

TOWARDS OVERCOMING THE CURSE OF DIMENSIONALITY IN PREDICTIVE MODELLING AND UNCERTAINTY QUANTIFICATION

Dan G. Cacuci¹

¹University of South Carolina
300 Main Street, Columbia, SC 29208, USA

cacuci@cec.sc.edu

ABSTRACT

This invited presentation summarizes new methodologies developed by the author for performing high-order sensitivity analysis, uncertainty quantification and predictive modeling. The presentation commences by summarizing the newly developed 3rd-Order Adjoint Sensitivity Analysis Methodology (3rd-ASAM) for linear systems, which overcomes the “curse of dimensionality” for sensitivity analysis and uncertainty quantification of a large variety of model responses of interest in reactor physics systems. The use of the exact expressions of the 2nd-, and 3rd-order sensitivities computed using the 3rd-ASAM is subsequently illustrated by presenting 3rd-order formulas for the first three cumulants of the response distribution, for quantifying response uncertainties (covariance, skewness) stemming from model parameter uncertainties. The use of the 1st-, 2nd-, and 3rd-order sensitivities together with the formulas for the first three cumulants of the response distribution are subsequently used in the newly developed 2nd/3rd-BERRU-PM (“Second/Third-Order Best-Estimated Results with Reduced Uncertainties Predictive Modeling”), which aims at overcoming the curse of dimensionality in predictive modeling. The 2nd/3rd-BERRU-PM uses the maximum entropy principle to eliminate the need for introducing a subjective user-defined “cost functional quantifying the discrepancies between measurements and computations.” By utilizing the 1st-, 2nd- and 3rd-order response sensitivities to combine experimental and computational information in the joint phase-space of responses and model parameters, the 2nd/3rd-BERRU-PM generalizes the current data adjustment/assimilation methodologies. Even though all of the 2nd- and 3rd-order are comprised in the mathematical framework of the 2nd/3rd-BERRU-PM formalism, the computations underlying the 2nd/3rd-BERRU-PM require the inversion of a single matrix of dimensions equal to the number of considered responses, thus overcoming the curse of dimensionality which would affect the inversion of hessian and higher-order matrices in the parameter space.

KEYWORDS: 3rd-order adjoint sensitivity analysis methodology; uncertainty quantification and reduction; predictive modeling; curse of dimensionality.

1. INTRODUCTION

This invited presentation summarizes ongoing work aimed at overcoming the “curse of dimensionality” in sensitivity analysis, uncertainty quantification and predictive modeling. The computation of higher-order sensitivities by conventional methods is limited in practice by the so-called “curse of dimensionality,” since the number of such large-scale computations increases exponentially with the order of the response sensitivities. For the exact computation of the 1st- and 2nd-order response sensitivities to parameters, the “curse of dimensionality” has been overcome by the Second-Order Adjoint Sensitivity Analysis Methodology (2nd-ASAM) conceived and developed by

Cacuci [1]. Generalizing the 2nd-ASAM, Section 2 of this work presents the Third-Order Adjoint Sensitivity Analysis Methodology (3rd-ASAM) for linear systems which computes efficiently and exactly expressions of the 3rd-order functional derivatives (“sensitivities”) of a scalar-valued system response with respect to all of the parameters that characterize the respective system. Such responses are often encountered when representing mathematically detector responses and reaction rates in reactor physics problems. The 1st-, 2nd-, and 3rd-order sensitivities computed using the 3rd-ASAM are incorporated in the new formulas, presented in Section 3.1, for computing the first four cumulants of the response distribution in the phase-space of model parameters. Section 3.2 presents a new mathematical formalism for [predictive modeling, which will be called the “Second/Third-Order Best-Estimated Results with Reduced Uncertainties Predictive Modeling (2nd/3rd-BERRU-PM).” Set in the joint phase-space of model responses and parameters, the 2nd/3rd-BERRU-PM incorporates experimental and computational information, including the complete set of 1st-, 2nd-, and 3rd-order sensitivities of model responses to model parameters. Thus, the 2nd/3rd-BERRU-PM extends the “BERRU Predictive Modeling” methodology presented in [2], thereby generalizing and including, as particular cases, similar formulas used in data adjustment methodologies [3], Bayesian linear statistics [4], and data assimilation [5,6] methodologies. The 2nd/3rd-BERRU-PM uses the maximum entropy (MaxEnt) principle to eliminate the need for introducing and “minimizing” a user-chosen “cost functional quantifying the discrepancies between measurements and computations.” Incorporating correlations, including those between the imprecisely known model parameters and computed model responses, the 2nd/3rd-BERRU-PM also provides a quantitative metric, constructed from sensitivity and covariance matrices, for determining the degree of agreement among the various computational and experimental data and helping eliminate discrepant information. Section 4 summarizes the significance of this work’s novel results in the quest to overcome the curse of dimensionality in sensitivity analysis, uncertainty quantification and predictive modeling.

2. THIRD-ORDER ADJOINT SENSITIVITY ANALYSIS METHODOLOGY (3rd-ASAM) FOR LINEAR SYSTEMS

The system’s response considered in this work is a scalar-valued nonlinear functional of the forward state-function (e.g., the particle flux in a neutron/gamma transport equation)

$\phi(\mathbf{x}) \triangleq [\varphi_1(\mathbf{x}), \dots, \varphi_{N_u}(\mathbf{x})]^{\dagger}$. Such functionals represent detector responses and/or reaction rates in reactor physics problems, and will be denoted in inner-product form as $R[\phi(\mathbf{x}); \alpha] \triangleq \langle S(\phi; \alpha), 1 \rangle$,

where $S(\phi; \alpha)$ denotes a suitably differentiable function of its arguments. The inner product has the

form $\langle \phi(\mathbf{x}), \psi(\mathbf{x}) \rangle \triangleq \sum_{i=1}^{N_u} \int_{\Omega_x} \varphi_i(\mathbf{x}) \psi_i(\mathbf{x}) d\mathbf{x}$, and the forward function $\phi(\mathbf{x})$ is the solution of the

following operator equations, in which the equality hold in the weak (distributional) sense:

$$\mathbf{L}[\alpha(\mathbf{x})]\phi(\mathbf{x}) = \mathbf{Q}(\mathbf{x}), \quad \mathbf{x} \in \Omega_x, \quad \mathbf{B}_F(\alpha)\phi(\mathbf{x}) - \mathbf{C}_F(\alpha) = \mathbf{0}, \quad \mathbf{x} \in \partial\Omega_x. \quad (1)$$

