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Editorial

Sensitivity Analysis, Uncertainty Quantification and Predictive Modeling of Nuclear Energy Systems

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The Special Issue "Sensitivity Analysis, Uncertainty Quantification and Predictive Modeling of Nuclear Energy Systems" comprises nine articles that present important applications of concepts for performing sensitivity analyses and uncertainty quantifications of models of nuclear energy systems. These models of nuclear systems include a stochastic point kinetic reactor model [1], a reduced-order model for fuel burnup analysis [2], and an OECD/NEA reactor physics benchmark [3–8]. The ninth article in this Special Issue presents [9] a new methodology aimed at overcoming the curse of dimensionality [10] in sensitivity analysis, uncertainty quantification, and predictive modeling.

A mixed spectral technique was used in [1] to quantify uncertainties in a stochastic point-kinetics reactor model with six groups of delayed neutrons, comprising noise and uncertain parameters. This stochastic model was decomposed into a system of deterministic ordinary differential equations by using a Wiener–Ito expansion (WIE) to handle the noise and by using a first-order Gaussian expansion to handle the model's random parameters. The simplified deterministic model thus derived was solved using deterministic methods for solving ordinary differential equations. The solution of this simplified model was subsequently used to compute the average neutronic power and the average delayed neutron precursors, as well as the standard deviations in these quantities due to various levels of noise, random parameters, and combinations thereof. The power was found to be more sensitive to noise variations rather than to the standard deviations assumed for the random parameters. For large deviations of the random parameters, the power decreased with increasing the assumed parameter's standard deviation, which is a counterintuitive result whose correctness was not proven. The results presented in [1] were not validated by comparisons to actual experiments.

A reduced order model (ROM) aimed at finding a compromise between computational cost and solution accuracy in fuel burnup analysis has been presented in [2]. This ROM has been constructed by using an offline/online strategy as follows:

(i) The offline stage commences by using proper orthogonal decomposition (POD) to select, via singular value decomposition, the largest eigenvalues of a matrix generated by using the solutions ("snapshots") of the "full order model" (FOM) of a Monte Carlo simulation of the burnup process. The largest eigenvalues are assumed to correspond to the most significant features of the full order model (FOM). For the time-evolution of the neutron fluxes and burnup matrices, a "snapshot" is a burnup-step between two time points, for a burnup region at a specific power level. For the time-evolution of the nuclide concentrations, a snapshot is provided by the concentrations at each time point, including the concentrations at the end of the burnup history. Subsequently, a low-dimensional approximation of the FOM was obtained by a Galerkin projection onto the space spanned by the POD basis functions.

(ii) In the online stage, the ROM simulation is run repeatedly, as needed.

The above strategy was used to reproduce the time-evolution of the reactivity and nuclide densities over 4 years of burnup of the TMI-1 unit cell benchmark by reconstructing

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fuel materials and burnup matrices over time with different levels of approximation. It was found that the benchmark's effective multiplication factor and nuclide concentrations displayed reasonably good agreement (hundreds of percent per mille of reactivity) with the FOM-results if over 50 basis-functions were used, but the results for the multiplication factor were unphysical when fewer than 20 basis-functions were used. This indicates that a monotonic behavior of the error between the POD and the FOM as a function of the number of basis-functions included in the ROM is not guaranteed. The results presented in [2] illustrate both the advantages (in terms of the reduced memory and computational time requirements) as well as the disadvantages (in terms of accuracy and extrapolation capabilities) of using a ROM instead of a FOM.

The sequence of works [3–8] presents a very large (probably the largest ever) application of the Second-Order Adjoint Sensitivity Analysis Methodology conceived by Cacuci [11–13] to compute *exactly* the 21,976 first-order sensitivities and 482,944,576 second-order sensitivities of the leakage response of a polyethylene-reflected plutonium (PERP) OECD/NEA reactor physics benchmark [14] with respect to the benchmark's imprecisely known nuclear cross sections, isotopic number densities, number of neutrons per fission, fission spectrum, and source parameters. The PERP benchmark consists of an inner sphere containing α-phase plutonium surrounded by a spherical shell reflector made of polyethylene; the benchmark comprises the constitutive materials specified in Table 1.

Table 1. Dimensions and material composition of the PERP benchmark.

