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Power uprates
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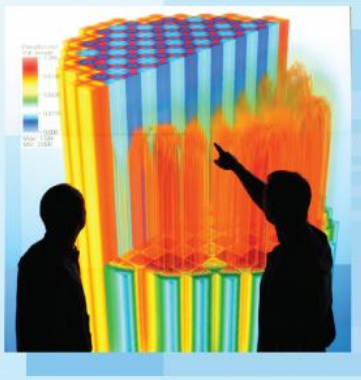

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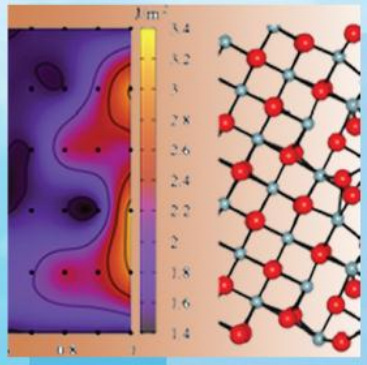
computing



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HIGH-ORDER QUANTITATIVE MODEL VALIDATION METRICS INTEGRATING EXPERIMENTAL AND COMPUTATIONAL DATA FOR LARGE-SCALE TIME-INDEPENDENT NONLINEAR SYSTEMS

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ABSTRACT

Model validation is the process of confirming that the predictions of a computer code adequately represent measured physical phenomena. This work presents novel quantitative multivariate covariance, skewness and kurtosis metrics, constructed from model sensitivities combined with computational and experimental uncertainties, for validating results produced by large-scale nonlinear multi-scale multi-physics models. These new validation metrics also provide indicators for quantifying deviations of the system under consideration from a multivariate normal distribution. Furthermore, the new validation metrics also indicate the consistency among parameters and responses, providing quantitative measures for acceptance or rejection of information.

I. INTRODUCTION

It is well known that the true values of measured and computed data are impossible to know exactly because of various uncontrollable errors and uncertainties arising in the data measurement and interpretation reduction processes. Hence, all inferences, predictions, engineering computations, and other applications of measured and/or computed data are necessarily based on weighted averages over the possibly true values, with weights indicating the degree of plausibility of each value. Furthermore, combination of data from different sources involves a weighted propagation (e.g., via sensitivities) of all uncertainties, requiring reasoning from incomplete information and using probability theory for extracting optimal values together with "best-estimate" uncertainties from often sparse, incomplete, error-afflicted, and occasionally discrepant data. A wide range of probability theory concepts and tools is employed in data evaluation and assimilation, from deductive statistics involving mainly frequencies and sample tallies to inductive inference for assimilating non-frequency data and a priori knowledge.

If the results of separate measurements of the same quantity differ from one another, and the respective differences cannot be predicted individually, then the error stemming from this scatter of the results is called *random error*. Random errors can be identified by repeatedly measuring the same quantity under the same conditions. The scatter in results cannot be always tested in practice, particularly for large-scale modern experiments, where it may be impractical to provide sufficient repetition in order to satisfy the explicit needs for quantifying the random errors based on strict statistical requirements. Nevertheless, reasonable estimates of random errors can often be made, particularly when the nature of the underlying probability distribution can be inferred from previous experience. A subtle issue regarding random errors stems the fact that such errors may contain correlated components: whether an error

component is correlated or not within a particular data set depends upon the role that the associated random variable plays in the respective physical problem.

In contradistinction to a random error, a *systematic error* is defined as a measurement error that remains constant or changes in a regular fashion when the measurements of that quantity are repeated. Such errors arise because of inherent flaws in the investigative process itself, and they lead to bias. Although systematic errors are difficult to distinguish from blunders, particularly when the impact of a blunder is small, the most reliable way to uncover systematic errors is by using a more accurate measuring instrument and/or by comparing a given result with a measurement of the same quantity but performed by a different method. Each distinct approach leads to results that differ somewhat from those obtained in other ways. These differences exhibit a pattern (i.e., are systematic) no matter how many times each approach is repeated because the inherent systematic deficiencies of each method cannot be avoided by mere repetition. When the errors are truly systematic, statistical regularity will emerge from the ensemble of all measurements. Such a statistical regularity will not emerge when the data sets are afflicted with blunders since blunders are generally one-time occurrences that can be detected if a particular procedure is repeated. Consequently, redundancy within a given investigative procedure is desirable not only to improve precision but also to clear the results of blunders and unintended mistakes (e.g., overlooking or miscalculating important corrections, equipment failure or improper calibration, bugs in computer codes, etc.) that can produce defective data. Although such defective data are not uncertainties, data points that exhibit atypical behavior need to be carefully scrutinized since outright rejection may not necessarily be appropriate. In nuclear data analysis and evaluation, for example, a differential cross-section point on an excitation curve might appear to be anomalous but could nevertheless be correct because of the effect of a previously unidentified

resonance. Such data points need to be well understood prior to subjecting the entire data set to extensive statistical analysis for quantifying the associated uncertainties.

In practice, measurements are affected by both random and systematic errors. Typical systematic errors in the nuclear field, for example, can arise from cross sections used for neutron fluence determination, sample material standards, detector calibrations, shortcomings in deriving corrections (e.g., neutron multiple scattering, background) or nuclear decay properties. Once the sources of systematic error have been identified, it is necessary to estimate their respective magnitudes, corresponding to a consistent level of confidence. This is a very difficult task since the applicable probability distribution laws are often unknown, and only an estimate of the ranges of possibilities for the variables in question may be available. The issue of confidence is important because the various error components must ultimately be combined to generate covariance matrices, and if the specific errors conform to widely different confidence levels, their combination may lead to misleading results.

The current state-of-the-art data assimilation/model calibration methodologies [see, e.g., D. G. Cacuci, and M. Ionescu-Bujor, (2010), ”Best-Estimate Model Calibration and Prediction through Experimental Data Assimilation: I. Mathematical Framework”, *Nucl. Sci. Eng*., **165**, 18-44, 2010; and W. Lahoz, B. Khattatov, and R. Ménard (Eds.), “*Data Assimilation: Making Sense of Observations*”, Springer-Verlag Berlin/Heidelberg, 2010] for large-scale nonlinear systems cannot take into account uncertainties higher-order than second-order (i.e., covariances) thereby failing to quantify the deviations of the problem under consideration from a normal (Gaussian) multivariate distribution. Such deviations would be quantified by the third- and fourth-order moments (namely: skewness and kurtosis) of the model’s predicted results (responses). These higher-order moments would be constructed by combining modeling and experimental uncertainties (which also incorporate the corresponding skewness and kurtosis information), using derivatives (sensitivities) of the model responses with respect to the model’s parameters. Notably, model calibration methodologies currently employed in large-scale nuclear engineering applications can quantify only the first-order predictions. Furthermore, none of the model calibration methodologies currently employed in large-scale nuclear

engineering applications can account for unrecognized modeling errors (omitting or incomplete modeling of physical phenomena). Our ongoing research aims at addressing and overcoming all of these current shortcomings.

This report is organized as follows: Section II introduces metrics for the *a priori verification and validation* of the covariance matrices for the measured responses and model parameters, respectively, taking also into account possible correlations between parameters and responses. As is well known, *covariance matrices must be positive definite*, since they represent physical uncertainties. Section II also addresses the fundamental issue of data consistency, and introduces quantitative indicators for assessing consistency among n measurements and/or computations of the same (unknown) quantity μ, which yielded data $x_1 \pm \sigma_1, \ldots, x_n \pm \sigma_n$, where x_i denotes the measured or computed mean value of response i, and σ_i denotes the corresponding standard deviation for response i. When the distance, $\left|x_i - x_j\right|$, between any two values is smaller than or comparable to the sum $\left(\sigma_i + \sigma_j\right)$ of the corresponding uncertainties, the data is customarily considered to be "consistent" or to agree "within error bars". However, *if the distances* $\left|x_j - x_k\right|$ *are larger than* $\left(\sigma_j + \sigma_k\right)$, *the respective data could be inconsistent* (*discrepant*). Inconsistencies can be caused by unrecognized or ill-corrected experimental effects (e.g., background, dead time of the counting electronics, instrumental resolution, sample impurities, calibration errors, etc.). Although there is a non-zero probability that apparently discrepant data are actually not discrepant [e.g., for Gaussian sampling distributions with standard deviation σ, the probability that two equally precise measurements would yield a separation greater than $\sigma_i + \sigma_j = 2\sigma$ is $erfc(1) \simeq 0.157$], it *is much more likely* (about 84% probability) *that apparently discrepant data actually indicate the presence of unrecognized errors* ε_j. Section II recalls the recent procedure of Cacuci and Ionescu-Bujor (*NS&E*, **165**, pp 1-17, 2010) for combining consistent and possibly mildly inconsistent data to determine the

marginal posterior distributions for unrecognized errors, if present, thereby recommending mean values and covariances for subsequent model validation.