The quantities appearing in Eq. (1) are defined as follows: (i) $\alpha \triangleq (\alpha_1, \dots, \alpha_{N_\alpha})^{\dagger}$ denotes a N_α -dimensional column vector whose components are the physical system’s imprecisely known parameters, which are subject to uncertainties; (ii) $\mathbf{x} \triangleq (x_1, \dots, x_{N_x})^{\dagger} \in \mathbb{R}^{N_x}$ denotes the N_x -dimensional phase-space position vector, defined on a phase-space domain denoted as Ω_x ; (iii)

$\phi(\mathbf{x}) \triangleq [\varphi_1(\mathbf{x}), \dots, \varphi_{N_u}(\mathbf{x})]^{\dagger}$ denotes a N_u -dimensional column vector whose components represent the system’s dependent variables (also called “state functions”); (iv) $\mathbf{Q}(\alpha) \triangleq [Q_1(\alpha), \dots, Q_{N_u}(\alpha)]^{\dagger}$ denotes a N_u -dimensional column vector; the components of \mathbf{Q} are operators acting on α and \mathbf{x} ; (v)

$\mathbf{L}(\boldsymbol{\alpha}) \triangleq [L_1(\boldsymbol{\alpha}), \dots, L_{N_u}(\boldsymbol{\alpha})]^\top$ denotes a N_u -component column vector whose components are operators acting linearly on $\boldsymbol{\phi}(\mathbf{x})$; the forward function $\boldsymbol{\phi}(\mathbf{x})$ is subject to forward initial and/or boundary conditions denoted as $\mathbf{B}_F(\boldsymbol{\alpha})\boldsymbol{\phi}(\mathbf{x}) - \mathbf{C}_F(\boldsymbol{\alpha}) = \mathbf{0}$, $\mathbf{x} \in \partial\Omega_x$, where the subscript “F” indicates “forward”. Due to space limitations, only the final form of the 1st-, 2nd-, and 3rd-order response sensitivities will be presented in this work. Thus, the I^{st} -order response sensitivity $R_i^{(1)}[\boldsymbol{\phi}; \boldsymbol{\psi}_1^{(1)}; \boldsymbol{\alpha}]$ of $R[\boldsymbol{\phi}(\mathbf{x}); \boldsymbol{\alpha}]$ with respect to a parameter α_i , $i = 1, \dots, N_\alpha$, has the following expression:

$$R_i^{(1)}[\boldsymbol{\phi}; \boldsymbol{\psi}_1^{(1)}; \boldsymbol{\alpha}] = \frac{\partial R[\boldsymbol{\phi}; \boldsymbol{\psi}_1^{(1)}; \boldsymbol{\alpha}]}{\partial \alpha_i} + \left\langle \frac{\partial S(\boldsymbol{\phi}; \boldsymbol{\alpha})}{\partial \alpha_i}, 1 \right\rangle + \left\langle \boldsymbol{\psi}_1^{(1)}, \frac{\partial [\mathbf{Q}(\boldsymbol{\alpha}) - \mathbf{L}(\boldsymbol{\alpha})\boldsymbol{\phi}(\mathbf{x})]}{\partial \alpha_i} \right\rangle - \frac{\partial \hat{P}^{(1)}}{\partial \alpha_i}, \quad (2)$$

where $\hat{P}^{(1)}$ denotes the bilinear concomitant on $\partial\Omega_x$, and the 1st-level adjoint function $\boldsymbol{\psi}_1^{(1)}(\mathbf{x})$ is the solution of the following I^{st} -Level Adjoint Sensitivity System (1st-LASS):

$$\mathbf{L}^+(\boldsymbol{\alpha})\boldsymbol{\psi}_1^{(1)}(\mathbf{x}) = [\partial S(\boldsymbol{\phi}; \boldsymbol{\alpha})/\partial \boldsymbol{\phi}]^\top, \quad \mathbf{B}_A^{(1)}[\boldsymbol{\phi}(\mathbf{x}); \boldsymbol{\psi}_1^{(1)}(\mathbf{x}); \boldsymbol{\alpha}] = \mathbf{0}, \quad \mathbf{x} \in \partial\Omega_x. \quad (3)$$

where the subscript “A” indicates “adjoint”. The expression of the 2nd-order sensitivity of $R[\boldsymbol{\phi}(\mathbf{x}); \boldsymbol{\alpha}]$ with respect to parameters α_i and α_j is as follows:

$$R_{ij}^{(2)}[\boldsymbol{\phi}; \boldsymbol{\psi}_1^{(1)}; \boldsymbol{\psi}_{1,i}^{(2)}(\mathbf{x}), \boldsymbol{\psi}_{2,i}^{(2)}(\mathbf{x}); \boldsymbol{\alpha}] \triangleq \frac{\partial R_i^{(1)}(\boldsymbol{\phi}; \boldsymbol{\psi}_1^{(1)}; \boldsymbol{\alpha})}{\partial \alpha_j} - \frac{\partial \hat{P}^{(2)}}{\partial \alpha_j} + \left\langle \boldsymbol{\psi}_{1,i}^{(2)}(\mathbf{x}), \frac{\partial [\mathbf{Q}[\boldsymbol{\alpha}(\mathbf{x})] - \mathbf{L}(\boldsymbol{\alpha})\boldsymbol{\phi}(\mathbf{x})]}{\partial \alpha_j} \right\rangle + \left\langle \boldsymbol{\psi}_{2,i}^{(2)}(\mathbf{x}), \frac{\partial^2 S(\boldsymbol{\phi}; \boldsymbol{\alpha})}{\partial \boldsymbol{\phi} \partial \alpha_j} - \frac{\partial [\mathbf{L}^+(\boldsymbol{\alpha})\boldsymbol{\psi}_1^{(1)}(\mathbf{x})]}{\partial \alpha_j} \right\rangle, \quad i = 1, \dots, N_\alpha; \quad j = 1, \dots, i, \quad (4)$$

where $\hat{P}^{(2)}$ denotes the bilinear concomitant on $\partial\Omega_x$, and the 2nd-level adjoint functions $\boldsymbol{\psi}_{1,i}^{(2)}(\mathbf{x}), \boldsymbol{\psi}_{2,i}^{(2)}(\mathbf{x})$ are the solutions of the following 2nd-Level Adjoint Sensitivity system (2nd-LASS):

