Resource allocation for code development in partitioned models

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Abstract

Purpose – Physical phenomena interact with each other in ways that one cannot be analyzed without considering the other. To account for such interactions between multiple phenomena, partitioning has become a widely implemented computational approach. Partitioned analysis involves the exchange of inputs and outputs from constituent models (partitions) via iterative coupling operations, through which the individually developed constituent models are allowed to affect each other's inputs and outputs. Partitioning, whether multi-scale or multi-physics in nature, is a powerful technique that can yield coupled models that can predict the behavior of a system more complex than the individual constituents themselves. The paper aims to discuss these issues.

Design/methodology/approach – Although partitioned analysis has been a key mechanism in developing more realistic predictive models over the last decade, its iterative coupling operations may lead to the propagation and accumulation of uncertainties and errors that, if unaccounted for, can severely degrade the coupled model predictions. This problem can be alleviated by reducing uncertainties and errors in individual constituent models through further code development. However, finite resources may limit code development efforts to just a portion of possible constituents, making it necessary to prioritize constituent model development for efficient use of resources. Thus, the authors propose here an approach along with its associated metric to rank constituents by tracing uncertainties and errors in coupled model predictions back to uncertainties and errors in constituent model predictions.

Findings – The proposed approach evaluates the deficiency (relative degree of imprecision and inaccuracy), importance (relative sensitivity) and cost of further code development for each constituent model, and combines these three factors in a quantitative prioritization metric. The benefits of the proposed metric are demonstrated on a structural portal frame using an optimization-based uncertainty inference and coupling approach.

Originality/value – This study proposes an approach and its corresponding metric to prioritize the improvement of constituents by quantifying the uncertainties, bias contributions, sensitivity analysis, and cost of the constituent models.

Keywords Resource allocation, Uncertainty propagation, Code development, Coupled simulations, Model calibration, Model validation

Paper type Research paper

1. Introduction

Partitioned analysis enables independently developed constituent models to affect each other's input and output through iterative coupling operations (Matthies and Steindorf, 2002a, b; Matthies *et al.*, 2006) making it possible to take the interactions between physical phenomena into account during numerical analysis. Thus, partitioned approaches can eliminate the need for strong and occasionally unwarranted assumptions about the effects of phenomena on each other (Lieber and Wolke, 2008)

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and result in more dependable representations of reality (Heil, 2004; Döscher *et al.*, 2002). The result is a coupled model that can predict the response of a system more complex than the individual constituents themselves.

If the constituents of a coupled model accurately represent the underlying engineering or physics principles, the prediction of the coupled model can be expected to be accurate, provided that errors are not introduced at interfaces between constituents. However, numerical models are only approximate representations of reality and thus, a level of disagreement inevitably exists between constituent model predictions and true responses – henceforth referred to as model form error (MFE) (Draper, 1995; Kennedy and O'Hagan, 2001). The MFE of the constituent models propagate through the interfaces during coupling iterations and ultimately result in MFE in the coupled model (Bunya *et al.*, 2010; Dietrich *et al.*, 2010).

It should be intuitive that improving the predictive ability of the constituent models would improve the predictive abilities of the coupled model, and that reducing the MFE of each constituent model would affect the MFE of the coupled model differently. The latter becomes an important factor as the finite resources limit the extent of code development efforts necessitating prioritization of constituents. As a result, decision makers are left with a natural quandary: which constituent model must be improved to most effectively reduce the MFE of the coupled model? In this manuscript, the authors intend to answer precisely this question.

