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# MULTI-PRED: A Software Module for Predictive Modeling of Coupled Multi-Physics Systems

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**Abstract** — *The software module MULTI-PRED implements the methodology for predictive modeling of coupled multi-physics systems (PM-CMPS) formulated by Cacuci [Ann. Nucl. Energy, Vol. 70, p, 266 (2014)]. This methodology fully takes into account the coupling terms between the systems but requires only the computational resources that would be needed to perform predictive modeling on each system separately. The PM-CMPS methodology uses the maximum entropy principle to construct an optimal approximation of the unknown a priori distribution based on a priori known mean values and uncertainties characterizing the experimental and computational parameters and results of interest responses called for the multi-physics models under consideration. This maximum entropy a priori distribution is combined, using Bayes' theorem, with the likelihood provided by the multi-physics simulation models to obtain a formal posterior distribution. Subsequently, the posterior distribution thus obtained is evaluated using the saddle-point method to obtain analytical expressions for the optimally predicted values for the multi-physics model parameters and responses along with corresponding reduced uncertainties. Noteworthy, the predictive modeling methodology for the coupled systems is constructed such that the systems can be considered sequentially rather than simultaneously, while preserving exactly the same results as if the systems were treated simultaneously. Consequently, very large coupled systems, which could perhaps exceed available computational resources if treated simultaneously, can be treated with the PM-CMPS methodology presented in this work sequentially and without any loss of generality or information, requiring just the resources that would be needed if the systems were treated sequentially.*

*The PM-CMPS methodology can be applied to reduce uncertainties in both forward and inverse problems. Three demonstration problems are provided to illustrate the application of the PM-CMPS methodology. The first problem presents the application of the PM-CMPS methodology to a simple particle diffusion problem which admits a closed-form analytical solution which facilitates a rapid understanding of this methodology and its predicted results. The second demonstration problem presents the application of the PM-CMPS methodology to the problem of inverse prediction, from detector responses in the presence of counting uncertainties, of the thickness of a homogeneous slab of material containing uniformly distributed gamma-emitting sources for optically thin and thick slabs. This problem highlights the essential role played by the relative uncertainties (or, conversely, accuracies) of measured and computed responses. The third demonstration problem presents the application of the PM-CMPS methodology to the F-Area cooling towers at the Savannah River National Lab. This problem demonstrates that the PM-CMPS methodology reduces the predicted response uncertainties not only at locations where measurements are available, but also at locations where measurements are not available.*

*MULTI-PRED is written in Fortran and runs on Linux and Windows systems. A C++ version will also become available.*

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**Keywords** — *Predictive modeling, data assimilation, model calibration, reduced predicted uncertainties, optimally predicted best-estimate values for mode parameters and responses.*

**Note** — *Some figures may be in color only in the electronic version.*

## I. INTRODUCTION

The results of measurements inevitably reflect the influence of experimental errors, imperfect instruments, and imperfectly known calibration standards. Around any reported experimental value, therefore, there always exists a range of values that may also be plausibly representative of the true but unknown value of the measured quantity. On the other hand, computations are also imperfect, since they are afflicted by errors stemming from numerical procedures, uncertain model parameters, boundary and initial conditions, and/or imperfectly known physical processes or problem geometry. Therefore, nominal values for experimentally measured or computed quantities are insufficient, by themselves, for applications. The quantitative uncertainties accompanying the measurements and computations are also needed, along with the respective nominal values. Extracting best-estimate values for model parameters and predicted results (responses), together with best-estimate uncertainties for these parameters and responses, requires the combination of experimental and computational data and their uncertainties. This combination process often requires reasoning from incomplete, error-afflicted, and occasionally, discrepant information.

The discrepancies between experimental and computational results provide the basic motivation for performing quantitative model verification, validation, qualification, and predictive estimation. Loosely speaking, code verification means: “Are you solving the mathematical model correctly?” Code validation means: “Does the model represent reality?” Code qualification means certifying that a proposed simulation/design methodology/system satisfies all performance and safety specifications. Model validation addresses issues of (1) assessing model accuracy when several system response quantities have been measured and compared and (2) comparing system response quantities from multiple realizations of the experiment with computational results that are characterized by probability distributions. Model validation and qualification require selected benchmarking, including sensitivity and uncertainty analyses.

Predictive modeling commences with the identification and characterization of uncertainties from all steps in the sequence of modeling and simulation processes that lead to a computational model prediction. This includes (1) data error or uncertainty (input data such as cross sections; model

parameters such as reaction-rate coefficients, initial conditions, and boundary conditions; and forcing functions such as external loading), (2) numerical discretization error, and (3) uncertainty in (e.g., lack of knowledge of) the processes being modeled. The result of the predictive modeling analysis is a probabilistic description of possible future outcomes based on all recognized errors and uncertainties.

Predictive modeling combines/assimilates computational and experimental information using response sensitivities to perform model calibration, model extrapolation, and estimation of the validation domain. Model calibration addresses the integration of experimental data for the purpose of updating the data of the computer model. Important components include the estimation of discrepancies in the data and of the biases between model predictions and experimental data. The state-of-the-art of model calibration is fairly well developed, but current methods are still hampered in practice by the significant computational effort required. Reducing the computational effort is paramount, and methods based on adjoint models show great promise in this regard. Model extrapolation addresses the prediction 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. Extrapolation of models and the resulting increase of uncertainty are poorly understood, particularly the estimation of uncertainty that results from nonlinear coupling of two or more physical phenomena that were not coupled in the existing validation database. The quantification of the validation domain underlying the models of interest requires estimation of contours of constant uncertainty in the high-dimensional space that characterizes the application of interest. In practice, this involves the identification of areas where the predictive estimation of uncertainty meets specified requirements for the performance, reliability, or safety of the system of interest.

The software module MULTI-PRED implements the methodology for predictive modeling of coupled multi-physics systems (PM-CMPS) formulated by Cacuci.<sup>1</sup> The PM-CMPS methodology generalizes the work of Cacuci and Ionescu-Bujor<sup>2,3</sup> on predictive modeling of a single time-dependent multi-physics system, and also generalizes and significantly extends the data adjustment methods customarily used in nuclear engineering, as well as those underlying the so-called

4D-VAR data assimilation procedures in the geophysical sciences.<sup>4,5</sup> The PM-CMPS provides a quantitative indicator, constructed from sensitivity and covariance matrices, for determining the consistency (agreement or disagreement) among the a priori computational and experimental data (parameters and responses). This consistency indicator measures, in the corresponding metric, the deviations between the experimental and nominally computed responses. Note that this consistency indicator can be evaluated directly from the originally given data (i.e., given parameters and responses, together with their original uncertainties) once the response sensitivities have been computed. Preferably, the PM-CMPS utilizes the exactly and efficiently computed response sensitivities using the adjoint sensitivity analysis methodology as generally formulated by Cacuci.<sup>6-11</sup> When the numerical value of this consistency indicator is close to unity (per degrees of freedom), the respective data are considered to be consistent within the respective error norms (usually under quadratic loss). However, when the numerical value of this consistency indicator differs considerably from unity, which usually occurs when the distance between the mean values of two (sets of) measurements or two (sets of) computations of the same quantity are larger than the sum of the two accompanying standard deviations, the respective (measured or computed) data points are considered to be inconsistent or discrepant. This means that there is a nonzero probability that two nondiscrepant (i.e., belonging to the same distribution) measurements that are separated by more than  $2\sigma$  (thus giving the appearance of being discrepant) could actually occur in practice. Recall that for a Gaussian sampling distribution, the probability that two equally precise measurements would be separated by more than  $2\sigma$  is 15.7%. However, this probability is rather small; therefore, it is much more likely that apparently discrepant data actually indicate the presence of unrecognized errors. Methods for treating unrecognized errors have been developed by Cacuci and Ionescu-Bujor,<sup>12</sup> by applying the maximum entropy principle under quadratic loss to the discrepant data.

The PM-CMPS methodology is constructed such that the systems can be treated sequentially rather than simultaneously, while preserving exactly the same results as if the systems had been treated simultaneously. Consequently, very large coupled systems, which could perhaps exceed available computational resources if treated simultaneously, can be treated with the PM-CMPS methodology sequentially, without any loss of generality or information, requiring just the resources that would be needed as if the systems had been

treated separately. The PM-CMPS methodology has been successfully applied to reducing the predicted uncertainties in model parameters and responses in several forward and inverse problems.<sup>13-18</sup> The MULTI-PRED software module provides three illustrative problems: (1) a simple neutron diffusion problem,<sup>19</sup> (2) an inverse problem in particle transport,<sup>18</sup> and (3) a predictive modeling of the F-Area cooling towers at the Savannah River National Laboratory.<sup>16,17</sup> Sections II and III describe the quantities required as inputs to MULTI-PRED, along with the optimally predicted best-estimate values for the model responses and model parameters, with reduced predicted uncertainties, which are obtained as the outputs of MULTI-PRED.

## II. PM-CMPS: MATHEMATICAL FRAMEWORK

### II.A. MULTI-PRED Input: A Priori Information for Two Multi-Physics Models

Consider a multi-physics model, henceforth called model A comprising  $N_\alpha$  system (model) parameters  $\alpha_n$ . Model A is used to compute results, henceforth called responses, which can also be measured experimentally. Consider now a second physical system, henceforth called model B, comprising  $N_\beta$  system (model) parameters  $\beta_m$ , and which is also used to compute responses that can be measured experimentally. Model A and model B are considered to be coupled. In reactor analysis and design, for example, model A may comprise the neutron transport and depletion equations which are coupled to model B which computes the thermal-hydraulic conservation (mass, momentum, energy) equations.

Consider next that there are  $N_r$  experimentally measured responses  $r_i$  associated mostly, but not necessarily exclusively, with model A. Furthermore, consider also that there are  $N_q$  experimentally measured responses  $q_j$  associated mostly, but not necessarily exclusively, with model B. For example, measurement of reaction rates and power (or flux) distributions could be considered to be responses of type  $r_i$ , while measurements of flow rates and temperature distributions could be considered responses of type  $q_j$ . In the same spirit, cross sections can be considered to be model parameters of type  $\alpha_n$ , while heat transfer correlations can be considered model parameters of type  $\beta_m$ . Parameters modeling the geometry of the system (e.g., rod and assembly dimensions, core dimensions), for example, could be considered to belong to either type of model parameters (i.e., either  $\alpha_n$  or  $\beta_m$ ), since they affect both the neutron transport equation and the thermal-hydraulic conservation equations.

