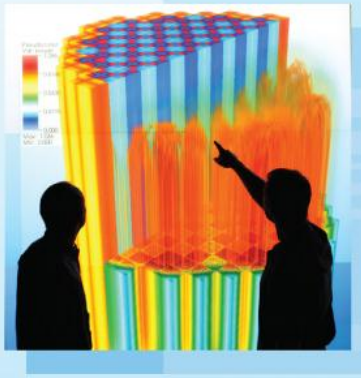
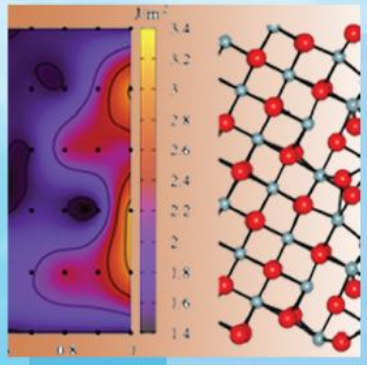
CASL-U-2011-0055-000

Power uprates
and plant life extension



Engineering design
and analysis

Science-enabling
high performance
computing



Fundamental science

Plant operational data

Consortium for Advanced Simulation of LWRs

L3:VUQ.VVDA.P2-2.01

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U.S. DEPARTMENT OF ENERGY | Nuclear Energy

BEST ESTIMATE PLUS REDUCED UNCERTAINTIES (BERU) PREDICTIONS

VUQ.Y1.02	Enable generalized data assimilation and model calibration for VERA.	06/30/2011	All

VUQ.VVDA.Y1-2.01	Develop mathematical data assimilation framework	06/30/2011	VUQ.Y1.02

Dan G. Cacuci (April 3, 2011)

NOTE: This report is based on the work by :

Dan G. Cacuci and Mihaela Ionescu-Bujor, "*Model Calibration and Best-Estimate Prediction Through Experimental Data Assimilation: I. Mathematical Framework*", ***Nucl. Sci. Eng.***, **165**, 18 - 44, 2010.

Repeated measurements of the same physical quantity yield values that differ from each other, as well as from the true but unknown value of that quantity. This variation in results is due to experimental errors, imperfect instruments, and imperfectly known calibration standards. Hence, around any reported experimental value, there always exists a range of values that may also be plausibly representative of the true value. In turn, this means that all inferences, predictions, engineering computations, and other applications of measured data are necessarily founded on weighted averages over all the possibly true values, with weights indicating the degree of plausibility of each value. These weights and weighted averages are what we call probabilities and expectation values. Hence, probabilities encode incomplete

information, in that persons possessing different information or knowledge would assign different probabilities, and would update the respective probabilities whenever new information became available. Thus, since the true value of physical quantities cannot be measured exactly, nominally measured values are insufficient, by themselves, for applications; the quantitative uncertainties accompanying the measurements are also needed, along with the respective nominal values. Combination of data from different sources involves a weighted propagation (e.g., using sensitivities) of various uncertainties, requiring reasoning from incomplete information for extracting "best" values together with "best" uncertainties from often sparse, incomplete, error-afflicted, and occasionally discrepant experimental data. A wide range of probability-theory concepts and tools are 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.

Since the combination of data from different sources involves a weighted propagation (e.g., using sensitivities) of various, data evaluation is intrinsically intertwined with uncertainty analysis, requiring reasoning from incomplete information and using probability theory for extracting "best" values together with "best" uncertainties from often sparse, incomplete, error-afflicted, and occasionally discrepant experimental data. The probabilistic description of possible future computational and experimental outcomes, based on all recognized errors and uncertainties, is the aim of *"best estimates plus reduced uncertainties" (BERU) predictions.* BERU-predictions relies on the assimilation of experimental data ("data assimilation") for updating (i.e., "calibrating" or "adjusting") the parameters characterizing a computational model. The procedures for model calibration must encompass the propagation of all relevant uncertainties, including:

(i) data uncertainties (input data, model parameters, initial and boundary conditions, forcing functions, etc);

(ii) numerical discretization errors;

(iii) discrepancies within the experimental data and/or discrepancies between data and model predictions; and

(iv) uncertainties in the physics of the modeled processes (e.g., due to incomplete knowledge).

The results of BERU-predictions are best-estimated values for parameters and predicted responses, as well as best-estimate reduced uncertainties (i.e., "smaller" values for the variance-covariance matrices) for the predicted best-estimate parameters and responses, provided all elements involved in the calibration process are consistent with each other.

This paper presents a new and rigorous mathematical methodology for predictive estimation through data assimilation and simultaneous calibration of model parameters and responses for a generic time-dependent physical system, generalizing and setting on a rigorous basis the pioneering work originally presented in Refs. 3 and 4, as well as the data assimilation methodologies currently used in geophysical sciences (see, e.g., Refs. 5 and 6). This methodology also provides quantitative indicators (based on uncertainties and sensitivities) for determining the degree of agreement (or disagreement) relevant to the assimilation and best-estimate adjustment of computational and experimental parameters and responses. The paper is structured as follows: Section II introduces the mathematical and physical basis for assigning prior probability distributions under incomplete information. Section III presents the mathematical framework for data assimilation and simultaneous calibration of model parameters and responses, for a generic time-dependent physical system; of course, time independent systems are included as a particular case within this framework. Furthermore, this framework also encompasses the basic elements for *quantitative model extrapolation* (i.e., 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) and *estimation of the validation domain*. The data assimilation and best-estimate model calibration methodology presented in Section III also includes quantitative indicators (based on uncertainties and sensitivities) for determining the degree of agreement (or disagreement) relevant to the assimilation and best-estimate adjustment of parameters and responses, of computations and experiments. An illustrative application of the methodology presented in Sections III to a paradigm transient thermal-hydraulics system of benchmark quality for reactor safety codes is presented in the accompanying PART II[7] of this paper. Section IV presents the fundamental indicators for data consistency and rejection criteria. Finally, Section V offers concluding remarks, addressing further work needed to alleviate the current limitations of the best-estimate predictive methodology presented in this work.

III. EXPERIMENTAL DATA ASSIMILATION FOR MODEL CALIBRATION AND PREDICTIVE ESTIMATION

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).

The time-dependent generic physical system to be analyzed in the sequel is considered to comprise N_α^ν model parameters and N_r^ν distinct responses, respectively, at every time node $\nu = 1, 2, \ldots, N_t$. Hence, at every time node ν, the (column) vector $\boldsymbol{\alpha}^\nu$ of J_α^ν system parameters, and the (column) vector $\mathbf{r}^\nu$ of J_r^ν measured responses can be represented in component form as

$$\boldsymbol{\alpha}^\nu = \left\{ \alpha_n^\nu \,|\, n = 1, \ldots N_\alpha^\nu \right\}, \quad \mathbf{r}^\nu = \left\{ r_i^\nu \,|\, i = 1, \ldots, N_r^\nu \right\}, \quad \nu = 1, \ldots, N_t . \tag{III.1}$$

At any time node ν, the system parameters are considered to be variates with mean values $\left(\boldsymbol{\alpha}^0\right)^\nu$. Furthermore, the correlations between two parameters α_i^ν and α_j^μ, at two time nodes μ and ν, have the general form

$$c_{\alpha,ij}^{\nu\mu} \equiv \left\langle \left[\alpha_i^\nu - \left(\alpha_i^\nu\right)^0 \right] \left[\alpha_j^\mu - \left(\alpha_j^\mu\right)^0 \right] \right\rangle, \tag{III.2}$$

The above covariances constitute the elements of symmetric covariance matrices of the form

$$\mathbf{C}_\alpha^{\mu\nu} \triangleq \left\langle \left(\boldsymbol{\alpha} - \boldsymbol{\alpha}^0\right)^\mu \left[\left(\boldsymbol{\alpha} - \boldsymbol{\alpha}^0\right)^\nu \right]^\dagger \right\rangle = \left(\mathbf{C}_\alpha^{\mu\nu}\right)^\dagger = \mathbf{C}_\alpha^{\nu\mu} = \left(\mathbf{C}_\alpha^{\nu\mu}\right)^\dagger . \tag{III.3}$$

Similarly, the *measured* responses are characterized by mean values $\left(\mathbf{r}_m\right)^\nu$ at a time node ν, and by symmetric covariance matrices between two time nodes μ and ν defined as

$$\mathbf{C}_m^{\mu\nu} \triangleq \left\langle \left(\mathbf{r}-\mathbf{r}_m\right)^{\mu}\left[\left(\mathbf{r}-\mathbf{r}_m\right)^{\nu}\right]^{\dagger}\right\rangle = \left(\mathbf{C}_m^{\mu\nu}\right)^{\dagger} = \mathbf{C}_m^{\nu\mu} = \left(\mathbf{C}_m^{\nu\mu}\right)^{\dagger}. \qquad \text{(III.4)}$$

In the most general case, the measured responses may be correlated to the parameters through symmetric *response-parameter uncertainty* matrices of the form

$$\mathbf{C}_{r\alpha}^{\mu\nu} \triangleq \left\langle \left(\mathbf{r}-\mathbf{r}_m\right)^{\mu}\left[\left(\boldsymbol{\alpha}-\boldsymbol{\alpha}^0\right)^{\nu}\right]^{\dagger}\right\rangle = \left(\mathbf{C}_{r\alpha}^{\mu\nu}\right)^{\dagger} = \mathbf{C}_{r\alpha}^{\nu\mu} = \left(\mathbf{C}_{r\alpha}^{\nu\mu}\right)^{\dagger}. \qquad \text{(III.5)}$$

Note that the matrices $\mathbf{C}_{r\alpha}^{\mu\nu}$ are *not* bona-fide variance-covariance matrices, in that they are not necessarily square positive matrices (often, they are rectangular), and the elements on the their respective main diagonals (if they happen to be square) are also covariances (or correlations) rather that variances.

At any given time node ν, a response r_i^{ν} can be a function of not only the system parameters at time node ν, but also of the system parameters at all previous time nodes μ, $1 \le \mu \le \nu$; this means that $\mathbf{r}^{\nu} = \mathbf{R}^{\nu}\left(\mathbf{p}^{\nu}\right)$, where $\mathbf{p}^{\nu} \triangleq \left(\boldsymbol{\alpha}^1,\ldots,\boldsymbol{\alpha}^{\mu},\ldots,\boldsymbol{\alpha}^{\nu}\right)$. In general, the response computed using the model depends nonlinearly and implicitly (in an analytically intractable form) on the model parameters. Furthermore, the uncertainties in parameters and modeling induce uncertainties in the computed responses, and can be computed either by means of statistical methods (for relatively simple models with few parameters) or deterministically, by using the well-known propagation of moments (errors) method (see, e.g., Ref 16). In this method, the computed response is linearized via a functional Taylor-series expansion around the nominal values, $\mathbf{p}_0^{\nu} \triangleq \left(\left(\boldsymbol{\alpha}^0\right)^1,\ldots,\left(\boldsymbol{\alpha}^0\right)^{\mu},\ldots,\left(\boldsymbol{\alpha}^0\right)^{\nu}\right)$, of the parameters $\mathbf{p}^{\nu}$, as follows:

$$\mathbf{r}^{\nu} = \mathbf{R}^{\nu}\left(\mathbf{p}^{\nu}\right) = \mathbf{R}^{\nu}\left(\mathbf{p}_0^{\nu}\right) + \sum_{\mu=1}^{\nu} \mathbf{S}^{\nu\mu}\left(\mathbf{p}_0^{\mu}\right)\left[\boldsymbol{\alpha}^{\mu} - \left(\boldsymbol{\alpha}^0\right)^{\mu}\right] + \ldots, \ \nu = 1,\ldots,N_t, \qquad \text{(III.6)}$$

where $\mathbf{R}^{\nu}\left(\mathbf{p}_0^{\nu}\right)$ denotes the vector of computed responses at a time node ν, at the nominal parameter values $\mathbf{p}_0^{\nu}$, while $\mathbf{S}^{\nu\mu}\left(\mathbf{p}_0^{\mu}\right)$, $1 \le \mu \le \nu$, represents the $\left(J_r^{\nu} \times J_{\alpha}^{\mu}\right)$-dimensional matrix containing the first Gateaux-derivatives of the computed responses with respect to the parameters, defined as

$$\mathbf{S}^{\nu\mu}\left(\mathbf{p}_0^{\mu}\right) \triangleq \begin{pmatrix} s_{11}^{\nu\mu} & \cdots & s_{1N}^{\nu\mu} \\ \vdots & s_{in}^{\nu\mu} & \vdots \\ s_{I1}^{\nu\mu} & \cdots & s_{IN}^{\nu\mu} \end{pmatrix} \triangleq \begin{pmatrix} \dfrac{\partial R_1^{\nu}\left(\mathbf{p}_0^{\mu}\right)}{\partial \alpha_1^{\mu}} & \cdots & \dfrac{\partial R_1^{\nu}\left(\mathbf{p}_0^{\mu}\right)}{\partial \alpha_N^{\mu}} \\ \vdots & \dfrac{\partial R_i^{\nu}}{\partial \alpha_n^{\mu}} & \vdots \\ \dfrac{\partial R_I^{\nu}\left(\mathbf{p}_0^{\mu}\right)}{\partial \alpha_1^{\mu}} & \cdots & \dfrac{\partial R_I^{\nu}\left(\mathbf{p}_0^{\mu}\right)}{\partial \alpha_N^{\mu}} \end{pmatrix}, \ 1 \le \mu \le \nu . \qquad \text{(III.7)}$$

Since the response $\mathbf{R}^{\nu}\left(\mathbf{p}_0^{\nu}\right)$ at time node ν can depend only on parameters $\left(\boldsymbol{\alpha}^0\right)^{\mu}$ which appear up to the current time node ν, it follows that $\mathbf{S}^{\nu\mu} = \mathbf{0}$ when $\mu > \nu$, and hence non-zero terms in the expansion shown in Eq. (III.6) can only occur in the range $1 \le \mu \le \nu$. By introducing the block matrix

$$\mathbf{S} \triangleq \begin{pmatrix} \mathbf{S}^{11} & \cdots & \mathbf{0} \\ \vdots & \ddots & \vdots \\ \mathbf{S}^{N_t 1} & \cdots & \mathbf{S}^{N_t N_t} \end{pmatrix}, \qquad \text{(III.8)}$$

and the (block) column vectors

$$\boldsymbol{\alpha} \triangleq \left(\boldsymbol{\alpha}^1,\ldots,\boldsymbol{\alpha}^\mu,\ldots,\boldsymbol{\alpha}^{N_t}\right), \qquad \mathbf{r} \triangleq \left(\mathbf{r}^1,\ldots,\mathbf{r}^\mu,\ldots,\mathbf{r}^{N_t}\right), \mathbf{R}\left(\boldsymbol{\alpha}^0\right) \triangleq \left(\mathbf{R}^1,\ldots,\mathbf{R}^\mu,\ldots,\mathbf{R}^{N_t}\right), \quad \text{(III.9)}$$

the system shown in Eq. (III.6) can be written in the form

$$\mathbf{r} = \mathbf{R}\left(\boldsymbol{\alpha}^0\right) + \mathbf{S}\left(\boldsymbol{\alpha} - \boldsymbol{\alpha}^0\right) + \textit{higher order terms}. \qquad \text{(III.10)}$$

Applying the propagation of errors method (see, e.g., Ref 16) to Eq. (III.10), which involves the formal integration of the over the unknown joint distributions of the parameters $\boldsymbol{\alpha}$, yields the following expressions for the expectation value, $\langle \mathbf{r} \rangle$, of the response $\mathbf{r}$, and the corresponding covariance matrix, $\mathbf{C}_{rc}\left(\boldsymbol{\alpha}^0\right)$, of the computed responses, respectively

$$\langle \mathbf{r} \rangle = \mathbf{R}\left(\boldsymbol{\alpha}^0\right), \qquad \text{(III.11)}$$

and

$$\mathbf{C}_{rc}\left(\boldsymbol{\alpha}^0\right) \triangleq \left\langle \delta\mathbf{r}\delta\mathbf{r}^\dagger \right\rangle = \left[\mathbf{S}\left(\boldsymbol{\alpha}^0\right)\right]\left\langle \delta\boldsymbol{\alpha}\delta\boldsymbol{\alpha}^\dagger \right\rangle\left[\mathbf{S}\left(\boldsymbol{\alpha}^0\right)\right]^\dagger = \left[\mathbf{S}\left(\boldsymbol{\alpha}^0\right)\right]\mathbf{C}_\alpha\left[\mathbf{S}\left(\boldsymbol{\alpha}^0\right)\right]^\dagger. \qquad \text{(III.12)}$$

The covariance matrix of the computed responses, $\mathbf{C}_{rc}$, has the symmetric structure

$$\mathbf{C}_{rc} \triangleq \begin{pmatrix} \mathbf{C}_{rc}^{11} & \cdots & \mathbf{C}_{rc}^{1N_t} \\ \vdots & \ddots & \vdots \\ \mathbf{C}_{rc}^{N_t 1} & \cdots & \mathbf{C}_{rc}^{N_t N_t} \end{pmatrix} \qquad \mathbf{C}_{rc}^{\nu\mu} = \sum_{\eta=1}^{\nu}\sum_{\rho=1}^{\mu} \mathbf{S}^{\nu\eta}\mathbf{C}_\alpha^{\eta\rho}\left(\mathbf{S}^{\mu\rho}\right)^\dagger = \left(\mathbf{C}_{rc}^{\mu\nu}\right)^\dagger; \quad \nu,\mu = 1,\ldots,N_t. \quad \text{(III.13)}$$

As indicated by Eq. (III.11), the expectation value of the computed responses for linearized models in which the numerical errors are neglected is given by the value of the response computed at the nominal parameter-values.