Answering this question requires the evaluation of the predictive abilities of the constituent models using separate-effect experiments (see Figure 1) those that are conducted in each of the constituents' domain in an isolated manner without considering the interactions between constituents. However, prioritizing constituents based solely on MFE may guide code developers to dedicate resources to a constituent

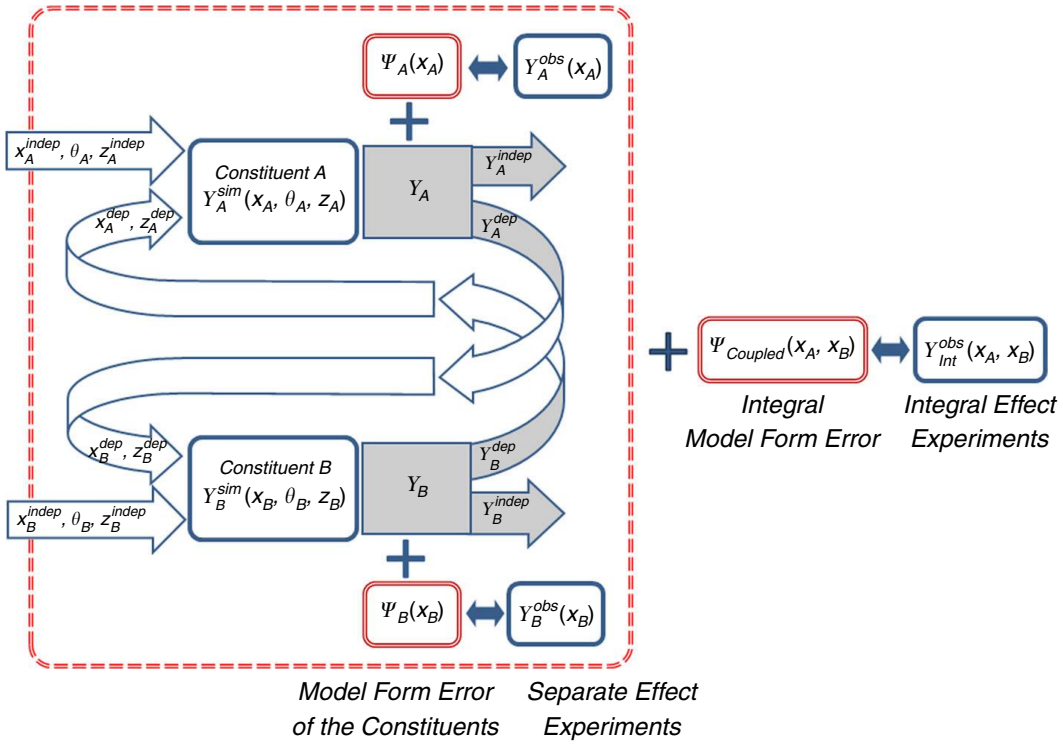

Figure 1.
Schematic diagram of the coupled models

with the highest MFE, but with little influence on the coupled model output. Hence, it is also necessary to consider the sensitivity of the coupled model MFEs to the MFEs of constituent models (Kumar and Ghoniem, 2012a, b). This requires an evaluation of the predictive abilities of coupled models using integral-effect experiments (Döscher *et al.*, 2002; Li *et al.*, 2012) those that are conducted on the coupled system taking the interactions between constituents into account (Hegenderfer and Atamturktur, 2013).

Earlier studies conducted to solve the problem of prioritization of code development efforts were based on the principles of the well-known Phenomena Identification and Ranking Table (PIRT). Alvin and Reese (2000) for instance, implemented PIRT for complex mechanical systems considering separable physics and fully coupled effects to rank the physical phenomena according to their importance. Their approach utilized protocols, such as peer review, error estimation, and uncertainty quantification, where the validation of the constituents and coupled system are conducted in separate steps. Although valuable in compiling expert opinion, Alvin and Reese's (2000) approach is qualitative and dependent upon the subjective opinion of the expert. Similarly, founded on the PIRT concept, Hegenderfer and Atamturktur (2013) proposed a quantitative code prioritization metric for partitioned analysis. Constituent models are ranked according to their priority for further improvement using three criteria: current knowledge level (uncertainty), importance (sensitivity), and error analysis (initial error). The quantitative approach of Hegenderfer and Atamturktur (2013), however, has focused strictly on integral-effect experiments, neglecting the benefits that can be gained from separate-effect experiments while determining the constituent model errors (Figure 1). Furthermore, neither of these two studies considered the cost of further code development in their ranking schemes, another key factor in resource allocation.