In practice, the values of the parameters  $\alpha_n$  and  $\beta_m$  are determined experimentally. Therefore, these parameters cannot be known exactly, but can be considered to behave stochastically, obeying some probability distribution function which is seldom known. Such stochastic quantities will be called variates in this work; thus, the parameters  $\alpha_n$  and  $\beta_m$  as well as the measured responses  $r_i$  and  $q_j$  are variates. To simplify the mathematical derivations to follow in this section, the model parameters  $\alpha_n$  will be considered to constitute the components of the (column) vector  $\boldsymbol{\alpha}$ , defined as

$$\boldsymbol{\alpha} \triangleq (\alpha_1, \dots, \alpha_{N_\alpha}), \quad (1)$$

while the model parameters  $\beta_m$  will be considered to constitute the components of the (column) vector  $\boldsymbol{\beta}$  defined as

$$\boldsymbol{\beta} \triangleq (\beta_1, \dots, \beta_{N_\beta}). \quad (2)$$

By convention, all of the vectors considered in this work (e.g.,  $\boldsymbol{\alpha}$  and  $\boldsymbol{\beta}$ ) are column vectors. A dagger  $\dagger$  will be used to denote transposition; thus, the quantities  $\boldsymbol{\alpha}^\dagger$  and  $\boldsymbol{\beta}^\dagger$  are row vectors. Similarly, the  $N_r$  experimentally measured responses  $r_i$  will be considered to be components of the column vector:

$$\mathbf{r} \triangleq (r_1, \dots, r_{N_r}), \quad (3)$$

while the  $N_q$  experimentally measured responses  $q_j$  will be considered to be components of the column vector:

$$\mathbf{q} \triangleq (q_1, \dots, q_{N_q}). \quad (4)$$

Most generally, the parameters  $\alpha_n$  and  $\beta_m$ , as well as the responses  $r_i$  and  $q_j$  can be considered to obey some a priori probability distribution function  $P(\boldsymbol{\alpha}, \boldsymbol{\beta}, \mathbf{r}, \mathbf{q})$ . For large-scale systems, as customarily encountered in practice, the probability distribution  $P(\boldsymbol{\alpha}, \boldsymbol{\beta}, \mathbf{r}, \mathbf{q})$  is unknown. The information usually available in practice comprises the mean values of the model parameters and responses together with the corresponding uncertainties (standard deviations and, occasionally, correlations) about the respective mean values. For notational simplicity, angular brackets  $\langle f \rangle$  will be used to denote the integral of the quantity  $f(\boldsymbol{\alpha}, \boldsymbol{\beta}, \mathbf{r}, \mathbf{q})$  over the joint probability distribution  $P(\boldsymbol{\alpha}, \boldsymbol{\beta}, \mathbf{r}, \mathbf{q})$ , i.e.,

$$\langle f \rangle \triangleq \int f(\boldsymbol{\alpha}, \boldsymbol{\beta}, \mathbf{r}, \mathbf{q}) P(\boldsymbol{\alpha}, \boldsymbol{\beta}, \mathbf{r}, \mathbf{q}) d\boldsymbol{\alpha} d\boldsymbol{\beta} d\mathbf{r} d\mathbf{q}. \quad (5)$$

Using the above convention, the mean values of the model parameters  $\alpha_n$  will be denoted using the superscript zero, i.e., as  $\alpha_n^0 \triangleq \langle \alpha_n \rangle$ ; these mean values are considered to constitute the components of the vector  $\boldsymbol{\alpha}^0$  defined as

$$\boldsymbol{\alpha}^0 \triangleq (\alpha_1^0, \dots, \alpha_{N_\alpha}^0). \quad (6)$$

Similarly, the mean values of the parameters  $\beta_n$  are considered to be known and will be denoted as  $\beta_n^0 \triangleq \langle \beta_n \rangle$ . These mean values are considered to be the components of the vector  $\boldsymbol{\beta}^0$  defined as

$$\boldsymbol{\beta}^0 \triangleq (\beta_1^0, \dots, \beta_{N_\beta}^0). \quad (7)$$

The parameters' second-order central moments, namely the standard deviations and correlations, are also considered to be known. For the parameters  $\alpha_n$ , the second-order central moments are the components of covariance matrices  $\mathbf{C}_{\alpha\alpha}^{(N_\alpha \times N_\alpha)}$  defined as

$$\begin{aligned} \mathbf{C}_{\alpha\alpha}^{(N_\alpha \times N_\alpha)} &\triangleq [\text{cov}(\alpha_i, \alpha_j)]_{N_\alpha \times N_\alpha} \\ &\triangleq \langle (\alpha_i - \alpha_i^0)(\alpha_j - \alpha_j^0) \rangle_{N_\alpha \times N_\alpha}; \quad (8) \\ i, j &= 1, \dots, N_\alpha, \end{aligned}$$

while the second-order central moments (i.e., the standard deviations and correlations) for the parameters  $\beta_m$  form covariance matrices  $\mathbf{C}_{\beta\beta}^{(N_\beta \times N_\beta)}$  defined as

$$\begin{aligned} \mathbf{C}_{\beta\beta}^{(N_\beta \times N_\beta)} &\triangleq [\text{cov}(\beta_i, \beta_j)]_{N_\beta \times N_\beta} \\ &\triangleq \langle (\beta_i - \beta_i^0)(\beta_j - \beta_j^0) \rangle_{N_\beta \times N_\beta}; \quad (9) \\ i, j &= 1, \dots, N_\beta. \end{aligned}$$

In general, the components of the vectors  $\boldsymbol{\alpha}$  and  $\boldsymbol{\beta}$  may be correlated. The correlations among the parameters  $\boldsymbol{\alpha}$  and  $\boldsymbol{\beta}$  are quantified by correlation matrices  $\mathbf{C}_{\alpha\beta}^{(N_\alpha \times N_\beta)}$  defined as

$$\begin{aligned} \mathbf{C}_{\alpha\beta}^{(N_\alpha \times N_\beta)} &\triangleq \langle (\boldsymbol{\alpha} - \boldsymbol{\alpha}^0)(\boldsymbol{\beta} - \boldsymbol{\beta}^0)^\dagger \rangle \\ &\triangleq \left[ \mathbf{C}_{\beta\alpha}^{(N_\beta \times N_\alpha)} \right]^\dagger. \quad (10) \end{aligned}$$

The experimentally measured responses are also considered to be characterized by known mean measured values and measured variances and covariances. Thus, for the  $N_r$  experimentally measured responses  $r_i$ , the mean measured values will be denoted as  $r_i^m$  and will be considered to constitute the components of the vector  $\mathbf{r}^m$  defined as

$$\mathbf{r}^m \triangleq (r_1^m, \dots, r_{N_r}^m), \quad r_i^m \triangleq \langle r_i \rangle, \quad (11)$$

$$i = 1, \dots, N_r,$$

while the corresponding measured covariance matrix, denoted as  $\mathbf{C}_{rr}^{(N_r \times N_r)}$ , is defined as

$$\mathbf{C}_{rr}^{(N_r \times N_r)} \triangleq \left\langle (r_i - r_i^m)(r_j - r_j^m) \right\rangle_{N_r \times N_r}, \quad (12)$$

$$i, j = 1, \dots, N_r.$$

Similarly, the  $N_q$  experimentally measured responses  $q_j$  are characterized by mean measured values, denoted as  $q_j^m$ , and constituting the components of the vector  $\mathbf{q}^m$  defined as

$$\mathbf{q}^m \triangleq (q_1^m, \dots, q_{N_q}^m), \quad q_j^m \triangleq \langle q_j \rangle, \quad (13)$$

$$j = 1, \dots, N_q,$$

and by the measured covariance matrix  $\mathbf{C}_{qq}^{(N_q \times N_q)}$  defined as

$$\mathbf{C}_{qq}^{(N_q \times N_q)} \triangleq \left\langle (q_i - q_i^m)(q_j - q_j^m) \right\rangle_{N_q \times N_q}, \quad (14)$$

$$i, j = 1, \dots, N_q.$$

Furthermore, the responses  $\mathbf{r}$  and  $\mathbf{q}$  may also be correlated; such correlations would be quantified by correlation matrices defined as

$$\mathbf{C}_{rq}^{(N_r \times N_q)} \triangleq \left\langle (\mathbf{r} - \mathbf{r}^m)(\mathbf{q} - \mathbf{q}^m)^\dagger \right\rangle$$

$$\triangleq \left[ \mathbf{C}_{qr}^{(N_q \times N_r)} \right]^\dagger. \quad (15)$$

In the most general case, correlations may also exist among all parameters and responses. Such correlations would be quantified through matrices defined as follows:

$$\mathbf{C}_{ar}^{(N_a \times N_r)} \triangleq \left\langle (\boldsymbol{\alpha} - \boldsymbol{\alpha}^0)(\mathbf{r} - \mathbf{r}^m)^\dagger \right\rangle$$

$$\triangleq \left[ \mathbf{C}_{ra}^{(N_r \times N_a)} \right]^\dagger, \quad (16)$$

$$\mathbf{C}_{aq}^{(N_a \times N_q)} \triangleq \left\langle (\boldsymbol{\alpha} - \boldsymbol{\alpha}^0)(\mathbf{q} - \mathbf{q}^m)^\dagger \right\rangle$$

$$\triangleq \left[ \mathbf{C}_{qa}^{(N_q \times N_a)} \right]^\dagger, \quad (17)$$

$$\mathbf{C}_{\beta r}^{(N_\beta \times N_r)} \triangleq \left\langle (\boldsymbol{\beta} - \boldsymbol{\beta}^0)(\mathbf{r} - \mathbf{r}^m)^\dagger \right\rangle$$

$$\triangleq \left[ \mathbf{C}_{r\beta}^{(N_r \times N_\beta)} \right]^\dagger, \quad (18)$$

and

$$\mathbf{C}_{\beta q}^{(N_\beta \times N_q)} \triangleq \left\langle (\boldsymbol{\beta} - \boldsymbol{\beta}^0)(\mathbf{q} - \mathbf{q}^m)^\dagger \right\rangle$$

$$\triangleq \left[ \mathbf{C}_{q\beta}^{(N_q \times N_\beta)} \right]^\dagger. \quad (19)$$

## II.B. MULTI-PRED Output: Optimally Predicted Values of Model Parameters and Responses

The following quantities are computed and provided as outputs of MULTI-PRED:

1. Covariance matrices of the computed responses for model A arising from the uncertainties in the model parameters of model A:

$$\mathbf{C}_{rr}^{comp} \triangleq \left\langle [\mathbf{r} - \mathbf{r}^c(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0)] [\mathbf{r} - \mathbf{r}^c(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0)]^\dagger \right\rangle$$

$$= \mathbf{S}_{r\alpha} \mathbf{C}_{\alpha\alpha} \mathbf{S}_{r\alpha}^\dagger + 2\mathbf{S}_{r\alpha} \mathbf{C}_{\alpha\beta} \mathbf{S}_{r\beta}^\dagger + \mathbf{S}_{r\beta} \mathbf{C}_{\beta\beta} \mathbf{S}_{r\beta}^\dagger. \quad (20)$$

2. Covariance matrices of the computed responses for model B arising from the uncertainties in the model parameters of model B:

$$\mathbf{C}_{qq}^{comp} \triangleq \left\langle [\mathbf{q} - \mathbf{q}^c(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0)] [\mathbf{q} - \mathbf{q}^c(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0)]^\dagger \right\rangle$$

$$= \mathbf{S}_{q\alpha} \mathbf{C}_{\alpha\alpha} \mathbf{S}_{q\alpha}^\dagger + 2\mathbf{S}_{q\alpha} \mathbf{C}_{\alpha\beta} \mathbf{S}_{q\beta}^\dagger + \mathbf{S}_{q\beta} \mathbf{C}_{\beta\beta} \mathbf{S}_{q\beta}^\dagger. \quad (21)$$