In practice, the exact first-order response derivatives ("sensitivities") with respect to model parameters can be computed most efficiently for large-scale nonlinear systems by using the *"adjoint sensitivity analysis procedure" (ASAP).* However, the computation of the second-order derivatives severely strains computational resources, while third- and higher-order response derivatives with respect to model parameters are practically unavailable for large-scale systems. Section III presents, in premiere, *explicit expressions for skewness and kurtosis of computed responses,* thereby permitting *quantification of the deviations of the computed response uncertainties from multivariate normality.* This Section also presents *a new and most efficient procedure for computing the second-order response derivatives with respect to model parameters using the "adjoint sensitivity analysis procedure" (ASAP).*

Loosely speaking, model validation means "Does the model represent physical reality?" More formally: "*Validation is the process of confirming that the predictions of a computer code adequately represent measured physical phenomena*", or "*Model validation is the process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model*". Physical reality is represented by experiments, which are accompanied by experimental uncertainties. Computational results are also accompanied by uncertainties. Hence, model validation requires comparing computations to experiments, in the presence of both computational and experimental uncertainties. Validation experiments must be designed to allow conclusive quantitative comparisons of computations with experimental data for quantifying model fidelity and credibility. Section IV provides *quantitative second-, third-, and fourth-order metrics (denoted as* $C_k - metrics$, *for* $k = 2,3,4$ *), which combine experimental and modeling uncertainties with first- and*

second-order response sensitivities, for determining the degree of validation and agreement (or disagreement) among the experimentally measured and computed parameters and responses, as well as quantifying the deviations from multivariate normality of the combined experimental-computational distribution functions. These $C_k - metrics$ allow *quantification of the validation domain* and provide the basic elements for *quantitative model extrapolation*, namely the prediction of uncertainty in new environments or conditions of interest, including both untested parts of the parameter space and higher levels of system complexity in the validation hierarchy. Finally, Section V highlights the importance and wide applicability for model validation of the new high-order $C_k - metrics$ introduced in this report.

II. A PRIORI DATA CONSISTENCY VERIFICATION AND VALIDATION: UNCERTAIN MODEL PARAMETERS AND MEASURED RESPONSES

In general, a physical system and/or the result of an indirect experimental measurement is modeled mathematically in terms of:

(a) A system of linear and/or nonlinear equations that relate the system's independent variables and parameters to the system's state (i.e., dependent) variables;

(b) Inequality and/or equality constraints that delimit the ranges of the system's parameters;

(c) One or several quantities, customarily referred to as system responses (or objective functions, or indices of performance), which are computed using the mathematical model; and

(d) Experimentally measured responses, with their respective nominal (mean) values and uncertainties (covariance matrices).

II.A. Verification of "A Priori" Measured Response Covariance Matrix: Consistent and Discrepant Measurements

Consider that the model under consideration is used to compute N_r *responses* (or results), denoted generically by the vector

$$\boldsymbol{r} = \{r_i \,|\, i = 1,\ldots,N_r\}. \tag{II.1}$$

Consider also that measurements are available for the computed responses; these *measured responses* are characterized by mean values, denoted as

$$\boldsymbol{r}^m = \left\{ r_i^m \,|\, i = 1,\ldots,N_r \right\}, \quad r_i^m \equiv \left\langle r_i \right\rangle, \tag{II.2}$$

and by symmetric positive-definite covariance matrices $\boldsymbol{C}^{rr}$ of dimension $N_r \times N_r$ of the form

$$\boldsymbol{C}^{rr} \equiv \left\langle \left(\boldsymbol{r} - \boldsymbol{r}^m \right) \left(\boldsymbol{r} - \boldsymbol{r}^m \right)^\dagger \right\rangle, \tag{II.3}$$

comprising elements c_{ij}^m defined as

$$c_{ij}^m \equiv \left\langle \left(r_i - r_i^m \right) \left(r_j - r_j^m \right) \right\rangle. \tag{II.4}$$

The covariance matrix $\boldsymbol{C}^{rr}$ of measured responses must be *positive definite* (otherwise, it would not qualify as a bon-fide covariance matrix). This means that the measured response correlations must satisfy the Cauchy-Schwartz inequality

$$-1 \le \frac{c_{ij}^m}{\sqrt{c_{ii}^m c_{jj}^m}} \le 1, \tag{II.5}$$

while $\boldsymbol{C}^{rr}$ must admit the Cholesky decomposition

$$\boldsymbol{C}^{rr} = \boldsymbol{L}^{rr} \left(\boldsymbol{L}^{rr} \right)^\dagger = \left(\boldsymbol{U}^{rr} \right)^\dagger \boldsymbol{U}^{rr}, \tag{II.6}$$

with $\boldsymbol{L}^{rr}$ (respectively $\boldsymbol{U}^{rr}$) being a nonsingular lower (respectively upper) triangular matrix with positive entries on its diagonal.

If $\boldsymbol{C}^{rr}$ is not positive definite or, worse, is singular, most Cholesky-decomposition algorithms will not perform the decomposition and will exit with a warning message. In such cases, it is imperative to examine the elements of $\boldsymbol{C}^{rr}$ to quantify possible *multi-colinearity* among them.

Multi-colinearity occurs when the elements of $\boldsymbol{C}^{rr}$ are moderately to highly correlated, and causes $\boldsymbol{C}^{rr}$ to be ill-conditioned or singular (in case of linear dependence among its elements). As detailed in [B. G. Tabachnik and L. S. Fiddel, *Using Multivariate Statistics*, 4th Ed, Allyn and Bacon, Boston, 2001], multi-colinearity can be diagnosed by using either or all of the following quantifiers:

(i) *variance inflation factors*, which indicate whether there is a strong linear relation between a measured response and all of the remaining measurements;

(ii) the so-called *tolerance* value, which quantifies the degree to which one measured response can itself be predicted by the other measured responses; and

(iii) the so-called *condition index* in conjunction with the *variance proportions*, to assess the dependency of one measurement on the others.

Highly correlated measurements must be combined to alleviate multi-colinearity, thereby ensuring that $\boldsymbol{C}^{rr}$ is a bona-fide, positive definite, covariance matrix.

The covariance matrix $\boldsymbol{C}^{rr}$ may also be affected by *influential data points* and/or *outliers* (which may be influential or not) which can affect or even falsify subsequent analyses involving $\boldsymbol{C}^{rr}$. A value greater than unity for *Cook's distance*, for example, would generally indicate an influential measurement [see, e.g., J. P.Stevens, *Applied Multivariate Statistics for the Social Sciences*, 4th Ed., LEA, Mahwah, NJ]. The identification of outliers usually relies on the assumption of an underlying model for the respective measurements, since a measurement value can considered to be an outlier only relative to some assumed model. There are several classical methods for identifying outliers [see, e.g., V. Barnett and T. Lewis, *Outliers in Statistical Data*, 2nd Ed., John Wiley & Sons, New York, 1984], although none of them are guaranteed to perform perfectly, particularly in the presence of *masking* or *swamping* caused my multiple outliers in multivariate data. A well-known robust criterion for detecting outliers

in multivariate data is when the squared Mahalanobis distance, D_i^2, exceeds some appropriate critical value $\left(D_i^2\right)_{crit}$. The Mahalanobis distance D_i is defined for N observations in a p-variable data set $\boldsymbol{x}_i$ with mean $\bar{\boldsymbol{x}}_N$ and covariance matrix $\boldsymbol{C}_N$ as

$$D_i \equiv \left[\left(\boldsymbol{x}_i - \bar{\boldsymbol{x}}_N\right)^{\dagger} \boldsymbol{C}_N^{-1} \left(\boldsymbol{x}_i - \bar{\boldsymbol{x}}_N\right)\right]^{1/2}. \tag{II.7}$$

Based on the asymptotic distribution of the Mahalanobis distance for large samples (i.e., large N), an observation $\boldsymbol{x}_i$ can be considered to be an outlier if

$$D_i^2 > \chi^2_{p;1-\alpha/N};\ \ \alpha \in (0,1),\ \ N = \text{large}, \tag{II.8}$$

where $\chi^2_{p;1-\alpha/N}$ denotes the $(1-\alpha/N)$ quantile of the χ_p^2 for a (large) sample of size N, and typically $\alpha = 1\%$ or $\alpha = 5\%$. For smaller samples (i.e., small N), the recommended critical value for $\left(D_i^2\right)_{crit}$ is [see, e.g., C. Becker and U. Gather, "The Masking Breakdown Point of Multivariate Outlier Identification Rules", *J. Am. Stat. Assoc*, **94**, 947-955, 1999]

$$D_i^2 > \frac{p(n-1)^2 F_{p,n-p-1;\alpha/N}}{n\left(n-p-1+pF_{p,n-p-1;\alpha/N}\right)};\ \ \alpha \in (0,1),\ \ N = \text{small}, \tag{II.9}$$