Applying now the maximum entropy algorithm described in Section II [cf. Eq. (II.18)] to the computational and experimental information described above indicates that the most objective probability distribution for this information is a multivariate Gaussian of the form

$$p\left(\mathbf{z}\,|\,\mathbf{C}\right)d\left(\mathbf{z}\right)=\frac{\exp\left[-\frac{1}{2}Q\left(\mathbf{z}\right)\right]}{\det\left(2\pi\mathbf{C}\right)^{1/2}}\,d\left(\mathbf{z}\right),\ Q\left(\mathbf{z}\right)\equiv\mathbf{z}^{\dagger}\,\mathbf{C}^{-1}\mathbf{z}\ ,-\infty<z_j<\infty\,, \qquad \text{(III.14)}$$

where:

$$\mathbf{z}\equiv\begin{pmatrix}\boldsymbol{\alpha}-\boldsymbol{\alpha}^0\\ \mathbf{r}-\mathbf{r}_m\end{pmatrix},\ \ \boldsymbol{\alpha}^0\triangleq\left(\left(\boldsymbol{\alpha}^0\right)^1,\ldots,\left(\boldsymbol{\alpha}^0\right)^{\mu},\ldots,\left(\boldsymbol{\alpha}^0\right)^{N_t}\right)\quad, \qquad \text{(III.15)}$$

$$\mathbf{C}\equiv\begin{pmatrix}\mathbf{C}_{\alpha} & \mathbf{C}_{\alpha r}\\ \mathbf{C}_{r\alpha} & \mathbf{C}_{m}\end{pmatrix},\qquad \mathbf{C}_{\alpha}=\begin{pmatrix}\mathbf{C}_{\alpha}^{11} & \mathbf{C}_{\alpha}^{12} & \ldots & \ldots\\ \mathbf{C}_{\alpha}^{21} & \mathbf{C}_{\alpha}^{22} & \ldots & \ldots\\ \ldots & \ldots & \ldots & \ldots\\ \ldots & \ldots & \ldots & \mathbf{C}_{\alpha}^{N_tN_t}\end{pmatrix}\qquad \mathbf{C}_{\alpha r}=\begin{pmatrix}\mathbf{C}_{\alpha r}^{11} & \mathbf{C}_{\alpha r}^{12} & \ldots & \ldots\\ \mathbf{C}_{\alpha r}^{21} & \mathbf{C}_{\alpha r}^{22} & \ldots & \ldots\\ \ldots & \ldots & \ldots & \ldots\\ \ldots & \ldots & \ldots & \mathbf{C}_{\alpha r}^{N_tN_t}\end{pmatrix}$$

$$\mathbf{C}_{x}=\begin{pmatrix}\mathbf{C}_{x}^{11} & \mathbf{C}_{x}^{12} & \ldots & \ldots\\ \mathbf{C}_{x}^{21} & \mathbf{C}_{x}^{22} & \ldots & \ldots\\ \ldots & \ldots & \ldots & \ldots\\ \ldots & \ldots & \ldots & \mathbf{C}_{x}^{N_tN_t}\end{pmatrix} \qquad \text{(III.16)}$$

The posterior information contained in Eqs. (III.14) and (III.10) can now be condensed into a recommended best-estimate value $\left(\mathbf{z}^{be}\right)^{\nu}$ at a time node ν for the parameters $\boldsymbol{\alpha}^{\nu}$ and responses $\mathbf{r}^{\nu}$, together with corresponding best-estimate recommended uncertainties for these

quantities. If a loss function is given, decision theory[7] indicates how these best-estimate quantities are to be computed. If no specific loss function is provided, the recommended best-estimate updated posterior mean vector $\left(\mathbf{z}^{be}\right)^{\nu}$ and its respective best-estimate posterior covariance matrix are usually evaluated by assuming "quadratic loss". In such a case, the bulk of the contribution to the distribution $p\left(\mathbf{z}\,|\mathbf{C}\right)$ in Eq. (III.14) is extracted by computing it at the point in phase space where the respective exponent attains its minimum, subject to the relation provided by Eq. (III.10). When, in addition to *neglecting the higher-order terms*, the *numerical errors are also neglected* in Eq. (III.10), this relation is imposed as a hard constraint, which can be conveniently written in the form

$$\mathbf{Z}\left(\boldsymbol{\alpha}^{0}\right)\mathbf{z}+\mathbf{d}=\mathbf{0}\,,\quad \mathbf{d}\triangleq\mathbf{R}\left(\boldsymbol{\alpha}^{0}\right)-\mathbf{r}_{m}\,, \tag{III.17}$$

where $\mathbf{r}_{m}\triangleq\left(\mathbf{r}_{m}^{1},\ldots,\mathbf{r}_{m}^{\mu},\ldots,\mathbf{r}_{m}^{N_t}\right)$ is the vector comprising all of the experimentally measured responses, $\mathbf{d}\triangleq\mathbf{R}\left(\boldsymbol{\alpha}^{0}\right)-\mathbf{r}_{m}$ is a vector of "deviations" reflecting the discrepancies between the nominal computations and the nominally measured responses, while $\mathbf{Z}$ denotes the partitioned matrix

$$\mathbf{Z}\triangleq\left(\mathbf{S}\quad\mathbf{U}\right);\quad \mathbf{U}\triangleq\begin{pmatrix}-\mathbf{I}^{11} & \cdots & \mathbf{0}\\ \vdots & \ddots & \vdots\\ \mathbf{0} & \cdots & -\mathbf{I}^{N_tN_t}\end{pmatrix}, \tag{III.18}$$

where $\mathbf{I}^{\nu\nu}$, $\nu=1,\ldots,N_t$, denotes the identity matrix of corresponding dimensions.

Computing the stationary point of $Q(\mathbf{z})$ subject to Eq. (III.17) poses a constrained minimization problem which can be solved by introducing Lagrange multipliers, $\boldsymbol{\lambda}$, to construct the augmented Lagrangian functional $P(\mathbf{z},\boldsymbol{\lambda})$ defined as

$$P(\mathbf{z},\boldsymbol{\lambda}) \equiv Q(\mathbf{z}) + 2\boldsymbol{\lambda}^{\dagger}\left[\mathbf{Z}(\boldsymbol{\alpha}^{0})\mathbf{z} + \mathbf{d}\right] = \min,\ \ at\ \mathbf{z} = \mathbf{z}^{be} \equiv \begin{pmatrix} \boldsymbol{\alpha}^{be} - \boldsymbol{\alpha}^{0} \\ \mathbf{r}^{be} - \mathbf{r}_{m} \end{pmatrix}. \tag{III.19}$$

where $\boldsymbol{\lambda} = \left(\boldsymbol{\lambda}^{1},...,\boldsymbol{\lambda}^{\nu},...,\boldsymbol{\lambda}^{N_t}\right)$ denotes the corresponding vector of Lagrange multipliers. In the above expression, the superscript "*be*" denotes "*best-estimated values*", and the factor "2" was introduced for convenience in front of $\boldsymbol{\lambda}$ in order to simplify the subsequent algebraic derivations. The point $\mathbf{z}^{be}$ where the functional $P(\mathbf{z},\boldsymbol{\lambda})$ attains its extremum (minimum) is defined implicitly through the conditions

$$\nabla_{\mathbf{z}} P(\mathbf{z},\boldsymbol{\lambda}) = \mathbf{0}, \quad \nabla_{\boldsymbol{\lambda}} P(\mathbf{z},\boldsymbol{\lambda}) = \mathbf{0}, \quad at\ \mathbf{z} = \mathbf{z}^{be}. \tag{III.20}$$

The solution to the above constrained minimization problem is detailed in the Appendix. The final results for the predictive best-estimate parameters, responses, and their corresponding reduced uncertainties (covariance matrices) are as follows:

(i) The best-estimate predicted nominal values for the calibrated (adjusted) parameters:

$$\boldsymbol{\alpha}^{be} = \boldsymbol{\alpha}^{0} + \left(\mathbf{C}_{\alpha r} - \mathbf{C}_{\alpha}\left[\mathbf{S}(\boldsymbol{\alpha}^{0})\right]^{\dagger}\right)\left[\mathbf{C}_{d}(\boldsymbol{\alpha}^{0})\right]^{-1}\mathbf{d} \tag{III.21}$$

In component form, the above expression for the calibrated best-estimate parameter values becomes

$$\left(\boldsymbol{\alpha}^{be}\right)^{\nu}=\left(\boldsymbol{\alpha}^{0}\right)^{\nu}+\sum_{\mu=1}^{N_t}\left\{\left[\mathbf{C}_{\alpha r}^{\nu\mu}-\sum_{\rho=1}^{\mu}\mathbf{C}_{\alpha}^{\nu\rho}\left(\mathbf{S}^{\dagger}\right)^{\mu\rho}\right]\left[\sum_{\eta=1}^{N_t}\mathbf{K}_{d}^{\mu\eta}\mathbf{d}^{\eta}\right]\right\},\quad \nu=1,\ldots,N_t\,. \tag{III.22}$$

where $\mathbf{K}_d^{\nu\eta}$ denotes the corresponding (ν,η)-element of the block-matrix $\mathbf{C}_d^{-1}$, with the block-matrix $\mathbf{C}_d\left(\boldsymbol{\alpha}^0\right)$ defined as follows:

$$\begin{aligned}\mathbf{C}_d\left(\boldsymbol{\alpha}^0\right)&\triangleq\left\langle\mathbf{d}\mathbf{d}^{\dagger}\right\rangle=\left\langle\left(\delta\mathbf{r}-\mathbf{S}\left(\boldsymbol{\alpha}^0\right)\delta\boldsymbol{\alpha}\right)\left(\delta\mathbf{r}^{\dagger}-\delta\boldsymbol{\alpha}^{\dagger}\left[\mathbf{S}\left(\boldsymbol{\alpha}^0\right)\right]^{\dagger}\right)\right\rangle\\&=\mathbf{C}_{rc}\left(\boldsymbol{\alpha}^0\right)-\mathbf{C}_{r\alpha}\left[\mathbf{S}\left(\boldsymbol{\alpha}^0\right)\right]^{\dagger}-\left[\mathbf{S}\left(\boldsymbol{\alpha}^0\right)\right]\mathbf{C}_{\alpha r}+\mathbf{C}_m\end{aligned} \tag{III.23}$$

In component form, the matrix $\mathbf{C}_d$ is expressed as

$$\begin{aligned}\mathbf{C}_d&\triangleq\begin{pmatrix}\mathbf{C}_d^{11}&\cdots&\mathbf{C}_d^{1N_t}\\\vdots&\ddots&\vdots\\\mathbf{C}_d^{N_t1}&\cdots&\mathbf{C}_d^{N_tN_t}\end{pmatrix}=\begin{pmatrix}\mathbf{C}_{rc}^{11}+\mathbf{C}_m^{11}&\cdots&\mathbf{C}_{rc}^{1N_t}+\mathbf{C}_m^{1N_t}\\\vdots&\ddots&\vdots\\\mathbf{C}_{rc}^{N_t1}+\mathbf{C}_m^{N_t1}&\cdots&\mathbf{C}_{rc}^{N_tN_t}+\mathbf{C}_m^{N_tN_t}\end{pmatrix}\\&-\begin{pmatrix}\mathbf{C}_{r\alpha}^{11}\left(\mathbf{S}^{\dagger}\right)^{11}+\mathbf{S}^{11}\mathbf{C}_{\alpha r}^{11}&\cdots&\mathbf{S}^{11}\mathbf{C}_{\alpha r}^{1N_t}+\sum_{\rho=1}^{N_t}\mathbf{C}_{r\alpha}^{1\rho}\left(\mathbf{S}^{\dagger}\right)^{N_t\rho}\\\vdots&\ddots&\vdots\\\mathbf{C}_{r\alpha}^{N_t1}\left(\mathbf{S}^{\dagger}\right)^{11}+\sum_{\rho=1}^{N_t}\mathbf{S}^{N_t\rho}\mathbf{C}_{\alpha r}^{\rho1}&\cdots&\sum_{\rho=1}^{N_t}\left[\mathbf{C}_{r\alpha}^{N_t\rho}\left(\mathbf{S}^{\dagger}\right)^{N_t\rho}+\mathbf{S}^{N_t\rho}\mathbf{C}_{\alpha r}^{\rho N_t}\right]\end{pmatrix}.\end{aligned} \tag{III.24}$$

(ii) The best-estimate predicted nominal values for the calibrated (adjusted) responses:

$$\mathbf{r}\left(\boldsymbol{\alpha}^{be}\right)=\mathbf{r}_m+\left(\mathbf{C}_m-\mathbf{C}_{r\alpha}\left[\mathbf{S}\left(\boldsymbol{\alpha}^0\right)\right]^{\dagger}\right)\left[\mathbf{C}_d\left(\boldsymbol{\alpha}^0\right)\right]^{-1}\mathbf{d} \tag{III.25}$$

At a specific time node ν, each component $\left(\mathbf{r}^{be}\right)^{\nu}$ of $\mathbf{r}\left(\boldsymbol{\alpha}^{be}\right)$ has the explicit form

$$\left(\mathbf{r}^{be}\right)^{\nu}=\left(\mathbf{r}_m\right)^{\nu}+\sum_{\mu=1}^{N_t}\left\{\left[\mathbf{C}_{m}^{\nu\mu}-\sum_{\rho=1}^{\mu}\mathbf{C}_{r\alpha}^{\nu\rho}\left(\mathbf{S}^{\dagger}\right)^{\mu\rho}\right]\left[\sum_{\eta=1}^{N_t}\mathbf{K}_{d}^{\mu\eta}\mathbf{d}^{\eta}\right]\right\},\quad \nu=1,\ldots,N_t\,. \tag{III.26}$$

(iii) The expressions for the best-estimate predicted covariances $\mathbf{C}_{\alpha}^{be}$ and $\mathbf{C}_{r}^{be}$, corresponding to the best-estimate parameters $\boldsymbol{\alpha}^{be}$ and responses $\mathbf{r}\left(\boldsymbol{\alpha}^{be}\right)$, together with the predicted best-estimate parameter-response covariance matrix $\mathbf{C}_{\alpha r}^{be}$ are as follows:

$$\mathbf{C}_{\alpha}^{be} \triangleq \left\langle \left(\boldsymbol{\alpha}-\boldsymbol{\alpha}^{be}\right)\left(\boldsymbol{\alpha}-\boldsymbol{\alpha}^{be}\right)^{\dagger} \right\rangle = \mathbf{C}_{\alpha} - \left[\mathbf{C}_{\alpha d}\left(\boldsymbol{\alpha}^{0}\right)\right]\left[\mathbf{C}_{d}\left(\boldsymbol{\alpha}^{0}\right)\right]^{-1}\left[\mathbf{C}_{\alpha d}\left(\boldsymbol{\alpha}^{0}\right)\right]^{\dagger}, \tag{III.27}$$

$$\mathbf{C}_{r}^{be} \triangleq \left\langle \left(\mathbf{r}-\mathbf{r}\left(\boldsymbol{\alpha}^{be}\right)\right)\left(\mathbf{r}-\mathbf{r}\left(\boldsymbol{\alpha}^{be}\right)\right)^{\dagger} \right\rangle = \mathbf{C}_{m} - \left[\mathbf{C}_{r d}\left(\boldsymbol{\alpha}^{0}\right)\right]\left[\mathbf{C}_{d}\left(\boldsymbol{\alpha}^{0}\right)\right]^{-1}\left[\mathbf{C}_{r d}\left(\boldsymbol{\alpha}^{0}\right)\right]^{\dagger}, \tag{III.28}$$

$$\mathbf{C}_{r\alpha}^{be} = \mathbf{C}_{\alpha r}^{be} \triangleq \left\langle \left(\boldsymbol{\alpha}-\boldsymbol{\alpha}^{be}\right)\left(\mathbf{r}-\mathbf{r}\left(\boldsymbol{\alpha}^{be}\right)\right)^{\dagger} \right\rangle = \mathbf{C}_{r\alpha} - \left[\mathbf{C}_{r d}\left(\boldsymbol{\alpha}^{0}\right)\right]\left[\mathbf{C}_{d}\left(\boldsymbol{\alpha}^{0}\right)\right]^{-1}\left[\mathbf{C}_{\alpha d}\left(\boldsymbol{\alpha}^{0}\right)\right]^{\dagger}, \tag{III.29}$$

where

$$\mathbf{C}_{rd}\left(\boldsymbol{\alpha}^{0}\right) \triangleq \left\langle \left(\mathbf{r}-\mathbf{r}_{m}\right)\mathbf{d}^{\dagger} \right\rangle = \left(\mathbf{C}_{m} - \mathbf{C}_{r\alpha}\left[\mathbf{S}\left(\boldsymbol{\alpha}^{0}\right)\right]^{\dagger}\right), \tag{III.30}$$

$$\mathbf{C}_{\alpha d}\left(\boldsymbol{\alpha}^{0}\right) \triangleq \left\langle \left(\boldsymbol{\alpha}-\boldsymbol{\alpha}^{0}\right)\mathbf{d}^{\dagger} \right\rangle = \left(\mathbf{C}_{\alpha r} - \mathbf{C}_{\alpha}\left[\mathbf{S}\left(\boldsymbol{\alpha}^{0}\right)\right]^{\dagger}\right), \tag{III.31}$$

For completeness, the block-matrix components, which correlate two (distinct or not) time-nodes, of the above calibrated best-estimate covariance matrices are given below:

$$\left(\mathbf{C}_{\alpha}^{be}\right)^{\nu\mu} = \mathbf{C}_{\alpha}^{\nu\mu} - \sum_{\eta=1}^{N_t}\sum_{\rho=1}^{N_t}\left[\mathbf{C}_{\alpha r}^{\nu\rho} - \sum_{\pi=1}^{\rho}\mathbf{C}_{\alpha}^{\nu\pi}\left(\mathbf{S}^{\dagger}\right)^{\rho\pi}\right]\mathbf{K}_{d}^{\rho\eta}\left[\mathbf{C}_{r\alpha}^{\eta\mu} - \sum_{\pi=1}^{\eta}\mathbf{S}^{\eta\pi}\mathbf{C}_{\alpha}^{\pi\mu}\right]. \tag{III.32}$$

$$\left(\mathbf{C}_{r}^{be}\right)^{\nu\mu} = \mathbf{C}_{m}^{\nu\mu} - \sum_{\eta=1}^{N_t}\sum_{\rho=1}^{N_t}\left[\mathbf{C}_{m}^{\nu\rho} - \sum_{\pi=1}^{\rho}\mathbf{C}_{r\alpha}^{\nu\pi}\left(\mathbf{S}^{\dagger}\right)^{\rho\pi}\right]\mathbf{K}_{d}^{\rho\eta}\left[\mathbf{C}_{m}^{\eta\mu} - \sum_{\pi=1}^{\eta}\mathbf{S}^{\eta\pi}\mathbf{C}_{\alpha r}^{\pi\mu}\right]. \tag{III.33}$$

$$\left(\mathbf{C}_{r\alpha}^{be}\right)^{\nu\mu} = \mathbf{C}_{r\alpha}^{\nu\mu} - \sum_{\eta=1}^{N_t}\sum_{\rho=1}^{N_t}\left[\mathbf{C}_{m}^{\nu\rho} - \sum_{\pi=1}^{\rho}\mathbf{C}_{r\alpha}^{\nu\pi}\left(\mathbf{S}^{\dagger}\right)^{\rho\pi}\right]\mathbf{K}_{d}^{\rho\eta}\left[\mathbf{C}_{\alpha r}^{\eta\mu} - \sum_{\pi=1}^{\eta}\mathbf{S}^{\eta\pi}\mathbf{C}_{\alpha}^{\pi\mu}\right]. \qquad \text{(III.34)}$$

Note in Eq. (III.27) that a symmetric positive matrix is subtracted from the initial parameter covariance matrix $\mathbf{C}_{\alpha}$; hence, in this sense, *the best-estimate predicted parameter uncertainty matrix* $\mathbf{C}_{\alpha}^{be}$ *has been reduced by the calibration (adjustment) procedure, through the introduction of new information from experiments*. Similarly in Eq. (III.28), a symmetric positive matrix is subtracted from the initial covariance matrix $\mathbf{C}_{m}$ of the experimental-responses; hence, *the best-estimate predicted response covariance matrix* $\mathbf{C}_{r}^{be}$ *has been improved (reduced) through the introduction of new experimental information*. Furthermore, Eq. (III.29) indicates that the calibration (adjustment) procedure will introduce correlations between the calibrated (adjusted) parameters and responses even if the parameters and response were initially uncorrelated, since $\mathbf{C}_{r\alpha}^{be} \neq 0$ even if $\mathbf{C}_{r\alpha} = 0$, i.e.,

$$\mathbf{C}_{r\alpha}^{be} = \mathbf{C}_{m}\left[\mathbf{C}_{rc}\left(\boldsymbol{\alpha}^{0}\right) + \mathbf{C}_{m}\right]^{-1}\left[\mathbf{S}\left(\boldsymbol{\alpha}^{0}\right)\right]\mathbf{C}_{\alpha}\text{, when } \mathbf{C}_{r\alpha} = 0. \qquad \text{(III.35)}$$

As the above expression indicates, the adjustment (calibration) modifies the correlations among the parameters through couplings introduced by the sensitivities of the participating responses. In the calibration procedure, the sensitivities play the role of weighting functions for propagating the initial parameter-covariances and experimental-response covariances to the adjusted best-estimate predicted quantities. Thus, as indicated by Eqs. (III.27) through (III.29), the incorporation of additional (experimental) information in the adjustment (calibration) process reduces the variances of the adjusted parameters and responses while also modifying their correlations.