3. Correlation matrices of the computed responses for models A and B arising from the uncertainties in the model parameters of models A and B:

$$\begin{aligned}
 \mathbf{C}_{rq}^{comp} &\triangleq \left\langle [\mathbf{r} - \mathbf{r}^c(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0)] [\mathbf{q} - \mathbf{q}^c(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0)]^\dagger \right\rangle \\
 &= \mathbf{S}_{r\alpha} \mathbf{C}_{\alpha\alpha} \mathbf{S}_{q\alpha}^\dagger + \mathbf{S}_{r\alpha} \mathbf{C}_{\alpha\beta} \mathbf{S}_{q\beta}^\dagger + \mathbf{S}_{r\beta} \mathbf{C}_{\alpha\beta}^\dagger \mathbf{S}_{q\alpha}^\dagger \\
 &\quad + \mathbf{S}_{r\beta} \mathbf{C}_{\beta\beta} \mathbf{S}_{q\beta}^\dagger. \quad (22)
 \end{aligned}$$

4. Optimally predicted best-estimate values for the parameters of model A (model calibration):

$$\begin{aligned}
 \boldsymbol{\alpha}^{pred} &= \boldsymbol{\alpha}^0 - [\mathbf{X}_\alpha \mathbf{D}_{11} + \mathbf{Y}_\alpha \mathbf{D}_{12}^\dagger] \mathbf{r}^d(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0) \\
 &\quad - [\mathbf{X}_\alpha \mathbf{D}_{12} + \mathbf{Y}_\alpha \mathbf{D}_{22}] \mathbf{q}^d(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0). \quad (23)
 \end{aligned}$$

5. Optimally predicted best-estimate values for the parameters of model B (model calibration):

$$\begin{aligned}
 \boldsymbol{\beta}^{pred} &= \boldsymbol{\beta}^0 - [\mathbf{X}_\beta \mathbf{D}_{11} + \mathbf{Y}_\beta \mathbf{D}_{12}^\dagger] \mathbf{r}^d(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0) \\
 &\quad - [\mathbf{X}_\beta \mathbf{D}_{12} + \mathbf{Y}_\beta \mathbf{D}_{22}] \mathbf{q}^d(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0). \quad (24)
 \end{aligned}$$

6. Optimally predicted best-estimate values for the responses of model A:

$$\begin{aligned}
 \mathbf{r}^{pred} &= \mathbf{r}^m - [\mathbf{X}_r \mathbf{D}_{11} + \mathbf{Y}_r \mathbf{D}_{12}^\dagger] \mathbf{r}^d(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0) \\
 &\quad - [\mathbf{X}_r \mathbf{D}_{12} + \mathbf{Y}_r \mathbf{D}_{22}] \mathbf{q}^d(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0). \quad (25)
 \end{aligned}$$

7. Optimally predicted best-estimate values for the responses of model B:

$$\begin{aligned}
 \mathbf{q}^{pred} &= \mathbf{q}^m - [\mathbf{X}_q \mathbf{D}_{11} + \mathbf{Y}_q \mathbf{D}_{12}^\dagger] \mathbf{r}^d(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0) \\
 &\quad - [\mathbf{X}_q \mathbf{D}_{12} + \mathbf{Y}_q \mathbf{D}_{22}] \mathbf{q}^d(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0). \quad (26)
 \end{aligned}$$

8. Optimally predicted best-estimate values for components of the covariance matrix  $\mathbf{C}_{\alpha\alpha}^{pred}$  for the parameters  $\boldsymbol{\alpha}$  of model A:

$$\begin{aligned}
 \mathbf{C}_{\alpha\alpha}^{pred} &\triangleq \left\langle (\boldsymbol{\alpha} - \boldsymbol{\alpha}^{pred})(\boldsymbol{\alpha} - \boldsymbol{\alpha}^{pred})^\dagger \right\rangle \\
 &= \mathbf{C}_{\alpha\alpha} - [\mathbf{X}_\alpha (\mathbf{D}_{11} \mathbf{X}_\alpha^\dagger + \mathbf{D}_{12} \mathbf{Y}_\alpha^\dagger) \\
 &\quad + \mathbf{Y}_\alpha (\mathbf{D}_{21} \mathbf{X}_\alpha^\dagger + \mathbf{D}_{22} \mathbf{Y}_\alpha^\dagger)]. \quad (27)
 \end{aligned}$$

9. Optimally predicted best-estimate values for the components of the predicted covariance matrix  $\mathbf{C}_{rr}^{pred}$  for the responses  $\mathbf{r}$  of model A:

$$\begin{aligned}
 \mathbf{C}_{rr}^{pred} &\triangleq \left\langle (\mathbf{r} - \mathbf{r}^{pred})(\mathbf{r} - \mathbf{r}^{pred})^\dagger \right\rangle \\
 &= \mathbf{C}_{rr} - [\mathbf{X}_r (\mathbf{D}_{11} \mathbf{X}_r^\dagger + \mathbf{D}_{12} \mathbf{Y}_r^\dagger) \\
 &\quad + \mathbf{Y}_r (\mathbf{D}_{21} \mathbf{X}_r^\dagger + \mathbf{D}_{22} \mathbf{Y}_r^\dagger)]. \quad (28)
 \end{aligned}$$

10. Optimally predicted best-estimate values for the components of the predicted correlation matrix  $\mathbf{C}_{\alpha r}^{pred}$  for the parameters  $\boldsymbol{\alpha}$  and  $\mathbf{r}$  responses of model A:

$$\begin{aligned}
 \mathbf{C}_{\alpha r}^{pred} &\triangleq \left\langle (\boldsymbol{\alpha} - \boldsymbol{\alpha}^{pred})(\mathbf{r} - \mathbf{r}^{pred})^\dagger \right\rangle \\
 &= \mathbf{C}_{\alpha r} - [\mathbf{X}_\alpha (\mathbf{D}_{11} \mathbf{X}_r^\dagger + \mathbf{D}_{12} \mathbf{Y}_r^\dagger) \\
 &\quad + \mathbf{Y}_\alpha (\mathbf{D}_{21} \mathbf{X}_r^\dagger + \mathbf{D}_{22} \mathbf{Y}_r^\dagger)]. \quad (29)
 \end{aligned}$$

11. Optimally predicted best-estimate values for the components of the predicted covariance matrix  $\mathbf{C}_{\beta\beta}^{pred}$  for the parameters  $\boldsymbol{\beta}$  of model B:

$$\begin{aligned}
 \mathbf{C}_{\beta\beta}^{pred} &\triangleq \left\langle (\boldsymbol{\beta} - \boldsymbol{\beta}^{pred})(\boldsymbol{\beta} - \boldsymbol{\beta}^{pred})^\dagger \right\rangle \\
 &= \mathbf{C}_{\beta\beta} - [\mathbf{X}_\beta (\mathbf{D}_{11} \mathbf{X}_\beta^\dagger + \mathbf{D}_{12} \mathbf{Y}_\beta^\dagger) \\
 &\quad + \mathbf{Y}_\beta (\mathbf{D}_{21} \mathbf{X}_\beta^\dagger + \mathbf{D}_{22} \mathbf{Y}_\beta^\dagger)]. \quad (30)
 \end{aligned}$$

12. Optimally predicted best-estimate values for the components of the predicted covariance matrix  $\mathbf{C}_{qq}^{pred}$  for the responses  $\mathbf{q}$  of model B are obtained as

$$\begin{aligned}
 \mathbf{C}_{qq}^{pred} &\triangleq \left\langle (\mathbf{q} - \mathbf{q}^{pred})(\mathbf{q} - \mathbf{q}^{pred})^\dagger \right\rangle \\
 &= \mathbf{C}_{qq} - [\mathbf{X}_q (\mathbf{D}_{11} \mathbf{X}_q^\dagger + \mathbf{D}_{12} \mathbf{Y}_q^\dagger) \\
 &\quad + \mathbf{Y}_q (\mathbf{D}_{21} \mathbf{X}_q^\dagger + \mathbf{D}_{22} \mathbf{Y}_q^\dagger)]. \quad (31)
 \end{aligned}$$

13. Optimally predicted best-estimate values for the components of the predicted correlation matrix  $\mathbf{C}_{\beta q}^{pred}$  for the parameters  $\boldsymbol{\beta}$  and the responses  $\mathbf{q}$  of model B:

$$\begin{aligned}
 \mathbf{C}_{\beta q}^{opt} &\triangleq \left\langle (\boldsymbol{\beta} - \boldsymbol{\beta}^{pred})(\mathbf{q} - \mathbf{q}^{pred})^\dagger \right\rangle \\
 &= \mathbf{C}_{\beta q} - [\mathbf{X}_\beta (\mathbf{D}_{11} \mathbf{X}_q^\dagger + \mathbf{D}_{12} \mathbf{Y}_q^\dagger) \\
 &\quad + \mathbf{Y}_\beta (\mathbf{D}_{21} \mathbf{X}_q^\dagger + \mathbf{D}_{22} \mathbf{Y}_q^\dagger)]. \quad (32)
 \end{aligned}$$

14. Optimally predicted best-estimate values for the components of the predicted correlation matrix

$\mathbf{C}_{\alpha\beta}^{pred}$  for the parameters  $\boldsymbol{\alpha}$  of model A and the parameters  $\boldsymbol{\beta}$  of model B:

$$\begin{aligned}\mathbf{C}_{\alpha\beta}^{pred} &\triangleq \left\langle (\boldsymbol{\alpha} - \boldsymbol{\alpha}^{pred})(\boldsymbol{\beta} - \boldsymbol{\beta}^{pred})^\dagger \right\rangle \\ &= \mathbf{C}_{\alpha\beta} - \left[ \mathbf{X}_\alpha (\mathbf{D}_{11} \mathbf{X}_\beta^\dagger + \mathbf{D}_{12} \mathbf{Y}_\beta^\dagger) \right. \\ &\quad \left. + \mathbf{Y}_\alpha (\mathbf{D}_{21} \mathbf{X}_\beta^\dagger + \mathbf{D}_{22} \mathbf{Y}_\beta^\dagger) \right].\end{aligned}\quad (33)$$

15. Optimally predicted best-estimate values for the components of the predicted correlation matrix  $\mathbf{C}_{\alpha q}^{pred}$  for the parameters  $\boldsymbol{\alpha}$  of model A and the responses  $\mathbf{q}$  of model B:

$$\begin{aligned}\mathbf{C}_{\alpha q}^{pred} &\triangleq \left\langle (\boldsymbol{\alpha} - \boldsymbol{\alpha}^{pred})(\mathbf{q} - \mathbf{q}^{pred})^\dagger \right\rangle \\ &= \mathbf{C}_{\alpha q} - \left[ \mathbf{X}_\alpha (\mathbf{D}_{11} \mathbf{X}_q^\dagger + \mathbf{D}_{12} \mathbf{Y}_q^\dagger) \right. \\ &\quad \left. + \mathbf{Y}_\alpha (\mathbf{D}_{21} \mathbf{X}_q^\dagger + \mathbf{D}_{22} \mathbf{Y}_q^\dagger) \right].\end{aligned}\quad (34)$$

16. Optimally predicted best-estimate values for the components of the predicted correlation matrix  $\mathbf{C}_{\beta r}^{pred}$  for the parameters  $\boldsymbol{\beta}$  of model B and the responses  $\mathbf{r}$  of model A:

$$\begin{aligned}\mathbf{C}_{\beta r}^{pred} &\triangleq \left\langle (\boldsymbol{\beta} - \boldsymbol{\beta}^{pred})(\mathbf{r} - \mathbf{r}^{pred})^\dagger \right\rangle \\ &= \mathbf{C}_{\beta r} - \left[ \mathbf{X}_\beta (\mathbf{D}_{11} \mathbf{X}_r^\dagger + \mathbf{D}_{12} \mathbf{Y}_r^\dagger) \right. \\ &\quad \left. + \mathbf{Y}_\beta (\mathbf{D}_{21} \mathbf{X}_r^\dagger + \mathbf{D}_{22} \mathbf{Y}_r^\dagger) \right].\end{aligned}\quad (35)$$