If a measurement is grossly inconsistent with the rest, it should be eliminated from further consideration. However, if inconsistencies are mild, then the respective measurements should be combined with other appropriately chosen measurements, just as in the case of highly correlated measurements, in order to ensure that $\boldsymbol{C}^{rr}$ is a bona-fide (physically and

mathematically) covariance matrix. For example, if the distance, $\left|r_i - r_j\right|$, between the nominal values of two measured responses is smaller than or comparable to the sum $\left(\sigma_i + \sigma_j\right)$ of the corresponding standard deviations, the respective responses can be considered to be "consistent" or to agree "within error bars". On the other hand, if the distances $\left|r_i - r_j\right|$ are larger than $\left(\sigma_j + \sigma_k\right)$, the respective measurements might be consistent (since about 17% of the members of the same normal distribution do lie outside an interval of two standard deviations) or might indicate the possible presence of unrecognized errors ε_j. A method for combining measurements has been recently presented by Cacuci and Ionescu-Bujor (2010.a), who consider n measurements of the same unknown mean-value (i.e., "location parameter") r, such that each measurement yielded data $x_1 \pm \sigma_1, \ldots, x_n \pm \sigma_n$, where x_i denotes the measured mean value while σ_i denotes the corresponding measured standard deviation obtained in measurement (or computation) i. Considering both recognized and unrecognized errors, Cacuci and Ionescu-Bujor [D. G. Cacuci, and M. Ionescu-Bujor, "On the Evaluation of Discrepant Scientific Data with Unrecognized Errors", *Nucl. Sci. Eng.*, **165**, 1-17, 2010] employed the maximum entropy principle to derive optimal (under quadratic loss) mean values and marginal posterior distributions that are uniformly valid for the combined data. The unknown true variance of the unrecognized errors ε_j was considered to be of the form $var\left(\varepsilon_j\right) = \left\langle \varepsilon_j^2 \right\rangle = \tau_i^2 / s$, where τ_i^2 denotes an *estimate of the unknown variance* of ε_i (estimated, for example, from the accuracy of the techniques employed) and s *is an adjustable common scale parameter* with a prior distribution $p(s)ds$. *If nothing is known about the adjustable common scale parameter* s, Cacuci and Ionescu-Bujor (2010) employed Jeffrey's prior $p(s)ds = ds/s$ to obtain the following marginal posterior distribution for the location parameter r, given $\boldsymbol{\sigma} = \left(\sigma_1, \ldots, \sigma_n\right)$, $\boldsymbol{x} = \left(x_1, \ldots, x_n\right)$, and $\boldsymbol{\tau} = \left(\tau_1, \ldots, \tau_n\right)$:

$$p\left(r\,|\,\boldsymbol{\sigma},\boldsymbol{x},\boldsymbol{\tau}\right)dr \propto dr\frac{\left(s^{*}\right)^{\frac{n}{2}-1}}{\prod_{j=1}^{n}\left(s^{*}\sigma_j^2+\tau_j^2\right)^{1/2}}exp\left[-\frac{s^{*}}{2}\sum_{j=1}^{n}\frac{\left(r-x_j\right)^2}{s^{*}\sigma_j^2+\tau_j^2}\right], \tag{II.10}$$

where s^{*} is the solution of the following nonlinear algebraic equation:

$$s^{*}=\left(n-2\right)\left[\sum_{j=1}^{n}\frac{\sigma_j^2}{s^{*}\sigma_j^2+\tau_j^2}+\sum_{j=1}^{n}\frac{\tau_j^2\left(r-x_j\right)^2}{\left(s^{*}\sigma_j^2+\tau_j^2\right)^2}\right]^{-1}, \quad for \quad n>2. \tag{II.11}$$

On the other hand, it can be argued that the scale factor s would be expected to be close to unity; since the values τ_i are the best available estimates of the uncertainties caused by unrecognized errors. In such a case, the mean value of s would also be expected to be close to unity, i.e., $\langle s\rangle=1$, and the maximum-entropy argument can be used with the constraint $\langle s\rangle=1$ to obtain the exponential prior $p\left(s\right)ds=e^{-s}ds,\ \ 0<s<\infty$. This prior is almost as noncommittal as Jeffreys' prior $\left(ds/s\right)$, decreasing also monotonically as s increases, but gives less weight to the extreme values approaching the two ends of the positive real axis. For this (exponential) prior, Cacuci and Ionescu-Bujor (2010) have obtained the following marginal posterior distribution for the location parameter r:

$$p\left(r\,|\,\boldsymbol{\sigma},\boldsymbol{x},\boldsymbol{\tau}\right)dr \propto dr\frac{\left(s^{*}\right)^{\frac{n}{2}}}{\prod_{j=1}^{n}\left(s^{*}\sigma_j^2+\tau_j^2\right)^{1/2}}exp\left\{\left(-s^{*}\right)\left[1+\frac{1}{2}\sum_{j=1}^{n}\frac{\left(r-x_j\right)^2}{s^{*}\sigma_j^2+\tau_j^2}\right]\right\}. \tag{II.12}$$

where s^{*} that is the solution of the following nonlinear algebraic equation:

$$s^* = \frac{n}{2}\left[1 + \frac{1}{2}\sum_{j=1}^{n}\frac{\sigma_j^2}{s^*\sigma_j^2 + \tau_j^2} + \frac{1}{2}\sum_{j=1}^{n}\frac{\tau_j^2\left(r - x_j\right)^2}{\left(s^*\sigma_j^2 + \tau_j^2\right)^2}\right]^{-1}, \quad for \quad n > 1. \tag{II.13}$$

In view of the expectation that the scale factor s would be close to unity, a reasonable starting value for solving Eq. (II.11) or (II.13) iteratively, e.g., by Picard or Newton-like procedures, would be $s_0 = 1$. Replacing this value in either Eq. (II.10) or (II.12) would yield a Gaussian of the form "starting expression" for the distribution the location parameter r

$$p\left(r \mid \boldsymbol{\sigma}, \boldsymbol{x}, \boldsymbol{\tau}, s_0 = 1\right) = \frac{exp\left[-\frac{1}{2}\sum_{j=1}^{n}\frac{\left(r - x_j\right)^2}{\sigma_j^2 + \tau_j^2}\right]}{\int_{-\infty}^{\infty} dr\, exp\left[-\frac{1}{2}\sum_{j=1}^{n}\frac{\left(r - x_j\right)^2}{\sigma_j^2 + \tau_j^2}\right]}, \tag{II.14}$$

as the "starting expression" for the distribution the location parameter r. Using Eq. (II.14) would yield the following "starting" expressions for the mean, $\langle r \rangle_{s_0=1}$, and variance, $var\left(r\right)_{s_0=1}$, of the unknown location parameter r:

$$\langle r \rangle_{s_0=1} = \frac{\sum_{k=1}^{n}\left(\sigma_k^2 + \tau_k^2\right)^{-1} x_k}{\sum_{k=1}^{n}\left(\sigma_k^2 + \tau_k^2\right)^{-1}}, \quad var\left(r\right)_{s_0=1} = \frac{1}{\sum_{k=1}^{n}\left(\sigma_k^2 + \tau_k^2\right)^{-1}}. \tag{II.15}$$

As the above expressions indicate, the initial estimate $s_0 = 1$ (for the scale factor s) would give equal importance to both the recognized and unrecognized errors. Of course, subsequent iterations of Eq. (II.11) or (II.13), for obtaining improved estimates $s_k \xrightarrow{k=1,2,\ldots} s^*$ would lead to non-Gaussian distributions $p\left(r \mid \boldsymbol{\sigma}, \boldsymbol{x}, \boldsymbol{\tau}\right)$.

In the limiting case when there are no unrecognized errors ($\tau_j = 0$), i.e., all the errors are known, both the distribution in Eq. (II.10) and that in Eq. (II.12) reduce to the well-known Gaussian that describes the evaluation of an unknown location parameter r using known scale parameters (variances), namely:

$$p\left(r \mid \boldsymbol{\sigma}, \boldsymbol{x}, \boldsymbol{\tau} \to \boldsymbol{0}\right) dr = \frac{exp\left[-\frac{\left(r - \langle r \rangle_{\tau=0}\right)^2}{2\, var\left(r\right)_{\tau=0}}\right]}{\left[2\pi\, var\left(r\right)_{\tau=0}\right]^{1/2}} dr\,, \quad -\infty < r < \infty\,. \tag{II.16}$$

characterized by the mean value $\langle r \rangle_{\tau=0}$ and variance , $var\left(r\right)_{\tau=0}$, of the form

$$\langle r \rangle_{\tau=0} = \left(\sum_{k=1}^{n} \sigma_k^{-2} x_k\right)\left(\sum_{k=1}^{n} \sigma_k^{-2}\right)^{-1}, \quad var\left(r\right)_{\tau=0} = \left(\sum_{k=1}^{n} \sigma_k^{-2}\right)^{-1}. \tag{II.17}$$

In the opposite limit when *the recognized uncertainties are unimportant,* $\sigma_j \to 0$, Eq. (II.10) reduces uniformly to a Student's-distribution of the form

$$p\left(r \mid \boldsymbol{\sigma} \to \boldsymbol{0}, \boldsymbol{x}, \boldsymbol{\tau}\right) dr \;\propto\; St\left(r \middle| \langle r \rangle_{\sigma=0}, (n-1)A, n-1\right) dr;$$

$$\langle r \rangle_{\sigma=0} = \left(\sum_{i=1}^{n} x_i \tau_i^{-2}\right)\left(\sum_{i=1}^{n} \tau_i^{-2}\right)^{-1}, \quad for\ n > 2; \tag{II.18}$$

$$A \equiv \left(\sum_{i=1}^{n} x_i^2 \tau_i^{-2}\right)\left(\sum_{i=1}^{n} \tau_i^{-2}\right)^{-1} - \left[\langle r \rangle_{\sigma=0}\right]^2,$$

with mean $\langle r \rangle_{\sigma=0}$ and variance

$$var\left(r\right)_{\sigma=0} = \frac{A}{n-3}, \quad for \;\; n > 3, \tag{II.19}$$