The goal of this paper is to develop a code prioritization algorithm and its corresponding metric, in which resources are dedicated to constituent models to most efficiently improve the predictive capability of the coupled model. The proposed algorithm can incorporate both separate-effect and integral-effect experiments to infer not only uncertain input parameters but also discrepancy bias of the constituent models as well as the coupled model (see Figure 1). Uncertainty inference and coupling of constitutive models are achieved simultaneously using an optimization-based approach previously introduced in Farajpour and Atamturktur (2014). Moreover, a sensitivity analysis is conducted to determine the relative importance of the incompleteness and inexactness of each constituent model on the MFE of the coupled model. Furthermore, a cost assessment is completed by evaluating the time and effort requirements of incorporating the missing physics and/or engineering principles to the constituent models. Based on the uncertainty inference, sensitivity analysis and cost assessment, a quantitative metric is defined to rank each constituent according to its potential to yield improvement in the accuracy of the coupled model predictions.

The paper is organized as follows. First, a mathematical formulation of the proposed code prioritization methodology is discussed considering MFE; sensitivity; and development cost of each constituent in the partitioned analysis. Then, the applicability of the proposed methodology along with its associated metric is demonstrated through a proof-of-concept study on a portal frame. The paper concludes with a summary of main findings, limitations of the proposed methodology and suggestions for future studies.

2. Mathematical formulation and background

Figure 1 represents the schematic diagram of the propagation of MFEs between the two constituents, A and B of a strongly coupled system. In this figure, y_A^{obs} and y_B^{obs} represent separate-effect experiments that are acquired by conducting isolated experiments on the constituents, while y_{Int}^{obs} represents integral-effect experiments that are acquired by conducting experiments on the coupled system. Correspondingly, Ψ_A and Ψ_B represent the MFE of each constituent model, and $\Psi_{Coupled}$ represents the MFE of the coupled model. A functional relationship exists between the MFE of the coupled model and the MFEs of the constituents as given in Equation (1). This functional relationship is unknown, but can be evaluated numerically, which will be discussed in detail later in Section 11:

$$\Psi_{Coupled} = f(\Psi_A, \Psi_B) \tag{1}$$

Inferring the MFEs in the constituents and coupled system is the first necessary step in estimating the effect of constituent MFE on the coupled system MFE. Estimating this effect will help identify the critical constituents that require improvement.

Let us consider two simulation models, A and B, in which the output response of the constituent models, M_A and M_B, can be defined as functions of input parameters as follows:

$$Y_*^{sim} = M_*(x_*, \theta_*, z_*); \quad * \in \{A, B\}, \tag{2}$$

where Y^{sim} is the output response, and x, θ, and z are the input parameters of the constituent models, M. The constituent models could be either closed form representations in the form of explicit mathematical equations or numerical evaluations of input/output relationships. The x variables indicate a subset of input parameters that are known to the analyst and can be controlled during experimental testing. These x variables, referred to as the control parameters, define the domain of applicability. In contrast, the θ variables indicate a subset of input parameters that cannot be controlled during experimental testing. The θ variables, known as the calibration parameters, represent uncertain parameters that exhibit significant influence on the simulation results and are selected for parameter calibration. The z variables represent all other input parameters that are neither control nor calibration parameters.

In coupled systems, constituents have common input/output parameters, in which the input of one constituent model is dependent to the output of another. To differentiate these common parameters from the rest, the input parameters of the coupled models can be divided into categories: dependent, and independent parameters. Dependent parameters rely on the output of other constituents and thus, must be updated in each iteration, while independent parameters remain constant during coupling iterations. Equation (2) can therefore be rewritten as follows:

$$Y_*^{sim} = \left[Y_*^{dep} || Y_*^{indep}\right] = M_*\left(x_*^{dep}, x_*^{indep}, \theta_*, z_*^{dep}, z_*^{indep}\right); * \in \{A, B\} \tag{3}$$