17. Optimally predicted best-estimate values for the components of the predicted correlation matrix  $\mathbf{C}_{rq}^{pred}$  for the responses  $\mathbf{r}$  of model A and the responses  $\mathbf{q}$  of model B:

$$\begin{aligned}\mathbf{C}_{rq}^{pred} &\triangleq \left\langle (\mathbf{r} - \mathbf{r}^{pred})(\mathbf{q} - \mathbf{q}^{pred})^\dagger \right\rangle \\ &= \mathbf{C}_{rq} - \left[ \mathbf{X}_r (\mathbf{D}_{11} \mathbf{X}_q^\dagger + \mathbf{D}_{12} \mathbf{Y}_q^\dagger) \right. \\ &\quad \left. + \mathbf{Y}_r (\mathbf{D}_{21} \mathbf{X}_q^\dagger + \mathbf{D}_{22} \mathbf{Y}_q^\dagger) \right].\end{aligned}\quad (36)$$

18. The validation metric  $V$ :

$$\begin{aligned}V &\triangleq \chi^2 \\ &= (\mathbf{r}^c - \mathbf{r}^m)^\dagger \mathbf{D}_{11} (\mathbf{r}^c - \mathbf{r}^m) \\ &\quad + 2(\mathbf{r}^c - \mathbf{r}^m)^\dagger \mathbf{D}_{12} (\mathbf{q}^c - \mathbf{q}^m) \\ &\quad + (\mathbf{q}^c - \mathbf{q}^m)^\dagger \mathbf{D}_{22} (\mathbf{q}^c - \mathbf{q}^m).\end{aligned}\quad (37)$$

The validation metric  $V$  can be evaluated directly from the originally given data (i.e., from given parameters and responses, together with their original uncertainties). The validation metric  $V$  is distributed according to the  $\chi^2$  (chi-square)-distribution with  $n$  degrees of freedom of the continuous variable  $x$ ,  $0 \leq x < \infty$  and is defined as

$$\begin{aligned}P(x < \chi^2 < x + dx) dx &= \frac{1}{2^{n/2} \Gamma(n/2)} x^{n/2-1} e^{-x/2} dx, \\ x > 0, \quad (n = 1, 2, \dots).\end{aligned}\quad (38)$$

The mean and variance of  $x$  are  $\langle x \rangle = n$  and  $\text{var}(x) = 2n$ . Since the  $\chi^2$ -distribution is a measure of the deviation of a true distribution (in this case, the distribution of experimental responses) from the hypothetic one (in this case, a Gaussian), the value of  $V = \chi^2$  computed using Eq. (37) provides a very valuable quantitative indicator for investigating the agreement between the computed and experimental responses, measuring essentially the consistency of the experimental responses with the model parameters.

The various quantities appearing in Eqs. (20) through (37) are defined as follows:

1. The matrices  $\mathbf{S}_{r\alpha}(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0)$ ,  $\mathbf{S}_{r\beta}(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0)$ ,  $\mathbf{S}_{q\alpha}(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0)$ , and  $\mathbf{S}_{q\beta}(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0)$  comprise first-order response-derivatives with respect to the model parameters, computed at the nominal parameter values  $(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0)$ , and are defined as follows:

$$\mathbf{S}_{r\alpha}^{N_r \times N_\alpha} \equiv \begin{bmatrix} \frac{\partial r_1}{\partial \alpha_1} & \dots & \frac{\partial r_1}{\partial \alpha_{N_\alpha}} \\ \vdots & \ddots & \vdots \\ \frac{\partial r_{N_r}}{\partial \alpha_1} & \dots & \frac{\partial r_{N_r}}{\partial \alpha_{N_\alpha}} \end{bmatrix},\quad (39a)$$

$$\mathbf{S}_{r\beta}^{N_r \times N_\beta} \equiv \begin{bmatrix} \frac{\partial r_1}{\partial \beta_1} & \dots & \frac{\partial r_1}{\partial \beta_{N_\beta}} \\ \vdots & \ddots & \vdots \\ \frac{\partial r_{N_r}}{\partial \beta_1} & \dots & \frac{\partial r_{N_r}}{\partial \beta_{N_\beta}} \end{bmatrix}\quad (39b)$$



$$\mathbf{S}_{q\alpha}^{N_q \times N_\alpha} \equiv \begin{bmatrix} \frac{\partial q_1}{\partial \alpha_1} & \cdots & \frac{\partial q_1}{\partial \alpha_{N_\alpha}} \\ \vdots & \ddots & \vdots \\ \frac{\partial q_{N_q}}{\partial \alpha_1} & \cdots & \frac{\partial q_{N_q}}{\partial \alpha_{N_\alpha}} \end{bmatrix}, \quad (40a)$$

$$\mathbf{S}_{q\beta}^{N_q \times N_\beta} \equiv \begin{bmatrix} \frac{\partial q_1}{\partial \beta_1} & \cdots & \frac{\partial q_1}{\partial \beta_{N_\beta}} \\ \vdots & \ddots & \vdots \\ \frac{\partial q_{N_q}}{\partial \beta_1} & \cdots & \frac{\partial q_{N_q}}{\partial \beta_{N_\beta}} \end{bmatrix}. \quad (40b)$$

2. The vectors  $\mathbf{r}^d(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0)$  and  $\mathbf{q}^d(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0)$  measure the differences (deviations) between the computed and measured responses, and are defined as follows:

$$\mathbf{r}^d(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0) \triangleq \mathbf{r}^c(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0) - \mathbf{r}^m \quad (41)$$

and

$$\mathbf{q}^d(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0) \triangleq \mathbf{q}^c(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0) - \mathbf{q}^m.$$

3. The matrix  $\mathbf{D}_{rr}$ , having  $\dim \mathbf{D}_{rr} = (N_r \times N_r)$ , is actually the covariance matrix of the vector of response deviations for model A, i.e.,

$$\begin{aligned} \mathbf{D}_{rr} &\triangleq \mathbf{S}_{r\alpha} \left( \mathbf{C}_{\alpha\alpha} \mathbf{S}_{r\alpha}^\dagger + \mathbf{C}_{\alpha\beta} \mathbf{S}_{r\beta}^\dagger - \mathbf{C}_{\alpha r} \right) \\ &+ \mathbf{S}_{r\beta} \left( \mathbf{C}_{\alpha\beta}^\dagger \mathbf{S}_{r\alpha}^\dagger + \mathbf{C}_{\beta\beta} \mathbf{S}_{r\beta}^\dagger - \mathbf{C}_{\beta r} \right) \\ &- \mathbf{C}_{\alpha r}^\dagger \mathbf{S}_{r\alpha}^\dagger - \mathbf{C}_{\beta r}^\dagger \mathbf{S}_{r\beta}^\dagger + \mathbf{C}_{rr} \\ &= \left\langle \mathbf{r}^d(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0) [\mathbf{r}^d(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0)]^\dagger \right\rangle. \end{aligned} \quad (42)$$

4. The matrix  $\mathbf{D}_{qq}$ , having  $\dim \mathbf{D}_{qq} = (N_q \times N_q)$ , is actually the covariance matrix of the vector of response deviations for model B, i.e.,

$$\begin{aligned} \mathbf{D}_{qq} &\triangleq \mathbf{S}_{q\alpha} \left( \mathbf{C}_{\alpha\alpha} \mathbf{S}_{q\alpha}^\dagger + \mathbf{C}_{\alpha\beta} \mathbf{S}_{q\beta}^\dagger - \mathbf{C}_{\alpha q} \right) \\ &+ \mathbf{S}_{q\beta} \left( \mathbf{C}_{\alpha\beta}^\dagger \mathbf{S}_{q\alpha}^\dagger + \mathbf{C}_{\beta\beta} \mathbf{S}_{q\beta}^\dagger - \mathbf{C}_{\beta q} \right) \\ &- \mathbf{C}_{\alpha q}^\dagger \mathbf{S}_{q\alpha}^\dagger - \mathbf{C}_{\beta q}^\dagger \mathbf{S}_{q\beta}^\dagger + \mathbf{C}_{qq} \\ &= \left\langle \mathbf{q}^d(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0) [\mathbf{q}^d(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0)]^\dagger \right\rangle. \end{aligned} \quad (43)$$

5. The matrix  $\mathbf{D}_{rq} = \mathbf{D}_{rq}^\dagger$ , having  $\dim \mathbf{D}_{rq} = \mathbf{D}_{rq}^\dagger = (N_q \times N_r)$ , is actually the correlation matrix between the vector of response deviations for model A and model B, i.e.,

$$\begin{aligned} \mathbf{D}_{qr} &\triangleq \mathbf{S}_{q\alpha} \left( \mathbf{C}_{\alpha\alpha} \mathbf{S}_{r\alpha}^\dagger + \mathbf{C}_{\alpha\beta} \mathbf{S}_{r\beta}^\dagger - \mathbf{C}_{\alpha r} \right) \\ &+ \mathbf{S}_{q\beta} \left( \mathbf{C}_{\alpha\beta}^\dagger \mathbf{S}_{r\alpha}^\dagger + \mathbf{C}_{\beta\beta} \mathbf{S}_{r\beta}^\dagger - \mathbf{C}_{\beta r} \right) \\ &- \mathbf{C}_{\alpha q}^\dagger \mathbf{S}_{r\alpha}^\dagger - \mathbf{C}_{\beta q}^\dagger \mathbf{S}_{r\beta}^\dagger + \mathbf{C}_{rq} \\ &= \left\langle \mathbf{r}^d(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0) [\mathbf{q}^d(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0)]^\dagger \right\rangle = \mathbf{D}_{rq}^\dagger \end{aligned} \quad (44)$$

and

$$\begin{aligned} \mathbf{D}_{rq} &\triangleq \mathbf{S}_{r\alpha} \left( \mathbf{C}_{\alpha\alpha} \mathbf{S}_{q\alpha}^\dagger + \mathbf{C}_{\alpha\beta} \mathbf{S}_{q\beta}^\dagger - \mathbf{C}_{\alpha q} \right) \\ &+ \mathbf{S}_{r\beta} \left( \mathbf{C}_{\alpha\beta}^\dagger \mathbf{S}_{q\alpha}^\dagger + \mathbf{C}_{\beta\beta} \mathbf{S}_{q\beta}^\dagger - \mathbf{C}_{\beta q} \right) \\ &- \mathbf{C}_{\alpha r}^\dagger \mathbf{S}_{q\alpha}^\dagger - \mathbf{C}_{\beta r}^\dagger \mathbf{S}_{q\beta}^\dagger + \mathbf{C}_{rq} \\ &= \left\langle \mathbf{q}^d(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0) [\mathbf{r}^d(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0)]^\dagger \right\rangle. \end{aligned} \quad (45)$$