It is noteworthy that the result shown in Eq. (II.18) is the same as would be obtained if the *unknown location parameter* μ *were estimated from a sample drawn from a Gaussian distribution with unknown variance (i.e., unknown scale parameter).*

The distribution in Eq. (II.12) also reduces uniformly to a Student's-distribution when the recognized uncertainties are unimportant (i.e., $\sigma_j \to 0$), namely

$$p\left(r \mid \boldsymbol{\sigma} \to \boldsymbol{0}, \boldsymbol{x}, \boldsymbol{\tau}\right) dr \propto St\left(r \left| \langle r \rangle_{\sigma=0}, \left(n+1\right) B,\ n+1 \right.\right) dr; \tag{II.20}$$

having the same mean $\langle r \rangle_{\sigma=0}$ as before, but with variance

$$var\left(r\right)_{\sigma=0} = \frac{B}{n-1}, \quad for \quad n>1;\ B \equiv \left[2\left(\sum_{j=1}^{n} \tau_j^{-2} \right)^{-1} + \left\langle x^2 \right\rangle - \left\langle x \right\rangle^2 \right]^{-1}. \tag{II.21}$$

Comparing Eqs. (II.20) with Eq. (II.18) indicates that the mean $,\langle r \rangle_{\sigma=0}$, for discrepant experiments obtained when using the exponential prior for the scale factor s is the same as the mean obtained by using Jeffreys' prior for s; this mean is given by the sample average with weights proportional to τ_j^{-2}, and is valid already when two experiments are available. Comparing now the corresponding expressions for $var\left(r\right)_{\sigma=0}$ in Eq. (II.20) and Eq. (II.18), respectively, indicates that the use of the exponential distribution for the scale factor s brings in the additional term $\left(\sum_{j=1}^{n} \tau_j^{-2} \right)^{-1}$ in Eq. (II.21), but extends the validity of the latter to two experiments (as opposed to minimum four experiments, as required when Jeffryes' prior is used for the scale factor s).

II.B. Verification of "A Priori" Parameter Covariance Matrix

In general, the model parameters are experimentally derived quantities and are therefore subject to uncertainties. Specifically, consider that the model comprises N_α uncertain parameters α_n, which constitute the components of the (column) vector $\boldsymbol{\alpha}$ of *model parameters*, defined as

$$\boldsymbol{\alpha} = \{\alpha_n \,|n = 1,\ldots,N_\alpha\}\ . \tag{II.22}$$

In practice, the mean values of the model parameters are known together with uncertainties (correlations and standard deviations) computed about the respective mean values. The vector $\boldsymbol{\alpha}^0 = \{\alpha_n^0 \,|n = 1,\ldots,N_\alpha\}$ of mean values of the model parameters has components denoted as

$$\alpha_i^0 \equiv \langle \alpha_j \rangle,\ \ \langle f \rangle \equiv \int f(\boldsymbol{\alpha},\boldsymbol{r})\, p(\boldsymbol{\alpha},\boldsymbol{r})\, d\boldsymbol{\alpha} dr, \tag{II.23}$$

where the angular brackets denote integration of a generic function $f(\boldsymbol{\alpha},\boldsymbol{r})$ over the *unknown* joint probability distribution $p(\boldsymbol{\alpha},\boldsymbol{r})$ of parameters and responses. The parameter correlations are defined as

$$c_{ij}^{\alpha} \equiv \left\langle \left(\alpha_i - \alpha_i^0\right)\left(\alpha_j - \alpha_j^0\right) \right\rangle, \tag{II.24}$$

and constitute the elements of a symmetric, positive-definite parameter covariance matrix, denoted here as $\boldsymbol{C}^{\alpha\alpha}$, of dimension $N_\alpha \times N_\alpha$ defined as

$$\boldsymbol{C}^{\alpha\alpha} \equiv \left\langle \left(\boldsymbol{\alpha} - \boldsymbol{\alpha}^0\right)\left(\boldsymbol{\alpha} - \boldsymbol{\alpha}^0\right)^{\dagger} \right\rangle \,, \tag{II.25}$$

where the dagger denotes "transposition". Since the elements of $\boldsymbol{C}^{\alpha\alpha}$ are obtained, in practice, by a variety of experimental, empirical, and/or theoretical methods, it is imperative to ensure, at the outset, that the covariance matrix $\boldsymbol{C}^{\alpha\alpha}$ fulfills the physical and mathematical properties required of a covariance matrix. Thus, $\boldsymbol{C}^{\alpha\alpha}$ must be positive definite and the correlations $\rho_{ij}^{\alpha} \equiv c_{ij}^{\alpha}\left(c_{ii}^{\alpha} c_{jj}^{\alpha}\right)^{-1/2}$ must satisfy the Cauchy-Schwartz inequality

$$-1 \le \frac{c_{ij}^{\alpha}}{\sqrt{c_{ii}^{\alpha} c_{jj}^{\alpha}}} \le 1 \,. \tag{II.26}$$

As is well known, *the trace, the determinant, and the principal minors of a positive definite matrix are positive*, so that these properties must be satisfied, in particular, by $\boldsymbol{C}^{\alpha\alpha}$. As is also well known, an equivalent necessary and sufficient condition for $\boldsymbol{C}^{\alpha\alpha}$ to be positive definite is that it admit the *Cholesky decomposition*

$$\boldsymbol{C}^{\alpha\alpha} = \boldsymbol{L}^{\alpha\alpha}\left(\boldsymbol{L}^{\alpha\alpha}\right)^{\dagger} = \left(\boldsymbol{U}^{\alpha\alpha}\right)^{\dagger}\boldsymbol{U}^{\alpha\alpha} \,, \tag{II.27}$$

where $\boldsymbol{L}^{\alpha\alpha}$ (respectively $\boldsymbol{U}^{\alpha\alpha}$) is a nonsingular lower (respectively upper) triangular matrix with positive entries on its diagonal. It is very important to perform the Cholesky decomposition on a given covariance matrix at the outset, not only to ensure that the respective covariance data makes physical and mathematical sense but also to simplify and facilitate subsequent computations involving $\boldsymbol{C}^{\alpha\alpha}$.

It is very unlikely that higher-order (i.e., triple, quadruple) correlations among parameters would be available in practice; nevertheless, the *skewness* $\mu_3(\alpha_i) \equiv \left\langle \left(\alpha_i - \alpha_i^0\right)^3 \right\rangle$ and *kurtosis* $\mu_4(\alpha_i) \equiv \left\langle \left(\alpha_i - \alpha_i^0\right)^4 \right\rangle$ for individual parameters α_i could be obtained if the forms of the corresponding individual probability distributions are known or can be approximately surmized.

II.C. Verification of "A Priori" Parameter - Response Covariance Matrix

Finally note that in the most general case, the measured responses may be correlated to the parameters through *response-parameter uncertainty* matrices of dimension $N_\alpha \times N_r$ denoted as

$$\boldsymbol{C}^{\alpha r} \equiv \left\langle \left(\boldsymbol{\alpha} - \boldsymbol{\alpha}^0\right)\left(\boldsymbol{r} - \boldsymbol{r}^m\right)^\dagger \right\rangle, \tag{II.28}$$

comprising elements $c_{ij}^{\alpha r}$ defined as

$$c_{ij}^{\alpha r} \equiv \left\langle \left(\alpha_i - \alpha_i^m\right)\left(r_j - r_j^m\right) \right\rangle, \tag{II.29}$$

Note that the matrix $\boldsymbol{C}^{\alpha r}$ is *not* a bona-fide variance-covariance matrix, since it is generally rectangular and the elements on its main diagonal (if it happens to be square) are correlations rather that variances.

III. COMPUTATION OF HIGH-ORDER MODEL RESPONSE SENSITIVITIES AND UNCERTAINTIES

When the numerical and/or modeling errors are not explicitly taken into account, but are considered to be amenable to treatment via uncertain model parameters that are included among the components of $\boldsymbol{\alpha}$, the most general representation of a the vector of responses, $\boldsymbol{r}$, as a function of the parameters, $\boldsymbol{\alpha}$, is

$$\boldsymbol{r} = \boldsymbol{r}^c\left(\boldsymbol{\alpha}\right), \tag{III.1}$$

where $\boldsymbol{r}^c\left(\boldsymbol{\alpha}\right)$ denotes the *computed* response value for a given, but otherwise arbitrary, set of numerical values for the parameters $\boldsymbol{\alpha}$.