Note that Eq. (III.28) expresses the best-estimate response covariance matrix $\mathbf{C}_r^{be}$ in terms of the initial covariance matrix $\mathbf{C}_m$ of the experimental-responses. Alternatively, it is of interest to derive the expression of the computed best-estimate response covariance matrix, $\mathbf{C}_{rc}^{be}$, directly from the model (the subscript "rc", denotes "computed response", to distinguish it from the covariance $\mathbf{C}_r^{be}$, which is obtained directly from the calibration/adjustment process). The starting point for computing $\mathbf{C}_{rc}^{be}$ is the linearization of the model, similar to that shown in Eq. (III.10), but around $\boldsymbol{\alpha}^{be}$ instead of $\boldsymbol{\alpha}^0$, i.e.

$$\mathbf{r} = \mathbf{R}\left(\boldsymbol{\alpha}^{be}\right) + \mathbf{S}\left(\boldsymbol{\alpha}^{be}\right)\left(\boldsymbol{\alpha} - \boldsymbol{\alpha}^{be}\right) + \textit{higher order terms}\,. \tag{III.36}$$

It follows from Eqs. (III.36) that

$$\begin{aligned}
\mathbf{C}_{rc}^{be} &= \left\langle \left(\mathbf{r} - \mathbf{R}\left(\boldsymbol{\alpha}^{be}\right)\right)\left(\mathbf{r} - \mathbf{R}\left(\boldsymbol{\alpha}^{be}\right)\right)^{\dagger} \right\rangle \triangleq \left[\mathbf{S}\left(\boldsymbol{\alpha}^{be}\right)\right]\left\langle \left(\boldsymbol{\alpha} - \boldsymbol{\alpha}^{be}\right)\left(\boldsymbol{\alpha} - \boldsymbol{\alpha}^{be}\right)^{\dagger} \right\rangle \left[\mathbf{S}\left(\boldsymbol{\alpha}^{be}\right)\right]^{\dagger} \\
&= \left[\mathbf{S}\left(\boldsymbol{\alpha}^{be}\right)\right]\mathbf{C}_{\alpha}^{be}\left[\mathbf{S}\left(\boldsymbol{\alpha}^{be}\right)\right]^{\dagger} \\
&= \left[\mathbf{S}\left(\boldsymbol{\alpha}^{be}\right)\right]\left[\mathbf{C}_{\alpha} - \left(\mathbf{C}_{\alpha r} - \mathbf{C}_{\alpha}\left[\mathbf{S}\left(\boldsymbol{\alpha}^{0}\right)\right]^{\dagger}\right)\left[\mathbf{C}_{d}\left(\boldsymbol{\alpha}^{0}\right)\right]^{-1}\left(\mathbf{C}_{\alpha r} - \left[\mathbf{S}\left(\boldsymbol{\alpha}^{0}\right)\right]\mathbf{C}_{\alpha}\right)\right]\left[\mathbf{S}\left(\boldsymbol{\alpha}^{be}\right)\right]^{\dagger}
\end{aligned} \tag{III.37}$$

Comparing Eq. (III.37) to Eq. (III.28) reveals that, in general, $\mathbf{C}_{rc}^{be} \neq \mathbf{C}_r^{be}$ since $\mathbf{S}\left(\boldsymbol{\alpha}^{be}\right) \neq \mathbf{S}\left(\boldsymbol{\alpha}^{0}\right)$. Nevertheless, *when the model is "perfect" (i.e., free of numerical errors) and exactly linear, then the sensitivity matrix* $\mathbf{S}$ *is independent of the parameter values* $\boldsymbol{\alpha}$, i.e.,

$$\mathbf{S}\left(\boldsymbol{\alpha}^{be}\right) = \mathbf{S}\left(\boldsymbol{\alpha}^{0}\right) = \mathbf{S}\text{, for "perfect" and linear models,} \tag{III.38}$$

As shown in the Appendix, it follows from Eqs (III. 37) and (III. 38) that

$$\begin{aligned}\mathbf{C}_{rc}^{be} &= \mathbf{S}\left[\mathbf{C}_{\alpha} - \left(\mathbf{C}_{\alpha r} - \mathbf{C}_{\alpha}\mathbf{S}^{\dagger}\right)\mathbf{C}_{d}^{-1}\left(\mathbf{C}_{\alpha r} - \mathbf{S}\mathbf{C}_{\alpha}\right)\right]\mathbf{S}^{\dagger} \\ &= \mathbf{C}_{rc} - \left(\mathbf{C}_{rc} - \mathbf{S}\mathbf{C}_{\alpha r}\right)\left[\mathbf{C}_{rc} + \mathbf{C}_{e} - \mathbf{C}_{r\alpha}\mathbf{S}^{\dagger} - \mathbf{S}\mathbf{C}_{\alpha r}\right]^{-1}\left(\mathbf{C}_{rc} - \mathbf{C}_{\alpha r}\mathbf{S}^{\dagger}\right) \\ &= \mathbf{C}_{r}^{be}, \quad \textbf{for "}\textit{perfect}\textbf{" linear models.}\end{aligned} \tag{III.39}$$

It is important to note that the computation of the best estimate parameter and response values, together with their corresponding best-estimate uncertainties, cf, Eqs. (III.21), (III.25), (III.27), (III.28) and (III.29) require the inversion of a single matrix, namely the matrix $\mathbf{C}_{d}\left(\boldsymbol{\alpha}^{0}\right)$ defined in Eq. (III.24). This is usually advantageous in practice, since the order of the matrix $\mathbf{C}_{d}\left(\boldsymbol{\alpha}^{0}\right)$ is given by the number of measured (or computed responses), which is most often considerably smaller that the number of model parameters under consideration.

On the other hand, when the number of parameter exceeds the number of responses, it is possible to derive alternative expressions for the best-estimate calibrated parameters and their corresponding best-estimate covariances, by performing all derivations in the "parameter space" rather than in "response space". This entails using Eq. (III.10) to eliminate the response (variables) $\mathbf{r}$ at the outset, and carrying out the minimization procedure solely for the parameters (variables) $\boldsymbol{\alpha}$. Equivalently, as shown in the Appendix, the Sherman-Morrison-Woodbury extension can be employed to obtain the alternative expression

$$\begin{aligned}\mathbf{C}_{d}^{-1} &\triangleq \left(\mathbf{C}_{rc} - \mathbf{C}_{r\alpha}\mathbf{S}^{\dagger} - \mathbf{S}\mathbf{C}_{\alpha r} + \mathbf{C}_{m}\right)^{-1} \\ &= \mathbf{A}^{-1} - \mathbf{A}^{-1}\mathbf{S}\left(\mathbf{C}_{\alpha}^{-1} + \mathbf{S}^{\dagger}\mathbf{A}^{-1}\mathbf{S}\right)^{-1}\mathbf{S}^{\dagger}\mathbf{A}^{-1}; \quad \mathbf{A} \triangleq \mathbf{C}_{m} - \mathbf{C}_{r\alpha}\mathbf{S}^{\dagger} - \mathbf{S}\mathbf{C}_{\alpha r}.\end{aligned} \tag{III.40}$$

The above expression provides the bridge between the “response-space” and “parameter-space” formulations. This expression also highlights the fact that the response-space formulation requires a single inversion of a square symmetric matrix (namely, the matrix $\mathbf{C}_d$) of the same dimensions as the number of responses. In contradistinction, the “parameter space” formulation requires the inversion of three symmetric matrices, two of which have dimensions equal to the number of parameters and one of dimensions equal to the number of responses. Hence, from a computational standpoint, the “response-space” formulations should be used whenever possible.

In view of Eq. (III.24), it is important to note that the inverse matrix, $\mathbf{C}_d^{-1}$, incorporates simultaneously all of the available information about the system parameters and responses, at all time nodes [i.e., $\nu = 1, 2, ..., N_t$]. Specifically, at any time node ν, $\mathbf{C}_d^{-1}$ incorporates information not only from time nodes prior in time to ν (i.e., information regarding the "past" and "present" states of the system) but also from time nodes posterior in time to ν (i.e., information about the “future” states of the system). Through the matrix $\mathbf{C}_d^{-1}$, at any specified time node ν, the calibrated best-estimates parameters $\left(\boldsymbol{\alpha}^{be}\right)^{\nu}$ and responses $\mathbf{r}\left(\boldsymbol{\alpha}^{be}\right) \triangleq \mathbf{r}^{be}$, together with the corresponding calibrated best-estimate covariance matrices $\left(\mathbf{C}_{\alpha}^{be}\right)^{\nu\mu}$, $\left(\mathbf{C}_{r}^{be}\right)^{\nu\mu}$, and $\left(\mathbf{C}_{\alpha r}^{be}\right)^{\nu\mu}$ will also incorporate automatically all of the available information about the system parameters and responses at all time nodes [i.e., $\nu = 1, 2, ..., N_t$].

In this respect, the methodology presented in this section is conceptually related to the "foresight" aspects encountered in decision analysis. It is also important to note that, in practice, the application of the methodology developed in this section involves two distinct computational stages. A complete sensitivity data base (i.e., sensitivities $s_{ni}^{\nu\mu}$ at all times nodes

$\nu, \mu = 1, \ldots, N_t$) needs to be generated prior to performing the "data assimilation" and "model calibration" (or data adjustment) stage, since all of the sensitivities are needed in order to perform data assimilation and model calibration. These stages are performed subsequently, together with the computation of calibrated best-estimate covariance matrices (the "uncertainty analysis" stage), by combining the sensitivities with covariance matrices.

Because of the "foresight" and "off-line" characteristics, the methodology presented in this Section can be called the "off-line with foresight" data assimilation and adjustment (model calibration) methodology, underscoring that all sensitivities are generated separately, prior to performing the uncertainty analysis, and that foresight characteristics are included in the procedure. Since the incorporation of foresight effects involves the inversion of the matrix $\mathbf{C}_d$, this methodology is best suited for problems involving relatively few time nodes. For large-scale highly nonlinear problems involving many time nodes, the matrix $\mathbf{C}_d$ becomes very large, requiring large amounts of computer storage; the inversion of $\mathbf{C}_d$ may become prohibitively expensive in such cases. These difficulties can be reduced at the expense of using less than the complete information available at any specific time node. For example, even in time-dependent problems in which the entire time history is known (e.g., transient behavior of reactor systems), one may nevertheless choose to use only information up to the current time index, and disregard the information about "future" system states.

On the other hand, in dynamical problems such as climate or weather prediction, in which the time variable advances continuously and states beyond the current time are not known, information about future states cannot be reliably accounted for anyway. Thus, the most common way of reducing the dimensionality of the data assimilation and model calibration problem is to disregard information about future states and limit the amount of information

assimilated about “past states”. Data assimilation and model calibration procedure using such a limited amount of information can be performed either off-line or on-line, assimilating the new data as the time index advances.

The simplest case of dynamic data assimilation and model calibration is when these operations are performed by using information on-line from only two successive time-steps. In this particular case, the expressions given by Eqs. (III.22), (III.26), (III.32), (III.33) and (III.34) for the best-estimate predicted calibrated quantities reduce (see the Appendix for details) to the following explicit formulas:

(i) The components $\left(\boldsymbol{\alpha}^{be}\right)^{k}$, representing the calibrated best-estimates for the system parameters at time node k, can be written in a particular form of Eq. (III.22), as follows:

$$\left(\boldsymbol{\alpha}^{be}\right)^{k} = \left(\boldsymbol{\alpha}^{0}\right)^{k} + \sum_{\mu=k-1}^{k} \left\{ \left[\mathbf{C}_{\alpha r}^{k\mu} - \sum_{\rho=k-1}^{\mu} \mathbf{C}_{\alpha}^{k\rho} \left(\mathbf{S}^{\dagger}\right)^{\mu\rho} \right] \left[\sum_{\eta=k-1}^{k} \mathbf{K}_{d}^{\mu\eta} \mathbf{d}^{\eta} \right] \right\}, \quad k = 1, 2, ..., N_t. \qquad \text{(III.41)}$$

(ii) The vector $\left(\mathbf{r}^{be}\right)^{k}$, representing the best-estimates predicted values for the system parameters at a time node k, take on the following particular form of Eq. (III.26):

$$\left(\mathbf{r}^{be}\right)^{k} = \left(\mathbf{r}_{m}\right)^{k} + \sum_{\mu=k-1}^{k} \left\{ \left[\mathbf{C}_{m}^{k\mu} - \sum_{\rho=k-1}^{\mu} \mathbf{C}_{r\alpha}^{k\rho} \left(\mathbf{S}^{\dagger}\right)^{\mu\rho} \right] \left[\sum_{\eta=k-1}^{k} \mathbf{K}_{d}^{\mu\eta} \mathbf{d}^{\eta} \right] \right\}, \quad k = 1, 2, ..., N_t. \qquad \text{(III.42)}$$

(iii) The components $\left(\mathbf{C}_{\alpha}^{be}\right)^{\nu\mu}$, $\left(\nu, \mu = k-1, k\right)$, of the calibrated best-estimate covariance matrix, $\mathbf{C}_{\alpha}^{be}$, for the calibrated best-estimates system parameters is obtained by particularizing Eq. (III.32) to two consecutive time nodes $\left(k-1, k\right)$, $k = 1, 2, ..., N_t$, leading to

$$\left(\mathbf{C}_{\alpha}^{be}\right)^{\nu\mu} = \mathbf{C}_{\alpha}^{\nu\mu} - \sum_{\eta=k-1}^{k}\sum_{\rho=k-1}^{k}\left[\mathbf{C}_{\alpha r}^{\nu\rho} - \sum_{\pi=k-1}^{\rho}\mathbf{C}_{\alpha}^{\nu\pi}\left(\mathbf{S}^{\dagger}\right)^{\rho\pi}\right]\mathbf{K}_{d}^{\rho\eta}\left[\mathbf{C}_{r\alpha}^{\eta\mu} - \sum_{\pi=k-1}^{\eta}\mathbf{S}^{\eta\pi}\mathbf{C}_{\alpha}^{\pi\mu}\right]. \quad \text{(III.43)}$$
$$for \quad \nu = k-1, k; \quad and \quad \mu = k-1, k; \quad k = 1, 2, ..., N_t.$$

(iv) The components $\left(\mathbf{C}_{r}^{be}\right)^{\nu\mu}$, $\left(\nu, \mu = k-1, k\right)$, of the calibrated best-estimate covariance matrix $\mathbf{C}_{r}^{be}$, for the best-estimate responses takes on the following particular form of Eq. (III.33):

$$\left(\mathbf{C}_{r}^{be}\right)^{\nu\mu} = \mathbf{C}_{m}^{\nu\mu} - \sum_{\eta=k-1}^{k}\sum_{\rho=k-1}^{k}\left[\mathbf{C}_{m}^{\nu\rho} - \sum_{\pi=k-1}^{\rho}\mathbf{C}_{r\alpha}^{\nu\pi}\left(\mathbf{S}^{\dagger}\right)^{\rho\pi}\right]\mathbf{K}_{d}^{\rho\eta}\left[\mathbf{C}_{m}^{\eta\mu} - \sum_{\pi=k-1}^{\eta}\mathbf{S}^{\eta\pi}\mathbf{C}_{\alpha r}^{\pi\mu}\right]. \quad \text{(III.44)}$$
$$for \quad \nu = k-1, k; \quad and \quad \mu = k-1, k; \quad k = 1, 2, ..., N_t.$$

(v) The components $\left(\mathbf{C}_{\alpha r}^{be}\right)^{\nu\mu}$, $\left(\nu, \mu = k-1, k\right)$, of the best-estimate response-parameter covariance matrix $\mathbf{C}_{\alpha r}^{be}$ take on the following particular form of Eq. (III.34):

$$\left(\mathbf{C}_{r\alpha}^{be}\right)^{\nu\mu} = \mathbf{C}_{r\alpha}^{\nu\mu} - \sum_{\eta=k-1}^{k}\sum_{\rho=k-1}^{k}\left[\mathbf{C}_{m}^{\nu\rho} - \sum_{\pi=k-1}^{\rho}\mathbf{C}_{r\alpha}^{\nu\pi}\left(\mathbf{S}^{\dagger}\right)^{\rho\pi}\right]\mathbf{K}_{d}^{\rho\eta}\left[\mathbf{C}_{r\alpha}^{\eta\mu} - \sum_{\pi=k-1}^{\eta}\mathbf{S}^{\eta\pi}\mathbf{C}_{\alpha}^{\pi\mu}\right]. \quad \text{(III.45)}$$
$$for \quad \nu = k-1, k; \quad and \quad \mu = k-1, k; \quad k = 1, 2, ..., N_t.$$

For each time node, $k = 1, 2, ..., N_t$, the quantities $\mathbf{K}_{d}^{\nu\eta}$ which appear in Eqs. (III. 41) through (III. 45) have the following expressions:

$$\begin{aligned}\mathbf{K}_d^{k-1,k-1} &= \left[\mathbf{C}_d^{k-1,k-1} - \mathbf{C}_d^{k-1,k}\left(\mathbf{C}_d^{k,k}\right)^{-1}\mathbf{C}_d^{k,k-1}\right]^{-1} \\ &= \left(\mathbf{C}_d^{k-1,k-1}\right)^{-1} + \left(\mathbf{C}_d^{k-1,k-1}\right)^{-1}\mathbf{C}_d^{k-1,k}\mathbf{K}_d^{k,k}\mathbf{C}_d^{k,k-1}\left(\mathbf{C}_d^{k-1,k-1}\right)^{-1}\end{aligned} \tag{III.46}$$

$$\begin{aligned}\mathbf{K}_d^{k-1,k} &= -\left(\mathbf{C}_d^{k-1,k-1}\right)^{-1}\mathbf{C}_d^{k-1,k}\left[\mathbf{C}_d^{k,k} - \mathbf{C}_d^{k,k-1}\left(\mathbf{C}_d^{k-1,k-1}\right)^{-1}\mathbf{C}_d^{k-1,k}\right]^{-1} \\ &= -\left(\mathbf{C}_d^{k-1,k-1}\right)^{-1}\mathbf{C}_d^{k-1,k}\mathbf{K}_d^{k,k}\end{aligned} \tag{III.47}$$

$$\begin{aligned}\mathbf{K}_d^{k,k} &= \left[\mathbf{C}_d^{k,k} - \mathbf{C}_d^{k,k-1}\left(\mathbf{C}_d^{k-1,k-1}\right)^{-1}\mathbf{C}_d^{k-1,k}\right]^{-1} \\ &= \left(\mathbf{C}_d^{k,k}\right)^{-1} + \left(\mathbf{C}_d^{k,k}\right)^{-1}\mathbf{C}_d^{k,k-1}\mathbf{K}_d^{k-1,k-1}\mathbf{C}_d^{k-1,k}\left(\mathbf{C}_d^{k,k}\right)^{-1}\end{aligned} \tag{III.48}$$

$$\begin{aligned}\mathbf{K}_d^{k,k-1} &= -\left(\mathbf{C}_d^{k,k}\right)^{-1}\mathbf{C}_d^{k,k-1}\left[\mathbf{C}_d^{k-1,k-1} - \mathbf{C}_d^{k-1,k}\left(\mathbf{C}_d^{k,k}\right)^{-1}\mathbf{C}_d^{k,k-1}\right]^{-1} \\ &= -\left(\mathbf{C}_d^{k,k}\right)^{-1}\mathbf{C}_d^{k,k-1}\mathbf{K}_d^{k-1,k-1}\end{aligned} \tag{III.49}$$

For *time-independent* problems, the time-dependent results derived in the forgoing reduce to expressions that are formally identical to Eqs. (III.21), (III.25), (III.27), (III.28) and (III.29); hence, these expressions can be used directly to obtain the best-estimate predicted values for parameters, responses, and their respective covariances. It is also important to note that although modeling errors have not been considered explicitly in this Section, they can be treated in a manner similar to parameter uncertainties by including the discretization intervals in the vector of model parameters, as shown in Refs. 16 and 17.