6. The matrices  $\mathbf{D}_{11}$ ,  $\mathbf{D}_{12}$ , and  $\mathbf{D}_{22}$  are defined as follows:

$$\mathbf{D}_{11} \triangleq \mathbf{D}_{rr}^{-1} + \mathbf{D}_{rr}^{-1} \mathbf{D}_{rq} \mathbf{D}_{22} \mathbf{D}_{rq}^\dagger \mathbf{D}_{rr}^{-1}, \quad (46)$$

$$\mathbf{D}_{12} \triangleq -\mathbf{D}_{rr}^{-1} \mathbf{D}_{rq} \mathbf{D}_{22}, \quad (47)$$

$$\mathbf{D}_{12}^\dagger \triangleq -\mathbf{D}_{22} \mathbf{D}_{rq}^\dagger \mathbf{D}_{rr}^{-1}, \quad (48)$$

and

$$\mathbf{D}_{22} \triangleq \left( \mathbf{D}_{qq} - \mathbf{D}_{rq}^\dagger \mathbf{D}_{rr}^{-1} \mathbf{D}_{rq} \right)^{-1}. \quad (49)$$

7. The vectors  $\mathbf{X}_\alpha$ ,  $\mathbf{Y}_\alpha$ ,  $\mathbf{X}_\beta$ ,  $\mathbf{Y}_\beta$ ,  $\mathbf{X}_r$ ,  $\mathbf{Y}_r$ ,  $\mathbf{X}_q$ , and  $\mathbf{Y}_q$  are defined as follows:

$$\mathbf{X}_\alpha \triangleq \mathbf{C}_{\alpha\alpha} \mathbf{S}_{r\alpha}^\dagger + \mathbf{C}_{\alpha\beta} \mathbf{S}_{r\beta}^\dagger - \mathbf{C}_{\alpha r}, \quad (50)$$

$$\mathbf{Y}_\alpha \triangleq \mathbf{C}_{\alpha\alpha} \mathbf{S}_{q\alpha}^\dagger + \mathbf{C}_{\alpha\beta} \mathbf{S}_{q\beta}^\dagger - \mathbf{C}_{\alpha q}, \quad (51)$$

$$\mathbf{X}_\beta \triangleq \mathbf{C}_{\alpha\beta}^\dagger \mathbf{S}_{r\alpha}^\dagger + \mathbf{C}_{\beta\beta} \mathbf{S}_{r\beta}^\dagger - \mathbf{C}_{\beta r}, \quad (52)$$

$$\mathbf{Y}_\beta \triangleq \mathbf{C}_{\beta\alpha} \mathbf{S}_{q\alpha}^\dagger + \mathbf{C}_{\beta\beta} \mathbf{S}_{q\beta}^\dagger - \mathbf{C}_{\beta q}, \quad (53)$$

$$\mathbf{X}_r \triangleq \mathbf{C}_{\alpha r}^\dagger \mathbf{S}_{r\alpha}^\dagger + \mathbf{C}_{\beta r}^\dagger \mathbf{S}_{r\beta}^\dagger - \mathbf{C}_{rr}, \quad (54)$$

$$\mathbf{Y}_r \triangleq \mathbf{C}_{ar}^\dagger \mathbf{S}_{q\alpha}^\dagger + \mathbf{C}_{\beta r}^\dagger \mathbf{S}_{q\beta}^\dagger - \mathbf{C}_{rq}, \quad (55)$$

$$\mathbf{X}_q \triangleq \mathbf{C}_{\alpha q}^\dagger \mathbf{S}_{r\alpha}^\dagger + \mathbf{C}_{\beta q}^\dagger \mathbf{S}_{r\beta}^\dagger - \mathbf{C}_{rq}^\dagger, \quad (56)$$

and

$$\mathbf{Y}_q \triangleq \mathbf{C}_{\alpha q}^\dagger \mathbf{S}_{q\alpha}^\dagger + \mathbf{C}_{\beta q}^\dagger \mathbf{S}_{q\beta}^\dagger - \mathbf{C}_{qq}. \quad (57)$$

## II.C. Discussion and Particular Cases

The derivations in Sec. II.B were carried out in the response space because in large-scale practical problems, the number of measured responses is smaller than the number of model parameters. The only matrix inversions required are the inversion of the matrix  $\mathbf{D}_{rr}$  of size  $N_r$  in Eq. (46) and the inversion of the matrix  $(\mathbf{D}_{qq} - \mathbf{D}_{rq}^\dagger \mathbf{D}_{rr}^{-1} \mathbf{D}_{rq})$ , which is of size  $N_q$  in Eq. (49). Both of these matrix inversions are performed in the respective response spaces.

The PM-CMPS methodology can also be used if one starts with the data assimilation and model calibration for one of the models (either model A or model B) and subsequently couples the second model to the first one. Without the PM-CMPS methodology, when the second model (e.g., model B) is coupled to the first one (e.g., model A), both models would have to be calibrated anew, simultaneously, and the work performed initially for calibrating model A alone would become useless. Using the PM-CMPS methodology, however, the work initially performed for calibrating model A would not become useless, but would simply be augmented by the specific additional terms arising from model B, thus performing PM-CMPS in a sequential and more efficient way.

It is also important to note that the explicit separation, in Eq. (37), of contributions from model A and model B to the overall validation metric  $V$  enables the explicit evaluation of adding or subtracting measured responses. Large contributions to  $V$  indicate that the respective responses may be inconsistent or discrepant, and such discrepancies warrant further investigations.

It often happens in practice that, after one has already performed a model calibration, e.g., using model A (involving  $N_\alpha$  model parameters  $\alpha_n$  and  $N_r$  experimentally measured responses  $r_i$ ), additional measurements may become available and/or additional parameters (which were not considered in the initial data

assimilation/model calibration/predictive modeling procedure) may need to be taken into account (e.g., model parameters for which quantified uncertainties became available only after the initial data assimilation/model calibration/predictive modeling procedure was already performed), all for the same model A. The PM-CMPS predictive modeling methodology can also be used as a most efficient procedure for systematically adding or subtracting responses and/or parameters for performing a subsequent data assimilation/model calibration/predictive modeling procedure on the same model, without “wasting” the information already obtained in previous predictive modeling computations that involved a different (higher or lower) number of responses and/or model parameters. Adding and/or subtracting measurements (responses) and/or model parameters to the same model without needing to discard previous predictive modeling computations are described in Secs. III.C.1, III.C.2, and III.C.3 as particular cases of the general PM-CMPS methodology.

### II.C.1. Predictive Modeling for a Single Multi-Physics Model

In the case of applying the PM-CMPS methodology for the predictive modeling of a single multi-physics model (e.g., model A, involving  $N_\alpha$  model parameters  $\alpha_n$  and  $N_r$  experimentally measured responses  $r_i$ ), the predictive modeling equations Eqs. (20) through (37) reduce to the final results presented originally by Cacuci and Ionescu-Bujor,<sup>3</sup> namely,

$$\boldsymbol{\alpha}^{pred} = \boldsymbol{\alpha}^0 - (\mathbf{C}_{\alpha\alpha} \mathbf{S}_{r\alpha}^\dagger - \mathbf{C}_{ar}) [\mathbf{D}_{rr}]^{-1} \mathbf{r}^d(\boldsymbol{\alpha}^0), \quad (58)$$

$$\mathbf{r}^{pred} = \mathbf{r}^m - (\mathbf{C}_{ar}^\dagger \mathbf{S}_{r\alpha}^\dagger - \mathbf{C}_{rr}) [\mathbf{D}_{rr}]^{-1} \mathbf{r}^d(\boldsymbol{\alpha}^0), \quad (59)$$

$$\mathbf{C}_{\alpha\alpha}^{pred} = \mathbf{C}_{\alpha\alpha} - (\mathbf{C}_{\alpha\alpha} \mathbf{S}_{r\alpha}^\dagger - \mathbf{C}_{ar}) [\mathbf{D}_{rr}]^{-1} (\mathbf{C}_{\alpha\alpha} \mathbf{S}_{r\alpha}^\dagger - \mathbf{C}_{ar})^\dagger, \quad (60)$$

$$\mathbf{C}_{rr}^{pred} = \mathbf{C}_{rr} - (\mathbf{C}_{ar}^\dagger \mathbf{S}_{r\alpha}^\dagger - \mathbf{C}_{rr}) [\mathbf{D}_{rr}]^{-1} (\mathbf{C}_{ar}^\dagger \mathbf{S}_{r\alpha}^\dagger - \mathbf{C}_{rr})^\dagger, \quad (61)$$

and

$$\mathbf{C}_{ar}^{pred} = \mathbf{C}_{ar} - (\mathbf{C}_{\alpha\alpha} \mathbf{S}_{r\alpha}^\dagger - \mathbf{C}_{ar}) [\mathbf{D}_{rr}]^{-1} (\mathbf{C}_{ar}^\dagger \mathbf{S}_{r\alpha}^\dagger - \mathbf{C}_{rr})^\dagger \quad (62)$$

Note that if the model is perfect (i.e.,  $\mathbf{C}_{\alpha\alpha} = \mathbf{0}$  and  $\mathbf{C}_{\alpha r} = \mathbf{0}$ ), then Eqs. (58) through (62) would yield  $\mathbf{a}^{pred} = \mathbf{a}^0$  and  $\mathbf{r}^{pred} = \mathbf{r}^c(\mathbf{a}^0, \mathbf{\beta}^0)$ , predicted perfectly without any accompanying uncertainties (i.e.,  $\mathbf{C}_{rr}^{pred} = \mathbf{0}$ ,  $\mathbf{C}_{\alpha\alpha}^{pred} = \mathbf{0}$ , and  $\mathbf{C}_{\alpha r}^{pred} = \mathbf{0}$ ). In other words, for a perfect model, the PM-CMPS methodology predicts values for the responses and the parameters that coincide with the model's values (assumed to be perfect), and the experimental measurements would have no effect on the predictions (as would be expected, since imperfect measurements could not possibly improve the perfect model's predictions).

On the other hand, if the measurements are perfect (i.e.,  $\mathbf{C}_{rr} = \mathbf{0}$  and  $\mathbf{C}_{\alpha r} = \mathbf{0}$ ), but the model is imperfect, then Eqs. (58) through (62) would yield  $\mathbf{a}^{pred} = \mathbf{a}^0 - \mathbf{C}_{\alpha\alpha}$   $\mathbf{S}_{r\alpha}^\dagger [\mathbf{S}_{r\alpha} \mathbf{C}_{\alpha\alpha} \mathbf{S}_{r\alpha}^\dagger]^{-1} \mathbf{r}^d(\mathbf{a}^0)$ ,  $\mathbf{C}_{\alpha\alpha}^{pred} = \mathbf{C}_{\alpha\alpha} - \mathbf{C}_{\alpha\alpha} \mathbf{S}_{r\alpha}^\dagger [\mathbf{S}_{r\alpha} \mathbf{C}_{\alpha\alpha} \mathbf{S}_{r\alpha}^\dagger]^{-1} \mathbf{S}_{r\alpha} \mathbf{C}_{\alpha\alpha}$ ,  $\mathbf{r}^{pred} = \mathbf{r}^m$ ,  $\mathbf{C}_{rr}^{pred} = \mathbf{0}$ , and  $\mathbf{C}_{\alpha r}^{pred} = \mathbf{0}$ . In other words, in the case of perfect measurements, the PM-CMPS predicted values for the responses would coincide with the measured values (assumed to be perfect), but the model's uncertain parameters would be calibrated by taking the measurements into account to yield improved nominal values and reduced parameter uncertainties.

