Truchet et al., 2014a, b; Truchet, 2015). In view of a future release of the code, we have developed first-order reactivity perturbations and *k*-eigenvalue sensitivity analysis capabilities

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[1] Contribution-Linked eigenvalue sensitivity/Uncertainty estimation via Track-length importance CHaracterization.

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based on the IFP method [2]. In this work we will illustrate the new features of TRIPOLI-4® in this domain and compare our findings to those coming from other Monte Carlo methods and codes, so as to validate our implementation and to elucidate the respective advantages and drawbacks of the existing perturbation and sensitivity techniques. Multi-method comparisons have been previously attempted for perturbations (see, e.g., Nagaya and Mori (2005), Kiedrowski and Brown (2011)) and sensitivities (see, e.g., Kiedrowski and Brown (2013), Qiu et al. (2016)). Moreover, the equivalence between the first-order differential operator sampling method including the fission source perturbation and the IFP-based SPT has been shown in Shim et al. (2011).

In this work, we will first contrast the reactivity perturbations obtained by the IFP-based Standard Perturbation Theory (IFP-SPT) with the correlated sampling method already available in TRIPOLI-4® and to the second-order Taylor differential operator perturbation method available in MCNP6 [3]. For this purpose, we will consider a few significant benchmark configurations, including Godiva (ICSBEP Handbook 2016) and Stacy (Nagaya and Mori, 2005). Verification tests will be also performed for neutron multiplicity perturbations. Then, we will examine first-order sensitivity coefficients and profiles for some benchmark configurations including Jezebel, Stacy, Godiva, Flattop and a MOX fuel lattice (ICSBEP Handbook, 2016), and contrast our results with those coming from MCNP6 (Kiedrowski et al., 2011; Kiedrowski and Brown, 2013) and KENO (Rearden, 2000). Our main finding is that TRIPOLI-4® produces very similar results to MCNP6 when the same techniques are used. Finally, uncertainty propagation will be examined by resorting to the COMAC [4] covariance data library (Archier et al., 2014).

The paper is organized as follows: in Section 2 we provide the algorithms and implementation choices for IFP-based reactivity and sensitivity analysis functionalities in TRIPOLI-4®. In Section 3 we examine reactivity perturbations due to density, cross section and neutron multiplicity in several reactor configurations by using the different methods available in TRIPOLI-4® and MCNP6. In Section 4 we illustrate the comparison between TRIPOLI-4®, MCNP6 and KENO for sensitivity analysis calculations, and we provide results concerning nuclear data uncertainty propagation. Conclusions are drawn in Section 5.

2. Implementing IFP-based SPT in TRIPOLI-4®

In this Section we describe the choices that have been made for the development of SPT functionalities in TRIPOLI-4®, based on a generalization of the IFP method that has been recently implemented for adjoint-weighted kinetics parameters (Truchet et al., 2015; Terranova and Zoia, 2017). The importance π_i of an ancestor i beginning an IFP cycle at generation g is estimated at a later generation $g+M+1$, where the number M of latent generations defines the length of an IFP cycle within the Monte Carlo power iteration. An overlapping-cycles algorithm has been proposed in TRIPOLI-4®, where a new IFP cycle begins at each generation and each neutron carries M distinct importance contributions (Truchet et al., 2015; Terranova and Zoia, 2017). This improves the statistics by a factor $\sqrt{M}$, although inter-cycle correlations may possibly increase (Truchet et al., 2015).

2.1. Reactivity perturbations

According to SPT, the first-order reactivity variation $\Delta\rho$ due to a system perturbation is given by

$$\Delta\rho = \frac{\langle \varphi^\dagger, (\Delta\mathcal{S} + \frac{1}{k}\Delta\mathcal{F} - \Delta\mathcal{C})\varphi\rangle}{\langle \varphi^\dagger, \mathcal{F}\varphi\rangle}, \tag{1}$$

where $\Delta\mathcal{S}, \Delta\mathcal{C}$ and $\Delta\mathcal{F}$ are the variations in the scattering, collision and fission operators, respectively[5]. For our implementation of first-order reactivity perturbations in TRIPOLI-4®, we have basically followed the strategy proposed in Kiedrowski et al. (2011). By resorting to IFP, the reactivity change $\Delta\rho_{\mathcal{A}}$ due to the generic perturbation $\Delta\mathcal{A} = \mathcal{A}_* - \mathcal{A}$ of an operator $\mathcal{A}$ is obtained by using

$$\Delta\rho_{\mathcal{A}} = \frac{\langle \varphi^\dagger, \Delta\mathcal{A}\varphi\rangle}{\langle \varphi^\dagger, \mathcal{F}\varphi\rangle} = \frac{\sum_i \pi_i T_i}{k\sum_i \pi_i}, \tag{4}$$