Materials	Isotopes	Weight Fraction	Density (g/cm^3)	Zones
Material 1 (plutonium metal)	Isotope 1 (^{239}Pu)	9.3804×10^{-1}	19.6	Material 1 is assigned to zone 1, which has a radius of 3.794 cm.
	Isotope 2 (^{240}Pu)	5.9411×10^{-2}		
	Isotope 3 (^{69}Ga)	1.5152×10^{-3}		
	Isotope 4 (^{71}Ga)	1.0346×10^{-3}		
Material 2 (polyethylene)	Isotope 5 (C)	8.5630×10^{-1}	0.95	Material 2 is assigned to zone 2, which has an inner radius of 3.794 cm and an outer radius of 7.604 cm.
	Isotope 6 (^{1}H)	1.4370×10^{-1}		

The neutron distribution within the PERP benchmark was modeled by means of the six-dimensional linear integro-differential neutron transport equation, which was solved numerically by using the PARTISN [15] multigroup discrete ordinates transport code. The response of interest for the PERP benchmark was the total leakage of neutrons leaving its outer surface (numerical value: 1.7648×10^6 neutrons/s). The numerical model of the PERP benchmark included 21,976 imprecisely known (uncertain) parameters, as presented below in Table 2.

Table 2. Summary of imprecisely known parameters for the PERP benchmark.

Symbol	Parameter Name	Number of Parameters
$\sigma_{t,i}^{g}$	Multigroup microscopic total cross section for isotope i and energy group g	180; $for\ i = 1,\ldots,6;\ g = 1,\ldots,30$
$\sigma_{s,l,i}^{g' \to g}$	Multigroup microscopic scattering cross section for $l-$ th order Legendre expansion, from energy group g' into energy group g, for isotope i	21,600; $for\ l = 0,\ldots,3;\ i = 1,\ldots,6;\ g, g' = 1,\ldots,30$
$\sigma_{f,i}^{g}$	Multigroup microscopic fission cross section i and energy group g	60; $for\ i = 1,2;\ g = 1,\ldots,30$
ν_i^g	Average number of neutrons per fission for isotope i and energy group g	60; $for\ i = 1,2;\ g = 1,\ldots,30$
χ_i^g	Fission spectrum for isotope i and energy group g	60; $for\ i = 1,2;\ g = 1,\ldots,30$
q_j	Source parameters : $\lambda_1, \lambda_2; F_1^{SF}, F_2^{SF}; a_1, a_2; b_1, b_2; \nu_1^{SF}, \nu_2^{SF}$	10
$N_{i,m}$	Isotopic number density for isotope i and material m	6; $N_{1,1}, N_{2,1}, N_{3,1}, N_{4,1}, N_{5,2}, N_{6,2}$
J_α	Total number of parameters:	21,976

It was found [3–8] that most of the first-order relative sensitivities of the leakage response with respect to the model parameters were negligibly small, with absolute val-

ues less than 0.1. The most important (i.e., largest) sensitivities of the leakage response are with respect to the group-averaged total microscopic cross sections, followed by the sensitivities of the leakage response with respect to the isotopic number densities. Additionally important were the first-order relative sensitivities of the leakage response with respect to several source parameters for the isotope ^{240}Pu. The first-order sensitivities of the leakage response with respect to the fission spectrum were negligibly small. Several tens of the 1st-order sensitivities, particularly with respect to the microscopic total cross sections, were found to have absolute values between 0.1 and 1.0, thirteen of which had values larger than 1.0. The largest first-order sensitivities have the following values: $S^{(1)}\left(\sigma^{30}_{t,i=6}\right) = -9.366$, $S^{(1)}(N_{1,1}) = 5.963$, $S^{(1)}\left(\sigma^{12}_{t,i=1}\right) = -1.320$, $S^{(1)}(N_{2,1}) = 1.220$, $S^{(1)}\left(\nu^{12}_{i=1}\right) = 1.215$, $S^{(1)}\left(\sigma^{17}_{t,i=6}\right) = -1.173$, $S^{(1)}\left(\sigma^{16}_{t,i=6}\right) = -1.164$, $S^{(1)}\left(\sigma^{13}_{t,i=1}\right) = -1.154$, $S^{(1)}\left(\sigma^{18}_{t,i=6}\right) = -1.141$, $S^{(1)}\left(\sigma^{19}_{t,i=6}\right) = -1.094$, $S^{(1)}\left(\sigma^{20}_{t,i=6}\right) = -1.033$, $S^{(1)}(N_{6,2}) = 1.001$, $S^{(1)}(\lambda_2) = S^{(1)}\left(F^{SF}_2\right) = S^{(1)}\left(\nu^{SF}_2\right) = S^{(1)}(N_{2,1}) = 0.9998$.

