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Uncertainty analysis of assembly and core-level calculations with application to CASMO-4E and SIMULATE-3

Maria Pusa [a,*], Aarno Isotalo [b]

[a] VTT Technical Research Centre of Finland, P.O. Box 1000, FI-02044 VTT, Finland
[b] Aalto University, Department of Applied Physics, P.O. Box 14100, FI-00076 AALTO, Finland

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ABSTRACT

The topic of this paper is the development of sensitivity and uncertainty analysis capability to the CASMO-4/CASMO-4E – SIMULATE-3 code sequence in the context of the OECD/NEA benchmark 'Uncertainty Analysis in Best-Estimate Modelling for Design, Operation and Safety Analysis of LWRs' (UAM). The developed capability uses a two-step approach. In the first step, Uncertainties in nuclear data are propagated to two-group cross sections, diffusion coefficients, and assembly discontinuity factors. This is carried out using deterministic, perturbation-theory-based uncertainty analysis methodology. In the second step, a global covariance matrix, characterizing the uncertainties of the group constants, is formed, and the uncertainties are propagated through a full core SIMULATE calculation using a stochastic approach. This system enables the analysis of nuclear data related uncertainties in assembly-homogenized group constants, assembly discontinuity factors, and pin powers, as well as full core results such as multiplication factor and power distribution. The mathematical background of the deterministic uncertainty analysis methodology is reviewed and the main conclusions related to the implementation are summarized. Numerical results are presented for the full core Three Mile Island model in exercise I-3 of the UAM benchmark at hot zero power with all rods out and inserted. The computational efficiency of the calculations is discussed.

1. Introduction

The topic of this paper is the development of sensitivity and uncertainty analysis capability to the CASMO-4/CASMO-4E – SIMULATE-3 code sequence (Rhodes and Edenius, 2001; Rhodes et al., 2004; Studsvik Scandpower, 2003) in the context of the 'Uncertainty Analysis in Best-Estimate Modelling for Design, Operation and Safety Analysis of LWRs' (UAM) benchmark (Ivanov et al., 2007).

The UAM benchmark was initiated in 2006 to establish the current state and needs of sensitivity and uncertainty analysis with the goal of being able to propagate uncertainty through all stages of coupled neutronics/thermal-hydraulics calculations with a special emphasis on the uncertainty related to nuclear data. The first phase of the benchmark concentrates on stand-alone neutronics calculations in group constant generation and in subsequent full core analyses using the generated constants. At VTT, CASMO-4 and CASMO-4E are the standard tools for assembly-level calculations, while SIMULATE is often used for core-level analysis. Therefore it was decided to begin developing uncertainty analysis capability for this calculation sequence.

Uncertainty analysis methods can be divided into stochastic and deterministic methods. In stochastic methods, the values of the uncertain parameters are repeatedly sampled from their uncertainty distributions and the calculation is repeated with each perturbed set of parameters to obtain a sample from the uncertainty distribution of the system responses under consideration. This approach is simple and universally applicable, but computationally expensive. In deterministic methods, on the other hand, the sensitivity profiles of the responses with respect to uncertain parameters are computed first, after which the parameter uncertainty is propagated by the Sandwich rule by combining the sensitivity profiles with the covariance matrices of the parameters. These sensitivity profiles can be computed efficiently by solving the corresponding generalized adjoint systems. This approach is generally well-suited when the number of responses is small compared to the number of uncertain parameters. It is also beneficial that this type of uncertainty analysis yields detailed information on the sources of uncertainty in the computation.

Reactor core analyses are generally based on a computation sequence, where the level of detail and physical complexity is

* Corresponding author.
E-mail address: maria.pusa@vtt.fi (M. Pusa).

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reduced and the scale of the modelled system is increased at every step. In lattice physics calculations, the neutron transport eigenvalue problem is solved on the assembly-level in different operating conditions, and the solutions are used to homogenize and collapse assembly data for the following nodal calculations. The power distribution in the reactor core is then solved from the diffusion equation based on these constants obtained from the lattice calculations. In this work, the adjoint-based approach (perturbation theory) was applied to the sensitivity analysis of the assembly-level calculations and stochastic sampling to the uncertainty analysis of the core-level calculations. This framework is sometimes called the two-step method (Yankov et al., 2012).

This paper is organized as follows. Section 2 reviews the theoretical background for the two-step method with emphasis on the adjoint-based sensitivity analysis. The implementation and the processing of covariance matrices are discussed in Section 3. Numerical results are presented and analyzed in Section 4.