Finally, it is important to emphasize that the explicit formulas presented in this Section are based on the linearized relationship between responses and parameters that customarily underlies the “propagation of moments” method, i.e., Eq. (III.10), without considering

nonlinearities explicitly. Nevertheless, this limitation is not as severe as it may appear at first glance, since nonlinear relations between computed responses and model parameters can be treated by considering Eq. (III.10) iteratively, starting with the known nominal values of the quantities involved. The first iteration (in such an iterative procedure) would yield all of the major explicit results derived in Eqs. (III.21), (III.25), (III.27), (III.28) and (III.29). The subsequent iteration would the results of Eqs. (III.21), (III.25), (III.27), (III.28) and (III.29) as the "prior information" in a second application of these formulas, and compute the new ("second-iteration") best-estimate quantities by using once again these formulas. This iterative procedure would then be repeated until the best-estimated values would not change any longer, thereby indicating convergence of the nonlinear iterative procedure.

IV. DATA CONSISTENCY AND REJECTION CRITERIA

The actual application of the model calibration (adjustment) algorithms, cf. Eqs. (III.21), (III.25), (III.27), (III.28) and (III.29), to the a physical system characterized by nominal values and uncertainties for model parameters together with the computed and measured responses is straightforward, in principle, although it can become computationally very demanding on both data handling and computational speed. It is also important to note that the indiscriminate incorporation of all (seemingly relevant) experimental-response data could produce a set of calibrated (adjusted) parameter values that might differ unreasonably much from the corresponding original nominal values. Worse yet, the indiscriminate use of information might even fail to improve the agreement between the calculated and measured values of some of the very responses by which the library was calibrated (adjusted). When calibrating (adjusting) a library of model parameters, it is tacitly assumed that the given parameters are basically "correct," except that they are not sufficiently accurate for the

objective at hand. The calibration procedure uses additional data (e.g., experimental responses) for improving the parameter values while reducing their uncertainties. Although such additional information induces modifications of the original parameter values, the adjusted parameters are still generally expected to remain consistent with their original nominal values, within the range of their original uncertainties. However, calibration of model parameters by experimental responses which significantly deviate from their respective computed values would significantly modify the resulting adjusted parameters, perhaps even violating the restriction of linearity underlying the calibration procedure, cf. Eq. (III.10). Such unlikely adjustments would most probably lead to failure of even reproducing the original experimental responses.

On the other hand, calibrating a parameter library by using measured responses that are very close to their respective computed values would cause minimal parameter modifications and a nearly perfect reproduction of the given responses by the adjusted library (as would be expected). In such a case, the given responses would be considered as being consistent with the parameter library, in contradistinction to adjustment by inconsistent experimental information, in which case the adjustment could fail because of inconsistencies. These considerations clearly underscore the need for using a quantitative indicator to measure the mutual and joint consistency of the information available for model calibration.

As shown in the Appendix, the minimum value, $Q_{\min} \equiv Q\left(\mathbf{z}^{be}\right)$, of $Q\left(\mathbf{z}\right)$ takes on the following expression:

$$Q_{\min} \equiv Q\left(\mathbf{z}^{be}\right) = \mathbf{d}^{\dagger}\left[\mathbf{C}_{d}\left(\boldsymbol{\alpha}^{0}\right)\right]^{-1}\mathbf{d}\,,\mathbf{d} \triangleq \mathbf{R}\left(\boldsymbol{\alpha}^{0}\right) - \mathbf{r}_{x} \ . \qquad \text{(IV.1)}$$

As the above expression indicates, $Q_{\min} \equiv Q\left(\mathbf{z}^{be}\right)$ represents the square of the length of the vector $\mathbf{d}$, measuring (in the corresponding metric) the deviations between the experimental and nominally computed responses. Note that $Q_{\min} \equiv Q\left(\mathbf{z}^{be}\right)$ can be evaluated directly from the given data (i.e., given parameters and responses, together with their original uncertainties) after having inverted the deviation-vector uncertainty matrix $\mathbf{C}_d\left(\boldsymbol{\alpha}^0\right)$. It is also very important to note that $Q_{\min} \equiv Q\left(\mathbf{z}^{be}\right)$ is independent of calibrating (or adjusting) the original data. As the dimension of $\mathbf{d}$ indicates, the number of degrees of freedom characteristic of the calibration under consideration is equal to the number of experimental responses. In the extreme case of absence of experimental responses, no actual calibration takes place since $\mathbf{d} = \mathbf{R}\left(\boldsymbol{\alpha}^0\right)$, so that the best-estimate parameter values are just the original nominal values, i.e., $\left(\boldsymbol{\alpha}^{be}\right)^k = \left(\boldsymbol{\alpha}^0\right)^k$; an actual adjustment occurs only when at least one experimental response is included.

Replacing Eq. (IV.1) in Eq. (III.14) shows that the bulk of the contribution to the joint posterior probability distribution, which comes from the point $\mathbf{z} = \mathbf{z}^{be}$, takes on the form of the following multivariate Gaussian distribution:

$$p\left(\mathbf{z}^{be} \,|\mathbf{C}\right) \sim \exp\left[-\frac{1}{2}Q\left(\mathbf{z}^{be}\right)\right] = \exp\left\{-\frac{1}{2}\left[\mathbf{r}_x - \mathbf{R}\left(\boldsymbol{\alpha}^0\right)\right]^{\dagger}\left[\mathbf{C}_d\left(\boldsymbol{\alpha}^0\right)\right]^{-1}\left[\mathbf{r}_x - \mathbf{R}\left(\boldsymbol{\alpha}^0\right)\right]\right\}. \quad \text{(IV.2)}$$

The above relation indicates that experimental responses can be considered as random variables approximately described by a multivariate Gaussian distribution with means located at the nominal values of the computed responses, and with a covariance matrix $\mathbf{C}_d\left(\boldsymbol{\alpha}^0\right)$. In turn, the random variable $Q_{\min} \equiv Q\left(\mathbf{z}^{be}\right)$ obeys a χ^2-distribution with n degrees of freedom,

where n denotes the total number of experimental responses considered in the calibration (adjustment) procedure. Since $Q_{\min} \equiv Q\left(\mathbf{z}^{be}\right)$ is the "χ^2 of the calibration (adjustment) at hand", it can be used as an indicator of the agreement between the computed and experimental responses, measuring essentially the consistency of the experimental responses with the model parameters. Recall that the χ^2 (chi-square) distribution with n degrees of freedom of the continuous variable ($0 \le x < \infty$) is defined as

$$P\left(x < \chi^2 < x + dx\right) \triangleq k_n\left(x\right)dx = \frac{1}{2^{n/2}\Gamma\left(n/2\right)} x^{n/2-1} e^{-x/2} dx,\ x > 0,\ \left(n = 1, 2, \ldots\right). \quad \text{(IV.3)}$$

The χ^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 mean and variance of x are $\langle x \rangle = n$ and $\mathrm{var}\left(x\right) = 2n$. Further practically useful asymptotic properties of the χ^2 - distribution for $n \to \infty$ are as follows: (i) x is asymptotically normal with mean n and variance $2n$; (ii) x/n is asymptotically normal with mean 1 and variance $2/n$; (iii) $\sqrt{2x}$ is asymptotically normal with mean $\sqrt{2n-1}$ and variance 1. Although the χ^2- distribution is extensively tabulated, the notation is not uniform in the literature for the various derived quantities (in particular, for the corresponding cumulative distribution functions and fractiles). The cumulative distributions, denoted here by $P_n\left(\chi^2\right)$ and $Q_n\left(\chi^2\right)$, are defined as

$$P_n\left(\chi_0^2\right) \triangleq P\left(\chi^2 \le \chi_0^2\right) \triangleq \int_0^{\chi_0^2} k_n\left(t\right)dt; \quad Q_n\left(\chi_0^2\right) \triangleq P\left(\chi^2 \ge \chi_0^2\right) \triangleq \int_{\chi_0^2}^{\infty} k_n\left(t\right)dt = 1 - P_n\left(\chi_0^2\right). \quad \text{(IV.4)}$$

In practice, one rejects a hypothesis using the χ^2- distribution when, for a given significance level α and number of degrees of freedom n, the value of $Q_{\min} \equiv \chi^2$ exceeds a chosen critical fractile value $\chi^2_\alpha(n)$. Published tables often show $\chi^2_{1-\alpha}(n)$ versus α. When the number of degrees of freedom is large ($n > 30$), a useful asymptotic approximation is $\chi^2_\alpha(n) \approx 1/2\left(\sqrt{2n-1} + z_{2\alpha}\right)^2$, with $z_{2\alpha}$ denoting the corresponding fractile of the standard normal distribution $\Phi_0(z)$, computed by solving the equation $2\Phi_0(z_{2\alpha}) = 1 - 2\alpha$, using the tabulated tables for $\Phi_0(z)$. For large or small values of α, a more accurate approximation is $\chi^2_\alpha(n) \approx n\left(1 - \frac{2}{9m} + z_{2\alpha}\sqrt{\frac{2}{9m}}\right)^3$. It may be often more convenient to transform χ^2 to the variate $t = \chi^2/n$ (i.e., " χ^2 per degree of freedom"), in which case the transformed distribution, $g_n(t)$, becomes $g_n(t) = nk_n(nt)$, with mean value $\langle t \rangle = 1$ and variance $2/n$.

For model calibration (adjustment), it is important to assess if: (i) the response and data measurements are free of gross errors (blunders such as wrong settings, mistaken readings, etc), and (ii) the measurements are consistent with the assumptions regarding the respective means, variances, and covariances. For example if $\chi^2/n \simeq 1$, then that the measurements are very likely to be both free of gross errors and consistent with the assumptions. However, if $\chi^2/n \gg 1$ or $\chi^2/n \ll 1$, the measurements (or at least some measurements), the assumptions, or both are suspect. In particular, unusually large values $\chi^2/n \gg 1$ could be obtained when the original variances are underestimated; increasing them beyond their assumed nominal values would cause the adjusted values of χ^2/n and $P_n(\chi^2)$ to decrease accordingly. The reverse argument would apply if the a priori values of χ^2/n and $P_n(\chi^2)$ were unusually small (e.g., $\chi^2/n \ll 1$, $P_n(\chi^2) \sim 10^{-4}$), which could be the result of a priori overestimated

variances. A practical quantitative criterion for *the "acceptance" (or "rejection") of experimental results in conjunction with a given "theoretical" model* (i.e., in conjunction with the assumptions regarding the variates underlying the model) *is to accept the value of* χ^2/n *whenever* $0.15 < P_n\left(\chi^2\right) < 0.85$, in analogy to the "$1\sigma$" range of normal distributions. Note that, when setting an acceptance criterion for χ^2/n of the general form

$$\alpha < P_n\left(\chi^2\right) < 1-\alpha, \tag{IV.5}$$

the exact value of α is not essential and is subject to personal judgment. This is because the probability $P_n\left(\chi^2\right)$ is still sensitive to the value of χ^2/n due to the fact that $\chi^2/n \simeq 1 \pm \sqrt{(2/n)}$ (except for few degrees of freedom, e.g., for $n \leq 5$), so the acceptable range of χ^2/n narrows as $1/\sqrt{n}$ (see also the previously noted asymptotic forms for χ^2_α/n). In other words, moderate changes in χ^2/n lead to significant relative changes in $P_n\left(\chi^2\right)$. For example, the central 50%-range of $\chi^2/20$ is (0.77, 1.19), and the corresponding 90%-range is (0.54, 1.57), implying that values of $\chi^2/20$ below $\simeq 0.4$ or above $\simeq 2.0$ would be definitely unacceptable.

In addition to measuring the overall consistency of a given set of parameters and responses, the quantity χ^2/n also measures the consistency among the measured responses. Hence, an entire data set (model parameters and/or experimental responses) should not be indiscriminately disqualified because of too high or too low value of χ^2/n, since even a single "outlying" response could significantly degrade the set's overall consistency. Note that a simple-minded assessment and ranking of "questionable responses" according to the values

of the "individual consistencies" (i.e., the values of χ^2 obtained for each response as if it were the only response available for calibrating the entire set of parameters), would be very likely misleading. This is because the sum of the respective "individual consistencies" [which would numerically be obtained by dividing the squares of the deviations, d_i^2, through the sum of the respective variances of the computed and measured responses $\mathrm{var}\left(r_i^{comp}\right)+\mathrm{var}\left(r_i^{\exp}\right)$], would not be equal to the "joint consistency" (i.e., the joint χ^2) of the entire set of experimental responses. This is because the deviation-vector uncertainty matrix $\mathbf{C}_d\left(\boldsymbol{\alpha}^0\right)\triangleq\mathbf{C}_{rc}\left(\boldsymbol{\alpha}^0\right)-\mathbf{C}_{r\alpha}\left[\mathbf{S}\left(\boldsymbol{\alpha}^0\right)\right]^{\dagger}-\left[\mathbf{S}\left(\boldsymbol{\alpha}^0\right)\right]\mathbf{C}_{\alpha r}+\mathbf{C}_x$ is generally non-diagonal, even if both $\mathbf{C}_{rc}\left(\boldsymbol{\alpha}^0\right)$ and $\mathbf{C}_x$ are diagonal. On the other hand, verifying the consistency of *all* partial sets of the array of n responses with respect to their consistency with the given library is usually impractical, since the number of partial sets of an array of n responses is 2^n-1; hence, such a verification would be practically feasible only when the number of measured responses is very small.

A procedure that has been successfully used to identify successively the responses which are least consistent with a given library of parameters is based on leaving out one response at a time and evaluating $\chi_{n-1}^2(1)$ for the remaining $n-1$ responses. The response left out is subsequently returned to the response set, another response (response "two") is eliminated, and the corresponding $\chi_{n-1}^2(2)$ is evaluated. This procedure is continued until all remaining $\chi_{n-1}^2(i), i=3,\ldots,n,$ are successively evaluated. The response that yields the lowest χ_{n-1}^2 when eliminated is considered to be "the least consistent", and is thus ranked "last" in the consistency sequence, and eliminated from further consideration. The evaluation procedure is then repeated for the remaining $n-1$ ("more consistent") responses, to identify the "second least consistent response", which is then ranked next-to-last. The procedure is then repeatedly

applied to the successive, fewer and fewer, partial response sets until establishing the complete consistency sequence. Establishing such a consistency sequence requires only $n(n+1)/2$ computations of χ^2, as compared to (2^n-1) calculations needed to assign χ^2 values to all possible partial sets of n responses.

The quantity χ^2/n measures the consistency of any set of n experimentally measured responses with a given library of model parameters, in the sense that if χ_1^2 refers to a specific set of n experimental responses and χ_2^2 to another set of n responses, then $\chi_1^2 < \chi_2^2$ means that the first set is more consistent with the library than the second. On the other hand, when varying the number of responses, it is not a priori obvious whether the set yielding a smaller χ^2/n is also necessarily the most consistent with the given parameters. As an example, consider the value $P_n(\chi^2) = 0.85$, which can correspond to both $\chi^2/5 = 1.623$ and also to $\chi^2/10 = 1.453$. If, for example, one set of 5 responses would give a computed value $\chi^2/5 = 1.6$, and second set of 10 responses would give $\chi^2/10 = 1.5$, the first set would be considered to be the "more consistent", for it falls within the "central 70% range," whereas the second does not. In such situations, it is preferable to use the quantity $Q_n(\chi^2) = 1 - P_n(\chi^2)$, as an additional measure of consistency.

Quite generally, therefore, the calibration (adjustment) of a set of model parameters and experimental responses must include the verification of their mutual consistency, which is performed by first generating the consistency sequence, and then determining the probabilities $Q_i(\chi^2)$, when $i = 1, 2, \ldots, n$, while generating the sequence. The less consistent responses will show up at the end of the sequence, and the probabilities $Q_i(\chi^2)$ will generally decrease as i

approaches the total number of responses, n . Such an analysis would identify the significantly less-consistent responses, and would also indicate the level of consistency of all response subsets along the consistency sequence.

In parallel, the irregular model parameters, if any, must also be identified. This can be done by computing not only χ^2 for any response subset, but also computing from Eq. (III.21) the corresponding best-estimate parameters $\boldsymbol{\alpha}^{be} = \boldsymbol{\alpha}^0 + \left(\mathbf{C}_{\alpha r} - \mathbf{C}_{\alpha}\left[\mathbf{S}\left(\boldsymbol{\alpha}^0\right)\right]^{\dagger}\right)\left[\mathbf{C}_d\left(\boldsymbol{\alpha}^0\right)\right]^{-1}\mathbf{d}$. This way, the actual individual parameter adjustments induced by the respective response subset are also examined while proceeding step-by-step along the consistency sequence, noting which parameters vary more than others, and by how much. Usually, the parameter-adjustments induced by the more consistent subsets of responses tend to be marginal. The less-consistent responses and the questionable parameters would tend to undergo larger adjustments, requiring specific further examinations.

V. CONCLUDING REMARKS

This work has presented a general mathematical framework for simultaneously calibrating (adjusting) model parameters and responses through the assimilation of experimental data, leading to “best-estimate” values with reduced uncertainties for both parameters and responses in a generic time-dependent system. When only first and second moments of model parameters and experimental responses are a priori available, as is most often the case in practice, the maximum entropy principle of statistical mechanics was employed in conjunction with information theory to construct a Gaussian prior distribution that takes all of the available information into account while minimizing (in the sense of quadratic loss) the

introduction of spurious information. This prior distribution comprises also any correlations among model parameters and responses, thus generalizing the state-of-the-art data assimilation algorithms used in the geosciences[5,6].

The posterior distribution for the best-estimate calibrated model parameters and responses has been constructed by using Bayes' theorem. The best-estimate predicted mean values and reduced covariances, which are customarily needed when employing decision theory under "quadratic loss", were computed by extracting the bulk contributions via the saddle-point method. In particular, this procedure yields the same Gaussian posterior distribution as would be obtained by using the maximum likelihood method. The minimum value of the quadratic form appearing in the exponent of the Gaussian posterior distribution also provides the "χ^2 of the calibration (adjustment) at hand". This quadratic form can therefore be used as an indicator of the agreement between the computed and experimentally measured responses, indicating essentially the consistency of the measured responses with the model parameters. When all information is consistent, the posterior probability density function yields reduced best-estimate uncertainties for the best-estimate model parameters and responses. The accompanying PART II[7] will present typical results obtained by applying the methodology presented in this work to an illustrative paradigm time-dependent thermal-hydraulic system.

The model calibration methodology presented in this work provides a rigorous mathematical foundation for similar methodologies used in geophysical sciences, while extending these methodologies in several directions:

(i) Simultaneous calibration of all parameters and responses (as opposed to just initial conditions, as usually performed in geophysical sciences);

(ii) Treatment of systems involving correlated parameters and responses (as opposed to no parameter-response correlations, e.g., in geophysical sciences);

(iii) Simultaneous calibration over all time intervals; the usual two-step time advancement procedures used in geophysical sciences simply becomes a consequence, as a particular case, of the general methodology presented in this work.