*II.C.2. Predictive Modeling for Model A with  $\beta$  Additional Parameters, But No Additional Responses*

In this case, the predictive modeling formulation in the response space allows the consideration of additional parameters for a model without increasing the size of the matrix  $\mathbf{D}_{rr}$  to be inverted. This is clearly demonstrated as Eqs. (20) through (57) become

$$\mathbf{D}_{rq} = \mathbf{0}, \mathbf{D}_{qr} = \mathbf{0}, \mathbf{D}_{qq} = \mathbf{0}, \tag{63}$$

$$\begin{aligned} \mathbf{D}_{rr} = & \mathbf{S}_{r\alpha} \left( \mathbf{C}_{\alpha\alpha} \mathbf{S}_{r\alpha}^\dagger + \mathbf{C}_{\alpha\beta} \mathbf{S}_{r\beta}^\dagger - \mathbf{C}_{\alpha r} \right) \\ & + \mathbf{S}_{r\beta} \left( \mathbf{C}_{\alpha\beta}^\dagger \mathbf{S}_{r\alpha}^\dagger + \mathbf{C}_{\beta\beta} \mathbf{S}_{r\beta}^\dagger - \mathbf{C}_{\beta r} \right) \\ & - \mathbf{C}_{\alpha r}^\dagger \mathbf{S}_{r\alpha}^\dagger - \mathbf{C}_{\beta r}^\dagger \mathbf{S}_{r\beta}^\dagger + \mathbf{C}_{rr}, \end{aligned} \tag{64}$$

$$\mathbf{X}_\alpha \triangleq \mathbf{C}_{\alpha\alpha} \mathbf{S}_{r\alpha}^\dagger + \mathbf{C}_{\alpha\beta} \mathbf{S}_{r\beta}^\dagger - \mathbf{C}_{\alpha r}, \tag{65}$$

$$\mathbf{X}_\beta \triangleq \mathbf{C}_{\alpha\beta}^\dagger \mathbf{S}_{r\alpha}^\dagger + \mathbf{C}_{\beta\beta} \mathbf{S}_{r\beta}^\dagger - \mathbf{C}_{\beta r}, \tag{66}$$

$$\mathbf{X}_r \triangleq \mathbf{C}_{\alpha r}^\dagger \mathbf{S}_{r\alpha}^\dagger + \mathbf{C}_{\beta r}^\dagger \mathbf{S}_{r\beta}^\dagger - \mathbf{C}_{rr}, \tag{67}$$

$$\mathbf{X}_q \triangleq \mathbf{0}, \mathbf{Y}_\alpha \triangleq \mathbf{0}, \mathbf{Y}_r \triangleq \mathbf{0}, \mathbf{Y}_\beta \triangleq \mathbf{0}, \mathbf{Y}_q \triangleq \mathbf{0}, \tag{68}$$

$$\mathbf{D}_{11} \triangleq \mathbf{D}_{rr}^{-1}, \mathbf{D}_{12} = \mathbf{0}, \mathbf{D}_{12}^\dagger = \mathbf{0}, \mathbf{D}_{12}^\dagger = \mathbf{0}, \mathbf{D}_{22} = \mathbf{0}, \tag{69}$$

$$\mathbf{a}^{pred} = \mathbf{a}^0 - \mathbf{X}_\alpha \mathbf{D}_{11} \mathbf{r}^d(\mathbf{a}^0, \mathbf{\beta}^0), \tag{70}$$

$$\mathbf{\beta}^{pred} = \mathbf{\beta}^0 - \mathbf{X}_\beta \mathbf{D}_{11} \mathbf{r}^d(\mathbf{a}^0, \mathbf{\beta}^0), \tag{71}$$

$$\mathbf{r}^{pred} = \mathbf{r}^m - \mathbf{X}_r \mathbf{D}_{11} \mathbf{r}^d(\mathbf{a}^0, \mathbf{\beta}^0), \tag{72}$$

$$\mathbf{C}_{\alpha\alpha}^{pred} = \mathbf{C}_{\alpha\alpha} - \mathbf{X}_\alpha \mathbf{D}_{11} \mathbf{X}_\alpha^\dagger, \tag{73}$$

$$\mathbf{C}_{rr}^{pred} = \mathbf{C}_{rr} - \mathbf{X}_r \mathbf{D}_{11} \mathbf{X}_r^\dagger, \tag{74}$$

$$\mathbf{C}_{\alpha r}^{pred} = \mathbf{C}_{\alpha r} - \mathbf{X}_\alpha \mathbf{D}_{11} \mathbf{X}_r^\dagger, \tag{75}$$

$$\mathbf{C}_{\beta\beta}^{opt} = \mathbf{C}_{\beta\beta} - \mathbf{X}_\beta \mathbf{D}_{11} \mathbf{X}_\beta^\dagger, \tag{76}$$

$$\mathbf{C}_{\alpha\beta}^{pred} = \mathbf{C}_{\alpha\beta} - \mathbf{X}_\alpha \mathbf{D}_{11} \mathbf{X}_\beta^\dagger, \tag{77}$$

and

$$\mathbf{C}_{\beta r}^{pred} = \mathbf{C}_{\beta r} - \mathbf{X}_\beta \mathbf{D}_{11} \mathbf{X}_r^\dagger. \tag{78}$$

*II.C.3. Predictive Modeling for Model A with  $Q$  Additional Responses, But No Additional Parameters*

In this case, Eqs. (20) through (57) become

$$\begin{aligned} \mathbf{D}_{rr} = & \mathbf{S}_{r\alpha} \mathbf{C}_{\alpha\alpha} \mathbf{S}_{r\alpha}^\dagger - \mathbf{S}_{r\alpha} \mathbf{C}_{\alpha r} - \mathbf{C}_{\alpha r}^\dagger \mathbf{S}_{r\alpha}^\dagger \\ & + \mathbf{C}_{rr}, \text{Dim}(\mathbf{D}_{rr}) = (N_r \times N_r), \end{aligned} \tag{79}$$

$$\begin{aligned} \mathbf{D}_{rq} = & \mathbf{S}_{r\alpha} \mathbf{C}_{\alpha\alpha} \mathbf{S}_{q\alpha}^\dagger - \mathbf{S}_{r\alpha} \mathbf{C}_{\alpha q} - \mathbf{C}_{\alpha r}^\dagger \mathbf{S}_{q\alpha}^\dagger \\ & + \mathbf{C}_{rq}, \text{Dim}(\mathbf{D}_{rq}) = (N_r \times N_q), \end{aligned} \tag{80}$$

$$\begin{aligned} \mathbf{D}_{qr} = & \mathbf{S}_{q\alpha} \mathbf{C}_{\alpha\alpha} \mathbf{S}_{r\alpha}^\dagger - \mathbf{C}_{\alpha q}^\dagger \mathbf{S}_{r\alpha}^\dagger - \mathbf{S}_{q\alpha} \mathbf{C}_{\alpha r} \\ & + \mathbf{C}_{rq}^\dagger, \text{Dim}(\mathbf{D}_{qr}) = (N_q \times N_r), \end{aligned} \tag{81}$$

$$\begin{aligned} \mathbf{D}_{qq} = & \mathbf{S}_{q\alpha} \mathbf{C}_{\alpha\alpha} \mathbf{S}_{q\alpha}^\dagger - \mathbf{S}_{q\alpha} \mathbf{C}_{\alpha q} - \mathbf{C}_{\alpha q}^\dagger \mathbf{S}_{q\alpha}^\dagger \\ & + \mathbf{C}_{qq}, \text{Dim}(\mathbf{D}_{qq}) = (N_q \times N_q), \end{aligned} \tag{82}$$

$$\mathbf{X}_\alpha \triangleq \mathbf{C}_{\alpha\alpha} \mathbf{S}_{r\alpha}^\dagger - \mathbf{C}_{\alpha r}, \quad (83)$$

$$\mathbf{Y}_\alpha \triangleq \mathbf{C}_{\alpha\alpha} \mathbf{S}_{q\alpha}^\dagger - \mathbf{C}_{\alpha q}, \quad (84)$$

$$\mathbf{X}_\beta \triangleq \mathbf{0}, \quad \mathbf{Y}_\beta \triangleq \mathbf{0}, \quad (85)$$

$$\mathbf{X}_r \triangleq \mathbf{C}_{\alpha r}^\dagger \mathbf{S}_{r\alpha}^\dagger - \mathbf{C}_{rr}, \quad (86)$$

$$\mathbf{Y}_r \triangleq \mathbf{C}_{\alpha r}^\dagger \mathbf{S}_{q\alpha}^\dagger - \mathbf{C}_{rq}^\dagger \quad (87)$$

$$\mathbf{X}_q \triangleq \mathbf{C}_{\alpha q}^\dagger \mathbf{S}_{r\alpha}^\dagger - \mathbf{C}_{rq}^\dagger, \quad (88)$$

$$\mathbf{Y}_q \triangleq \mathbf{C}_{\alpha q}^\dagger \mathbf{S}_{q\alpha}^\dagger - \mathbf{C}_{qq}, \quad (89)$$

$$\begin{aligned} \boldsymbol{\alpha}^{pred} &= \boldsymbol{\alpha}^0 - [\mathbf{X}_\alpha \mathbf{D}_{11} + \mathbf{Y}_\alpha \mathbf{D}_{12}^\dagger] \mathbf{r}^d(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0) \\ &\quad - [\mathbf{X}_\alpha \mathbf{D}_{12} + \mathbf{Y}_\alpha \mathbf{D}_{22}] \mathbf{q}^d(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0), \end{aligned} \quad (90)$$

$$\begin{aligned} \mathbf{r}^{pred} &= \mathbf{r}^m - [\mathbf{X}_r \mathbf{D}_{11} + \mathbf{Y}_r \mathbf{D}_{12}^\dagger] \mathbf{r}^d(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0) \\ &\quad - [\mathbf{X}_r \mathbf{D}_{12} + \mathbf{Y}_r \mathbf{D}_{22}] \mathbf{q}^d(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0), \end{aligned} \quad (91)$$

$$\begin{aligned} \mathbf{q}^{pred} &= \mathbf{q}^m - [\mathbf{X}_q \mathbf{D}_{11} + \mathbf{Y}_q \mathbf{D}_{12}^\dagger] \mathbf{r}^d(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0) \\ &\quad - [\mathbf{X}_q \mathbf{D}_{12} + \mathbf{Y}_q \mathbf{D}_{22}] \mathbf{q}^d(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0), \end{aligned} \quad (92)$$

$$\begin{aligned} \mathbf{C}_{\alpha\alpha}^{pred} &= \mathbf{C}_{\alpha\alpha} - [\mathbf{X}_\alpha (\mathbf{D}_{11} \mathbf{X}_\alpha^\dagger + \mathbf{D}_{12} \mathbf{Y}_\alpha^\dagger) \\ &\quad + \mathbf{Y}_\alpha (\mathbf{D}_{21} \mathbf{X}_\alpha^\dagger + \mathbf{D}_{22} \mathbf{Y}_\alpha^\dagger)], \end{aligned} \quad (93)$$

$$\begin{aligned} \mathbf{C}_{rr}^{pred} &= \mathbf{C}_{rr} - [\mathbf{X}_r (\mathbf{D}_{11} \mathbf{X}_r^\dagger + \mathbf{D}_{12} \mathbf{Y}_r^\dagger) \\ &\quad + \mathbf{Y}_r (\mathbf{D}_{21} \mathbf{X}_r^\dagger + \mathbf{D}_{22} \mathbf{Y}_r^\dagger)], \end{aligned} \quad (94)$$