Although only 16 first-order sensitivities attained values larger than 0.99, many more 2nd-order sensitivities have values significantly larger than 1.0: 126 second-order relative sensitivities have values greater than 10.0, and 1853 second-order relative sensitivities have values between 1.0 and 10.0. The second-order sensitivities of the PERP model's leakage response to the model's group-averaged total microscopic cross sections were presented in [3]. It was found [3] that among the total of $32,400 = 180 \times 180$ second-order sensitivities involving the total microscopic cross sections, many of them are much larger than the corresponding first-order ones; in particular, 720 of these relative sensitivities have relative values greater than 1.0. The largest second-order sensitivities involve the total cross sections of ^{239}Pu and ^{1}H. The overall largest element is the unmixed second-order relative sensitivity $S^{(2)}\left(\sigma^{30}_{t,6}, \sigma^{30}_{t,6}\right) = 429.6$, which occurs in the lowest-energy group for ^{1}H. Neglecting these second-order sensitivities would cause an erroneous reporting of the response's expected value and a very large non-conservative error by the under-reporting of the response variance. For example, if the parameters were uncorrelated and had a uniform standard deviation of 10%, neglecting second (and higher) order sensitivities would cause a non-conservative error by the under-reporting of the response variance by a factor of 947%.

The results of the computations of the second-order sensitivities of the PERP benchmark's computed leakage response with respect to the benchmark's 21,600 parameters underlying the computed group-averaged isotopic scattering cross sections are presented in [4]. The numerical results obtained indicate that the vast majority of the $(21,600)^2$ second-order sensitivities with respect to the scattering cross sections are much smaller than the corresponding first-order ones. However, it was found that 52 of the mixed second-order sensitivities of the leakage response with respect to the scattering and total microscopic cross sections had values that were significantly larger than the unmixed second-order sensitivities of the leakage response with respect to the group-averaged scattering microscopic cross sections.

The second-order sensitivities of the leakage response of the PERP benchmark involving the group-averaged isotopic fission microscopic cross sections and the average number of neutrons per fission are presented in [5]. The numerical results obtained indicate that the vast majority of the 2nd-order unmixed sensitivities involving the fission cross sections are smaller than the corresponding 1st-order ones, but several 2nd-order sensitivities for isotope ^{239}Pu are significantly larger than the corresponding 1st-order sensitivities. It is shown that the effects of the 2nd-order sensitivities of the PERP benchmark's leakage response with respect to the benchmark's fission cross sections on the moments (expected value, variance, and skewness) of the PERP benchmark's leakage response distribution are negligible in comparison to the corresponding effects (on the response distribution) stemming from uncertainties in the total cross sections, but are larger than the corresponding effects (on the response distribution) stemming from uncertainties in the scattering

cross sections. It is also shown that the effects of the 2nd-order sensitivities of the PERP benchmark's leakage response with respect to the average number of neutrons per fission on the moments (expected value, variance, and skewness) of the PERP benchmark's leakage response distribution are negligible in comparison to the corresponding effects stemming from uncertainties in the microscopic total cross sections, but are larger than the corresponding effects stemming from uncertainties in the fission and scattering microscopic cross sections.

The results for the 2nd-order sensitivities of the PERP benchmark's leakage response with respect to the benchmark's imprecisely known source parameters are presented in [6]. These results indicate that the effects of the 1st- and 2nd-order sensitivities involving the benchmark's source parameters on the moments (expected value, variance, and skewness) of the benchmark's leakage response distribution are negligibly smaller than the corresponding effects involving the total, fission, and scattering microscopic cross sections.

The 2nd-order sensitivities of the PERP benchmark's leakage response involving the benchmark's imprecisely known isotopic number densities are presented in [7]. Many of these sensitivities turned out to have large values, particularly those involving the isotopic number density of ^{239}Pu and the microscopic total, scattering, or fission cross sections for the 12th or 30th energy groups of ^{239}Pu or ^{1}H, respectively. The largest in absolute value (of -94.91) is attained by the 2nd-order mixed sensitivity of the PERP leakage response involving the isotopic number density of ^{239}Pu and the microscopic total cross section for the 30th energy group of ^{1}H.

The overall impact of the 1st- and 2nd-order sensitivities on propagating uncertainties in the PERP's parameters to the PERP's leakage response is summarized in [8], underscoring the importance of 2nd-order sensitivities for the PERP benchmark in particular, as well as for other physical systems in general. For example, if the PERP's total cross sections were fully correlated, neglecting the 2nd-order sensitivities would cause an error as large as 2000% in the expected value of the leakage response, and up to 6000% in the variance of the leakage response for the microscopic total cross sections. Of course, neither the fully uncorrelated nor the fully correlated illustrative examples presented in [3–8] realistically describe the actual physical situations regarding the parameters describing the total and other microscopic cross section. The fully uncorrelated case underestimates reality while the fully correlated case overestimates it. In reality, cross sections are partially correlated, so reality falls in between the fully uncorrelated and fully correlated cases, which underscores the need for future experimental research aimed at obtaining values for the correlations that might exist among the various cross sections, which are unavailable at this time. In all cases, neglecting the second-order sensitivities would *erroneously* predict a Gaussian distribution in parameter space (for the PERP leakage response) centered about the computed value of the leakage response. In reality, the second-order sensitivities cause the leakage distribution in parameter space to be skewed towards positive values relative to the expected value, which, in turn, is significantly shifted to much larger positive values than the computed leakage value. The effects of the second-order sensitivities underscore the need for obtaining reliable data for correlations that might exist among the total cross sections; however, such data is unavailable at this time.