Computationally, the most intensive aspect of the methodology presented in this work is the computation of the sensitivities of responses to model parameters, which play a crucial role as weighting functions in all of the expressions for the best-estimated predicted values for parameters, responses and their associated best-estimated reduced uncertainties. For large-scale systems, the most efficient method for computing these sensitivities is the adjoint sensitivity procedure (ASAP), as detailed in Refs. 16 and 17. The other computationally intensive aspect in this mathematical formalism is the inversion of the covariance matrix $\mathbf{C}_d\left(\boldsymbol{\alpha}^0\right)$ associated with the vector $\mathbf{d} \triangleq \mathbf{R}\left(\boldsymbol{\alpha}^0\right) - \mathbf{r}_x$, which measures the deviations between the respective computed and experimentally-measured responses. Methods for efficiently inverting of this matrix, as well as for reducing its dimension, (e.g., reduced-order modeling using proper orthogonal decomposition methods) are of substantial interest.

The best-estimate calibrated values for model parameters obtained through the application of the mathematical framework presented in this work can also be used to estimate quantitatively the validation domain of the model under consideration, by computing contours of constant best-estimate uncertainties in the high-dimensional parameter-space. The best-estimate calibrated values can also be used to perform “model extrapolation”, by predicting uncertainties in new environments or conditions of interest. Extrapolation of large-scale models would address both untested parts of the parameter space and higher levels of system complexity in the validation hierarchy.

The explicit formulas presented in this work are based on the linearized relationship between responses and parameters that customarily underlies the "propagation of moments" method, without explicitly considering nonlinearities and modeling errors. Nevertheless, neither of these limitations is as severe as it may appear at first glance, since: (i) modeling errors can be treated in a manner similar to parameter uncertainties, as shown in Refs. 16 and 17, by including the discretization intervals in the vector of model parameters; and (ii) nonlinear relations between computed responses and model parameters can be treated iteratively, by considering Eq. (III.10), and hence, all of the major results derived explicitly in Sections III and IV, as the first step in an iterative procedure which starts with the known nominal values of the quantities involved. The subsequent step of such an iterative procedure would be to use the formulas for the best-estimate mean values and covariances for the parameters and responses obtained in Sections III and IV as the "prior information", and compute the new ("second-generation") best-estimate quantities by using once again the formulas of Sections III and IV. This iterative procedure would be repeated until the best-estimated values would not change any longer, thereby indicating convergence of the nonlinear iterative procedure.

Ongoing research is currently devoted to the explicit treatment of modeling errors, and to extending the results of Sections III and IV by including not only the sensitivities (i.e., first-order information) but also the Hessians (i.e., second-order information) of the responses. Additional work is also ongoing to remove the current restriction to Gaussian distributions. Actually, the de-facto limitation to Gaussian distribution is characteristic of all of the state-of-the-art procedures for data assimilation and model calibration, as evidenced by the scientific literature published thus far. Removing these limitations would contribute significantly to understanding the validation of coupled nonlinear multi-physics models (e.g., of two or more physical phenomena that were not coupled in the initial validation database), particularly the accompanying increase of uncertainty. Developing predictive experimentally validated "best-

estimate" numerical models is particularly important for designing new technologies and facilities based on novel processes, while striving to avoid, as much as possible, the costly and lengthy procedures of building representative mock-up experiments, which might confirm - but would not necessarily explain- the predictions of simulation tools.

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APPENDIX: SOLUTION OF THE CONSTRAINED MINIMIZATION PROBLEM EXPRESSED BY EQ. (III.19)

Recall that the augmented Lagrangian functional $P(\mathbf{z},\boldsymbol{\lambda})$ defined as

$$P(\mathbf{z},\boldsymbol{\lambda}) \equiv Q(\mathbf{z}) + 2\boldsymbol{\lambda}^{\dagger}\left[\mathbf{Z}(\boldsymbol{\alpha}^{0})\mathbf{z} + \mathbf{d}\right] = \min,\ \ at\ \mathbf{z} = \mathbf{z}^{be} \equiv \begin{pmatrix} \boldsymbol{\alpha}^{be} - \boldsymbol{\alpha}^{0} \\ \mathbf{r}^{be} - \mathbf{r}_{m} \end{pmatrix}. \tag{III.19}$$

where $\boldsymbol{\lambda} = \left(\boldsymbol{\lambda}^{1},...,\boldsymbol{\lambda}^{\nu},...,\boldsymbol{\lambda}^{N_t}\right)$ denotes the corresponding vector of Lagrange multipliers. In the above expression, the superscript "*be*" denotes "*best-estimated values*", and the factor "2" was introduced for convenience in front of $\boldsymbol{\lambda}$ in order to simplify the subsequent algebraic derivations. The point $\mathbf{z}^{be}$ where the functional $P(\mathbf{z},\boldsymbol{\lambda})$ attains its extremum (minimum) is defined implicitly through the conditions

$$\nabla_{\mathbf{z}} P(\mathbf{z},\boldsymbol{\lambda}) = \mathbf{0}, \quad \nabla_{\boldsymbol{\lambda}} P(\mathbf{z},\boldsymbol{\lambda}) = \mathbf{0}, \quad at\ \mathbf{z} = \mathbf{z}^{be}. \tag{III.20}$$

The condition $\nabla_{\boldsymbol{\lambda}} P(\mathbf{z},\boldsymbol{\lambda}) = \mathbf{0}$ ensures that the constraint $\mathbf{Z}(\boldsymbol{\alpha}^{0})\mathbf{z} + \mathbf{d} = \mathbf{0}$ is fulfilled at $\mathbf{z} = \mathbf{z}^{be}$, while the condition $\nabla_{\mathbf{z}} P(\mathbf{z},\boldsymbol{\lambda}) = \mathbf{0}$ yields

$$\begin{aligned} \nabla_{\mathbf{z}} P(\mathbf{z},\boldsymbol{\lambda}) &= \nabla_{\mathbf{z}}\left\{\mathbf{z}^{\dagger}\mathbf{C}^{-1}\mathbf{z} + 2\left[\boldsymbol{\lambda}^{\dagger}\mathbf{S}(\boldsymbol{\alpha}), -\boldsymbol{\lambda}^{\dagger}\right]\mathbf{z} + 2\boldsymbol{\lambda}^{\dagger}\mathbf{d}\right\} \\ &= 2\mathbf{C}^{-1}\mathbf{z} + 2\begin{pmatrix} \mathbf{S}^{\dagger}(\boldsymbol{\alpha})\boldsymbol{\lambda} \\ -\boldsymbol{\lambda} \end{pmatrix} = \mathbf{0}, \quad at\ \mathbf{z} = \mathbf{z}^{be}. \end{aligned} \tag{A.1}$$

Multiplying the last line of the above equation on the left by $\mathbf{C}$ and solving it for $\mathbf{z}^{be}$ gives:

$$\mathbf{z}^{be} = \mathbf{C}\begin{pmatrix} \mathbf{S}^{\dagger}(\boldsymbol{\alpha})\boldsymbol{\lambda} \\ -\boldsymbol{\lambda} \end{pmatrix} = \begin{pmatrix} \mathbf{C}_{\alpha} & \mathbf{C}_{\alpha r} \\ \mathbf{C}_{r\alpha} & \mathbf{C}_{m} \end{pmatrix}\begin{pmatrix} \mathbf{S}^{\dagger}(\boldsymbol{\alpha})\boldsymbol{\lambda} \\ -\boldsymbol{\lambda} \end{pmatrix}. \tag{A.2}$$

Writing the above expression in component form gives the following results for the calibrated best-estimate parameters and responses, respectively:

$$\boldsymbol{\alpha}^{be} = \boldsymbol{\alpha}^{0} + \left(\mathbf{C}_{\alpha r} - \mathbf{C}_{\alpha}\left[\mathbf{S}\left(\boldsymbol{\alpha}^{0}\right)\right]^{\dagger}\right)\boldsymbol{\lambda} \tag{A.3}$$

$$\mathbf{r}_{c}\left(\boldsymbol{\alpha}^{be}\right) = \mathbf{r}_{m} + \left(\mathbf{C}_{m} - \mathbf{C}_{r\alpha}\left[\mathbf{S}\left(\boldsymbol{\alpha}^{0}\right)\right]^{\dagger}\right)\boldsymbol{\lambda} \tag{A.4}$$

The Lagrange multiplier $\boldsymbol{\lambda}$ can be evaluated by using Eqs. (A.3) and (A.4) in Eq. (III.17) at $\mathbf{z}^{be}$, to obtain

$$\mathbf{d} \equiv \mathbf{R}\left(\boldsymbol{\alpha}^{0}\right) - \mathbf{r}_{m} = \left[\mathbf{C}_{rc}\left(\boldsymbol{\alpha}^{0}\right) - \mathbf{C}_{r\alpha}\left[\mathbf{S}\left(\boldsymbol{\alpha}^{0}\right)\right]^{\dagger} - \left[\mathbf{S}\left(\boldsymbol{\alpha}^{0}\right)\right]\mathbf{C}_{\alpha r} + \mathbf{C}_{m}\right]\boldsymbol{\lambda}. \tag{A.5}$$

In the above equation, the matrix-valued expression that multiplies $\boldsymbol{\lambda}$ is actually the covariance-matrix, $\mathbf{C}_{d}\left(\boldsymbol{\alpha}^{0}\right)$, of the vector of response-deviations, $\mathbf{d}$, namely:

$$\begin{aligned} \mathbf{C}_{d}\left(\boldsymbol{\alpha}^{0}\right) \triangleq \left\langle \mathbf{d}\mathbf{d}^{\dagger}\right\rangle &= \left\langle \left(\delta\mathbf{r} - \mathbf{S}\left(\boldsymbol{\alpha}^{0}\right)\delta\boldsymbol{\alpha}\right)\left(\delta\mathbf{r}^{\dagger} - \delta\boldsymbol{\alpha}^{\dagger}\left[\mathbf{S}\left(\boldsymbol{\alpha}^{0}\right)\right]^{\dagger}\right)\right\rangle \\ &= \mathbf{C}_{rc}\left(\boldsymbol{\alpha}^{0}\right) - \mathbf{C}_{r\alpha}\left[\mathbf{S}\left(\boldsymbol{\alpha}^{0}\right)\right]^{\dagger} - \left[\mathbf{S}\left(\boldsymbol{\alpha}^{0}\right)\right]\mathbf{C}_{\alpha r} + \mathbf{C}_{m} \end{aligned} \tag{A.6}$$

In component form, the matrix $\mathbf{C}_{d}$ is expressed as

$$
\mathbf{C}_d \triangleq \begin{pmatrix} \mathbf{C}_d^{11} & \cdots & \mathbf{C}_d^{1N_t} \\ \vdots & \ddots & \vdots \\ \mathbf{C}_d^{N_t 1} & \cdots & \mathbf{C}_d^{N_t N_t} \end{pmatrix} = \begin{pmatrix} \mathbf{C}_{rc}^{11} + \mathbf{C}_m^{11} & \cdots & \mathbf{C}_{rc}^{1N_t} + \mathbf{C}_m^{1N_t} \\ \vdots & \ddots & \vdots \\ \mathbf{C}_{rc}^{N_t 1} + \mathbf{C}_m^{N_t 1} & \cdots & \mathbf{C}_{rc}^{N_t N_t} + \mathbf{C}_m^{N_t N_t} \end{pmatrix}
$$

$$
- \begin{pmatrix} \mathbf{C}_{r\alpha}^{11} \left(\mathbf{S}^{\dagger}\right)^{11} + \mathbf{S}^{11}\mathbf{C}_{\alpha r}^{11} & \cdots & \mathbf{S}^{11}\mathbf{C}_{\alpha r}^{1N_t} + \sum_{\rho=1}^{N_t} \mathbf{C}_{r\alpha}^{1\rho} \left(\mathbf{S}^{\dagger}\right)^{N_t \rho} \\ \vdots & \ddots & \vdots \\ \mathbf{C}_{r\alpha}^{N_t 1} \left(\mathbf{S}^{\dagger}\right)^{11} + \sum_{\rho=1}^{N_t} \mathbf{S}^{N_t \rho}\mathbf{C}_{\alpha r}^{\rho 1} & \cdots & \sum_{\rho=1}^{N_t} \left[\mathbf{C}_{r\alpha}^{N_t \rho} \left(\mathbf{S}^{\dagger}\right)^{N_t \rho} + \mathbf{S}^{N_t \rho}\mathbf{C}_{\alpha r}^{\rho N_t} \right] \end{pmatrix}. \tag{A.7}
$$

Note that the second and third terms in Eq. (A.6), which are transposes of each other, are square matrices, which implies that the matrix $\mathbf{C}_d\left(\boldsymbol{\alpha}^0\right)$ is symmetric. In terms of the matrix $\mathbf{C}_d\left(\boldsymbol{\alpha}^0\right)$, Eq. (A.5) yields the following expression for the Lagrange multiplier $\boldsymbol{\lambda}$ at $\mathbf{z}^{be}$:

$$
\boldsymbol{\lambda} = \left[\mathbf{C}_d\left(\boldsymbol{\alpha}^0\right)\right]^{-1} \mathbf{d}\,. \tag{A.8}
$$

Replacing now Eq. (A.8) in Eq. (A.3) yields the following expressions for the nominal values of the calibrated (adjusted) best-estimate parameters:

$$
\boldsymbol{\alpha}^{be} = \boldsymbol{\alpha}^0 + \left(\mathbf{C}_{\alpha r} - \mathbf{C}_{\alpha}\left[\mathbf{S}\left(\boldsymbol{\alpha}^0\right)\right]^{\dagger}\right)\left[\mathbf{C}_d\left(\boldsymbol{\alpha}^0\right)\right]^{-1} \mathbf{d} \tag{A.9}
$$

In component form, the above expression for the calibrated best-estimate parameter values becomes

$$\begin{pmatrix} \left(\boldsymbol{\alpha}^{be}\right)^{1} \\ \vdots \\ \left(\boldsymbol{\alpha}^{be}\right)^{N_t} \end{pmatrix} = \begin{pmatrix} \left(\boldsymbol{\alpha}^{0}\right)^{1} \\ \vdots \\ \left(\boldsymbol{\alpha}^{0}\right)^{N_t} \end{pmatrix} + \begin{pmatrix} \mathbf{C}_{\alpha r}^{11} - \mathbf{C}_{\alpha}^{11}\left(\mathbf{S}^{\dagger}\right)^{11} & \cdots & \mathbf{C}_{\alpha r}^{1N_t} - \sum_{\rho=1}^{N_t}\mathbf{C}_{\alpha}^{1\rho}\left(\mathbf{S}^{\dagger}\right)^{N_t\rho} \\ \vdots & \ddots & \vdots \\ \mathbf{C}_{\alpha r}^{N_t 1} - \mathbf{C}_{\alpha}^{N_t 1}\left(\mathbf{S}^{\dagger}\right)^{11} & \cdots & \mathbf{C}_{\alpha r}^{N_t N_t} - \sum_{\rho=1}^{N_t}\mathbf{C}_{\alpha}^{N_t\rho}\left(\mathbf{S}^{\dagger}\right)^{N_t\rho} \end{pmatrix} \times \begin{pmatrix} \sum_{\eta=1}^{N_t}\mathbf{K}_{d}^{1\eta}\mathbf{d}^{\eta} \\ \vdots \\ \sum_{\eta=1}^{N_t}\mathbf{K}_{d}^{N_t\eta}\mathbf{d}^{\eta} \end{pmatrix} \tag{A.10}$$

where $\mathbf{K}_d^{\nu\eta}$ denotes the corresponding (ν,η)-element of the block-matrix $\mathbf{C}_d^{-1}$. As Eq. (A.10) indicates, each component $\left(\boldsymbol{\alpha}^{be}\right)^{\nu}$, representing the calibrated best-estimates for the system parameters at a specific time node ν, takes on the expression

$$\left(\boldsymbol{\alpha}^{be}\right)^{\nu} = \left(\boldsymbol{\alpha}^{0}\right)^{\nu} + \sum_{\mu=1}^{N_t}\left\{\left[\mathbf{C}_{\alpha r}^{\nu\mu} - \sum_{\rho=1}^{\mu}\mathbf{C}_{\alpha}^{\nu\rho}\left(\mathbf{S}^{\dagger}\right)^{\mu\rho}\right]\left[\sum_{\eta=1}^{N_t}\mathbf{K}_{d}^{\mu\eta}\mathbf{d}^{\eta}\right]\right\}, \quad \nu = 1,\ldots,N_t. \tag{A.11}$$

Similarly, replacing now Eq. (A.8) in Eq. (A.4) yields the following expressions for the nominal values of the calibrated (adjusted) best-estimate responses:

$$\mathbf{r}\left(\boldsymbol{\alpha}^{be}\right) = \mathbf{r}_m + \left(\mathbf{C}_m - \mathbf{C}_{r\alpha}\left[\mathbf{S}\left(\boldsymbol{\alpha}^{0}\right)\right]^{\dagger}\right)\left[\mathbf{C}_d\left(\boldsymbol{\alpha}^{0}\right)\right]^{-1}\mathbf{d} \tag{A.12}$$

or , in component form:

$$\begin{pmatrix} \left(\mathbf{r}^{be}\right)^{1} \\ \vdots \\ \left(\mathbf{r}^{be}\right)^{N_t} \end{pmatrix} = \begin{pmatrix} \left(\mathbf{r}_x\right)^{1} \\ \vdots \\ \left(\mathbf{r}_x\right)^{N_t} \end{pmatrix} + \begin{pmatrix} \mathbf{C}_m^{11} - \mathbf{C}_{r\alpha}^{11}\left(\mathbf{S}^{\dagger}\right)^{11} & \cdots & \mathbf{C}_m^{1N_t} - \sum_{\rho=1}^{N_t}\mathbf{C}_{r\alpha}^{1\rho}\left(\mathbf{S}^{\dagger}\right)^{N_t\rho} \\ \vdots & \ddots & \vdots \\ \mathbf{C}_m^{N_t 1} - \mathbf{C}_{r\alpha}^{N_t 1}\left(\mathbf{S}^{\dagger}\right)^{11} & \cdots & \mathbf{C}_m^{N_t N_t} - \sum_{\rho=1}^{N_t}\mathbf{C}_{r\alpha}^{N_t\rho}\left(\mathbf{S}^{\dagger}\right)^{N_t\rho} \end{pmatrix} \times \begin{pmatrix} \sum_{\eta=1}^{N_t}\mathbf{K}_d^{1\eta}\mathbf{d}^{\eta} \\ \vdots \\ \sum_{\eta=1}^{N_t}\mathbf{K}_d^{N_t\eta}\mathbf{d}^{\eta} \end{pmatrix} \tag{A.13}$$

As indicated by Eq. (A.13), each component $\left(\mathbf{r}^{be}\right)^{\nu}$, of calibrated best-estimates for the responses at a specific time node ν, becomes

$$\left(\mathbf{r}^{be}\right)^{\nu} = \left(\mathbf{r}_m\right)^{\nu} + \sum_{\mu=1}^{N_t}\left\{\left[\mathbf{C}_m^{\nu\mu} - \sum_{\rho=1}^{\mu}\mathbf{C}_{r\alpha}^{\nu\rho}\left(\mathbf{S}^{\dagger}\right)^{\mu\rho}\right]\left[\sum_{\eta=1}^{N_t}\mathbf{K}_d^{\mu\eta}\mathbf{d}^{\eta}\right]\right\}, \quad \nu = 1,\ldots,N_t. \tag{A.14}$$