where T_i is the estimator associated to $\Delta\mathcal{A}\varphi$ in the Monte Carlo simulation, evaluated during the first generation of the IFP cycle, π_i is the corresponding importance collected at the end of the IFP cycle, and the sum is extended over the ancestors (Kiedrowski et al., 2011). Normalization factors cancel out in the ratio of the two scalar products. For the reactivity change due to a perturbation in the collision operator, in TRIPOLI-4® a track estimator is used, namely,

$$\Delta\rho_{\mathcal{C}} = \frac{\langle \varphi^\dagger, \Delta\mathcal{C}\varphi\rangle}{\langle \varphi^\dagger, \mathcal{F}\varphi\rangle} = \frac{\sum_i \pi_i \sum_{\tau\in i} \Delta\Sigma_t l_\tau}{k\sum_i \pi_i}, \tag{5}$$

where $\Delta\Sigma_t$ is the change in the total cross section due to the system perturbation and l_τ is the length of the track τ followed by the ancestor i (Kiedrowski et al., 2011). The quantity $\Delta\Sigma_t l_\tau$ is then the estimator for $\Delta\mathcal{C}\varphi$, collected for the ancestor at each collision event, and 1 is the estimator for the term $\frac{1}{k}\mathcal{F}\varphi$ at the denominator. The contribution to a reactivity change due to a variation in the scattering operator is given by

$$\Delta\rho_{\mathcal{S}} = \frac{\langle \varphi^\dagger, \Delta\mathcal{S}\varphi\rangle}{\langle \varphi^\dagger, \mathcal{F}\varphi\rangle} = \frac{\sum_i \pi_i \sum_{\tau\in i} \frac{\Delta\Sigma_s}{\Sigma_s}}{k\sum_i \pi_i}, \tag{6}$$

where $\Delta\Sigma_s$ is the variation of the scattering cross section due to the system perturbation. For a perturbation in the fission operator, the corresponding reactivity variation is given by

$$\Delta\rho_{\mathcal{F}} = \frac{\langle \varphi^\dagger, \frac{1}{k}\Delta\mathcal{F}\varphi\rangle}{\langle \varphi^\dagger, \mathcal{F}\varphi\rangle} = \frac{\sum_i \pi_i \sum_{\tau\in i} \frac{\Delta(\nu\Sigma_f)}{\nu\Sigma_f}}{k\sum_i \pi_i}. \tag{7}$$

In TRIPOLI-4®, prompt and delayed fission contributions are singled out by separately computing the prompt $\Delta\rho_{\mathcal{F}_p}$ and delayed $\Delta\rho_{\mathcal{F}_d}$ fission terms. The total reactivity change is finally provided by

$$\Delta\rho = \Delta\rho_{\mathcal{S}} + \Delta\rho_{\mathcal{F}_p} + \Delta\rho_{\mathcal{F}_d} - \Delta\rho_{\mathcal{C}}. \tag{8}$$

A refinement of the first-order formulation would include a perturbed denominator in Eq. (1) (Gandini, 1981), namely,

$$\Delta\rho = \frac{\langle \varphi^\dagger, (\Delta\mathcal{S} + \frac{1}{k}\Delta\mathcal{F} - \Delta\mathcal{C})\varphi\rangle}{\langle \varphi^\dagger, \mathcal{F}_*\varphi\rangle}. \tag{9}$$

In order to take into account the perturbed fission operator $\mathcal{F}_*$ at the denominator of Eq. (9), a correction factor $(\nu\Sigma_f)_*/(\nu\Sigma_f)$ must be included in the Monte Carlo estimators for Eqs. (5)–(7), whose

[2] TRIPOLI-4® already has IFP-based adjoint-weighted scores for kinetics parameters (Truchet et al., 2015; Zoia and Brun, 2016; Zoia et al., 2016; Terranova and Zoia, 2017).

[3] We have used the version MCNP6.1 for all the simulation results presented in the following.

[4] COvariance MAtrices from Cadarache.

[5] We have used standard notation: the collision operator is simply $\mathcal{C}\varphi \equiv \Sigma_t\varphi$; the scattering operator reads

$$\mathcal{S}\varphi \equiv \int \Sigma_s(\mathbf{r}, E' \to E, \Omega' \to \Omega)\varphi(\mathbf{r}, E', \Omega')\,\mathrm{d}E'\mathrm{d}\Omega'; \tag{2}$$

and the fission operator reads

$$\mathcal{F}\varphi \equiv \frac{\chi(E)}{4\pi}\int \nu(E')\Sigma_f(\mathbf{r}, E')\varphi(\mathbf{r}, E', \Omega')\,\mathrm{d}E'\mathrm{d}\Omega'. \tag{3}$$