$$\begin{aligned} \mathbf{L}(\boldsymbol{\alpha})\boldsymbol{\psi}_{2,i}^{(2)}(\mathbf{x}) &= [\partial R_i^{(1)}(\boldsymbol{\phi}; \boldsymbol{\psi}_1^{(1)}; \boldsymbol{\alpha})/\partial \boldsymbol{\psi}_1^{(1)}]^\top, \quad i = 1, \dots, N_\alpha, \\ \mathbf{L}^+(\boldsymbol{\alpha})\boldsymbol{\psi}_{1,i}^{(2)}(\mathbf{x}) &= [\partial R_i^{(1)}(\boldsymbol{\phi}; \boldsymbol{\psi}_1^{(1)}; \boldsymbol{\alpha})/\partial \boldsymbol{\phi}]^\top + \frac{\partial^2 S(\boldsymbol{\phi}; \boldsymbol{\alpha})}{\partial \boldsymbol{\phi} \partial \boldsymbol{\phi}} \boldsymbol{\psi}_{2,i}^{(2)}(\mathbf{x}), \end{aligned} \quad (5)$$

subject to adjoint boundary conditions denoted as $\mathbf{B}_A^{(2)}[\boldsymbol{\phi}(\mathbf{x}); \boldsymbol{\psi}_1^{(1)}(\mathbf{x}); \boldsymbol{\psi}_{1,i}^{(2)}(\mathbf{x}); \boldsymbol{\psi}_{2,i}^{(2)}(\mathbf{x}); \boldsymbol{\alpha}] = \mathbf{0}$, $\mathbf{x} \in \partial\Omega_x$.

The exact computation of all of the partial second-order sensitivities requires at most N_α large-scale (adjoint) computations using the 2nd-LASS, rather than $O(N_\alpha^2)$ large-scale computations as would be required by forward methods. If the 2nd-LASS is solved N_α -times, the “off-diagonal” 2nd-order mixed sensitivities $R_{ij}^{(2)}[\boldsymbol{\phi}; \boldsymbol{\psi}_1^{(1)}; \boldsymbol{\psi}_{1,i}^{(2)}(\mathbf{x}), \boldsymbol{\psi}_{2,i}^{(2)}(\mathbf{x}); \boldsymbol{\alpha}]$ will be computed twice, using distinct 2nd-level adjoint functions, thereby providing an independent intrinsic numerical verification that the 1st- and 2nd-order sensitivities are computed accurately. In practice, it is useful to prioritize the computation of the 2nd-order sensitivities by using the rankings of the relative magnitudes of the 1st-order sensitivities as a “priority indicator”: the larger the magnitude of the relative 1st-order sensitivity, the higher the priority for computing the corresponding 2nd-order sensitivities. Also, since exactly-vanishing 1st-order sensitivities may indicate critical points of the response in the phase-space of model parameters, it is also of interest to compute the 2nd-order sensitivities that correspond to vanishing 1st-order

sensitivities. Information provided by the 1st-order sensitivities might indicate which 2nd-order sensitivities could be neglected.

The 3rd-order partial sensitivity of the response to the model parameters has the following expression:

$$\begin{aligned}
 R_{ijk}^{(3)}[\phi; \psi_1^{(1)}; \psi_{1,i}^{(2)}; \psi_{22,i}^{(2)}; \psi_{1,ij}^{(3)}, \dots, \psi_{4,ij}^{(3)}; \alpha] &\triangleq \frac{\partial R_{ij}^{(2)}(\phi; \dots; \alpha)}{\partial \alpha_k} + \left\langle \psi_{1,ij}^{(3)}, \frac{\partial [\mathbf{Q}(\alpha) - \mathbf{L}(\alpha)\phi]}{\partial \alpha_k} \right\rangle \\
 &+ \left\langle \psi_{2,ij}^{(3)}, \frac{\partial^2 S(\phi; \psi; \alpha)}{\partial \phi \partial \alpha_k} - \frac{\partial [\mathbf{L}^+(\alpha)\psi_1^{(1)}]}{\partial \alpha_k} \right\rangle + \left\langle \psi_{3,ij}^{(3)}, \frac{\partial}{\partial \alpha_k} \left[\frac{\partial R_i^{(1)}(\phi; \psi; \psi_1^{(1)}; \psi_2^{(1)}; \alpha)}{\partial \phi} \right]^\dagger - \mathbf{L}^+(\alpha)\psi_{1,i}^{(2)} \right. \\
 &\left. - \frac{\partial^2 S(\phi; \psi; \alpha)}{\partial \phi \partial \phi} \psi_{2,i}^{(2)} \right\rangle + \left\langle \psi_{4,ij}^{(3)}, \frac{\partial}{\partial \alpha_k} \left[\frac{\partial R_i^{(1)}(\phi; \psi; \psi_1^{(1)}; \psi_2^{(1)}; \alpha)}{\partial \psi_1^{(1)}} \right]^\dagger - \mathbf{L}(\alpha)\psi_{3,i}^{(2)} \right\rangle - \frac{\partial \hat{P}^{(3)}}{\partial \alpha_k}, \\
 &\text{for } i = 1, \dots, N_\alpha; j = 1, \dots, i; k = 1, \dots, j,
 \end{aligned} \tag{6}$$

where $\hat{P}^{(3)}$ denotes the bilinear concomitant on $\partial\Omega_x$, and the 3rd-level adjoint functions $\psi_{1,ij}^{(3)}, \dots, \psi_{4,ij}^{(3)}$, $i = 1, \dots, N_\alpha; j = 1, \dots, i$, are the solutions of the 3rd-Level Adjoint Sensitivity System (3rd-LASS) has the following structure:

$$\begin{aligned}
 \mathbf{L}(\alpha)\psi_{3,ij}^{(3)} &= [\partial R_{ij}^{(2)} / \partial \psi_{1,i}^{(2)}]^\dagger, \quad \mathbf{L}^+(\alpha)\psi_{4,ij}^{(3)} = [\partial R_{ij}^{(2)} / \partial \psi_{2,i}^{(2)}]^\dagger + \frac{\partial^2 S(\phi; \psi; \alpha)}{\partial \phi \partial \phi} \psi_{3,ij}^{(3)}, \tag{7} \\
 \mathbf{L}(\alpha)\psi_{2,ij}^{(3)} &= [\partial R_{ij}^{(2)} / \partial \psi_1^{(1)}]^\dagger + \left\{ \frac{\partial}{\partial \psi_1^{(1)}} \left[\frac{\partial R_i^{(1)}(\phi; \psi_1^{(1)}; \alpha)}{\partial \phi} \right]^\dagger \right\} \psi_{3,ij}^{(3)} + \left\{ \frac{\partial}{\partial \psi_1^{(1)}} \left[\frac{\partial R_i^{(1)}(\phi; \psi; \psi_1^{(1)}; \psi_2^{(1)}; \alpha)}{\partial \psi_1^{(1)}} \right]^\dagger \right\} \psi_{4,ij}^{(3)}, \tag{8} \\
 \mathbf{L}^+(\alpha)\psi_{1,ij}^{(3)} &= [\partial R_{ij}^{(2)} / \partial \phi]^\dagger + \frac{\partial^2 S(\phi; \psi; \alpha)}{\partial \phi \partial \phi} \psi_{2,ij}^{(3)} - \psi_{3,ij}^{(3)} \left\{ \frac{\partial^3 S(\phi; \psi; \alpha)}{\partial \phi \partial \phi \partial \phi} \psi_{2,i}^{(2)}(\mathbf{x}) \right. \\
 &\left. + \frac{\partial}{\partial \phi} \left[\frac{\partial R_i^{(1)}(\phi; \psi; \psi_1^{(1)}; \psi_2^{(1)}; \alpha)}{\partial \phi} \right]^\dagger \right\} + \left\{ \frac{\partial}{\partial \phi} \left[\frac{\partial R_i^{(1)}(\phi; \psi; \psi_1^{(1)}; \psi_2^{(1)}; \alpha)}{\partial \psi_1^{(1)}} \right]^\dagger \right\} \psi_{4,ij}^{(3)}. \tag{9}
 \end{aligned}$$

The boundary conditions for the adjoint functions $\psi_{1,ij}^{(3)}, \dots, \psi_{4,ij}^{(3)}$ can be represented in operator form as

$$\mathbf{B}_A^{(3)}[\phi(\mathbf{x}); \psi_1^{(1)}(\mathbf{x}); \psi_{1,i}^{(2)}(\mathbf{x}), \psi_{2,i}^{(2)}(\mathbf{x}); \psi_{1,ij}^{(3)}, \dots, \psi_{4,ij}^{(3)}; \alpha] = \mathbf{0}, \quad \mathbf{x} \in \partial\Omega_x.$$

Note that solving Eq. (7) would be performed by using the same forward and adjoint solvers (i.e., computer codes) as used for solving the original forward and adjoint systems, except that the right-sides of the respective solvers would have different as “sources,” thereby minimizing any need for new code development. Using the 3rd-LASS enables the specific computation of the 3rd-order sensitivities in the priority order set by the user, so that only the important 3rd-order partial sensitivities $R[\phi(\mathbf{x}), \psi(\mathbf{x}); \alpha]$ would be computed.

Information provided by the first- and second-order sensitivities might indicate which 3rd-order sensitivities could be neglected. The expressions provided above in Eqs. (2) through (9) are particular cases of those provided in [7].

3. 2nd/3rd-BERRU-PM: “SECOND/THIRD-ORDER BEST-ESTIMATED RESULTS WITH REDUCED UNCERTAINTIES PREDICTIVE MODELING WITH UNCERTAINTY ANALYSIS IN THE JOINT PHASE-SPACE OF RESPONSES AND PARAMETERS

Consider a computational model that comprises a total of N_α parameters, denoted as α_i , $i = 1, \dots, N_\alpha$. Since the values of the parameters α_i are determined experimentally they can be considered to behave stochastically, obeying a multivariate probability distribution function denoted as $p_\alpha(\alpha)$, which is seldom known in practice. The cumulants of $p_\alpha(\alpha)$ are defined as follows:

(i) The mean value of a parameter: $\alpha_i^0 \triangleq \langle \alpha_i \rangle_\alpha \triangleq \int_{D_\alpha} \alpha_i p_\alpha(\alpha) d\alpha$, $i = 1, \dots, N_\alpha$;

(ii) The covariance, $cov(\alpha_i, \alpha_j)$, of two parameters, α_i and α_j :

$\mu_2^{ij}(\alpha) \triangleq cov(\alpha_i, \alpha_j) \triangleq \langle (\alpha_i - \alpha_i^0)(\alpha_j - \alpha_j^0) \rangle_\alpha$, $i, j = 1, \dots, N_\alpha$. These covariances are considered to be the components of the parameter covariance matrix $C_\alpha \triangleq \langle (\alpha - \alpha^0)(\alpha - \alpha^0)^T \rangle_\alpha$. The

variance, $var(\alpha_i)$, of a parameter α_i , is defined as follows: $var(\alpha_i) \triangleq \langle (\alpha_i - \alpha_i^0)^2 \rangle_\alpha$, $i = 1, \dots, N_\alpha$;

the standard deviation, σ_i , of α_i , is defined as follows: $\sigma_i \triangleq \sqrt{var(\alpha_i)}$; The correlation, ρ_{ij} ,

between two parameters α_i and α_j , is defined as follows $\rho_{ij} \triangleq cov(\alpha_i, \alpha_j) / (\sigma_i \sigma_j)$; $i, j = 1, \dots, N_\alpha$

(iii) The 3rd-order moment, μ_3^{ijk} , of the multivariate parameter distribution function $p(\alpha)$, and the 3rd-order parameter correlation, t_{ijk} , respectively, are defined as follows:

$$\mu_3^{ijk}(\alpha) \triangleq \int_{D_\alpha} (\alpha_i - \alpha_i^0)(\alpha_j - \alpha_j^0)(\alpha_k - \alpha_k^0) p(\alpha) d\alpha \triangleq t_{ijk} \sigma_i \sigma_j \sigma_k, \quad i, j, k = 1, \dots, N_\alpha;$$

(iv) The 4th-order moment, μ_4^{ijkl} , of the multivariate parameter distribution function $p(\alpha)$, and the 4th-order parameter correlation, q_{ijkl} , respectively, are defined as follows:

$$\mu_4^{ijkl}(\alpha) \triangleq \int_{D_\alpha} (\alpha_i - \alpha_i^0)(\alpha_j - \alpha_j^0)(\alpha_k - \alpha_k^0)(\alpha_l - \alpha_l^0) p(\alpha) d\alpha \triangleq q_{ijkl} \sigma_i \sigma_j \sigma_k \sigma_l; \quad i, j, k, l = 1, \dots, N_\alpha.$$

3.1. Third-Order Expressions for the Expected Value, Covariance and Skewness of Response Multivariate Distributions in Parameter Space

Considering response sensitivities up to 3rd-order, it has been shown [1] that the expressions of the first three cumulants of the distribution in the phase-space of model parameters of N_r computed responses $r_i^c(\alpha)$, $i = 1, \dots, N_r$, are as follows:

(i) The expected (mean) value, denoted as $E[r_i^c(\alpha)]$, of a response $r_i^c(\alpha)$:

$$E[r_i^c(\alpha)] = r_i^c(\alpha^0) + \frac{1}{2} \sum_{i,j=1}^{N_\alpha} \left\{ \frac{\partial^2 r_i^c(\alpha)}{\partial \alpha_i \partial \alpha_j} \right\}_{\alpha^0} \rho_{ij} \sigma_i \sigma_j + \frac{1}{6} \sum_{i,j,k=1}^{N_\alpha} \left\{ \frac{\partial^3 r_i^c(\alpha)}{\partial \alpha_i \partial \alpha_j \partial \alpha_k} \right\}_{\alpha^0} t_{ijk} \sigma_i \sigma_j \sigma_k; \quad i = 1, \dots, N_r. \quad (10)$$

(ii) The covariance, denoted as $cov(r_{i_1}^c, r_{i_2}^c)$, of two responses, $r_{i_1}^c(\alpha)$ and $r_{i_2}^c(\alpha)$, $i_1, i_2 = 1, \dots, N_r$:

$$\begin{aligned} cov(r_{i_1}^c, r_{i_2}^c) &= \sum_{i=1}^{N_\alpha} \sum_{j=1}^{N_\alpha} \left(\frac{\partial r_{i_1}^c}{\partial \alpha_i} \frac{\partial r_{i_2}^c}{\partial \alpha_j} \right) \rho_{ij} \sigma_i \sigma_j + \frac{1}{2} \sum_{i=1}^{N_\alpha} \sum_{j=1}^{N_\alpha} \sum_{\mu=1}^{N_\alpha} \left(\frac{\partial^2 r_{i_1}^c}{\partial \alpha_i \partial \alpha_j} \frac{\partial r_{i_2}^c}{\partial \alpha_\mu} + \frac{\partial r_{i_1}^c}{\partial \alpha_i} \frac{\partial^2 r_{i_2}^c}{\partial \alpha_j \partial \alpha_\mu} \right) t_{ij\mu} \sigma_i \sigma_j \sigma_\mu \\ &+ \frac{1}{4} \sum_{i=1}^{N_\alpha} \sum_{j=1}^{N_\alpha} \sum_{\mu=1}^{N_\alpha} \sum_{\nu=1}^{N_\alpha} \left(\frac{\partial^2 r_{i_1}^c}{\partial \alpha_i \partial \alpha_j} \right) \left(\frac{\partial^2 r_{i_2}^c}{\partial \alpha_\mu \partial \alpha_\nu} \right) (q_{ij\mu\nu} - \rho_{ij} \rho_{\mu\nu}) \sigma_i \sigma_j \sigma_\mu \sigma_\nu \\ &+ \frac{1}{6} \sum_{i=1}^{N_\alpha} \sum_{j=1}^{N_\alpha} \sum_{\mu=1}^{N_\alpha} \sum_{\nu=1}^{N_\alpha} \left(\frac{\partial r_{i_1}^c}{\partial \alpha_i} \frac{\partial^3 r_{i_2}^c}{\partial \alpha_j \partial \alpha_\mu \partial \alpha_\nu} + \frac{\partial r_{i_2}^c}{\partial \alpha_j} \frac{\partial^3 r_{i_1}^c}{\partial \alpha_i \partial \alpha_\mu \partial \alpha_\nu} \right) q_{ij\mu\nu} \sigma_i \sigma_j \sigma_\mu \sigma_\nu. \end{aligned} \quad (11)$$

(iii) The covariance of a response, $r_{i_1}^c(\alpha)$ and a parameter α_ℓ , $i_1 = 1, \dots, N_r$ and $\ell = 1, \dots, N_\alpha$, which is denoted as $cov(r_{i_1}^c, \alpha_\ell)$ and is given by the following expression

$$\begin{aligned} cov(r_i^c, \alpha_\ell) &= \sum_{i=1}^{N_\alpha} \left\{ \frac{\partial r_i^c(\mathbf{a})}{\partial \alpha_i} \right\}_{\mathbf{a}^0} cov(\alpha_i, \alpha_\ell) + \frac{1}{2} \sum_{i,j=1}^{N_\alpha} \left\{ \frac{\partial^2 r_i^c(\mathbf{a})}{\partial \alpha_i \partial \alpha_j} \right\}_{\mathbf{a}^0} t_{ij\ell} \sigma_i \sigma_j \sigma_\ell \\ &+ \frac{1}{6} \sum_{i,j,k=1}^{N_\alpha} \left\{ \frac{\partial^3 r_i^c(\mathbf{a})}{\partial \alpha_i \partial \alpha_j \partial \alpha_k} \right\}_{\mathbf{a}^0} q_{ij\mu\nu} \sigma_i \sigma_j \sigma_k \sigma_\ell; \quad i_1 = 1, \dots, N_r; \quad \ell = 1, \dots, N_\alpha. \end{aligned} \tag{12}$$

(iv) The third-order cumulant for three responses, $r_{i_1}^c(\mathbf{a})$, $r_{i_2}^c(\mathbf{a})$ and $r_{i_3}^c(\mathbf{a})$, for $i_1, i_2, i_3 = 1, \dots, N_r$:

$$\begin{aligned} \mu_3(r_{i_1}^c, r_{i_2}^c, r_{i_3}^c) &\triangleq \left\langle \left[r_{i_1}^c - E(r_{i_1}^c) \right] \left[r_{i_2}^c - E(r_{i_2}^c) \right] \left[r_{i_3}^c - E(r_{i_3}^c) \right] \right\rangle_{\alpha} \\ &= \sum_{i=1}^{N_\alpha} \sum_{j=1}^{N_\alpha} \sum_{\mu=1}^{N_\alpha} \frac{\partial r_{i_1}^c}{\partial \alpha_i} \frac{\partial r_{i_2}^c}{\partial \alpha_j} \frac{\partial r_{i_3}^c}{\partial \alpha_\mu} t_{ij\mu} \sigma_i \sigma_j \sigma_\mu + \frac{1}{2} \sum_{i=1}^{N_\alpha} \sum_{j=1}^{N_\alpha} \sum_{\mu=1}^{N_\alpha} \sum_{\nu=1}^{N_\alpha} \frac{\partial r_{i_1}^c}{\partial \alpha_i} \frac{\partial r_{i_2}^c}{\partial \alpha_j} \frac{\partial^2 r_{i_3}^c}{\partial \alpha_\mu \partial \alpha_\nu} (q_{ij\mu\nu} - \rho_{ij} \rho_{\mu\nu}) \sigma_i \sigma_j \sigma_\mu \sigma_\nu \\ &+ \frac{1}{2} \sum_{i=1}^{N_\alpha} \sum_{j=1}^{N_\alpha} \sum_{\mu=1}^{N_\alpha} \sum_{\nu=1}^{N_\alpha} \frac{\partial r_{i_1}^c}{\partial \alpha_i} \frac{\partial^2 r_{i_2}^c}{\partial \alpha_j \partial \alpha_\mu} \frac{\partial r_{i_3}^c}{\partial \alpha_\nu} (q_{ij\mu\nu} - \rho_{i\nu} \rho_{j\mu}) \sigma_i \sigma_j \sigma_\mu \sigma_\nu \\ &+ \frac{1}{2} \sum_{i=1}^{N_\alpha} \sum_{j=1}^{N_\alpha} \sum_{\mu=1}^{N_\alpha} \sum_{\nu=1}^{N_\alpha} \frac{\partial^2 r_{i_1}^c}{\partial \alpha_i \partial \alpha_j} \frac{\partial r_{i_2}^c}{\partial \alpha_\mu} \frac{\partial r_{i_3}^c}{\partial \alpha_\nu} (q_{ij\mu\nu} - \rho_{ij} \rho_{\mu\nu}) \sigma_i \sigma_j \sigma_\mu \sigma_\nu. \end{aligned} \tag{13}$$

The first-order sensitivities contribute the leading terms to the 2nd-, 3rd-, and 4th-order moments of the response distribution, thus providing the leading contributions to the responses covariances, skewness, and kurtosis. Therefore, obtaining the exact and complete set of first-order sensitivities of responses to model parameters is of paramount importance for any analysis of a computational model. The 2nd-order sensitivities contribute the leading correction terms to the response's expected value (causing it to differ from the response's computed value), and also contribute to the response variances, covariances, and skewness. In particular, if the parameters follow a normal (Gaussian) multivariate distribution, the 2nd-order sensitivities contribute the leading terms to the response's 3rd-order cumulant. Thus, neglecting the 2nd-second-order response sensitivities to normally distributed parameters would nullify the 3rd-order response correlations and hence would nullify the skewness of a response. The 3rd-order sensitivities contribute the 3rd- and 4th-order (in parameter standard deviations) terms to the responses' mean values and covariances. The above formulas will be incorporated into the 2nd/3rd-BERRU-PM framework presented in the next Sub-section.

3.2. 2nd/3rd-BERRU-PM Framework

Consider that N_r system responses that have been experimentally measured. For the mathematical derivations to follow, it is convenient to denote each measured response as r_i^m , and to consider them as being the components of the N_r -dimensional column vector \mathbf{r}^m defined as $\mathbf{r}^m \triangleq (r_1^m, \dots, r_{N_r}^m)^\top$. The expected values of the measured responses are considered to be the components of the vector $E(\mathbf{r}^m)$, defined as $\mathbf{E}(\mathbf{r}^m) \triangleq [E(r_1^m), \dots, E(r_{N_r}^m)]^\top$. The covariance matrix of measured responses is defined as $\mathbf{C}_m \triangleq \left\langle \left[\mathbf{r}^m - \mathbf{E}(\mathbf{r}^m) \right] \left[\mathbf{r}^m - \mathbf{E}(\mathbf{r}^m) \right]^\top \right\rangle_r = [cov(r_i^m, r_j^m)]_{N_r \times N_r}$, $i, j = 1, \dots, N_r$. The computed responses $r_k^c(\mathbf{a})$, $k = 1, \dots, N_r$, are considered to be elements of an N_r -dimensional vector $\mathbf{r}^c(\mathbf{a}) \triangleq [r_1^c(\mathbf{a}), \dots, r_{N_r}^c(\mathbf{a})]^\top$. The expectation values $E[r_k^c(\mathbf{a})]$, given by Eq. (10), are considered to be the components of the following vector of "expected values of the computed response" $E[\mathbf{r}^c(\mathbf{a})] \triangleq [E(r_1^c), \dots, E(r_{N_r}^c)]^\top$. The response covariances defined in Eq. (11) are considered to be the components of a $(N_r \times N_r)$ -dimensional matrix defined as $\mathbf{C}_r \triangleq \left\langle \left[\mathbf{r}^c - E(\mathbf{r}^c) \right] \left[\mathbf{r}^c - E(\mathbf{r}^c) \right]^\top \right\rangle_{\alpha}$.

The covariances between the computed responses and the model parameters defined in Eq. (12) are considered to be the components of an $(N_r \times N_\alpha)$ -dimensional matrix denoted as

$$\mathbf{C}_{r\alpha} \triangleq \left\langle \left[\mathbf{r}^c - E(\mathbf{r}^c) \right] \left(\boldsymbol{\alpha} - \boldsymbol{\alpha}^0 \right)^\dagger \right\rangle_\alpha = \mathbf{C}_{\omega r}^\dagger.$$

The a priori information about the model parameters, computed and measured responses provided in the foregoing can be conveniently summarized by considering that the physical system under consideration is described mathematically by a

multivariate vector $\mathbf{x} \triangleq \left[\boldsymbol{\alpha}, \mathbf{r}^c(\boldsymbol{\alpha}), \mathbf{r}^m \right]^\dagger$ obeying an unknown joint multivariate distribution function

$p(\boldsymbol{\alpha}, \mathbf{r})$ in the combined phase-space of responses and parameters, having an expected value

denoted as $\mathbf{x}^0 \triangleq \left[\boldsymbol{\alpha}^0, E(\mathbf{r}^c), E(\mathbf{r}^m) \right]^\dagger$ and a covariance matrix denoted as \mathbf{C} and defined below. This

information can be used in conjunction with the ‘‘maximum entropy (MaxEnt)’’ principle to obtain the following ‘‘MaxEnt’’ approximation, denoted as $p_2(\mathbf{x} | \mathbf{x}^0, \mathbf{C})$, of the unknown distribution $p(\boldsymbol{\alpha}, \mathbf{r})$:

$$p_2(\mathbf{x} | \mathbf{x}^0, \mathbf{C}) d\mathbf{x} = \frac{\exp \left[-\frac{1}{2} (\mathbf{x} - \mathbf{x}^0)^\dagger \mathbf{C}^{-1} (\mathbf{x} - \mathbf{x}^0) \right] d\mathbf{x}}{\sqrt{\det(2\pi\mathbf{C})}}, \quad \mathbf{C} \triangleq \begin{pmatrix} \mathbf{C}_\alpha & \mathbf{C}_{\omega r} & \mathbf{0} \\ \mathbf{C}_{r\alpha} & \mathbf{C}_r & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{C}_m \end{pmatrix} \quad -\infty < x_j < \infty. \quad (14)$$