III.A. Computation of Model Response Uncertainties: Covariances, Skewness, and Kurtosis

The deterministic methods for propagating uncertainties in model parameters to computed responses rely on expanding formally the computed response in a Taylor series around $\boldsymbol{\alpha}^0$. In practice, first-order response derivatives ("sensitivities") with respect to model parameters can be computed most efficiently using the "adjoint sensitivity analysis procedure" (ASAP), but the second-order derivatives are seldom available for large-scale systems since they severely strain computational resources; third- and higher-order derivatives are practically unavailable. Reflecting these practicalities, only second-order derivatives of responses to model parameters will be explicitly taken into account in this work, implying a Taylor-series expansion of the form

$$\boldsymbol{r}(\boldsymbol{\alpha}) = \boldsymbol{r}^{c}(\boldsymbol{\alpha}^{0}) + \boldsymbol{S}^{r\alpha}(\boldsymbol{\alpha}^{0})(\boldsymbol{\alpha} - \boldsymbol{\alpha}^{0}) + \boldsymbol{\psi}(\boldsymbol{\alpha} - \boldsymbol{\alpha}^{0}) + O\left(\left|\boldsymbol{\alpha} - \boldsymbol{\alpha}^{0}\right|^{3}\right). \tag{III.2}$$

In the above expansion, $\boldsymbol{S}^{r\alpha}(\boldsymbol{\alpha})$ denotes the $N_r \times N_\alpha$ dimensional matrix of *response sensitivities* (to the model parameters) , with components defined as

$$\boldsymbol{S}^{r\alpha}(\boldsymbol{\alpha}) \equiv \begin{pmatrix} s_{11}^{r\alpha}(\boldsymbol{\alpha}) & \cdots & s_{1N_\alpha}^{r\alpha}(\boldsymbol{\alpha}) \\ \vdots & s_{ij}^{r\alpha}(\boldsymbol{\alpha}) & \vdots \\ s_{N_r 1}^{r\alpha}(\boldsymbol{\alpha}) & \cdots & s_{N_r N_\alpha}^{r\alpha}(\boldsymbol{\alpha}) \end{pmatrix} \equiv \begin{pmatrix} \dfrac{\partial r_1(\boldsymbol{\alpha})}{\partial \alpha_1} & \cdots & \dfrac{\partial r_1(\boldsymbol{\alpha})}{\partial \alpha_{N_\alpha}} \\ \vdots & \dfrac{\partial r_i(\boldsymbol{\alpha})}{\partial \alpha_j} & \vdots \\ \dfrac{\partial r_{N_r}(\boldsymbol{\alpha})}{\partial \alpha_1} & \cdots & \dfrac{\partial r_{N_r}(\boldsymbol{\alpha})}{\partial \alpha_{N_\alpha}} \end{pmatrix}. \tag{III.3}$$

As generally shown by Cacuci [*Sensitivity and Uncertainty Analysis: Theory*, **Volume 1**, Chapman & Hall/CRC, Boca Raton (2003); see also D.G. Cacuci, M. Ionescu-Bujor, and M.I. Navon, *Sensitivity and Uncertainty Analysis: Applications to Large Scale Systems*, **Volume 2**, Chapman & Hall/CRC, Boca Raton (2005)], the exact computation of the above first-order response sensitivities for large-scale nonlinear systems is performed most efficiently by using the *adjoint sensitivity analysis procedure (ASAP).*

Furthermore, the N_r-dimensional vector

$$\boldsymbol{\psi}(\boldsymbol{\alpha} - \boldsymbol{\alpha}^{0}) = \left[\psi_1(\boldsymbol{\alpha} - \boldsymbol{\alpha}^{0}), \ldots, \psi_{N_r}(\boldsymbol{\alpha} - \boldsymbol{\alpha}^{0})\right]^{\dagger}, \tag{III.4}$$

represents the second-order terms in $(\boldsymbol{\alpha} - \boldsymbol{\alpha}^{0})$, with components defined as follows:

$$\begin{aligned}\psi_k\left(\boldsymbol{\alpha}-\boldsymbol{\alpha}^0\right) &= \frac{1}{2}\sum_{i=1}^{N_\alpha}\sum_{j=1}^{N_\alpha}\left(\alpha_i-\alpha_i^0\right)\frac{\partial^2 r_k\left(\boldsymbol{\alpha}^0\right)}{\partial\alpha_i\partial\alpha_j}\left(\alpha_j-\alpha_j^0\right) \\ &= \frac{1}{2}\left(\boldsymbol{\alpha}-\boldsymbol{\alpha}^0\right)^\dagger\left[\nabla^2 r_k\left(\boldsymbol{\alpha}^0\right)\right]\left(\boldsymbol{\alpha}-\boldsymbol{\alpha}^0\right),\quad k=1,...,N_r,\end{aligned} \tag{III.5}$$

where $\nabla^2 r_k\left(\boldsymbol{\alpha}^0\right)$ denotes the Hessian matrix of the response r_k evaluated at $\boldsymbol{\alpha}^0$, i.e.,

$$\nabla^2 r_k\left(\boldsymbol{\alpha}^0\right)=\left[\frac{\partial^2 r_k\left(\boldsymbol{\alpha}^0\right)}{\partial\alpha_i\partial\alpha_j}\right],\quad i,j=1,...,N_\alpha;\ \ k=1,...,N_r. \tag{III.6}$$

The expected values, covariances, and higher-order correlations characterizing the computed responses can be obtained by formally integrating Eq.(III.2) over the unknown joint probability distribution $p\left(\boldsymbol{\alpha},\boldsymbol{r}\right)$. Thus, the expected value, $E\left(r_k\right)$, of the response r_k is obtained as

$$E\left(r_k\right)=r_k^c\left(\boldsymbol{\alpha}^0\right)+\frac{1}{2}\sum_{i=1}^{N_\alpha}\sum_{j=1}^{N_\alpha}\frac{\partial^2 r_k\left(\boldsymbol{\alpha}^0\right)}{\partial\alpha_i\partial\alpha_j}cov\left(\alpha_i,\alpha_j\right). \tag{III.7}$$

The $N_r\times N_r$ covariance matrix of the computed responses, denoted here as $\boldsymbol{C}_{rc}$, with elements $\left(\boldsymbol{C}^{rc}\right)_{ij}$ defined as

$$\left(\boldsymbol{C}^{rc}\right)_{ij}\equiv\left\langle\left[r_i-E\left(r_i\right)\right]\left[r_j-E\left(r_j\right)\right]\right\rangle;\ \ i,j=1,\ldots,N_r; \tag{III.8}$$

can obtained from Eqs. (III.2) and (III.7) by recalling the definitions

$$\mu_n\left(\alpha_i\right)\equiv\left\langle\left(\alpha_i-\alpha_i^0\right)^n\right\rangle,\ \ n=3,4, \tag{III.9}$$

and neglecting parameter cross-correlations of order higher than covariances. Carrying out the respective algebra leads to the following expressions for the elements $\left(\boldsymbol{C}^{rc}\right)_{ij}$:

$$\begin{aligned} cov\left(r_k,r_\ell\right) \equiv \left\langle \left[r_k - E\left(r_k\right)\right]\left[r_\ell - E\left(r_\ell\right)\right]\right\rangle &= \sum_{i=1}^{N_\alpha}\sum_{j=1}^{N_\alpha}\left(\frac{\partial r_k}{\partial \alpha_i}\frac{\partial r_\ell}{\partial \alpha_j}\right) cov\left(\alpha_i,\alpha_j\right) \\ &+\frac{1}{2}\sum_{i=1}^{N_\alpha}\left(\frac{\partial r_k}{\partial \alpha_i}\frac{\partial^2 r_\ell}{\partial \alpha_i^2}+\frac{\partial r_\ell}{\partial \alpha_i}\frac{\partial^2 r_k}{\partial \alpha_i^2}\right)\mu_3\left(\alpha_i\right)+\frac{1}{4}\sum_{i=1}^{N_\alpha}\left(\frac{\partial^2 r_k}{\partial \alpha_i^2}\frac{\partial^2 r_\ell}{\partial \alpha_i^2}\right)\mu_4\left(\alpha_i\right) \\ &-\frac{1}{4}\sum_{i=1}^{N_\alpha}\sum_{j=1}^{N_\alpha}\sum_{\mu=1}^{N_\alpha}\sum_{\nu=1}^{N_\alpha}\left(\frac{\partial^2 r_k}{\partial \alpha_i \partial \alpha_j}\right) cov\left(\alpha_i,\alpha_j\right)\left(\frac{\partial^2 r_\ell}{\partial \alpha_\mu \partial \alpha_\nu}\right) cov\left(\alpha_\mu,\alpha_\nu\right); \end{aligned} \tag{III.10}$$

In particular, Eq. (III-10) indicates that the variance, $var\left(r_k\right)$, of a response r_k has the expression

$$\begin{aligned} var\left(r_k\right) \equiv \left\langle \left[r_k - E\left(r_k\right)\right]^2\right\rangle &= \sum_{i=1}^{N_\alpha}\sum_{j=1}^{N_\alpha}\left(\frac{\partial r_k}{\partial \alpha_i}\frac{\partial r_k}{\partial \alpha_j}\right) cov\left(\alpha_i,\alpha_j\right)+\sum_{i=1}^{N_\alpha}\left(\frac{\partial r_k}{\partial \alpha_i}\frac{\partial^2 r_k}{\partial \alpha_i^2}\right)\mu_3\left(\alpha_i\right) \\ &+\frac{1}{4}\sum_{i=1}^{N_\alpha}\left(\frac{\partial^2 r_k}{\partial \alpha_i^2}\right)^2\mu_4\left(\alpha_i\right)-\frac{1}{4}\left[\sum_{i=1}^{N_\alpha}\sum_{j=1}^{N_\alpha}\left(\frac{\partial^2 r_k}{\partial \alpha_i \partial \alpha_j}\right) cov\left(\alpha_i,\alpha_j\right)\right]^2. \end{aligned} \tag{III.11}$$