The best-estimate covariances, $\mathbf{C}_{\alpha}^{be}$ and $\mathbf{C}_{r}^{be}$, corresponding to the best-estimate parameters $\boldsymbol{\alpha}^{be}$ and responses $\mathbf{r}\left(\boldsymbol{\alpha}^{be}\right)$, together with the new best-estimate parameter-response covariance matrix $\mathbf{C}_{\alpha r}^{be}$ are defined as follows:

$$\mathbf{C}_{\alpha}^{be} \triangleq \left\langle\left(\boldsymbol{\alpha} - \boldsymbol{\alpha}^{be}\right)\left(\boldsymbol{\alpha} - \boldsymbol{\alpha}^{be}\right)^{\dagger}\right\rangle, \tag{A.15}$$

$$\mathbf{C}_{r}^{be} \triangleq \left\langle\left(\mathbf{r} - \mathbf{r}\left(\boldsymbol{\alpha}^{be}\right)\right)\left(\mathbf{r} - \mathbf{r}\left(\boldsymbol{\alpha}^{be}\right)\right)^{\dagger}\right\rangle \tag{A.16}$$

$$\mathbf{C}_{r\alpha}^{be} = \mathbf{C}_{\alpha r}^{be} \triangleq \left\langle\left(\boldsymbol{\alpha} - \boldsymbol{\alpha}^{be}\right)\left(\mathbf{r} - \mathbf{r}\left(\boldsymbol{\alpha}^{be}\right)\right)^{\dagger}\right\rangle. \tag{A.17}$$

The explicit expression of $\mathbf{C}_{\alpha}^{be}$ is obtained by replacing Eq. (A.9) in Eq. (A.15), by carrying out the respective averaging procedure, and by noting that

$$\mathbf{d} \triangleq \mathbf{R}\left(\boldsymbol{\alpha}^{0}\right) - \mathbf{r}_{m} = \mathbf{r} - \mathbf{r}_{m} - \mathbf{S}\left(\boldsymbol{\alpha}^{0}\right)\left(\boldsymbol{\alpha} - \boldsymbol{\alpha}^{0}\right). \tag{A.18}$$

Performing the operations indicated above yields

$$\begin{aligned}\mathbf{C}_{\alpha}^{be} \triangleq & \left\langle \left(\boldsymbol{\alpha} - \boldsymbol{\alpha}^{0}\right)\left(\boldsymbol{\alpha} - \boldsymbol{\alpha}^{0}\right)^{\dagger} \right\rangle - \left\langle \left(\boldsymbol{\alpha} - \boldsymbol{\alpha}^{0}\right)\mathbf{d}^{\dagger} \right\rangle \left[\mathbf{C}_{d}\left(\boldsymbol{\alpha}^{0}\right)\right]^{-1}\left(\mathbf{C}_{\alpha r} - \left[\mathbf{S}\left(\boldsymbol{\alpha}^{0}\right)\right]\mathbf{C}_{\alpha}\right) \\ & - \left(\mathbf{C}_{\alpha r} - \mathbf{C}_{\alpha}\left[\mathbf{S}\left(\boldsymbol{\alpha}^{0}\right)\right]^{\dagger}\right)\left[\mathbf{C}_{d}\left(\boldsymbol{\alpha}^{0}\right)\right]^{-1}\left\langle \mathbf{d}\left(\boldsymbol{\alpha} - \boldsymbol{\alpha}^{0}\right)^{\dagger} \right\rangle \\ & + \left(\mathbf{C}_{\alpha r} - \mathbf{C}_{\alpha}\left[\mathbf{S}\left(\boldsymbol{\alpha}^{0}\right)\right]^{\dagger}\right)\left[\mathbf{C}_{d}\left(\boldsymbol{\alpha}^{0}\right)\right]^{-1}\left\langle \mathbf{d}\mathbf{d}^{\dagger} \right\rangle \left[\mathbf{C}_{d}\left(\boldsymbol{\alpha}^{0}\right)\right]^{-1}\left(\mathbf{C}_{\alpha r} - \left[\mathbf{S}\left(\boldsymbol{\alpha}^{0}\right)\right]\mathbf{C}_{\alpha}\right)\end{aligned} \tag{A.19}$$

The above expression can be simplified by recalling Eq. (A.6), and by noting that

$$\mathbf{C}_{\alpha d}\left(\boldsymbol{\alpha}^{0}\right) \triangleq \left\langle \left(\boldsymbol{\alpha} - \boldsymbol{\alpha}^{0}\right)\mathbf{d}^{\dagger} \right\rangle = \left(\mathbf{C}_{\alpha r} - \mathbf{C}_{\alpha}\left[\mathbf{S}\left(\boldsymbol{\alpha}^{0}\right)\right]^{\dagger}\right), \tag{A.20}$$

$$\mathbf{C}_{d\alpha}\left(\boldsymbol{\alpha}^{0}\right) \triangleq \left\langle \mathbf{d}\left(\boldsymbol{\alpha} - \boldsymbol{\alpha}^{0}\right)^{\dagger} \right\rangle = \left(\mathbf{C}_{\alpha r} - \left[\mathbf{S}\left(\boldsymbol{\alpha}^{0}\right)\right]\mathbf{C}_{\alpha}\right) = \left[\mathbf{C}_{\alpha d}\left(\boldsymbol{\alpha}^{0}\right)\right]^{\dagger}. \tag{A.21}$$

Replacing Eqs. (A.19) through (A.21) in the expression of $\mathbf{C}_{\alpha}^{be}$ leads to

$$\begin{aligned}\mathbf{C}_{\alpha}^{be} &= \mathbf{C}_{\alpha} - \left(\mathbf{C}_{\alpha r} - \mathbf{C}_{\alpha}\left[\mathbf{S}\left(\boldsymbol{\alpha}^{0}\right)\right]^{\dagger}\right)\left[\mathbf{C}_{d}\left(\boldsymbol{\alpha}^{0}\right)\right]^{-1}\left(\mathbf{C}_{\alpha r} - \left[\mathbf{S}\left(\boldsymbol{\alpha}^{0}\right)\right]\mathbf{C}_{\alpha}\right) \\ &= \mathbf{C}_{\alpha} - \left[\mathbf{C}_{\alpha d}\left(\boldsymbol{\alpha}^{0}\right)\right]\left[\mathbf{C}_{d}\left(\boldsymbol{\alpha}^{0}\right)\right]^{-1}\left[\mathbf{C}_{\alpha d}\left(\boldsymbol{\alpha}^{0}\right)\right]^{\dagger}\end{aligned} \tag{A.22}$$

Furthermore, noting that

$$\mathbf{C}_{rd}\left(\boldsymbol{\alpha}^0\right) \triangleq \left\langle \left(\mathbf{r}-\mathbf{r}_m\right)\mathbf{d}^\dagger \right\rangle = \left(\mathbf{C}_m - \mathbf{C}_{r\alpha}\left[\mathbf{S}\left(\boldsymbol{\alpha}^0\right)\right]^\dagger\right),$$

$$\mathbf{C}_{dr}\left(\boldsymbol{\alpha}^0\right) \triangleq \left\langle \mathbf{d}\left(\mathbf{r}-\mathbf{r}_m\right)^\dagger \right\rangle = \left(\mathbf{C}_m - \left[\mathbf{S}\left(\boldsymbol{\alpha}^0\right)\right]\mathbf{C}_{r\alpha}\right) = \left[\mathbf{C}_{rd}\left(\boldsymbol{\alpha}^0\right)\right]^\dagger . \qquad \text{(A.23)}$$

and replacing the above expressions in Eq. (A.16) gives the following expression for the best-estimate parameter covariance matrix:

$$\begin{aligned}\mathbf{C}_r^{be} &= \mathbf{C}_m - \left(\mathbf{C}_m - \mathbf{C}_{r\alpha}\left[\mathbf{S}\left(\boldsymbol{\alpha}^0\right)\right]^\dagger\right)\left[\mathbf{C}_d\left(\boldsymbol{\alpha}^0\right)\right]^{-1}\left(\mathbf{C}_m - \left[\mathbf{S}\left(\boldsymbol{\alpha}^0\right)\right]\mathbf{C}_{\alpha r}\right) \\ &= \mathbf{C}_m - \left[\mathbf{C}_{rd}\left(\boldsymbol{\alpha}^0\right)\right]\left[\mathbf{C}_d\left(\boldsymbol{\alpha}^0\right)\right]^{-1}\left[\mathbf{C}_{rd}\left(\boldsymbol{\alpha}^0\right)\right]^\dagger\end{aligned} \qquad \text{(A.24)}$$

A similar sequence of computations leads to the following expression for the best-estimate response-parameter covariance matrix:

$$\begin{aligned}\mathbf{C}_{r\alpha}^{be} = \mathbf{C}_{\alpha r}^{be} &= \mathbf{C}_{r\alpha} - \left(\mathbf{C}_m - \mathbf{C}_{r\alpha}\left[\mathbf{S}\left(\boldsymbol{\alpha}^0\right)\right]^\dagger\right)\left[\mathbf{C}_d\left(\boldsymbol{\alpha}^0\right)\right]^{-1}\left(\mathbf{C}_{\alpha r} - \left[\mathbf{S}\left(\boldsymbol{\alpha}^0\right)\right]\mathbf{C}_\alpha\right) \\ &= \mathbf{C}_{r\alpha} - \left[\mathbf{C}_{rd}\left(\boldsymbol{\alpha}^0\right)\right]\left[\mathbf{C}_d\left(\boldsymbol{\alpha}^0\right)\right]^{-1}\left[\mathbf{C}_{\alpha d}\left(\boldsymbol{\alpha}^0\right)\right]^\dagger\end{aligned} \qquad \text{(A.25)}$$

Note in Eq. (A.22) that a symmetric positive matrix is subtracted from the initial parameter covariance matrix $\mathbf{C}_\alpha$; hence, in this sense, *the best-estimate parameter uncertainty matrix* $\mathbf{C}_\alpha^{be}$ *has been reduced by the calibration (adjustment) procedure, through the introduction of new information from experiments*. Similarly in Eq. (A.24), a symmetric positive matrix is subtracted from the initial covariance matrix $\mathbf{C}_m$ of the experimental-responses; hence, *the best-estimate response covariance matrix* $\mathbf{C}_r^{be}$ *has been improved (reduced) through the introduction of new experimental information*. Furthermore, Eq. (A.25) indicates that the

calibration (adjustment) procedure will introduce correlations between the calibrated (adjusted) parameters and responses even if the parameters and response were initially uncorrelated, since $\mathbf{C}_{r\alpha}^{be} \neq 0$ even if $\mathbf{C}_{r\alpha} = 0$, i.e.,

$$\mathbf{C}_{r\alpha}^{be} = \mathbf{C}_m \left[\mathbf{C}_{rc}\left(\boldsymbol{\alpha}^0\right) + \mathbf{C}_m \right]^{-1} \left[\mathbf{S}\left(\boldsymbol{\alpha}^0\right) \right] \mathbf{C}_\alpha \text{, when } \mathbf{C}_{r\alpha} = 0 . \tag{A.26}$$

As the above expression indicates, the adjustment (calibration) modifies the correlations among the parameters through couplings introduced by the sensitivities of the participating responses; these sensitivities relate the initial parameter-covariances and experimental-response covariances. In summary, the incorporation of additional (experimental) information in the adjustment (calibration) process reduces the variances of the adjusted parameters and responses while also modifying their correlations.

Note that Eq. (A.24) expresses the best-estimate predicted response covariance matrix $\mathbf{C}_r^{be}$ in terms of the initial covariance matrix $\mathbf{C}_m$ of the experimental-responses. On the other hand, the expression of the computed best-estimate response covariance matrix, $\mathbf{C}_{rc}^{be}$, can be derived directly from the model (the subscript "rc", denotes "computed response", to distinguish it from the covariance $\mathbf{C}_r^{be}$, which is obtained directly from the calibration/adjustment process). The starting point for computing $\mathbf{C}_{rc}^{be}$ is the linearization of the model, similar to that shown in Eq. (III.10), but around $\boldsymbol{\alpha}^{be}$ instead of $\boldsymbol{\alpha}^0$, i.e.

$$\mathbf{r} = \mathbf{R}\left(\boldsymbol{\alpha}^{be}\right) + \mathbf{S}\left(\boldsymbol{\alpha}^{be}\right)\left(\boldsymbol{\alpha} - \boldsymbol{\alpha}^{be}\right) + \textit{higher order terms} . \tag{A.27}$$

It follows from Eqs. (A.27) that

$$
\begin{aligned}
\mathbf{C}_{rc}^{be} &= \left\langle \left(\mathbf{r}-\mathbf{R}\left(\boldsymbol{\alpha}^{be}\right)\right)\left(\mathbf{r}-\mathbf{R}\left(\boldsymbol{\alpha}^{be}\right)\right)^{\dagger} \right\rangle = \left[\mathbf{S}\left(\boldsymbol{\alpha}^{be}\right)\right]\left\langle \left(\boldsymbol{\alpha}-\boldsymbol{\alpha}^{be}\right)\left(\boldsymbol{\alpha}-\boldsymbol{\alpha}^{be}\right)^{\dagger} \right\rangle \left[\mathbf{S}\left(\boldsymbol{\alpha}^{be}\right)\right]^{\dagger} \\
&= \left[\mathbf{S}\left(\boldsymbol{\alpha}^{be}\right)\right]\mathbf{C}_{\alpha}^{be}\left[\mathbf{S}\left(\boldsymbol{\alpha}^{be}\right)\right]^{\dagger} \\
&= \left[\mathbf{S}\left(\boldsymbol{\alpha}^{be}\right)\right]\left[\mathbf{C}_{\alpha}-\left(\mathbf{C}_{\alpha r}-\mathbf{C}_{\alpha}\left[\mathbf{S}\left(\boldsymbol{\alpha}^{0}\right)\right]^{\dagger}\right)\left[\mathbf{C}_{d}\left(\boldsymbol{\alpha}^{0}\right)\right]^{-1}\left(\mathbf{C}_{\alpha r}-\left[\mathbf{S}\left(\boldsymbol{\alpha}^{0}\right)\right]\mathbf{C}_{\alpha}\right)\right]\left[\mathbf{S}\left(\boldsymbol{\alpha}^{be}\right)\right]^{\dagger}
\end{aligned}
\tag{A.28}
$$

Comparing Eq. (A.28) to Eq. (A.24) reveals that $\mathbf{C}_{rc}^{be} \neq \mathbf{C}_{r}^{be}$ since $\mathbf{S}\left(\boldsymbol{\alpha}^{be}\right) \neq \mathbf{S}\left(\boldsymbol{\alpha}^{0}\right)$, in general. Nevertheless, *when the model is "perfect" (i.e., free of numerical errors) and exactly linear, then the sensitivity matrix* $\mathbf{S}$ *is independent of the parameter values* $\boldsymbol{\alpha}$, i.e.,

$$
\mathbf{S}\left(\boldsymbol{\alpha}^{be}\right) = \mathbf{S}\left(\boldsymbol{\alpha}^{0}\right) = \mathbf{S}\text{, for "perfect" and linear models,} \tag{A.29}
$$

It consequently follows that

$$
\begin{aligned}
\mathbf{C}_{rc}^{be} &= \mathbf{S}\left[\mathbf{C}_{\alpha}-\left(\mathbf{C}_{\alpha r}-\mathbf{C}_{\alpha}\mathbf{S}^{\dagger}\right)\mathbf{C}_{d}^{-1}\left(\mathbf{C}_{\alpha r}-\mathbf{S}\mathbf{C}_{\alpha}\right)\right]\mathbf{S}^{\dagger} \\
&= \mathbf{C}_{rc}-\left(\mathbf{C}_{rc}-\mathbf{S}\mathbf{C}_{\alpha r}\right)\left[\mathbf{C}_{rc}+\mathbf{C}_{e}-\mathbf{C}_{r\alpha}\mathbf{S}^{\dagger}-\mathbf{S}\mathbf{C}_{\alpha r}\right]^{-1}\left(\mathbf{C}_{rc}-\mathbf{C}_{\alpha r}\mathbf{S}^{\dagger}\right) \\
&= \mathbf{C}_{r}^{be}, \quad \textbf{for "}\textit{perfect}\textbf{" linear models.}
\end{aligned}
\tag{A.30}
$$

The above equality can be demonstrated by using the following identity which holds for regular square matrices $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$,

$$
\mathbf{A}-\left(\mathbf{A}-\mathbf{C}^{\dagger}\right)\left(\mathbf{A}+\mathbf{B}-\mathbf{C}-\mathbf{C}^{\dagger}\right)^{-1}\left(\mathbf{A}-\mathbf{C}\right) = \mathbf{B}-\left(\mathbf{B}-\mathbf{C}\right)\left(\mathbf{A}+\mathbf{B}-\mathbf{C}-\mathbf{C}^{\dagger}\right)^{-1}\left(\mathbf{B}-\mathbf{C}^{\dagger}\right), \tag{A.31}
$$

and by effecting the replacements $\mathbf{A} \to \mathbf{C}_{rc}$, $\mathbf{B} \to \mathbf{C}_m$ $\mathbf{C} \to \mathbf{C}_{\alpha r}\mathbf{S}^{\dagger}$ in the above identity. For completeness, note that Eq. (A.31) can be obtained by starting from the identity

$$\mathbf{I} = \left(\mathbf{A} - \mathbf{C}^{\dagger}\right)\left(\mathbf{A} + \mathbf{B} - \mathbf{C} - \mathbf{C}^{\dagger}\right)^{-1} + \left(\mathbf{B} - \mathbf{C}\right)\left(\mathbf{A} + \mathbf{B} - \mathbf{C} - \mathbf{C}^{\dagger}\right)^{-1},$$

and by multiplying it on the right by $\left(\mathbf{A} - \mathbf{C}\right)$ to obtain

$$\begin{aligned}
\mathbf{A} - \mathbf{C} &= \left(\mathbf{A} - \mathbf{C}^{\dagger}\right)\left(\mathbf{A} + \mathbf{B} - \mathbf{C} - \mathbf{C}^{\dagger}\right)^{-1}\left(\mathbf{A} - \mathbf{C}\right) \\
&\quad + \left(\mathbf{B} - \mathbf{C}\right)\left(\mathbf{A} + \mathbf{B} - \mathbf{C} - \mathbf{C}^{\dagger}\right)^{-1}\left(\mathbf{A} - \mathbf{C} + \mathbf{B} - \mathbf{B} + \mathbf{C}^{\dagger} - \mathbf{C}^{\dagger}\right) \\
&= \left(\mathbf{A} - \mathbf{C}^{\dagger}\right)\left(\mathbf{A} + \mathbf{B} - \mathbf{C} - \mathbf{C}^{\dagger}\right)^{-1}\left(\mathbf{A} - \mathbf{C}\right) \\
&\quad + \left(\mathbf{B} - \mathbf{C}\right)\left(\mathbf{A} + \mathbf{B} - \mathbf{C} - \mathbf{C}^{\dagger}\right)^{-1}\left(\mathbf{A} + \mathbf{B} - \mathbf{C} - \mathbf{C}^{\dagger}\right) \\
&\quad - \left(\mathbf{B} - \mathbf{C}\right)\left(\mathbf{A} + \mathbf{B} - \mathbf{C} - \mathbf{C}^{\dagger}\right)^{-1}\left(\mathbf{B} - \mathbf{C}^{\dagger}\right)
\end{aligned}$$

a result which, after some minor rearrangements, reduces to Eq. (A.31).

It is important to note that the computation of the best estimate parameter and response values, together with their corresponding best-estimate uncertainties, cf. Eqs. (A.9), (A.12), (A.22), (A.24) and (A.25) require the inversion of a single matrix, namely the matrix $\mathbf{C}_d\left(\boldsymbol{\alpha}^0\right)$ defined in Eq. (A.6). This is often advantageous in practice, since the order of the matrix $\mathbf{C}_d\left(\boldsymbol{\alpha}^0\right)$ is given by the number of measured (or computed responses), which is most often considerably smaller that the number of model parameters under consideration.