2. Theoretical background

The purpose of uncertainty analysis is to estimate how the uncertainty related to the parameters of a mathematical model propagates to a response dependent on the solution of this model. Sensitivity analysis studies the changes in the responses due to perturbations in the parameters.

2.1. Adjoint-based sensitivity analysis

In deterministic uncertainty analysis, the response sensitivities are computed first, after which uncertainty is propagated in a deterministic manner by combining the sensitivity profiles of the responses with the covariance matrices characterizing the uncertainty of the model parameters.

Let us consider the neutron transport eigenvalue problem, which can be written in operator form as

$$\boldsymbol{A}\boldsymbol{\Phi} = \frac{1}{k}\boldsymbol{B}\boldsymbol{\Phi}, \tag{1}$$

where $\boldsymbol{\Phi} \in H_\Phi$ is the neutron flux, H_Φ is a Hilbert space and k is the critical eigenvalue. The uncertain parameters consist of nuclear data parameters, and they are denoted by the vector $\boldsymbol{\sigma} \in E_\sigma$. We will only consider functional responses dependent on the solution of Eq. (1). Since nuclear data parameters, such as neutron cross sections, are functions of energy and location, it is necessary to use a functional derivative to define the response sensitivities. We can define the sensitivity of the response R to the perturbation $\boldsymbol{h} = [\delta\boldsymbol{\Phi}, \delta\boldsymbol{\sigma}] \in D = H_\Phi \times E_\sigma$ at the point $\hat{\boldsymbol{e}} = [\hat{\boldsymbol{\Phi}}, \hat{\boldsymbol{\sigma}}] \in D$ as the Gâteaux variation:

$$\delta R(\hat{\boldsymbol{e}}; \boldsymbol{h}) = \lim_{t\to 0} \frac{R(\hat{\boldsymbol{e}} + t\boldsymbol{h}) - R(\hat{\boldsymbol{e}})}{t}. \tag{2}$$

In practice, however, Eq. (1) and the system responses are discretized, meaning that the sensitivity profiles to nuclear data are reduced to vectors containing conventional partial derivatives.

In perturbation theory, the sensitivities of system responses with respect to all uncertain parameters are computed based on solving one additional adjoint system for each response. The adjoint of Eq. (1) is defined as the system satisfying the following relation: [1]

$$\left\langle \boldsymbol{A}\boldsymbol{\Phi} - \frac{1}{k}\boldsymbol{B}\boldsymbol{\Phi},\ \boldsymbol{\Psi} \right\rangle = \left\langle \boldsymbol{\Phi},\ \boldsymbol{A}^*\boldsymbol{\Psi} - \frac{1}{k}\boldsymbol{B}^*\boldsymbol{\Psi} \right\rangle, \tag{3}$$

where the brackets $\langle \cdot, \cdot \rangle$ denote an inner product, i.e. integrals over energy, space and direction. The solution of the adjoint problem

$$\left(\boldsymbol{A}^* - \frac{1}{k}\boldsymbol{B}^*\right)\boldsymbol{\Psi} = 0 \tag{4}$$

is called the *fundamental adjoint*. In classical perturbation theory, the response under consideration is the critical eigenvalue k. By utilizing the fundamental adjoint we can derive the following expression for the relative sensitivity of k with respect to a perturbation $\delta\boldsymbol{\sigma}$ (for derivation, see e.g. Williams (1986) and Pusa (2012a)):

$$\frac{\delta k(\hat{\boldsymbol{e}}; \boldsymbol{h})}{k} = -\frac{\left\langle \left(\boldsymbol{A}'_\sigma(\hat{\boldsymbol{e}}) - \frac{1}{k}\boldsymbol{B}'_\sigma(\hat{\boldsymbol{e}})\right)\delta\boldsymbol{\sigma},\ \boldsymbol{\Psi}\right\rangle}{\left\langle \frac{1}{k}\boldsymbol{B}\boldsymbol{\Phi},\ \boldsymbol{\Psi}\right\rangle}. \tag{5}$$

For functional responses that are Fréchet-differentiable with the gradient orthogonal to the forward flux, we can define the *generalized adjoint* as the solution to the following inhomogeneous system

$$\left(\boldsymbol{A}^* - \frac{1}{k}\boldsymbol{B}^*\right)\boldsymbol{\Gamma} = \frac{\nabla_\Phi R}{R}. \tag{6}$$

If the generalized adjoint problem has a solution, it follows that an infinite number of solutions exist. Out of these solutions, it is possible to choose the one orthogonal to the forward fission source. For further details, see e.g. Pusa (2012b). This particular solution is denoted by $\boldsymbol{\Gamma}_p$ in this paper.