The third- and fourth-order moments $\mu_3\left(r_k\right)$ and $\mu_4\left(r_k\right)$ can also be obtained from Eqs. (III.2) and (III.7). Neglecting parameter cross-correlations of order higher than covariances leads to the following expressions:

$$\begin{aligned} \mu_3\left(r_k\right) &\equiv \left\langle \left[r_k - E\left(r_k\right)\right]^3\right\rangle \\ &= \frac{1}{2}\sum_{i=1}^{N_\alpha}\left(\frac{\partial^2 r_k}{\partial \alpha_i^2}\right)\mu_4\left(\alpha_i\right)\left[3\left(\frac{\partial r_k}{\partial \alpha_i}\right)^2-\frac{3}{4}\left(\frac{\partial^2 r_k}{\partial \alpha_i^2}\right)\sum_{\mu=1}^{N_\alpha}\sum_{\nu=1}^{N_\alpha}\left(\frac{\partial^2 r_k}{\partial \alpha_\mu \partial \alpha_\nu}\right) cov\left(\alpha_\mu,\alpha_\nu\right)\right] \\ &+\sum_{i=1}^{N_\alpha}\left(\frac{\partial r_k}{\partial \alpha_i}\right)\mu_3\left(\alpha_i\right)\left[\left(\frac{\partial r_k}{\partial \alpha_i}\right)^2-\frac{3}{2}\frac{\partial^2 r_k}{\partial \alpha_i^2}\sum_{\mu=1}^{N_\alpha}\sum_{\nu=1}^{N_\alpha}\left(\frac{\partial^2 r_k}{\partial \alpha_\mu \partial \alpha_\nu}\right) cov\left(\alpha_\mu,\alpha_\nu\right)\right] \\ &-\frac{3}{2}\left[\sum_{i=1}^{N_\alpha}\sum_{j=1}^{N_\alpha}\left(\frac{\partial r_k}{\partial \alpha_i}\frac{\partial r_k}{\partial \alpha_j}\right) cov\left(\alpha_i,\alpha_j\right)\right]\left[\sum_{\mu=1}^{N_\alpha}\sum_{\nu=1}^{N_\alpha}\left(\frac{\partial^2 r_k}{\partial \alpha_\mu \partial \alpha_\nu}\right) cov\left(\alpha_\mu,\alpha_\nu\right)\right] \\ &+\frac{1}{4}\left[\sum_{\mu=1}^{N_\alpha}\sum_{\nu=1}^{N_\alpha}\left(\frac{\partial^2 r_k}{\partial \alpha_\mu \partial \alpha_\nu}\right) cov\left(\alpha_\mu,\alpha_\nu\right)\right]^3; \end{aligned} \tag{III.12}$$

and

$$
\begin{aligned}
\mu_4(r_k) &\equiv \left\langle \left[r_k - E(r_k) \right]^4 \right\rangle \\
&= \sum_{i=1}^{N_\alpha} \mu_4(\alpha_i) \left\{ \left(\frac{\partial r_k}{\partial \alpha_i} \right)^4 + \frac{3}{8} \left(\frac{\partial^2 r_k}{\partial \alpha_i^2} \right)^2 \left[\sum_{\mu=1}^{N_\alpha} \sum_{\nu=1}^{N_\alpha} \left(\frac{\partial^2 r_k}{\partial \alpha_\mu \partial \alpha_\nu} \right) cov(\alpha_\mu, \alpha_\nu) \right]^2 \right. \\
&\quad \left. -3 \left(\frac{\partial r_k}{\partial \alpha_i} \right)^2 \left(\frac{\partial^2 r_k}{\partial \alpha_i^2} \right) \left[\sum_{\mu=1}^{N_\alpha} \sum_{\nu=1}^{N_\alpha} \left(\frac{\partial^2 r_k}{\partial \alpha_\mu \partial \alpha_\nu} \right) cov(\alpha_\mu, \alpha_\nu) \right] \right\} \\
&\quad + \sum_{i=1}^{N_\alpha} \mu_3(\alpha_i) \left(\frac{\partial r_k}{\partial \alpha_i} \right) \left[\sum_{\mu=1}^{N_\alpha} \sum_{\nu=1}^{N_\alpha} \left(\frac{\partial^2 r_k}{\partial \alpha_\mu \partial \alpha_\nu} \right) cov(\alpha_\mu, \alpha_\nu) \right] \times \\
&\quad \times \left\{ \frac{3}{2} \left(\frac{\partial^2 r_k}{\partial \alpha_i^2} \right) \left[\sum_{\mu=1}^{N_\alpha} \sum_{\nu=1}^{N_\alpha} \left(\frac{\partial^2 r_k}{\partial \alpha_\mu \partial \alpha_\nu} \right) cov(\alpha_\mu, \alpha_\nu) \right] - 2 \left(\frac{\partial r_k}{\partial \alpha_i} \right)^2 \right\} \\
&\quad - \frac{3}{16} \left[\sum_{\mu=1}^{N_\alpha} \sum_{\nu=1}^{N_\alpha} \left(\frac{\partial^2 r_k}{\partial \alpha_\mu \partial \alpha_\nu} \right) cov(\alpha_\mu, \alpha_\nu) \right]^4
\end{aligned}
\tag{III.13}
$$

III.B. An Efficient New Procedure for Computing Second-Order Response Derivatives and Uncertainties

Note that all of the derivatives appearing in the above expressions are evaluated at the nominal parameter values $\boldsymbol{\alpha}^0$. The quantity

$$
q_k(\rho_{ij}) \equiv \sum_{i=1}^{N_\alpha} \sum_{j=1}^{N_\alpha} \frac{\partial^2 r_k(\boldsymbol{\alpha}^0)}{\partial \alpha_i \partial \alpha_j} cov(\alpha_i, \alpha_j) = \sum_{i=1}^{N_\alpha} \sum_{j=1}^{N_\alpha} \frac{\partial^2 r_k(\boldsymbol{\alpha}^0)}{\partial \alpha_i \partial \alpha_j} \rho_{ij} \sigma_i \sigma_j , \tag{III.14}
$$

where ρ_{ij} denotes the correlation between parameters α_i and α_j, while σ_i and σ_j denote the standard deviations of the respective parameters, appears repeatedly in the expressions of $E(r_k)$, $cov(r_k, r_\ell)$, $var(r_k)$, $\mu_3(r_k)$ and $\mu_4(r_k)$. In general, the computation the mixed second-order response-derivatives $\partial^2 r_k / \partial \alpha_i \partial \alpha_j$ would require $O(N_\alpha)^2$ *large-scale computations using*

the original (forward) model for every response $r_k\left(\boldsymbol{\alpha}^0\right)$. In the special case when the parameters $\boldsymbol{\alpha}$ are fully correlated (i.e., all $\rho_{ij}=1$), however, the quantity $q_k\left(\rho_{ij}=1\right)$ can be computed very efficiently by following the following novel procedure. by considering the (column) vector of standard deviations

$$\boldsymbol{\sigma} \equiv \left(\sigma_1,\sigma_2,\ldots,\sigma_{N_\alpha}\right), \tag{III.15}$$

and by noting that the Hessian-vector product $\nabla^2 \boldsymbol{r}_k\left(\boldsymbol{\alpha}^0\right)\boldsymbol{\sigma}$ can be quantified most efficiently by using two computations of the gradients $\nabla_\alpha\left(\boldsymbol{r}_k\right)$, as follows:

$$\nabla^2 \boldsymbol{r}_k\left(\boldsymbol{\alpha}^0\right)\boldsymbol{\sigma} \cong b^{-1}\left\{\nabla_\alpha\left[\boldsymbol{r}_k\left(\boldsymbol{\alpha}^0+b\boldsymbol{\sigma}\right)\right]-\nabla_\alpha\left[\boldsymbol{r}_k\left(\boldsymbol{\alpha}^0\right)\right]\right\} \equiv \boldsymbol{y}_k\left(\boldsymbol{\alpha}^0\right),\ k=1,...,N_r. \tag{III.16}$$

where *b* is a small scalar quantity. As already mentioned, the gradients $\nabla_\alpha\left(\boldsymbol{r}_k\right)$ can be computed most efficiently using the *ASAP* (one adjoint model computation per response, yields all of the gradients $\nabla_\alpha\left(\boldsymbol{r}_k\right)$ with respect to the parameters $\boldsymbol{\alpha}$). Thus, the vector $\boldsymbol{y}_k\left(\boldsymbol{\alpha}^0\right)$ defined above can be obtained using two adjoint-model computations instead of $\left(N_\alpha\right)^2$ large-scale computations using the original (forward). Once $\boldsymbol{y}_k\left(\boldsymbol{\alpha}^0\right)$ has been obtained, the quantity $q_k\left(\rho_{ij}=1\right)$ can be obtained by an additional vector scalar-product computation of the form

$$q_k\left(\rho_{ij}=1\right)=\boldsymbol{\sigma}^\dagger \boldsymbol{y}_k\left(\boldsymbol{\alpha}^0\right). \tag{III.17}$$

In practice, however, the model parameters $\boldsymbol{\alpha}$ are extremely unlikely to be fully correlated. More likely, they are partially (positively or negatively) correlated or uncorrelated. In such

cases, it is still possible to reduce the number of computations required for obtaining the quantity $q_k\left(\rho_{ij}\right)$, from $O\left(N_\alpha\right)^2$ to at most $n_k \le \left(N_\alpha + 1\right)$ operations for each response $r_k\left(\boldsymbol{\alpha}^0\right)$, where n_k is a number to be determined as discussed below, by using Hessian-vector products of the same form as shown in Eq. (III.16).