Expressions such as shown in Eq. (14) can be evaluated to a high degree of accuracy (a priori controlled) by using the saddle-point method (also called Laplace approximation, or steepest descent method).

$$\mathbf{r}^{be} \triangleq \int_D \mathbf{r} p_2(\mathbf{x} | \mathbf{x}^0, \mathbf{C}) d\boldsymbol{\alpha} d\mathbf{r} = \mathbf{r}^m + \mathbf{C}_m (\mathbf{C}_m + \mathbf{C}_r)^{-1} \left[E(\mathbf{r}^c) - E(\mathbf{r}^m) \right], \quad (15)$$

$$\boldsymbol{\alpha}^{be} \triangleq \int_D \boldsymbol{\alpha} p_2(\mathbf{x} | \mathbf{x}^0, \mathbf{C}) d\boldsymbol{\alpha} d\mathbf{r} = \boldsymbol{\alpha}^0 - \mathbf{C}_{\omega r} (\mathbf{C}_m + \mathbf{C}_r)^{-1} \left[E(\mathbf{r}^c) - E(\mathbf{r}^m) \right]. \quad (16)$$

Since the components of the vector $E(\mathbf{r}^c)$, and the components of the matrices \mathbf{C}_r and $\mathbf{C}_{\omega r}$ contain 2nd-order and 3rd-order sensitivities, the formulas presented in Eqs. (15) and (16) generalize all of the previous formulas of this type found in data assimilation/assimilation procedures published to date (which contain at most first-order sensitivities), including the state-of-the-art ‘‘data adjustment’’ methodologies [3] used in reactor physics. The second-order moments of the posterior distribution $p(\boldsymbol{\alpha}, \mathbf{r})$ comprise the covariances between the best estimated response, which are denoted as \mathbf{C}_r^{be} , the covariances between the best-estimate parameters, which are denoted as \mathbf{C}_α^{be} , and the covariances between the best-estimate parameters and responses, which are denoted as $\mathbf{C}_{\omega r}^{be}$. The expression of the ‘‘best-estimate’’ posterior parameter covariance matrix \mathbf{C}_r^{be} for the best-estimate responses \mathbf{r}^{be} is derived by using the saddle-point method in conjunction with the results given in Eqs. (14) and (15) to obtain:

$$\mathbf{C}_r^{be} \triangleq \int_D (\mathbf{r} - \mathbf{r}^{be}) (\mathbf{r} - \mathbf{r}^{be})^\dagger p(\boldsymbol{\alpha}, \mathbf{r}) d\boldsymbol{\alpha} d\mathbf{r} = \mathbf{C}_m \left[\mathbf{I} - (\mathbf{C}_m + \mathbf{C}_r)^{-1} \mathbf{C}_m \right]. \quad (17)$$

As indicated in Eq. (17), the initial covariance matrix \mathbf{C}_m is multiplied by the matrix

$\left[\mathbf{I} - (\mathbf{C}_m + \mathbf{C}_r)^{-1} \mathbf{C}_m \right]$, which means that the variances contained on the diagonal of the best-estimate

matrix \mathbf{C}_r^{be} will be smaller than the experimentally measured variances contained in \mathbf{C}_m . Hence, the

addition of new experimental information has reduced the predicted best-estimate response variances in \mathbf{C}_r^{be} by comparison to the measured variances contained a priori in \mathbf{C}_m . Since the components of

the matrix \mathbf{C}_r contain 2nd-order and 3rd-order sensitivities, the formula presented in Eq. (17)

generalizes all of the previous formulas of this type found in data assimilation/assimilation procedures published to date (which contain at most first-order sensitivities).

The expression of the “best-estimate” posterior parameter covariance matrix \mathbf{C}_α^{be} for the best-estimate parameters $\boldsymbol{\alpha}^{be}$ is derived by using the saddle-point method in conjunction with the results given in Eqs. (14) and Eq. (16) to obtain:

$$\mathbf{C}_\alpha^{be} \triangleq \int_D (\boldsymbol{\alpha} - \boldsymbol{\alpha}^{be})(\boldsymbol{\alpha} - \boldsymbol{\alpha}^{be})^\dagger p(\boldsymbol{\alpha}, \mathbf{r}) d\boldsymbol{\alpha} d\mathbf{r} = \mathbf{C}_\alpha - \mathbf{C}_{\alpha r} (\mathbf{C}_m + \mathbf{C}_r)^{-1} \mathbf{C}_{r\alpha}. \quad (18)$$

Both matrices \mathbf{C}_α and $\mathbf{C}_{\alpha r} (\mathbf{C}_m + \mathbf{C}_r)^{-1} \mathbf{C}_{r\alpha}$ are symmetric and positive definite. Therefore, the subtraction indicated in Eq. (18) implies that the components of the main diagonal of \mathbf{C}_α^{be} must have smaller values than the corresponding elements of the main diagonal of \mathbf{C}_α . In this sense, the introduction of new computational and experimental information has reduced the best-estimate parameter variances on the diagonal of \mathbf{C}_α^{be} . Since the components of the matrices \mathbf{C}_α , $\mathbf{C}_{\alpha r}$, and \mathbf{C}_r contain 2nd-order and 3rd-order sensitivities, the formula presented in Eq. (18) generalizes all of the previous formulas of this type found in data assimilation/assimilation procedures published to date (which contain at most first-order sensitivities).