$$\begin{aligned} \mathbf{C}_{\alpha r}^{pred} &= \mathbf{C}_{\alpha r} - [\mathbf{X}_\alpha (\mathbf{D}_{11} \mathbf{X}_r^\dagger + \mathbf{D}_{12} \mathbf{Y}_r^\dagger) \\ &\quad + \mathbf{Y}_\alpha (\mathbf{D}_{21} \mathbf{X}_r^\dagger + \mathbf{D}_{22} \mathbf{Y}_r^\dagger)], \end{aligned} \quad (95)$$

$$\begin{aligned} \mathbf{C}_{qq}^{pred} &= \mathbf{C}_{qq} - [\mathbf{X}_q (\mathbf{D}_{11} \mathbf{X}_q^\dagger + \mathbf{D}_{12} \mathbf{Y}_q^\dagger) \\ &\quad + \mathbf{Y}_q (\mathbf{D}_{21} \mathbf{X}_q^\dagger + \mathbf{D}_{22} \mathbf{Y}_q^\dagger)], \end{aligned} \quad (96)$$

$$\begin{aligned} \mathbf{C}_{\alpha q}^{pred} &= \mathbf{C}_{\alpha q} - [\mathbf{X}_\alpha (\mathbf{D}_{11} \mathbf{X}_q^\dagger + \mathbf{D}_{12} \mathbf{Y}_q^\dagger) \\ &\quad + \mathbf{Y}_\alpha (\mathbf{D}_{21} \mathbf{X}_q^\dagger + \mathbf{D}_{22} \mathbf{Y}_q^\dagger)], \end{aligned} \quad (97)$$

$$\begin{aligned} \mathbf{C}_{r q}^{pred} &= \mathbf{C}_{r q} - [\mathbf{X}_r (\mathbf{D}_{11} \mathbf{X}_q^\dagger + \mathbf{D}_{12} \mathbf{Y}_q^\dagger) \\ &\quad + \mathbf{Y}_r (\mathbf{D}_{21} \mathbf{X}_q^\dagger + \mathbf{D}_{22} \mathbf{Y}_q^\dagger)], \end{aligned} \quad (98)$$

and

$$\mathbf{C}_{\alpha\beta}^{pred} = \mathbf{0}, \quad \mathbf{C}_{\beta\beta}^{opt} = \mathbf{0}, \quad \mathbf{C}_{\beta r}^{pred} = \mathbf{0}, \quad \mathbf{C}_{\beta q}^{opt} = \mathbf{0}. \quad (99)$$

Note also that (to first order in response sensitivities) the covariance matrices of the computed responses arising from the uncertainties in the model parameters become

$$\begin{aligned} \mathbf{C}_{rr}^{comp} &\triangleq \left\langle [\mathbf{r} - \mathbf{r}^c(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0)] [\mathbf{r} - \mathbf{r}^c(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0)]^\dagger \right\rangle \\ &= \mathbf{S}_{r\alpha} \mathbf{C}_{\alpha\alpha} \mathbf{S}_{r\alpha}^\dagger, \end{aligned} \quad (100)$$

$$\begin{aligned} \mathbf{C}_{qq}^{comp} &\triangleq \left\langle [\mathbf{q} - \mathbf{q}^c(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0)] [\mathbf{q} - \mathbf{q}^c(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0)]^\dagger \right\rangle \\ &= \mathbf{S}_{q\alpha} \mathbf{C}_{\alpha\alpha} \mathbf{S}_{q\alpha}^\dagger, \end{aligned} \quad (101)$$

and

$$\begin{aligned} \mathbf{C}_{r q}^{comp} &\triangleq \left\langle [\mathbf{r} - \mathbf{r}^c(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0)] [\mathbf{q} - \mathbf{q}^c(\boldsymbol{\alpha}^0, \boldsymbol{\beta}^0)]^\dagger \right\rangle \\ &= \mathbf{S}_{r\alpha} \mathbf{C}_{\alpha\alpha} \mathbf{S}_{q\alpha}^\dagger. \end{aligned} \quad (102)$$

### III. MULTI-PRED CODE MODULE

The equations expressing the results of the PM-CMPS methodology developed by Cacuci<sup>1</sup> namely, Eqs. (20) through (57), have been programed in the computational software module MULTI-PRED. All routines in MULTI-PRED are written in Fortran 90 and are compatible with most Linux systems, performing predictive modeling computations for the following four cases:

*Case 1: One Multi-Physics Model*—predictive modeling solely for model A with  $N_\alpha$  model parameters and  $N_r$  measured responses

*Case 2: One Multi-Physics Model with Additional Model Parameters*—predictive modeling for

model A with  $N_b$  additional model parameters, but no additional responses

*Case 3: One Multi-Physics Model with Additional Model Responses*—predictive modeling for model A with  $N_q$  additional responses, but no additional parameters

*Case 4: Two Coupled Multi-Physics Models*—predictive modeling for model A coupled with model B.

### III.A. Fortran Source Code for the Program MULTI-PRED

The program MULTI-PRED includes the following routines and modules:

1. *main program*: multi-pred.f90
2. *module*: ModuleGlobalParameters.f90
3. *module*: ModuleIO.f90
4. *module*: ModuleErrors.f90
5. *subroutine*: Files.f90
6. *module*: ModuleFiles.f90
7. *subroutine*: ReadInput.f90
8. *module*: ModuleReadWrite.f90
9. *subroutine*: MultiPredSolver.f90
10. *module*: ModuleMultiPred.f90
11. *module*: ModuleLapack.f90

The structure of the MULTI-PRED software module is organized as shown in Fig. 1.

### III.B. Directories

The computational software module MULTI-PRED comprises the following directories:

1. *multi-pred/source/*: This folder contains the source codes.
2. *multi-pred/examples/*: This folder contains five examples specified in the following subfolders:
  - a. *./Neutron\_Diffusion\_Model\_Case\_1/*: This folder contains the input/output (I/O) files for MULTI-PRED case 1 for a neutron diffusion model.
  - b. *./Cooling\_Tower\_Model\_Case\_1/*: This folder contains the I/O files for MULTI-PRED case 1 for the SRNL cooling tower model.
  - c. *./Cooling\_Tower\_Model\_Case\_2/*: This folder contains the I/O files for MULTI-PRED case 2 for the SRNL cooling tower model.
  - d. *./Cooling\_Tower\_Model\_Case\_3/*: This folder contains the I/O files for MULTI-PRED case 3 for the SRNL cooling tower model.
  - e. *./Cooling\_Tower\_Model\_Case\_4/*: This folder contains the I/O files for MULTI-PRED case 4 for the SRNL cooling tower model.

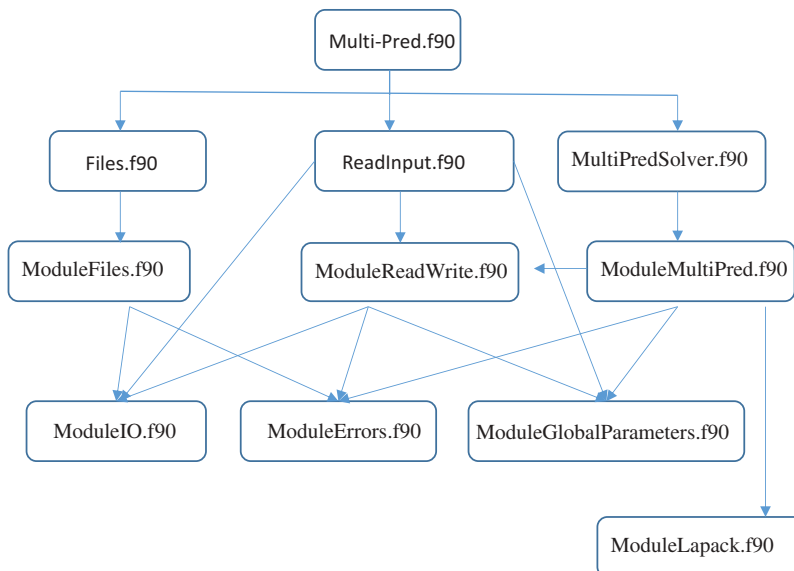


Fig. 1. MULTI-PRED code structure.

3. *multi-pred/matrix\_positive\_definite\_test/*: This folder contains the source code for a standalone program used to test if a symmetric matrix is positive definite (SPD).

Note that the covariance matrices  $\mathbf{C}_{aa}(N_a \times N_a)$ ,  $\mathbf{C}_{rr}(N_r \times N_r)$ ,  $\mathbf{C}_{bb}(N_b \times N_b)$ , and  $\mathbf{C}_{qq}(N_q \times N_q)$  must be SPD matrices. This program computes the Cholesky factorization of the matrix being tested. If it can be factorized, the program returns a flag indicating that the tested matrix is SPD. Running this test standalone program is optional, since the Cholesky factorization has also been implemented in MULTI-PRED. Also included in this folder is a large-scale matrix used for the SPD test. This matrix is a large SPD matrix, with a seemingly random sparsity pattern. It has a dimension of  $60\,000 \times 60\,000$  with 410 077 nonzero elements.<sup>a</sup>

### III.C. Code Compilation and Execution

Compilation and execution are accomplished as follows:

1. Compile the software program in Linux. Enter the *multi-pred/source/* directory and use the command *make*. An executable named *multi-pred* will be generated under the source directory. The compiler used in the *makefile* is ifort (version 12.1.6 and above). It can also be compiled with gfortran (version 4.47 and above). An example *makefile* with the gfortran compiler, named *makefile.gfortran*, is also included in the source directory.

2. Run the program. To run the program, copy the executable *multi-pred* into the example directories, then use the command: */multi-pred superfile.inp* where the argument *superfile.inp* contains all the I/O file names. Output files will be generated in the respective example folders.

### III.D. Input and Output File Organization

This section describes the I/O files within the MULTI-PRED module.

#### III.D.1. Super-File

The MULTI-PRED super-file is a text file that contains the names of I/O files and organizes the individual files for I/O operations. This super-file is read from the command line (UNIT = 5) as an argument. The first line of the super-file is reserved for an identifier card, MultiPredSup. After the

<sup>a</sup> Refer to the following website <http://www.cise.ufl.edu/research/sparse/matrices/Andrews/Andrews> for detailed information about this matrix.