For each response $r_k\left(\boldsymbol{\alpha}^0\right)$, $k = 1,...,N_r$, the new proposed procedure is as follows:

(i) Note from Eq. (III.11) that the main contribution to the variance $var\left(r_k\right)$ of a response $r_k\left(\boldsymbol{\alpha}^0\right)$ is provided by the quantity

$$\sum_{i=1}^{N_\alpha}\sum_{j=1}^{N_\alpha}\left(\frac{\partial r_k}{\partial \alpha_i}\frac{\partial r_k}{\partial \alpha_j}\right)cov\left(\alpha_i,\alpha_j\right) = \sum_{i=1}^{N_\alpha}\left(\frac{\partial r_k}{\partial \alpha_i}\right)^2\sigma_i^2 + \sum_{i=1}^{N_\alpha}\sum_{j\ne i}^{N_\alpha}\left(\frac{\partial r_k}{\partial \alpha_i}\frac{\partial r_k}{\partial \alpha_j}\right)\rho_{ij}\sigma_i\sigma_j \ . \quad \text{(III.18)}$$

(ii) Since a value of $\sigma_i^2 = 0$ would imply that the respective parameter is perfectly known, it is clear that all variances are positive, i.e., $\sigma_i^2 > 0$. Hence, each of the terms in the first sum on the rights side of Eq. (III.18) is positive, unless some response sensitivity happens to vanish, e.g., $\partial r_k / \partial \alpha_i = 0$. However, even when $\partial r_k / \partial \alpha_i = 0$ for some parameter α_i, the other sensitivities are non-zero (i.e., $\partial r_k / \partial \alpha_{j\ne i} \ne 0$), unless the response happens to be computed at a critical point $\boldsymbol{\alpha}^{crit}$. In such a highly unusual case, Eqs. (III.10) through (III.13) indicate that only terms containing second (and higher) order response derivatives would contribute to the response covariances, skewness and kurtosis. In this (highly unusual) case, the number n_k --to be used in the sequel-- would be set

to $n_k = N_\alpha$ since all of the second-order response derivatives would need to computed in order to quantify the response moments.

(iii) On the other hand, in the highly likely situation when $\boldsymbol{\alpha}^0 \neq \boldsymbol{\alpha}^{crit}$, not all of the sensitivities $\partial r_k / \partial \alpha_i$ would vanish. For the non-vanishing sensitivities, rank the relative sensitivities $t_{ki}^{r\alpha}\left(\boldsymbol{\alpha}^0\right) \equiv \left[\partial r_k\left(\boldsymbol{\alpha}^0\right)/\partial \alpha_i\right]\left[\alpha_i^0 / r_k\left(\boldsymbol{\alpha}^0\right)\right]$ in decreasing order of absolute magnitudes $\left|t_{ki}^{r\alpha}\left(\boldsymbol{\alpha}^0\right)\right|$. This ranking will also indicate the most important parameters α_i in contributing to the uncertainties in the response $r_k\left(\boldsymbol{\alpha}^0\right)$.

(iv) Compute the quantities $c_{ii}^k \equiv \left\{t_{ki}^{r\alpha}\left(\boldsymbol{\alpha}^0\right)\left[\alpha_i^0 / r_k\left(\boldsymbol{\alpha}^0\right)\right]\sigma_i\right\}^2$ and rank them in descending order of their magnitudes. As Eq.(III.18) indicates, c_{ii}^k represents the contribution to $var\left(r_k\right)$ stemming solely from uncertainties in parameter α_i.

(v) Based on the rankings of the partial variances c_{ii}^k, rank the standard deviations σ_i in order of importance in contribution to $\mathrm{var}\left(r_k\right)$, thus constructing the vector sequence $\left(\sigma_1, \sigma_2, \ldots, \sigma_{n_k}\right)$, with $n_k \leq \left(N_\alpha + 1\right)$, where σ_{n_k} denotes a user-defined cut-off value corresponding to a negligible (from the user's point of view) contribution to $var\left(r_k\right)$.

(vi) For each of selected variance in the sequence $\left(\sigma_1, \sigma_2, \ldots, \sigma_{n_k}\right)$, construct the n_k-dimensional column vectors $\boldsymbol{\sigma}_1 \equiv \left(\sigma_1, 0, \ldots, 0\right)$, …, $\boldsymbol{\sigma}_i \equiv \left(0, \ldots, \sigma_i, \ldots, 0\right)$, … $\boldsymbol{\sigma}_{n_k} \equiv \left(0, \ldots, 0, \ldots, \sigma_{n_k}\right)$, and use each of these, in turn, *in conjunction with one*

adjoint-model computation, to obtain the n_k -dimensional vector $\boldsymbol{t}^{ki} \equiv \left(t_1^{ki},\ldots,t_{n_k}^{ki}\right)^{\dagger}$ defined as

$$\begin{aligned}\boldsymbol{t}^{ki} \equiv \left(t_1^{ki},\ldots,t_{n_\alpha}^{ki}\right)^{\dagger} &\equiv \left(\frac{\partial^2 r_k\left(\boldsymbol{\alpha}^0\right)}{\partial\alpha_1\partial\alpha_i}\sigma_i,\ldots,\frac{\partial^2 r_k\left(\boldsymbol{\alpha}^0\right)}{\partial\alpha_{n_\alpha}\partial\alpha_i}\sigma_i\right)^{\dagger} \\ &= \nabla^2 \boldsymbol{r}_k\left(\boldsymbol{\alpha}^0\right)\boldsymbol{\sigma}_i \cong b^{-1}\left\{\nabla_\alpha\left[\boldsymbol{r}_k\left(\boldsymbol{\alpha}^0 + b\boldsymbol{\sigma}_i\right)\right] - \nabla_\alpha\left[\boldsymbol{r}_k\left(\boldsymbol{\alpha}^0\right)\right]\right\};\ i = 1,\ldots,n_\alpha;\end{aligned} \tag{III.19}$$

(vii) For each $i = 1,\ldots,n_k$, multiply the first component, t_1^{ki} , of the vector $\boldsymbol{t}^{ki} \equiv \left(t_1^{ki},\ldots,t_{n_k}^{ki}\right)^{\dagger}$ obtained in Eq. (III.19) by the correlation coefficient ρ_{i1}, the second component of this vector by the correlation coefficient ρ_{i2}, and so on, until the last component $t_{n_k}^{ki}$,which is to be multiplied by ρ_{in_k} , in order to construct the sequence of vectors

$$\left(t_1^{ki}\rho_{i1},\ldots,t_{n_k}^{ki}\rho_{in_k}\right)^{\dagger} = \left(\frac{\partial^2 r_k\left(\boldsymbol{\alpha}^0\right)}{\partial\alpha_1\partial\alpha_i}\sigma_i\rho_{i1},\ldots,\frac{\partial^2 r_k\left(\boldsymbol{\alpha}^0\right)}{\partial\alpha_{n_k}\partial\alpha_i}\sigma_i\rho_{in_k}\right)^{\dagger};\ i = 1,\ldots,n_k; \tag{III.20}$$

(viii) Sum up the corresponding components of the vectors in Eq. (III.20) to construct the column vector

$$\left(\sum_{i=1}^{n_k} t_1^{ki}\rho_{i1},\ldots,\sum_{i=1}^{n_k} t_{n_k}^{ki}\rho_{in_k}\right)^{\dagger} = \left(\sum_{i=1}^{n_k}\frac{\partial^2 r_k\left(\boldsymbol{\alpha}^0\right)}{\partial\alpha_1\partial\alpha_i}\sigma_i\rho_{i1},\ldots,\sum_{i=1}^{n_k}\frac{\partial^2 r_k\left(\boldsymbol{\alpha}^0\right)}{\partial\alpha_{n_k}\partial\alpha_i}\sigma_i\rho_{in_k}\right)^{\dagger}; \tag{III.21}$$

(ix) Form the scalar product of the above vector with the *row-vector* $\left(\sigma_1,\sigma_2,\ldots,\sigma_{n_k}\right)$ to obtain, finally, the sum of the retained first-order contributions to $\mathrm{var}\left(r_k\right)$, namely:

$$\left(\sigma_1,\sigma_2,\ldots,\sigma_{n_k}\right)\left(\sum_{i=1}^{n_k} t_1^{ki}\rho_{i1},\ldots,\sum_{i=1}^{n_\alpha} t_{n_k}^{ki}\rho_{in_k}\right)^\dagger = \sum_{i=1}^{n_k}\sum_{j=1}^{n_k}\frac{\partial^2 r_k\left(\boldsymbol{\alpha}^0\right)}{\partial\alpha_i\partial\alpha_j}\rho_{ij}\sigma_i\sigma_j\ ; \qquad \text{(III.22)}$$

Thus, the sum $\sum_{i=1}^{n_k}\sum_{j=1}^{n_k}\frac{\partial^2 r_k\left(\boldsymbol{\alpha}^0\right)}{\partial\alpha_i\partial\alpha_j}\rho_{ij}\sigma_i\sigma_j$, which comprises the major first-order contributions to the variance $var\left(r_k\right)$ can be computed most efficiently by needing only (large-scale) $n_k+1\le N_\alpha$ adjoint model computations, as opposed to at least $O\left(n_k\right)^2$, as would be needed to compute the second-order derivatives of r_k via forward large-scale model computations.