On the other hand, when the number of parameter exceeds the number of responses, it is possible to derive alternative expressions for the best-estimate calibrated parameters and their

corresponding best-estimate covariances, by performing all derivations in the "parameter space" rather than in "response space". This entails using Eq. (III.10) to eliminate the response (variables) $\mathbf{r}$ at the outset, and carrying out the minimization procedure solely for the parameters (variables) $\boldsymbol{\alpha}$. Alternatively, a considerable shortcut can be achieved by employing the Sherman-Morrison-Woodbury extension

$$\left(\mathbf{A}+\mathbf{CBD}^{\dagger}\right)^{-1}=\mathbf{A}^{-1}-\mathbf{A}^{-1}\mathbf{C}\left(\mathbf{B}^{-1}+\mathbf{D}^{\dagger}\mathbf{A}^{-1}\mathbf{C}\right)^{-1}\mathbf{D}^{\dagger}\mathbf{A}^{-1} \tag{A.32}$$

where $\mathbf{A}$ and $\mathbf{B}$ are invertible, and $\mathbf{D}=\mathbf{C}$, to rewrite the matrix $\left[\mathbf{C}_d\left(\boldsymbol{\alpha}^0\right)\right]^{-1}$, defined in Eq. (A.6), in the following alternative way

$$\begin{aligned}\mathbf{C}_d^{-1} &\triangleq \left(\mathbf{C}_{rc}-\mathbf{C}_{r\alpha}\mathbf{S}^{\dagger}-\mathbf{S}\mathbf{C}_{\alpha r}+\mathbf{C}_m\right)^{-1} \\ &= \mathbf{A}^{-1}-\mathbf{A}^{-1}\mathbf{S}\left(\mathbf{C}_{\alpha}^{-1}+\mathbf{S}^{\dagger}\mathbf{A}^{-1}\mathbf{S}\right)^{-1}\mathbf{S}^{\dagger}\mathbf{A}^{-1}, \quad \mathbf{A}\triangleq\mathbf{C}_m-\mathbf{C}_{r\alpha}\mathbf{S}^{\dagger}-\mathbf{S}\mathbf{C}_{\alpha r}\end{aligned} . \tag{A.33}$$

The above expression provides the bridge between the "response-space" and "parameter-space" formulations. This expression also highlights the fact that the response-space formulation requires a single inversion of a square symmetric matrix of the same dimensions as the number of responses. In contradistinction, the "parameter space" formulation requires the inversion of three symmetric matrices, two of which have dimensions equal to the number of parameters and one of dimensions equal to the number of responses. When the parameters and responses are initially uncorrelated, i.e., when $\mathbf{C}_{r\alpha}=\mathbf{0}$, the expressions in parameter space of the best-estimate calibrated (adjusted) quantities can be simplified somewhat by using the following special form of Eq. (A.32)

$$\mathbf{BC}^{\dagger}\left(\mathbf{A}+\mathbf{CBC}^{\dagger}\right)^{-1}=\left(\mathbf{B}^{-1}+\mathbf{C}^{\dagger}\mathbf{A}^{-1}\mathbf{C}\right)^{-1}\mathbf{C}^{\dagger}\mathbf{A}^{-1}, \tag{A.34}$$

in which case Eq. (A.33) can be rewritten in the form

$$\mathbf{C}_\alpha \mathbf{S}^\dagger \mathbf{C}_d^{-1} = \left(\mathbf{C}_\alpha^{-1} + \mathbf{S}^\dagger \mathbf{C}_m^{-1} \mathbf{S}\right)^{-1} \mathbf{S}^\dagger \mathbf{C}_m^{-1}, \text{ when } \mathbf{C}_{r\alpha} = \mathbf{0}. \tag{A.35}$$

In the above case, the "parameter-space" expressions for $\boldsymbol{\alpha}^{be}$ and $\mathbf{C}_\alpha^{be}$ become

$$\boldsymbol{\alpha}^{be} = \boldsymbol{\alpha}^0 - \left(\mathbf{C}_\alpha^{-1} + \mathbf{S}^\dagger \mathbf{C}_m^{-1} \mathbf{S}\right)^{-1} \mathbf{S}^\dagger \mathbf{C}_m^{-1} \mathbf{d}, \quad \text{when } \mathbf{C}_{r\alpha} = \mathbf{0}, \tag{A.36}$$

$$\mathbf{C}_\alpha^{be} = \left(\mathbf{C}_\alpha^{-1} + \mathbf{S}^\dagger \mathbf{C}_m^{-1} \mathbf{S}\right)^{-1}, \quad \text{when } \mathbf{C}_{r\alpha} = \mathbf{0}. \tag{A.37}$$

The computational evaluation of the above expressions still require the inversion of two matrices of dimensions equal to the number of parameters, and of one matrix of dimensions equal to the number of responses. Hence, from a computational standpoint, the "response-space" formulations should be used whenever possible.

For completeness, the calibrated best-estimated predicted covariance matrices, corresponding to the calibrated best-estimates system parameters, are given below in component form:

$$\begin{aligned}\mathbf{C}_\alpha^{be} \triangleq & \begin{pmatrix} \left(\mathbf{C}_\alpha^{be}\right)^{11} & \cdots & \left(\mathbf{C}_\alpha^{be}\right)^{1N_t} \\ \vdots & \ddots & \vdots \\ \left(\mathbf{C}_\alpha^{be}\right)^{N_t 1} & \cdots & \left(\mathbf{C}_\alpha^{be}\right)^{N_t N_t} \end{pmatrix} = \begin{pmatrix} \mathbf{C}_\alpha^{11} & \cdots & \mathbf{C}_\alpha^{1N_t} \\ \vdots & \ddots & \vdots \\ \mathbf{C}_\alpha^{N_t 1} & \cdots & \mathbf{C}_\alpha^{N_t N_t} \end{pmatrix} \\ & - \begin{pmatrix} \mathbf{C}_{\alpha d}^{11} & \cdots & \mathbf{C}_{\alpha d}^{1N_t} \\ \vdots & \ddots & \vdots \\ \mathbf{C}_{\alpha d}^{N_t 1} & \cdots & \mathbf{C}_{\alpha d}^{N_t N_t} \end{pmatrix} \begin{pmatrix} \mathbf{K}_d^{11} & \cdots & \mathbf{K}_d^{1N_t} \\ \vdots & \ddots & \vdots \\ \mathbf{K}_d^{N_t 1} & \cdots & \mathbf{K}_d^{N_t N_t} \end{pmatrix} \begin{pmatrix} \mathbf{C}_{\alpha d}^{11} & \cdots & \mathbf{C}_{\alpha d}^{1N_t} \\ \vdots & \ddots & \vdots \\ \mathbf{C}_{\alpha d}^{N_t 1} & \cdots & \mathbf{C}_{\alpha d}^{N_t N_t} \end{pmatrix}^\dagger \end{aligned} \tag{A.38}$$

where

$$\begin{pmatrix} \mathbf{C}_{\alpha d}^{11} & \cdots & \mathbf{C}_{\alpha d}^{1N_t} \\ \vdots & \ddots & \vdots \\ \mathbf{C}_{\alpha d}^{N_t 1} & \cdots & \mathbf{C}_{\alpha d}^{N_t N_t} \end{pmatrix} = \begin{pmatrix} \mathbf{C}_{\alpha r}^{11} - \mathbf{C}_{\alpha}^{11}\left(\mathbf{S}^{\dagger}\right)^{11} & \cdots & \mathbf{C}_{\alpha r}^{1N_t} - \sum_{\rho=1}^{N_t} \mathbf{C}_{\alpha}^{1\rho}\left(\mathbf{S}^{\dagger}\right)^{N_t\rho} \\ \vdots & \ddots & \vdots \\ \mathbf{C}_{\alpha r}^{N_t 1} - \mathbf{C}_{\alpha}^{N_t 1}\left(\mathbf{S}^{\dagger}\right)^{11} & \cdots & \mathbf{C}_{\alpha r}^{N_t N_t} - \sum_{\rho=1}^{N_t} \mathbf{C}_{\alpha}^{N_t\rho}\left(\mathbf{S}^{\dagger}\right)^{N_t\rho} \end{pmatrix} \tag{A.39}$$

The block-matrix expression in Eq. (A.38) can be written in component form, for the calibrated best-estimate parameter covariance matrix $\left(\mathbf{C}_{\alpha}^{be}\right)^{\nu\mu}$ between two (distinct or not) time-nodes, as follows

$$\left(\mathbf{C}_{\alpha}^{be}\right)^{\nu\mu} = \mathbf{C}_{\alpha}^{\nu\mu} - \sum_{\eta=1}^{N_t}\sum_{\rho=1}^{N_t}\left[\mathbf{C}_{\alpha r}^{\nu\rho} - \sum_{\pi=1}^{\rho}\mathbf{C}_{\alpha}^{\nu\pi}\left(\mathbf{S}^{\dagger}\right)^{\rho\pi}\right]\mathbf{K}_{d}^{\rho\eta}\left[\mathbf{C}_{r\alpha}^{\eta\mu} - \sum_{\pi=1}^{\eta}\mathbf{S}^{\eta\pi}\mathbf{C}_{\alpha}^{\pi\mu}\right]. \tag{A.40}$$

The expression of the calibrated best-estimate covariance block-matrix $\mathbf{C}_{r}^{be}$ for the best-estimate responses is:

$$\begin{aligned} \mathbf{C}_{r}^{be} \triangleq & \begin{pmatrix} \left(\mathbf{C}_{r}^{be}\right)^{11} & \cdots & \left(\mathbf{C}_{r}^{be}\right)^{1N_t} \\ \vdots & \ddots & \vdots \\ \left(\mathbf{C}_{r}^{be}\right)^{N_t 1} & \cdots & \left(\mathbf{C}_{r}^{be}\right)^{N_t N_t} \end{pmatrix} = \begin{pmatrix} \mathbf{C}_{m}^{11} & \cdots & \mathbf{C}_{m}^{1N_t} \\ \vdots & \ddots & \vdots \\ \mathbf{C}_{m}^{N_t 1} & \cdots & \mathbf{C}_{m}^{N_t N_t} \end{pmatrix} \\ & - \begin{pmatrix} \mathbf{C}_{rd}^{11} & \cdots & \mathbf{C}_{rd}^{1N_t} \\ \vdots & \ddots & \vdots \\ \mathbf{C}_{rd}^{N_t 1} & \cdots & \mathbf{C}_{rd}^{N_t N_t} \end{pmatrix} \begin{pmatrix} \mathbf{K}_{d}^{11} & \cdots & \mathbf{K}_{d}^{1N_t} \\ \vdots & \ddots & \vdots \\ \mathbf{K}_{d}^{N_t 1} & \cdots & \mathbf{K}_{d}^{N_t N_t} \end{pmatrix} \begin{pmatrix} \mathbf{C}_{rd}^{11} & \cdots & \mathbf{C}_{rd}^{1N_t} \\ \vdots & \ddots & \vdots \\ \mathbf{C}_{rd}^{N_t 1} & \cdots & \mathbf{C}_{rd}^{N_t N_t} \end{pmatrix}^{\dagger} \end{aligned} \tag{A.41}$$

where

$$\begin{pmatrix} \mathbf{C}_{rd}^{11} & \cdots & \mathbf{C}_{rd}^{1N_t} \\ \vdots & \ddots & \vdots \\ \mathbf{C}_{rd}^{N_t 1} & \cdots & \mathbf{C}_{rd}^{N_t N_t} \end{pmatrix} = \begin{pmatrix} \mathbf{C}_{m}^{11} - \mathbf{C}_{r\alpha}^{11}\left(\mathbf{S}^{\dagger}\right)^{11} & \cdots & \mathbf{C}_{m}^{1N_t} - \sum_{\rho=1}^{N_t}\mathbf{C}_{r\alpha}^{1\rho}\left(\mathbf{S}^{\dagger}\right)^{N_t\rho} \\ \vdots & \ddots & \vdots \\ \mathbf{C}_{m}^{N_t 1} - \mathbf{C}_{r\alpha}^{N_t 1}\left(\mathbf{S}^{\dagger}\right)^{11} & \cdots & \mathbf{C}_{m}^{N_t N_t} - \sum_{\rho=1}^{N_t}\mathbf{C}_{r\alpha}^{N_t\rho}\left(\mathbf{S}^{\dagger}\right)^{N_t\rho} \end{pmatrix} \tag{A.42}$$

The block-matrix expression given in Eq. (A.41) can be written in component form, for the calibrated best-estimate parameter covariance matrix $\left(\mathbf{C}_{r}^{be}\right)^{\nu\mu}$ between two (distinct or not) time-nodes as follows:

$$\left(\mathbf{C}_{r}^{be}\right)^{\nu\mu} = \mathbf{C}_{m}^{\nu\mu} - \sum_{\eta=1}^{N_t}\sum_{\rho=1}^{N_t}\left[\mathbf{C}_{m}^{\nu\rho} - \sum_{\pi=1}^{\rho}\mathbf{C}_{r\alpha}^{\nu\pi}\left(\mathbf{S}^{\dagger}\right)^{\rho\pi}\right]\mathbf{K}_{d}^{\rho\eta}\left[\mathbf{C}_{m}^{\eta\mu} - \sum_{\pi=1}^{\eta}\mathbf{S}^{\eta\pi}\mathbf{C}_{\alpha r}^{\pi\mu}\right]. \tag{A.43}$$

A similar sequence of computations leads to the following expression for the best-estimate response-parameter covariance block-matrix $\mathbf{C}_{\alpha r}^{be}$:

$$\begin{aligned} \mathbf{C}_{r\alpha}^{be} \triangleq & \begin{pmatrix} \left(\mathbf{C}_{r\alpha}^{be}\right)^{11} & \cdots & \left(\mathbf{C}_{r\alpha}^{be}\right)^{1N_t} \\ \vdots & \ddots & \vdots \\ \left(\mathbf{C}_{r\alpha}^{be}\right)^{N_t 1} & \cdots & \left(\mathbf{C}_{r\alpha}^{be}\right)^{N_t N_t} \end{pmatrix} = \begin{pmatrix} \mathbf{C}_{r\alpha}^{11} & \cdots & \mathbf{C}_{r\alpha}^{1N_t} \\ \vdots & \ddots & \vdots \\ \mathbf{C}_{r\alpha}^{N_t 1} & \cdots & \mathbf{C}_{r\alpha}^{N_t N_t} \end{pmatrix} \\ & - \begin{pmatrix} \mathbf{C}_{rd}^{11} & \cdots & \mathbf{C}_{rd}^{1N_t} \\ \vdots & \ddots & \vdots \\ \mathbf{C}_{rd}^{N_t 1} & \cdots & \mathbf{C}_{rd}^{N_t N_t} \end{pmatrix} \begin{pmatrix} \mathbf{K}_{d}^{11} & \cdots & \mathbf{K}_{d}^{1N_t} \\ \vdots & \ddots & \vdots \\ \mathbf{K}_{d}^{N_t 1} & \cdots & \mathbf{K}_{d}^{N_t N_t} \end{pmatrix} \begin{pmatrix} \mathbf{C}_{\alpha d}^{11} & \cdots & \mathbf{C}_{\alpha d}^{1N_t} \\ \vdots & \ddots & \vdots \\ \mathbf{C}_{\alpha d}^{N_t 1} & \cdots & \mathbf{C}_{\alpha d}^{N_t N_t} \end{pmatrix}^{\dagger} \end{aligned} \tag{A.44}$$

The block-matrices in the above expression can be written in component form, for the calibrated best-estimate parameter-response covariance matrix $\left(\mathbf{C}_{\alpha r}^{be}\right)^{\nu\mu}$ between two (distinct or not) time-nodes as follows:

$$\left(\mathbf{C}_{r\alpha}^{be}\right)^{\nu\mu} = \mathbf{C}_{r\alpha}^{\nu\mu} - \sum_{\eta=1}^{N_t}\sum_{\rho=1}^{N_t}\left[\mathbf{C}_{m}^{\nu\rho} - \sum_{\pi=1}^{\rho}\mathbf{C}_{r\alpha}^{\nu\pi}\left(\mathbf{S}^{\dagger}\right)^{\rho\pi}\right]\mathbf{K}_{d}^{\rho\eta}\left[\mathbf{C}_{\alpha r}^{\eta\mu} - \sum_{\pi=1}^{\eta}\mathbf{S}^{\eta\pi}\mathbf{C}_{\alpha}^{\pi\mu}\right]. \qquad \text{(A.45)}$$

Computing the calibrated best-estimate quantities by using Eqs. (A.11), (A.14), (A.40), (A.43), and (A.45) is clearly more advantageous in terms of storage requirements than the direct computations of the corresponding full block-matrices. The largest requirement of computational resources is involved when inverting the matrix $\mathbf{C}_d$. In view of Eq. (A.7), it is important to note that the inverse matrix, $\mathbf{C}_d^{-1}$, incorporates simultaneously all of the available information about the system parameters and responses at all time nodes [i.e., $\nu = 1, 2, ..., N_t$]. Specifically, at any time node ν, $\mathbf{C}_d^{-1}$ incorporates information not only from time nodes prior to ν (i.e., information regarding the "past" and "present" states of the system) but also from time nodes posterior to ν (i.e., information about the “future” states of the system). Through the matrix $\mathbf{C}_d^{-1}$, at any specified time node ν, the calibrated best-estimates parameters $\left(\boldsymbol{\alpha}^{be}\right)^{\nu}$ and responses $\mathbf{r}\left(\boldsymbol{\alpha}^{be}\right) \triangleq \mathbf{r}^{be}$, together with the corresponding calibrated best-estimate covariance matrices $\left(\mathbf{C}_{\alpha}^{be}\right)^{\nu\mu}$, $\left(\mathbf{C}_{r}^{be}\right)^{\nu\mu}$, and $\left(\mathbf{C}_{\alpha r}^{be}\right)^{\nu\mu}$ will also incorporate automatically all of the available information about the system parameters and responses at all time nodes [i.e., $\nu = 1, 2, ..., N_t$].

In this respect, the methodology presented in this section is conceptually related to the "foresight" aspects encountered in decision analysis. It is also important to note that, in practice, the application of the methodology developed in this section involves two distinct computational stages. A complete sensitivity data base (i.e., sensitivities $s_{ni}^{\nu\mu}$ at all times nodes $\nu, \mu = 1, \ldots, N_t$) needs to be generated prior to performing the “data assimilation” and “model calibration” (or data adjustment) stage, since all of the sensitivities are needed in order to

perform data assimilation and model calibration. These stages are performed subsequently, together with the computation of calibrated best-estimate covariance matrices (the "uncertainty analysis" stage), by combining the sensitivities with covariance matrices.