The expression of the “best-estimate” posterior parameter covariance matrix \mathbf{C}_α^{be} for the best-estimate parameters $\boldsymbol{\alpha}^{be}$ and best-estimate responses \mathbf{r}^{be} is derived similarly to obtain:

$$\mathbf{C}_{\alpha r}^{be} \triangleq \int_D (\boldsymbol{\alpha} - \boldsymbol{\alpha}^{be})(\mathbf{r} - \mathbf{r}^{be})^\dagger p(\boldsymbol{\alpha}, \mathbf{r}) d\boldsymbol{\alpha} d\mathbf{r} = \mathbf{C}_{\alpha r} (\mathbf{C}_m + \mathbf{C}_r)^{-1} \mathbf{C}_m. \quad (19)$$

As before, since the components of the matrices $\mathbf{C}_{\alpha r}$, and \mathbf{C}_r contain 2nd-order and 3rd-order sensitivities, the formula presented in Eq. (19) generalizes all of the previous formulas of this type found in data assimilation/assimilation procedures published to date (which contain at most first-order sensitivities). It is important to note from the results shown in Eqs. (15) through (19) that the computation of the best estimate parameter and response values, together with their corresponding best-estimate covariance matrices, only requires the computation of $(\mathbf{C}_m + \mathbf{C}_r)^{-1}$, which entails the inversion of a matrix of size $N_r \times N_r$. This is computationally very advantageous, since $N_r \ll N_\alpha$ (i.e., the number of responses is much less than the number of model parameters) in the overwhelming majority of practical situations. The minimum value, $Q_{min} \triangleq Q(\boldsymbol{\alpha}^{be}, \mathbf{r}^{be})$, of the exponent in Eq. (14)

has the expression $Q_{min} \triangleq Q(\boldsymbol{\alpha}^{be}, \mathbf{r}^{be}) = -\frac{1}{2} \mathbf{d}^\dagger (\mathbf{C}_m + \mathbf{C}_r)^{-1} \mathbf{d}$, where $\mathbf{d} \triangleq [E(\mathbf{r}^e) - E(\mathbf{r}^m)]$, and

provides a quantitative indicator for evaluating the degree of consistency of the given parameters and responses.

Although the expressions presented in Eqs. (15) through (19) look superficially similar to the expressions presented in [7, 19]. This superficial similarity stems from the fact that the 2nd/3rd-BERRU-PM methodology only includes means and covariances of the model parameters and computed and measured responses. However, contrary to previously published works, the 2nd/3rd-BERRU-PM methodology presented in in Eqs. (15) through (19) comprises all of the 2nd- and 3rd-order sensitivities of the computed responses with respect to the model parameters. None of the works published thus far include the complete set of 2nd- and 3rd-order sensitivities. Consequently, the 2nd/3rd-BERRU-PM methodology comprises, as particular cases, the previously published formulas used in predictive modeling [1], data adjustment [2], Bayesian linear statistics [3], and data assimilation [4,5].

4. CONCLUSIONS

This work has presented the Third-Order Adjoint Sensitivity Analysis Methodology (3rd-ASAM) for linear systems, which enables the efficient computation of the exact expressions of the 1st-, 2nd-, and 3rd-order functional derivatives (“sensitivities”) of a scalar-valued system response to all the parameters characterizing the respective system. Such responses are often encountered when representing mathematically detector responses and reaction rates in reactor physics problems. The 3rd-ASAM extends the 2nd-ASAM [1] in the quest to overcome the “curse of dimensionality” in

sensitivity analysis, uncertainty quantification and predictive modeling. Very importantly, the computation of the 2nd-level adjoint functions $\Psi_{1,j}^{(2)}, \Psi_{2,j}^{(2)}$, and of the 3rd-level adjoint functions, $\Psi_{1,ij}^{(3)}, \dots, \Psi_{4,ij}^{(3)}$, is performed by using the same forward and adjoint solvers (i.e., computer codes) as used for solving the original forward and adjoint systems. Thus, solving the 2nd-LASS and 3rd-ASAM would not require any significant code development, since the original forward and adjoint solvers (codes) would not need to be modified; only the right-sides (i.e., “sources”) for these solvers/codes would need to be programmed accordingly.

This work has also presented 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. These cumulants quantify the uncertainties (covariances, skewness) in the system response due to uncertainties in the system parameters. Using these new formulas for the response cumulants, this work also presents a new mathematical formalism, called the 2nd/3rd-BERRU-PM (“Second/Third-Order Best-Estimated Results with Reduced Uncertainties Predictive Modeling”), which combines experimental and computational information in the joint phase-space of responses and model parameters, including all of the 1st-order response sensitivities, the complete hessian matrix of 2nd-order second-sensitivities and also the complete set of 3rd-order sensitivities, all computed using the 3rd-ASAM. The 2nd/3rd-BERRU-PM formalism uses the maximum entropy principle to eliminate the need for introducing and “minimizing” a user-chosen “cost functional that quantifies the discrepancies between measurements and computations,” thus yielding results that are free of subjective user-interferences. The 2nd/3rd-BERRU-PM formalism generalizes and significantly extends the data adjustment/assimilation procedures. Incorporating correlations, including those between the imprecisely known model parameters and computed model responses, the 2nd/3rd-BERRU-PM formalism 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. The mathematical framework of the 2nd/3rd-BERRU-PM formalism requires the inversion of a single matrix of size $N_r \times N_r$, where N_r denotes the number of considered responses. In the overwhelming majority of practical situations, the number of responses is much less than the number of model parameters. Thus, the 2nd/3rd-BERRU-PM methodology overcomes the curse of dimensionality which affects the inversion of hessian and higher-order matrices in the parameter space. Ongoing work aims at developing the 3rd-ASAM for nonlinear systems, along with illustrative applications to large-scale practical problems.

REFERENCES

1. D.G. Cacuci, *The Second-Order Adjoint Sensitivity Analysis Methodology*, CRC Press, Taylor & Francis Group, Boca Raton, FL, USA (2018)
2. D.G. Cacuci, *BERRU Predictive Modeling: Best Estimate Results with Reduced Uncertainties*. Springer Heidelberg/New York (2018).
3. *Assessment of Existing Nuclear Data Adjustment Methodologies*, International Evaluation Cooperation, Intermediate Report of WPEC Subgroup 33, NEA/NSC/WPEC/DOC(2010)429, OECD/NEA, Paris (2011).
4. M. Goldstein and D. Woof, *Bayes Linear Statistics: Theory and Methods*. John Wiley & Sons, Chichester, England (2007).
5. W. Lahoz, B. Khattatov, and R. Ménard, *Data Assimilation: Making Sense of Observations*, Springer Verlag, New York (2010).
6. J. M. Lewis, S. Lakshmivarahan, and S.K. Dhall, *Dynamic Data Assimilation: A Least Square Approach*, Cambridge University Press, Cambridge (2006).
7. D.G. Cacuci, “Towards Overcoming the Curse of Dimensionality: The Third-Order Adjoint Method for Sensitivity Analysis of Response-Coupled Linear Forward/Adjoint Systems, with Applications to Uncertainty Quantification and Predictive Modeling,” *Energies*, *accepted*, November (2019).