In Equation (3), superscripts "*dep*" and "*indep*" stand for dependent and independent parameters in input/output of the constituent models, respectively. The notation || in the Equation (3) represents vector concatenation. Assuming that simulation models

are exact, coupling of the constituents can be achieved by solving the following system of equations:

$$\begin{pmatrix} M_A\left(x_A^{dep}, x_A^{indep}, \theta_A, z_A^{dep}, z_A^{indep}\right) - \left[Y_A^{dep} || Y_A^{indep}\right] = 0 \\ M_B\left(x_B^{dep}, x_B^{indep}, \theta_B, z_B^{dep}, z_B^{indep}\right) - \left[Y_B^{dep} || Y_B^{indep}\right] = 0 \\ Y_A^{dep} - \left[x_B^{dep} || z_B^{dep}\right] = 0 \\ Y_B^{dep} - \left[x_A^{dep} || z_A^{dep}\right] = 0 \end{pmatrix}. \quad (4)$$

In Equation (4), the first two equalities represent exact constituent models, while the last two equalities represent the coupling conditions. The coupling conditions reflect the dependent parameters that are transferred from simulation model A to B and from B to A, respectively. Y^{dep} in these equations then represents the combined set of values transferred from one constituent to another.

Several methods have been proposed to solve for the coupling conditions (Matthies *et al.*, 2006); for instance, Newton-like coupling methods (Matthies and Steindorf, 2002a, b, 2003; Fernandez and Moubachir, 2005), Block-Jacobi and Block-Gauss-Seidel methods (Joosten *et al.*, 2009), and optimization-based coupling (OBC) method (Farajpour and Atamturktur, 2012). The OBC method overcomes the divergence problems that classical coupling techniques, such as Block-Gauss-Seidel, may face. Furthermore, the simultaneous execution of constituent models makes OBC suitable for parallel computing (Farajpour and Atamturktur, 2012). Therefore, the OBC is preferable for this work.

In OBC, coupling is achieved by minimizing an objective function that satisfies the coupling conditions, where the dependent input parameters of the constituents $x_A^{dep}, z_A^{dep}, x_B^{dep}, z_B^{dep}$ are considered optimization variables. In most optimization techniques, initial estimates are made for optimization variables, which are then updated while minimizing the objective function. In Equation (5), it is clear that with these initial estimates, $\left(x_A^{dep}\right)_0, \left(z_A^{dep}\right)_0, \left(x_B^{dep}\right)_0, \left(z_B^{dep}\right)_0$, coupling conditions are not necessarily satisfied:

$$Y_A^{dep} - \left[\left(x_B^{dep}\right)_0 || \left(z_B^{dep}\right)_0\right] = R_0^{BA}; \quad Y_B^{dep} - \left[\left(x_A^{dep}\right)_0 || \left(z_A^{dep}\right)_0\right] = R_0^{AB} \quad (5)$$

Here R_0^{BA} and R_0^{AB} represent the residual vectors of the coupling equations for initial estimates of the dependent parameters. In a successfully coupled system, these residual vectors would ideally be 0[1]. Thus, the objective function of the OBC technique can be defined as the sum of the Euclidean norm of the residual vectors as follows:

$$Z_c = \|R^{AB}\| + \|R^{BA}\| = \|Y_A^{dep} - \left[x_B^{dep} || z_B^{dep}\right]\| + \|Y_B^{dep} - \left[x_A^{dep} || z_A^{dep}\right]\|, \quad (6)$$

where the notation $\|\ \|$ represents a suitable norm. By minimizing the objective function in Equation (6), the dependent input parameters of the constituents $x_A^{dep}, z_A^{dep}, x_B^{dep}, z_B^{dep}$ can be evaluated.