TABLE I  
MultiPredSup Super-File Format for MULTI-PRED  
Case 4: Two Coupled Multi-Physics Models

| Category   | File Name        |
|------------|------------------|
| 'dims'     | 'dimensions.inp' |
| 'a_nom'    | 'a.inp'          |
| 'r_mea'    | 'rm.inp'         |
| 'r_com'    | 'rc.inp'         |
| 'C_aa'     | 'Caa.inp'        |
| 'C_ar'     | 'Car.inp'        |
| 'C_rr'     | 'Crr.inp'        |
| 'S_ra'     | 'Sra.inp'        |
| 'b_nom'    | 'b.inp'          |
| 'q_mea'    | 'qm.inp'         |
| 'q_com'    | 'qc.inp'         |
| 'C_bb'     | 'Cbb.inp'        |
| 'C_bq'     | 'Cbq.inp'        |
| 'C_qq'     | 'Cqq.inp'        |
| 'S_qb'     | 'Sqb.inp'        |
| 'C_ab'     | 'Cab.inp'        |
| 'C_aq'     | 'Caq.inp'        |
| 'C_br'     | 'Cbr.inp'        |
| 'C_rq'     | 'Crq.inp'        |
| 'S_rb'     | 'Srb.inp'        |
| 'S_qa'     | 'Sqa.inp'        |
| 'a_BE'     | 'aBE.out'        |
| 'r_BE'     | 'rBE.out'        |
| 'C_aaBE'   | 'CaaBE.out'      |
| 'C_rrBE'   | 'CrrBE.out'      |
| 'C_arBE'   | 'CarBE.out'      |
| 'Crr_comp' | 'Crrcomp.out'    |
| 'b_BE'     | 'bBE.out'        |
| 'q_BE'     | 'qBE.out'        |
| 'C_bbBE'   | 'CbbBE.out'      |
| 'C_qqBE'   | 'CqqBE.out'      |
| 'C_bqBE'   | 'CbqBE.out'      |
| 'Cqq_comp' | 'Cqqcomp.out'    |
| 'C_abBE'   | 'CabBE.out'      |
| 'C_aqBE'   | 'CaqBE.out'      |
| 'C_brBE'   | 'CbrBE.out'      |
| 'C_rqBE'   | 'CrqBE.out'      |
| 'Crq_comp' | 'Crqcomp.out'    |
| 'chi2'     | 'chi2.out'       |

identifier line, each subsequent line is preceded by a category code and a file name. The category code and file name have to be enclosed in single quotes. The file names can be changed by the user. The second line of the super-file is also reserved for the dims category; the corresponding input file defines the dimensions of the matrices and vectors used in MULTI-PRED. The lines after the second line are for data files. There are no restrictions regarding the order of the data files and their corresponding categories. Table I shows the format and complete list of super-files for MULTI-PRED case 4: Two Coupled Multi-Physics Models.

TABLE II  
Summary of I/O Files for MULTI-PRED Case 4: Two Coupled Multi-Physics Models

| File                  | Unit | I/O    | Corresponding Vector/Matrix     | Description   |
|-----------------------|------|--------|---------------------------------|---|
| <i>superfile.inp</i>  | 5    | Input  |                                 | File organization   |
| <i>dimensions.inp</i> | 20   | Input  |                                 | Defines the case selection and dimensions control   |
| <i>a.inp</i>          | 21   | Input  | $\alpha(N_a)$                   | Nominal values of $N_a$ parameters of model A   |
| <i>rm.inp</i>         | 22   | Input  | $r_m(N_r)$                      | Nominal values of $N_r$ measured responses of model A   |
| <i>rc.inp</i>         | 23   | Input  | $r_c(N_r)$                      | Nominal values of $N_r$ computed responses of model A   |
| <i>Caa.inp</i>        | 24   | Input  | $C_{aa}(N_a \times N_a)$        | Covariance matrix of $N_a$ parameters of model A  |
| <i>Car.inp</i>        | 25   | Input  | $C_{ar}(N_a \times N_r)$        | Correlations between $N_a$ parameters and $N_r$ responses of model A                                      |
| <i>Crr.inp</i>        | 26   | Input  | $C_{rr}(N_r \times N_r)$        | Covariance matrix of $N_r$ responses of model A   |
| <i>Sra.inp</i>        | 27   | Input  | $S_{ra}(N_r \times N_a)$        | Absolute sensitivities of $N_r$ responses of model A with respect to $N_a$ parameters of model A          |
| <i>b.inp</i>          | 31   | Input  | $b(N_b)$                        | Nominal values of $N_b$ parameters of model B   |
| <i>qm.inp</i>         | 32   | Input  | $q_m(N_q)$                      | Nominal values of $N_q$ measured responses of model B   |
| <i>qc.inp</i>         | 33   | Input  | $q_c(N_q)$                      | Nominal values of $N_q$ computed responses of model B   |
| <i>Cbb.inp</i>        | 34   | Input  | $C_{bb}(N_b \times N_b)$        | Covariance matrix of $N_b$ parameters of model B  |
| <i>Cbq.inp</i>        | 35   | Input  | $C_{bq}(N_b \times N_q)$        | Correlations between $N_b$ parameters and $N_q$ responses of model B                                      |
| <i>Cqq.inp</i>        | 36   | Input  | $C_{qq}(N_q \times N_q)$        | Covariance matrix of $N_q$ responses of model B   |
| <i>Sqb.inp</i>        | 37   | Input  | $S_{qb}(N_q \times N_b)$        | Absolute sensitivities of $N_q$ responses of model B with respect to $N_b$ parameters of model B          |
| <i>Cab.inp</i>        | 41   | Input  | $C_{ab}(N_a \times N_b)$        | Correlation matrix between the $N_a$ parameters of model A and the $N_b$ parameters of model B            |
| <i>Caq.inp</i>        | 42   | Input  | $C_{aq}(N_a \times N_q)$        | Correlation matrix between the $N_a$ parameters and of model A and $N_q$ responses of model B             |
| <i>Cbr.inp</i>        | 43   | Input  | $C_{br}(N_b \times N_r)$        | Correlation matrix between the $N_b$ parameters of model B and $N_r$ responses of model A                 |
| <i>Crq.inp</i>        | 44   | Input  | $C_{rq}(N_r \times N_q)$        | Correlation matrix of between $N_r$ responses of model A and $N_q$ responses of model B                   |
| <i>Srb.inp</i>        | 45   | Input  | $S_{rb}(N_r \times N_b)$        | Absolute sensitivities of $N_r$ responses of model A with respect to $N_b$ parameters of model B          |
| <i>Sqa.inp</i>        | 46   | Input  | $S_{qa}(N_q \times N_a)$        | Absolute sensitivities of $N_q$ responses of model B with respect to $N_a$ parameters of model A          |
| <i>aBE.out</i>        | 51   | Output | $\alpha^{be}(N_a)$              | Best-estimate nominal values of parameters of model A   |
| <i>rBE.out</i>        | 52   | Output | $r^{be}(N_r)$                   | Best-estimate nominal values of responses of model A  |
| <i>CaaBE.out</i>      | 53   | Output | $C_{aa}^{be}(N_a \times N_a)$   | Predicted covariance matrix of $N_a$ parameters of model A  |
| <i>CrrBE.out</i>      | 54   | Output | $C_{rr}^{be}(N_r \times N_r)$   | Predicted covariance matrix of $N_r$ responses of model A   |
| <i>CarBE.out</i>      | 55   | Output | $C_{ar}^{be}(N_a \times N_r)$   | Predicted correlation matrix between the $N_a$ parameters and $N_r$ responses of model A                  |
| <i>Crrcomp.out</i>    | 56   | Output | $C_{rr}^{comp}(N_r \times N_r)$ | Covariance matrix of $N_r$ computed responses of model A  |
| <i>bBE.out</i>        | 61   | Output | $b^{be}(N_b)$                   | Best-estimate nominal values of parameters of model B   |
| <i>qBE.out</i>        | 62   | Output | $q^{be}(N_q)$                   | Best-estimate nominal values of responses of model B  |
| <i>CbbBE.out</i>      | 63   | Output | $C_{bb}^{be}(N_b \times N_b)$   | Predicted covariance matrix of $N_b$ parameters of model B  |
| <i>CqqBE.out</i>      | 64   | Output | $C_{qq}^{be}(N_q \times N_q)$   | Predicted covariance matrix of $N_q$ responses of model B   |
| <i>CbqBE.out</i>      | 65   | Output | $C_{bq}^{be}(N_b \times N_q)$   | Predicted correlation matrix between the $N_b$ parameters and $N_q$ responses of model B                  |
| <i>Cqqcomp.out</i>    | 66   | Output | $C_{qq}^{comp}(N_q \times N_q)$ | Covariance matrix of $N_q$ computed responses of model B  |
| <i>CabBE.out</i>      | 71   | Output | $C_{ab}^{be}(N_a \times N_b)$   | Predicted correlation matrix between the $N_a$ parameters of model A and the $N_b$ parameters for model B |

(Continued)

TABLE II (Continued)

| File               | Unit | I/O    | Corresponding Vector/Matrix     | Description   |
|--------------------|------|--------|---------------------------------|---|
| <i>CaqBE.out</i>   | 72   | Output | $C_{aq}^{be}(N_a \times N_q)$   | Predicted correlation matrix between the $N_a$ parameters and of model A and $N_q$ responses of model B |
| <i>CbrBE.out</i>   | 73   | Output | $C_{br}^{be}(N_b \times N_r)$   | Predicted correlation matrix between the $N_b$ parameters of model B and $N_r$ responses of model A     |
| <i>CrqBE.out</i>   | 74   | Output | $C_{rq}^{be}(N_r \times N_q)$   | Predicted correlation matrix of between $N_r$ responses of model A and $N_q$ responses of model B       |
| <i>Crqcomp.out</i> | 75   | Output | $C_{rq}^{comp}(N_r \times N_q)$ | Correlation matrix of $N_r$ computed responses of model A and $N_q$ computed responses of model B       |
| <i>chi2.out</i>    | 76   | Output | $\chi^2$ , scalar               | Value of the consistency indicator  |

TABLE III

Input Data Files for MULTI-PRED Case 4

| Input Data Files for Model A | Input Data Files for the Coupled Matrices Between Model A and Model B | Input Data Files for Model B |
|------------------------------|---|------------------------------|
| <i>a.inp</i>                 | –   | <i>b.inp</i>                 |
| <i>rm.inp</i>                | –   | <i>qm.inp</i>                |
| <i>rc.inp</i>                | –   | <i>qc.inp</i>                |
| <i>Caa.inp</i>               | <i>Cab.inp</i>  | <i>Cbb.inp</i>               |
| <i>Car.inp</i>               | <i>Caq.inp, Cbr.inp</i>   | <i>Cbq.inp</i>               |
| <i>Crr.inp</i>               | <i>Crq.inp</i>  | <i>Ccq.inp</i>               |
| <i>Sra.inp</i>               | <i>Sqa.inp, Srb.inp</i>   | <i>Sqb.inp</i>               |

III.D.2. Contents and Organization of I/O Files

The file *dimensions.inp* defines the following important control variables.

CaseNumber—Multi-Pred case selection:

- $N_a$ : number of parameters for model A
- $N_r$ : number of responses for model A
- $N_b$ : number of additional parameters for model A (case 2) or the number of parameters of model B (case 4)
- $N_q$ : number of additional responses for model A (case 3) or the number of responses of model B (case 4).

All data files are in the sparse triplet matrix file format, which is a commonly used ASCII file format for storing sparse matrices and is compatible with most files in the Matrix Market format.

The sparse triplet data structure simply records, for each nonzero entry of the matrix, the row, column, and value. The general format is as follows:

```

Line 1:      M      N      Nz
Line 2:      Row_index Col_index Val
Line 3:      Row_index Col_index Val
...
Line Nz + 1: Row_index Col_index Val
    
```

In the above format, the quantities **M** and **N** denote, respectively, the number of rows and columns in the original full matrix; **Nz** denotes total number of nonzero elements in the matrix; **Row\_index** and **Col\_index** denote the row and column indices of each nonzero element; and **VAL** denotes the value of the nonzero element.

Table II describes the contents of the I/O files specified within the MULTI-PRED super-files for case 4: Two Coupled Multi-Physics Models.

III.D.3. Input Data Files for MULTI-PRED Case 4

Table III presents the 20 input files required for MULTI-PRED case 4.



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