The sequence of works [3–8] has revealed that the 2nd-order mixed relative sensitivities of the PERP benchmark's leakage response to this benchmark's total cross sections exhibit a very large number of values that are greater than 1.0 (including many having values significantly larger than 10.0). This finding has motivated the quest to develop a methodology to enable the computation of 3rd-order sensitivities of model responses with respect to the model's uncertain parameters. The theoretical/mathematical framework for achieving this goal was provided in [9], which presented the Third-Order Adjoint Sensitivity Analysis Methodology (3rd-ASAM) for response-coupled forward and adjoint linear systems. The 3rd-ASAM enables the efficient computation of the exact expressions of the 3rd-order functional derivatives ("sensitivities") of a general system response, which depends on both the forward and adjoint state functions, with respect to all of the param-

eters underlying the respective forward and adjoint systems. Such responses are often encountered when mathematically representing detector responses and reaction rates in reactor physics problems. The 3rd-ASAM extends the 2nd-ASAM in the quest to overcome the "curse of dimensionality" in sensitivity analysis, uncertainty quantification, and predictive modeling. This work [9] also presents new formulas that incorporate the contributions of the 3rd-order sensitivities into the expressions of the first four cumulants of the response distribution in the phase-space of model parameters, which are employed in a new predictive modeling method (called the "Second/Third-Order Best-Estimated Results with Reduced Uncertainties Predictive Modeling") that combines experimental and computational information in the joint phase-space of responses and model parameters by using the maximum entropy principle. Eliminating the need for introducing and "minimizing" a user-chosen "cost functional quantifying the discrepancies between measurements and computations," this new predictive modeling methodology yields results that are free of subjective user-interferences while generalizing and significantly extending the so-called "4D-VAR" data assimilation procedures. This new predictive modeling methodology also provides a quantitative metric, constructed from sensitivity and covariance matrices, for determining the degree of agreement among the various computational and experimental data while eliminating discrepant information.

Regarding *open issues*: the work presented in [1] is a straightforward application of a first-order Gaussian expansion to handle the model's random parameters and the Wiener–Ito expansion (WIE) to handle noise, thus inheriting all of the benefits and drawbacks of these general procedures. Similarly, the work presented in [2] derives a reduced order model (ROM) using proper orthogonal decomposition (POD) to select, via singular value decomposition, the largest eigenvalues of a matrix generated by using solutions ("snapshots") produced by a full-order model (FOM) that uses the Monte Carlo method for solving the nuclide burnup equations. Similar to the work presented in [1], the work presented in [2] is an application of well-known methods, so the results presented in both works [1,2] inherited all of the computational advantages and the accuracy-related shortcomings of the respective methods. The specific applications presented in [1,2] leave no new open issues to be addressed.

The sequence of works [3–8] has presented the largest ever application of the second-order adjoint sensitivity analysis methodology conceived by Cacuci [11–13] to compute *exactly* and most efficiently the 21,976 first-order sensitivities and 482,944,576 second-order sensitivities of the leakage response of a polyethylene-reflected plutonium (PERP) OECD/NEA reactor physics benchmark [14] with respect to the benchmark's imprecisely known nuclear cross sections, isotopic number densities, number of neutrons per fission, fission spectrum, and source parameters. As has been mentioned in the foregoing discussion, the finding from the sequence of works [3–8] has motivated the quest to develop a methodology to enable the computation of the 3rd-order sensitivities of model responses with respect to the model's uncertain parameters, which was presented in [9]. Subsequently, the methodology developed in [9] was applied [16,17] to compute the largest 3rd-order sensitivities of the PERP benchmark's leakage response with respect to the benchmark's imprecisely known total cross sections. The results obtained in [16,17] indicated that many 3rd-order sensitivities were larger than the corresponding 2nd-order ones. This finding motivated the subsequent development of the 4th-order comprehensive adjoint sensitivity analysis of response-coupled linear forward/adjoint systems [18], which was applied [19,20] to compute the largest 4th-order sensitivities of the PERP benchmark's leakage response with respect to the benchmark's imprecisely known total cross sections. The results obtained in [19,20] indicated that that many 4th-order sensitivities were larger than the corresponding 3rd-order ones, dwarfing the effects of the lower-order sensitivities. These works were followed by the development of the arbitrarily-high-order comprehensive adjoint sensitivity analysis methodology for both linear systems [21] and nonlinear systems [22]. The new methodologies developed in [21,22] represent a fundamental break-

through in the quest for overcoming the curse of dimensionality [10] in sensitivity analysis, uncertainty quantification, and the predictive modeling of large-scale models.

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