A.1. Particular Case: Two-Step "On-Line" Mathematical Framework

If only information from two consecutive time nodes $\nu = k-1, k; \quad k = (1, 2, ..., N_t)$ is considered, then Eq. (III.6) becomes

$$\begin{pmatrix} \mathbf{r}^{k-1} \\ \mathbf{r}^{k} \end{pmatrix} = \begin{pmatrix} \mathbf{R}^{k-1} \\ \mathbf{R}^{k} \end{pmatrix} + \begin{pmatrix} \mathbf{S}^{k-1,k-1} & \mathbf{0} \\ \mathbf{S}^{k,k-1} & \mathbf{S}^{k,k} \end{pmatrix} \begin{pmatrix} \boldsymbol{\alpha}^{k-1} - \left(\boldsymbol{\alpha}^{0}\right)^{k-1} \\ \boldsymbol{\alpha}^{k} - \left(\boldsymbol{\alpha}^{0}\right)^{k} \end{pmatrix}. \tag{A.46}$$

Corresponding to the relation above, the "sandwich formula" $\mathbf{C}_{rc} \triangleq \mathbf{S}\mathbf{C}_{\alpha}\mathbf{S}^{\dagger}$, which yields the covariance matrix for the computed linearized responses, cf. Eq. (III.12), reduces to

$$\begin{pmatrix} \mathbf{C}_{rc}^{k-1,k-1} & \mathbf{C}_{rc}^{k-1,k} \\ \mathbf{C}_{rc}^{k,k-1} & \mathbf{C}_{rc}^{k,k} \end{pmatrix} = \begin{pmatrix} \mathbf{S}^{k-1,k-1} & \mathbf{0} \\ \mathbf{S}^{k,k-1} & \mathbf{S}^{k,k} \end{pmatrix} \begin{pmatrix} \mathbf{C}_{\alpha}^{k-1,k-1} & \mathbf{C}_{\alpha}^{k-1,k} \\ \mathbf{C}_{\alpha}^{k,k-1} & \mathbf{C}_{\alpha}^{k,k} \end{pmatrix} \begin{pmatrix} \left(\mathbf{S}^{k-1,k-1}\right)^{\dagger} & \left(\mathbf{S}^{k,k-1}\right)^{\dagger} \\ \mathbf{0} & \left(\mathbf{S}^{k,k}\right)^{\dagger} \end{pmatrix} \tag{A.47}$$

Carrying out the above matrix multiplications yields the following explicit expressions of the components of the covariance matrix, $\mathbf{C}_r$, of the computed responses:

$$\mathbf{C}_{rc}^{k-1,k-1} = \mathbf{S}^{k-1,k-1}\mathbf{C}_{\alpha}^{k-1,k-1}\left(\mathbf{S}^{k-1,k-1}\right)^{\dagger} = \left(\mathbf{C}_{rc}^{k-1,k-1}\right)^{\dagger} \tag{A.48}$$

$$\begin{aligned} \mathbf{C}_{rc}^{k-1,k} &= \mathbf{S}^{k-1,k-1}\left[\mathbf{C}_{\alpha}^{k-1,k-1}\left(\mathbf{S}^{k,k-1}\right)^{\dagger} + \mathbf{C}_{\alpha}^{k-1,k}\left(\mathbf{S}^{k,k}\right)^{\dagger}\right] \\ &= \left(\mathbf{C}_{rc}^{k,k-1}\right)^{\dagger} \end{aligned} \tag{A.49}$$

$$
\begin{aligned}
\mathbf{C}_{rc}^{k,k-1} &= \mathbf{S}^{k,k-1}\mathbf{C}_{\alpha}^{k-1,k-1}\left(\mathbf{S}^{k-1,k-1}\right)^{\dagger} + \mathbf{S}^{k,k}\mathbf{C}_{\alpha}^{k,k-1}\left(\mathbf{S}^{k-1,k-1}\right)^{\dagger} \\
&= \left(\mathbf{C}_{rc}^{k-1,k}\right)^{\dagger}
\end{aligned}
\tag{A.50}
$$

$$
\begin{aligned}
\mathbf{C}_{rc}^{k,k} &= \mathbf{S}^{k,k-1}\left[\mathbf{C}_{\alpha}^{k-1,k-1}\left(\mathbf{S}^{k,k-1}\right)^{\dagger} + \mathbf{C}_{\alpha}^{k-1,k}\left(\mathbf{S}^{k,k}\right)^{\dagger}\right] \\
&\quad + \mathbf{S}^{k,k}\left[\mathbf{C}_{\alpha}^{k,k-1}\left(\mathbf{S}^{k,k-1}\right)^{\dagger} + \mathbf{C}_{\alpha}^{k,k}\left(\mathbf{S}^{k,k}\right)^{\dagger}\right] \\
&= \left(\mathbf{C}_{rc}^{k,k}\right)^{\dagger}
\end{aligned}
\tag{A.51}
$$

Recall that the inversion of the symmetric matrix $\mathbf{C}_d \triangleq \mathbf{C}_{rc} - \mathbf{C}_{r\alpha}\mathbf{S}^{\dagger} - \mathbf{S}\mathbf{C}_{\alpha r} + \mathbf{C}_x$ plays a central role in the computation of the calibrated best estimate results. If only information from two consecutive time nodes $\nu = k-1, k; \quad k = (1, 2, ..., N_t)$ is considered, then the matrix $\mathbf{C}_d$ reduces to:

$$
\begin{aligned}
\mathbf{C}_d \triangleq \begin{pmatrix} \mathbf{C}_d^{k-1,k-1} & \mathbf{C}_d^{k-1,k} \\ \mathbf{C}_d^{k,k-1} & \mathbf{C}_d^{k,k} \end{pmatrix} &= \begin{pmatrix} \mathbf{C}_{rc}^{k-1,k-1} + \mathbf{C}_m^{k-1,k-1} & \mathbf{C}_{rc}^{k-1,k} + \mathbf{C}_m^{k-1,k} \\ \mathbf{C}_{rc}^{k,k-1} + \mathbf{C}_m^{k,k-1} & \mathbf{C}_{rc}^{k,k} + \mathbf{C}_m^{k,k} \end{pmatrix} \\
&- \begin{pmatrix} \mathbf{C}_{r\alpha}^{k-1,k-1}\left(\mathbf{S}^{\dagger}\right)^{k-1,k-1} + \mathbf{S}^{k-1,k-1}\mathbf{C}_{\alpha r}^{k-1,k-1} & \mathbf{S}^{k-1,k-1}\mathbf{C}_{\alpha r}^{k-1,k} + \sum_{\rho=k-1}^{k}\mathbf{C}_{r\alpha}^{k-1,\rho}\left(\mathbf{S}^{\dagger}\right)^{k\rho} \\ \mathbf{C}_{r\alpha}^{k,k-1}\left(\mathbf{S}^{\dagger}\right)^{k-1,k-1} + \sum_{\rho=k-1}^{k}\mathbf{S}^{k,\rho}\mathbf{C}_{\alpha r}^{\rho k-1} & \sum_{\rho=k-1}^{k}\left[\mathbf{C}_{r\alpha}^{k,\rho}\left(\mathbf{S}^{\dagger}\right)^{k\rho} + \mathbf{S}^{k\rho}\mathbf{C}_{\alpha r}^{\rho k}\right] \end{pmatrix}.
\end{aligned}
\tag{A.52}
$$

Since both $\mathbf{C}_d^{k-1,k-1}$ and $\mathbf{C}_d^{k,k}$ are nonsingular sub-matrices, the partitioned matrix $\mathbf{C}_d$ can be inverted directly ("by partitioning"); noting that

$$
\mathbf{C}_d^{-1} \triangleq \begin{pmatrix} \mathbf{K}_d^{k-1,k-1} & \mathbf{K}_d^{k-1,k} \\ \mathbf{K}_d^{k,k-1} & \mathbf{K}_d^{k,k} \end{pmatrix}, \tag{A.53}
$$

it follows that components $\mathbf{K}_d^{\nu\eta}$ can be computed using the following expressions:

$$\begin{aligned}\mathbf{K}_d^{k-1,k-1} &= \left[\mathbf{C}_d^{k-1,k-1} - \mathbf{C}_d^{k-1,k}\left(\mathbf{C}_d^{k,k}\right)^{-1}\mathbf{C}_d^{k,k-1}\right]^{-1} \\ &= \left(\mathbf{C}_d^{k-1,k-1}\right)^{-1} + \left(\mathbf{C}_d^{k-1,k-1}\right)^{-1}\mathbf{C}_d^{k-1,k}\mathbf{K}_d^{k,k}\mathbf{C}_d^{k,k-1}\left(\mathbf{C}_d^{k-1,k-1}\right)^{-1}\end{aligned} \tag{A.54}$$

$$\begin{aligned}\mathbf{K}_d^{k-1,k} &= -\left(\mathbf{C}_d^{k-1,k-1}\right)^{-1}\mathbf{C}_d^{k-1,k}\left[\mathbf{C}_d^{k,k} - \mathbf{C}_d^{k,k-1}\left(\mathbf{C}_d^{k-1,k-1}\right)^{-1}\mathbf{C}_d^{k-1,k}\right]^{-1} \\ &= -\left(\mathbf{C}_d^{k-1,k-1}\right)^{-1}\mathbf{C}_d^{k-1,k}\mathbf{K}_d^{k,k}\end{aligned} \tag{A.55}$$

$$\begin{aligned}\mathbf{K}_d^{k,k} &= \left[\mathbf{C}_d^{k,k} - \mathbf{C}_d^{k,k-1}\left(\mathbf{C}_d^{k-1,k-1}\right)^{-1}\mathbf{C}_d^{k-1,k}\right]^{-1} \\ &= \left(\mathbf{C}_d^{k,k}\right)^{-1} + \left(\mathbf{C}_d^{k,k}\right)^{-1}\mathbf{C}_d^{k,k-1}\mathbf{K}_d^{k-1,k-1}\mathbf{C}_d^{k-1,k}\left(\mathbf{C}_d^{k,k}\right)^{-1}\end{aligned} \tag{A.56}$$

$$\begin{aligned}\mathbf{K}_d^{k,k-1} &= -\left(\mathbf{C}_d^{k,k}\right)^{-1}\mathbf{C}_d^{k,k-1}\left[\mathbf{C}_d^{k-1,k-1} - \mathbf{C}_d^{k-1,k}\left(\mathbf{C}_d^{k,k}\right)^{-1}\mathbf{C}_d^{k,k-1}\right]^{-1} \\ &= -\left(\mathbf{C}_d^{k,k}\right)^{-1}\mathbf{C}_d^{k,k-1}\mathbf{K}_d^{k-1,k-1}\end{aligned} \tag{A.57}$$

The calibrated best-estimate parameter values are given by the following reduced form of. Eq. (A.10):

$$\begin{aligned}\begin{pmatrix}\left(\boldsymbol{\alpha}^{be}\right)^{k-1} \\ \left(\boldsymbol{\alpha}^{be}\right)^{k}\end{pmatrix} &= \begin{pmatrix}\left(\boldsymbol{\alpha}^{0}\right)^{k-1} \\ \left(\boldsymbol{\alpha}^{0}\right)^{k}\end{pmatrix} + \begin{pmatrix}\mathbf{C}_{\alpha r}^{k-1,k-1} - \mathbf{C}_{\alpha}^{k-1,k-1}\left(\mathbf{S}^{\dagger}\right)^{k-1,k-1} & \mathbf{C}_{\alpha r}^{k-1,k} - \sum_{\rho=k-1}^{k}\mathbf{C}_{\alpha}^{1,\rho}\left(\mathbf{S}^{\dagger}\right)^{k,\rho} \\ \mathbf{C}_{\alpha r}^{k,k-1} - \mathbf{C}_{\alpha}^{k,k-1}\left(\mathbf{S}^{\dagger}\right)^{k-1,k-1} & \mathbf{C}_{\alpha r}^{k.k} - \sum_{\rho=k-1}^{k}\mathbf{C}_{\alpha}^{k,\rho}\left(\mathbf{S}^{\dagger}\right)^{k,\rho}\end{pmatrix} \\ &\times \begin{pmatrix}\sum_{\eta=k-1}^{k}\mathbf{K}_d^{k-1,\eta}\mathbf{d}^{\eta} \\ \sum_{\eta=k-1}^{k}\mathbf{K}_d^{k,\eta}\mathbf{d}^{\eta}\end{pmatrix}\end{aligned} \tag{A.58}$$

As Eq. (A.58) indicates, the components $\left(\boldsymbol{\alpha}^{be}\right)^{k}$, representing the calibrated best-estimates for the system parameters at time node k, can be written in a particular form of Eq. (A.11), as follows:

$$\left(\boldsymbol{\alpha}^{be}\right)^{k} = \left(\boldsymbol{\alpha}^{0}\right)^{k} + \sum_{\mu=k-1}^{k} \left\{ \left[\mathbf{C}_{\alpha r}^{k\mu} - \sum_{\rho=k-1}^{\mu} \mathbf{C}_{\alpha}^{k\rho} \left(\mathbf{S}^{\dagger}\right)^{\mu\rho} \right] \left[\sum_{\eta=k-1}^{k} \mathbf{K}_{d}^{\mu\eta} \mathbf{d}^{\eta} \right] \right\}. \tag{A.59}$$

The calibrated best-estimate covariance matrix, $\mathbf{C}_{\alpha}^{be}$, for the above calibrated best-estimates system parameters is obtained by particularizing Eq. (A.38) to two consecutive time nodes $\left(k-1, k\right)$, which leads to

$$\begin{aligned} \mathbf{C}_{\alpha}^{be} \triangleq & \begin{pmatrix} \left(\mathbf{C}_{\alpha}^{be}\right)^{k-1,k-1} & \left(\mathbf{C}_{\alpha}^{be}\right)^{k-1,k} \\ \left(\mathbf{C}_{\alpha}^{be}\right)^{k,k-1} & \left(\mathbf{C}_{\alpha}^{be}\right)^{k,k} \end{pmatrix} = \begin{pmatrix} \mathbf{C}_{\alpha}^{k-1,k-1} & \mathbf{C}_{\alpha}^{k-1,k} \\ \mathbf{C}_{\alpha}^{k,k-1} & \mathbf{C}_{\alpha}^{k,k} \end{pmatrix} \\ & - \begin{pmatrix} \mathbf{C}_{\alpha d}^{k-1,k-1} & \mathbf{C}_{\alpha d}^{k-1,k} \\ \mathbf{C}_{\alpha d}^{k,k-1} & \mathbf{C}_{\alpha d}^{k,k} \end{pmatrix} \begin{pmatrix} \mathbf{K}_{d}^{k-1,k-1} & \mathbf{K}_{d}^{k-1,k} \\ \mathbf{K}_{d}^{k,k-1} & \mathbf{K}_{d}^{k,k} \end{pmatrix} \begin{pmatrix} \mathbf{C}_{\alpha d}^{k-1,k-1} & \mathbf{C}_{\alpha d}^{k-1,k} \\ \mathbf{C}_{\alpha d}^{k,k-1} & \mathbf{C}_{\alpha d}^{k,k} \end{pmatrix}^{\dagger} \end{aligned} \tag{A.60}$$

where

$$\begin{pmatrix} \mathbf{C}_{\alpha d}^{k-1,k-1} & \mathbf{C}_{\alpha d}^{k-1,k} \\ \mathbf{C}_{\alpha d}^{k,k-1} & \mathbf{C}_{\alpha d}^{k,k} \end{pmatrix} = \begin{pmatrix} \mathbf{C}_{\alpha r}^{k-1,k-1} - \mathbf{C}_{\alpha}^{k-1,k-1} \left(\mathbf{S}^{\dagger}\right)^{k-1,k-1} & \mathbf{C}_{\alpha r}^{k-1,k} - \sum_{\rho=k-1}^{k} \mathbf{C}_{\alpha}^{k-1,\rho} \left(\mathbf{S}^{\dagger}\right)^{k,\rho} \\ \mathbf{C}_{\alpha r}^{k,k-1} - \mathbf{C}_{\alpha}^{k,k-1} \left(\mathbf{S}^{\dagger}\right)^{k-1,k-1} & \mathbf{C}_{\alpha r}^{k,k} - \sum_{\rho=k-1}^{k} \mathbf{C}_{\alpha}^{k,\rho} \left(\mathbf{S}^{\dagger}\right)^{k.\rho} \end{pmatrix} \tag{A.61}$$

The components $\left(\mathbf{C}_{\alpha}^{be}\right)^{\nu\mu}$, $\left(\nu, \mu = k-1, k\right)$, of the (block) covariance matrix $\mathbf{C}_{\alpha}^{be}$ given by Eq. (A.60) can be written in the following particular form of Eq. (A.40):

$$\left(\mathbf{C}_{\alpha}^{be}\right)^{\nu\mu} = \mathbf{C}_{\alpha}^{\nu\mu} - \sum_{\eta=k-1}^{k}\sum_{\rho=k-1}^{k}\left[\mathbf{C}_{\alpha r}^{\nu\rho} - \sum_{\pi=k-1}^{\rho}\mathbf{C}_{\alpha}^{\nu\pi}\left(\mathbf{S}^{\dagger}\right)^{\rho\pi}\right]\mathbf{K}_{d}^{\rho\eta}\left[\mathbf{C}_{r\alpha}^{\eta\mu} - \sum_{\pi=k-1}^{\eta}\mathbf{S}^{\eta\pi}\mathbf{C}_{\alpha}^{\pi\mu}\right]. \tag{A.62}$$
$$for \quad \nu = k-1, k; \quad and \quad \mu = k-1, k;$$

The vector $\left(\mathbf{r}^{be}\right)^{k}$, representing the calibrated best-estimates for the system parameters at a time node k, is a particular form of Eq. (A.14), as follows:

$$\left(\mathbf{r}^{be}\right)^{k} = \left(\mathbf{r}_{m}\right)^{k} + \sum_{\mu=k-1}^{k}\left\{\left[\mathbf{C}_{m}^{k\mu} - \sum_{\rho=k-1}^{\mu}\mathbf{C}_{r\alpha}^{k\rho}\left(\mathbf{S}^{\dagger}\right)^{\mu\rho}\right]\left[\sum_{\eta=k-1}^{k}\mathbf{K}_{d}^{\mu\eta}\mathbf{d}^{\eta}\right]\right\}. \tag{A.63}$$

Similarly, the calibrated best-estimate covariance block-matrix $\mathbf{C}_{r}^{be}$ for the best-estimate responses takes on a particular form of Eq. (A.43), having in this case four components $\left(\mathbf{C}_{r}^{be}\right)^{\nu\mu}, \left(\nu, \mu = k-1, k\right)$, expressed as follows:

$$\left(\mathbf{C}_{r}^{be}\right)^{\nu\mu} = \mathbf{C}_{m}^{\nu\mu} - \sum_{\eta=k-1}^{k}\sum_{\rho=k-1}^{k}\left[\mathbf{C}_{m}^{\nu\rho} - \sum_{\pi=k-1}^{\rho}\mathbf{C}_{r\alpha}^{\nu\pi}\left(\mathbf{S}^{\dagger}\right)^{\rho\pi}\right]\mathbf{K}_{d}^{\rho\eta}\left[\mathbf{C}_{m}^{\eta\mu} - \sum_{\pi=k-1}^{\eta}\mathbf{S}^{\eta\pi}\mathbf{C}_{\alpha r}^{\pi\mu}\right]. \tag{A.64}$$
$$for \quad \nu = k-1, k; \quad and \quad \mu = k-1, k;$$

A similar sequence of computations leads to the following particular form of Eq. (A.45), for the four matrix-valued components $\left(\mathbf{C}_{\alpha r}^{be}\right)^{\nu\mu}, \left(\nu, \mu = k-1, k\right)$, of the best-estimate response-parameter covariance matrix $\mathbf{C}_{\alpha r}^{be}$:

$$\left(\mathbf{C}_{r\alpha}^{be}\right)^{\nu\mu} = \mathbf{C}_{r\alpha}^{\nu\mu} - \sum_{\eta=k-1}^{k}\sum_{\rho=k-1}^{k}\left[\mathbf{C}_{m}^{\nu\rho} - \sum_{\pi=k-1}^{\rho}\mathbf{C}_{r\alpha}^{\nu\pi}\left(\mathbf{S}^{\dagger}\right)^{\rho\pi}\right]\mathbf{K}_{d}^{\rho\eta}\left[\mathbf{C}_{r\alpha}^{\eta\mu} - \sum_{\pi=k-1}^{\eta}\mathbf{S}^{\eta\pi}\mathbf{C}_{\alpha}^{\pi\mu}\right]. \tag{A.65}$$
$$for \quad \nu = k-1, k; \quad and \quad \mu = k-1, k;$$