Note that the second-order derivatives $\partial^2 r_k/\partial\alpha_i^2$ of the response r_k can be computed by dividing each of the components of $\boldsymbol{t}^{ki}\equiv\left(t_1^{ki},\ldots,t_{n_k}^{ki}\right)^\dagger$ through σ_i, as follows:

$$\left(\frac{t_1^{ki}}{\sigma_i},\ldots,\frac{t_{n_k}^{ki}}{\sigma_i}\right)^\dagger = \left(\frac{\partial^2 r_k\left(\boldsymbol{\alpha}^0\right)}{\partial\alpha_1\partial\alpha_i},\ldots,\frac{\partial^2 r_k\left(\boldsymbol{\alpha}^0\right)}{\partial\alpha_{n_k}\partial\alpha_i}\right)^\dagger\ ;\ i=1,\ldots,n_k. \qquad \text{(III.23)}$$

Recall that the third-moment (skewness) and fourth-moment (kurtosis) of the standard Gaussian-distribution have values $\mu_3\left(Gaussian\right)=0$ and $\mu_4\left(Gaussian\right)=3$, respectively. Hence, comparing these moments to the third- and fourth-order moments $\mu_3\left(r_k\right)$ and $\mu_4\left(r_k\right)$ computed in Eqs. (III.12) and (III.13), respectively, provides a quantitative indicator of the non-Gaussian characteristics of the possible distribution of the response r_k.

IV. QUANTITATIVE MODEL VALIDATION METRICS: C_k – *METRICS* for k=2,3,4

Model validation is customarily defined as "*the process of confirming that the predictions of a computer code adequately represent measured physical phenomena*." This definition clearly indicates that the difference $\left[\boldsymbol{r}^m - \boldsymbol{r}^c\left(\boldsymbol{\alpha}^0\right)\right]$ between measured responses, $\boldsymbol{r}^m$, and the corresponding nominally computed responses, $\boldsymbol{r}^c\left(\boldsymbol{\alpha}^0\right)$, must play a fundamental role in model validation, a fact that has been recognized by several authors [ ].

IV.A. Model Validation Covariance Metric: $\boldsymbol{C}_2$

IV.A.1. Computed/Measured Responses Validation Metric $\boldsymbol{M}^{rr}\left(\boldsymbol{\alpha}^0\right)$

The difference $\left[\boldsymbol{r}^m - \boldsymbol{r}^c\left(\boldsymbol{\alpha}^0\right)\right]$ between the measured and the corresponding computed responses can be considered to be a multivariate vector quantity. It therefore follows that the covariance matrix of this multivariate vector quantity is, by definition, the $\left(N_r \times N_r\right)$-dimensional covariance matrix $\boldsymbol{M}^{rr}\left(\boldsymbol{\alpha}^0\right)$:

$$\boldsymbol{M}^{rr}\left(\boldsymbol{\alpha}^0\right) \equiv \left\langle \left[\boldsymbol{r}^m - \boldsymbol{r}^c\left(\boldsymbol{\alpha}^0\right)\right]\left[\boldsymbol{r}^m - \boldsymbol{r}^c\left(\boldsymbol{\alpha}^0\right)\right]^\dagger \right\rangle, \tag{IV.1}$$

with components

$$\left[\boldsymbol{M}^{rr}\left(\boldsymbol{\alpha}^0\right)\right]_{ij} \equiv \left\langle \left[r_i^m - r_i^c\left(\boldsymbol{\alpha}^0\right)\right]\left[r_j^m - r_j^c\left(\boldsymbol{\alpha}^0\right)\right] \right\rangle; \;\; i,j = 1,\ldots,N_r. \tag{IV.2}$$

Consistent with the assumption that full triple and quadruple parameter correlations are practically unavailable, except possibly for the skewness $\mu_3(\alpha_i) \equiv \left\langle \left(\alpha_i - \alpha_i^0\right)^3 \right\rangle$ and kurtosis $\mu_4(\alpha_i) \equiv \left\langle \left(\alpha_i - \alpha_i^0\right)^4 \right\rangle$ of single-variate parameters, triple correlations between responses and parameters of the form $\left\langle \left(\alpha_i - \alpha_i^0\right)\left(\alpha_j - \alpha_j^0\right)\left(r_k - r_k^m\right) \right\rangle$ would also be unavailable in practice and will therefore not be taken into account in this work. Consistent with these considerations, therefore, the expression of $\boldsymbol{M}^{rr}\left(\boldsymbol{\alpha}^0\right)$ can be determined from its definition in Eqs. (III.1) to obtain

$$\boldsymbol{M}^{rr}\left(\boldsymbol{\alpha}^0\right) = \boldsymbol{D}_2^{rr}\left(\boldsymbol{\alpha}^0\right) + \boldsymbol{D}_3^{rr}\left(\boldsymbol{\alpha}^0\right) + \boldsymbol{D}_4^{rr}\left(\boldsymbol{\alpha}^0\right), \tag{IV.3}$$

where

$$\boldsymbol{D}_2^{rr}\left(\boldsymbol{\alpha}^0\right) \equiv \boldsymbol{C}^{rr} + \boldsymbol{C}^{rc}\left(\boldsymbol{\alpha}^0\right) - \boldsymbol{S}^{r\alpha}\left(\boldsymbol{\alpha}^0\right)\boldsymbol{C}^{\alpha r} - \left[\boldsymbol{S}^{r\alpha}\left(\boldsymbol{\alpha}^0\right)\boldsymbol{C}^{\alpha r}\right]^{\dagger}, \tag{IV.4}$$

$$\boldsymbol{C}^{rc}\left(\boldsymbol{\alpha}^0\right) \equiv \boldsymbol{S}^{r\alpha}\left(\boldsymbol{\alpha}^0\right)\boldsymbol{C}^{\alpha\alpha}\left[\boldsymbol{S}^{r\alpha}\left(\boldsymbol{\alpha}^0\right)\right]^{\dagger}, \tag{IV.5}$$

$$\boldsymbol{D}_3^{rr}\left(\boldsymbol{\alpha}^0\right) \equiv \left[\left(D_3^{rr}\right)_{ij}\right]_{N_r \times N_r} \;;\; \left(D_3^{rr}\right)_{ij} \equiv \frac{1}{2}\sum_{m=1}^{N_\alpha}\left(\frac{\partial r_i}{\partial \alpha_m}\frac{\partial^2 r_j}{\partial \alpha_m^2} + \frac{\partial r_j}{\partial \alpha_m}\frac{\partial^2 r_i}{\partial \alpha_m^2}\right)\mu_3(\alpha_m), \tag{IV.6}$$

$$\boldsymbol{D}_4^{rr}\left(\boldsymbol{\alpha}^0\right) \equiv \left[\left(D_4^{rr}\right)_{ij}\right]_{N_r \times N_r} \;;\; \left(D_4^{rr}\right)_{ij} \equiv \frac{1}{4}\sum_{m=1}^{N_\alpha}\left(\frac{\partial^2 r_i}{\partial \alpha_m^2}\frac{\partial^2 r_j}{\partial \alpha_m^2}\right)\mu_4(\alpha_m). \tag{IV.7}$$

It can be readily verified that each of the $N_r \times N_r$-dimensional matrices $\boldsymbol{D}_i^{rr}\left(\boldsymbol{\alpha}^0\right); i = 2,3,4,$ is symmetric, which of course confirms that $\boldsymbol{M}^{rr}\left(\boldsymbol{\alpha}^0\right)$ is also a symmetric matrix of dimensions $N_r \times N_r$. **TO BE CONTINUED**

IV.A.2. Consistency Indicator of Computed and Measured Responses in the $\boldsymbol{C}_2$-Metric

IV.B. Model Validation Covariance Metric: $\boldsymbol{C}_3$

IV.C. Model Validation Covariance Metric: $\boldsymbol{C}_4$

V. CONCLUDING REMARKS

This work has presented has presented quantitative validation metrics for model validation. This work is part of ongoing research which will be published in peer reviewed journals; until so published, however, this work is to be referred to as:

D.G. Cacuci, *High-Order Quantitative Model Validation Metrics Integrating Experimental and Computational Data for Large-Scale Time-Independent Nonlinear Systems*, DOE/CASL Report #489: L3: VUQ.VVDA.P4.05 (VUQ.P4.02), December 31, 2011.

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