Generalized perturbation theory considers responses of the form

$$R(\boldsymbol{e}) = \frac{\langle \boldsymbol{\Phi},\ \boldsymbol{\Sigma}_1\rangle}{\langle \boldsymbol{\Phi},\ \boldsymbol{\Sigma}_2\rangle}, \tag{7}$$

where $\boldsymbol{\Sigma}_1, \boldsymbol{\Sigma}_2 \in H_\Phi$. In Eq. (7) it is assumed that Σ_1 and Σ_2 do not depend on Φ. It is straight-forward to show that in this case the relative gradient of the response can be written

$$\frac{\nabla_\Phi R}{R} = \frac{\boldsymbol{\Sigma}_1}{\langle \boldsymbol{\Phi},\ \boldsymbol{\Sigma}_1\rangle} - \frac{\boldsymbol{\Sigma}_2}{\langle \boldsymbol{\Phi},\ \boldsymbol{\Sigma}_2\rangle} \tag{8}$$

and that this gradient is orthogonal to the forward flux Φ. The following expression can now be derived for the sensitivity of a response in generalized perturbation theory (For derivation, see e.g. Williams (1986) and Pusa (2012b)):

$$\frac{\delta R(\hat{\boldsymbol{e}}, \boldsymbol{h})}{R} = \frac{R'_\sigma(\hat{\boldsymbol{e}})\,\delta\boldsymbol{\sigma}}{R} - \left\langle \boldsymbol{\Gamma},\ \left(\boldsymbol{A}'_\sigma(\hat{\boldsymbol{e}}) - \frac{1}{k}\boldsymbol{B}'_\sigma(\hat{\boldsymbol{e}})\right)\delta\boldsymbol{\sigma}\right\rangle_\Phi, \tag{9}$$

where the direct sensitivity term can further be written

$$\frac{R'_\sigma(\hat{\boldsymbol{e}})\,\delta\boldsymbol{\sigma}}{R} = \frac{\left\langle \frac{\partial}{\partial\sigma}\boldsymbol{\Sigma}_1(\hat{\boldsymbol{\sigma}})\delta\boldsymbol{\sigma}, \Phi\right\rangle}{\langle \boldsymbol{\Sigma}_1, \Phi\rangle} - \frac{\left\langle \frac{\partial}{\partial\sigma}\boldsymbol{\Sigma}_2(\hat{\boldsymbol{\sigma}})\delta\boldsymbol{\sigma}, \Phi\right\rangle}{\langle \boldsymbol{\Sigma}_2, \Phi\rangle}. \tag{10}$$

Homogenized two-group cross sections and pin powers can be written in the form of Eq. (7) and therefore Eqs. (8)–(10) can directly be applied to them. When diffusion coefficients are considered as responses, Eq. (8) needs to be modified. The energy and location dependent diffusion coefficient is generally defined as

$$D(\boldsymbol{r}, E) = \frac{1}{3\Sigma_{\mathrm{tr}}(\boldsymbol{r}, E)}, \tag{11}$$

where Σ_{tr} is the transport cross section. However, the two-group homogenized diffusion coefficients should not be computed by homogenizing and collapsing the energy- and space-dependent diffusion coefficient (Knott and Yamamoto, 2010). Instead, the transport cross section should be homogenized over the assembly. After this, two-group diffusion coefficients can be computed either by collapsing the homogenized transport cross section or the

[1] In some cases the adjoint relation needs to be written in the form $\langle \boldsymbol{A}\boldsymbol{\Phi} - \frac{1}{k}\boldsymbol{B}\boldsymbol{\Phi},\ \boldsymbol{\Psi}\rangle = \langle \Phi,\ \boldsymbol{A}^*\boldsymbol{\Psi} - \frac{1}{k}\boldsymbol{B}^*\boldsymbol{\Psi}\rangle + [\boldsymbol{P}(\boldsymbol{\Psi}, \boldsymbol{\Phi})]_{\boldsymbol{x}\in\partial\Omega}$, where $[\boldsymbol{P}(\boldsymbol{\Psi}, \boldsymbol{\Phi})]_{\boldsymbol{x}\in\partial\Omega}$ is a bilinear form associated with the system. We will only consider cases where it is straightforward to force this term to vanish.