If the simulation models are exact, the solution of Equation (6) represents the response of the coupled system. However, in reality, a level of inexactness exists in the constitutive models. Therefore, the true response of the physical system must be

represented as the summation of inexact simulation models, Y^{sim} and their corresponding MFEs, $\psi(x)$ as indicated in the following equation (Higdon *et al.*, 2008a, b):

$$\zeta_*(x_*) = Y_*^{sim}(x_*, \theta_*, z_*) + \psi_*(x_*, \alpha_*); \quad * \in \{A, B\}. \tag{7}$$

In Equation (7), α indicates the non-physical coefficients of the discrepancy model; and ζ represents the best estimate of truth. Thus, the system of equations for coupling the inexact constituents can be stated as follows:

$$\begin{pmatrix} M_A\left(x_A^{dep}, x_A^{indep}, \theta_A, z_A^{dep}, z_A^{indep}\right) + \psi_A(x_A, \alpha_A) - \zeta_A(x_A) = 0 \\ M_B\left(x_B^{dep}, x_B^{indep}, \theta_B, z_B^{dep}, z_B^{indep}\right) + \psi_B(x_B, \alpha_B) - \zeta_B(x_B) = 0 \\ Y_A^{dep} - \left[x_B^{dep} \,||\, z_B^{dep}\right] = 0 \\ Y_B^{dep} - \left[x_A^{dep} \,||\, z_A^{dep}\right] = 0 \end{pmatrix} \tag{8}$$

By solving Equation (8), we calculate the MFE of each constituent obtaining a quantitative estimate of the inexactness of constituent models and simultaneously, satisfy the coupling conditions. Once again, the first and second items in the Equation (8) address the estimation of the MFE in the constituents A and B, respectively. The third and fourth items satisfy the coupling condition of the constituents A and B. However, solving this system of equations is not a trivial task as discussed in detail in Farajpour and Atamturktur (2014). In their work, three possible configurations of integrating partitioned analysis with model validation are identified: first, coupling the constituent models followed by validation against experiments, second, validating the constituent models followed by coupling of constituents and third, simultaneously coupling and validating the constituent models. The first approach, being the most versatile of the three, is recommended in comparison to the second and third approaches, which require a prohibitively large number of experiments that are likely to be infeasible in practical applications (Farajpour and Atamturktur, 2014). Using this first approach, the MFE of the constituent models and coupled model can be trained, and the best estimate of truth for the coupled system, $\zeta_{Coupled}$, can be obtained as follows:

$$\zeta_{Coupled}(x_A, x_B) = M_{Coupled}\left(x_A^{indep}, \theta_A, z_A^{indep}, x_B^{indep}, \theta_B, z_B^{indep}\right) + \psi_{Coupled}\left(x_A, x_B, \alpha_{Coupled}\right), \tag{9}$$

where $M_{Coupled}$ is the inexact coupled model, a function of both the calibration parameters, θ_A , θ_B and independent input parameters of the constituents, $x_A^{indep}, z_A^{indep}, x_B^{indep}, z_B^{indep}$. Recall that $\psi_{Coupled}$ is the MFE of the coupled system, which is related to the MFE of the constituents as stated earlier in Equation (1).

While any suitable emulator can be used to approximate the MFE of the constituents and coupled system, in the present discussion polynomial functions are preferred due to their continuity and differentiability. Furthermore, as stated by the Weierstrass' approximation theorem, any real-valued continuous function can be approximated by polynomials to any desirable degree of accuracy (Atkinson and Han, 2009; Mastroianni and Milovanovic, 2008).

For example, for a model predicting in a two-dimensional domain (a domain defined by two control parameters), a two variable polynomial function as shown in Equation (10) can be used as an emulator. Note that this emulator would yield a three-dimensional surface as Ψ must be calculated for all sampled settings along both x_1 and x_2 axes:

$$\psi(x_1, x_2, \alpha) = \begin{bmatrix} 1 & x_1 & \cdots & x_1{}^p \end{bmatrix} \begin{bmatrix} \alpha_{11} & \alpha_{12} & \cdots & \alpha_{1(q+1)} \\ \alpha_{21} & \alpha_{22} & \cdots & \alpha_{2(q+1)} \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_{(p+1)1} & \alpha_{(p+1)2} & \cdots & \alpha_{(p+1)(q+1)} \end{bmatrix} \begin{bmatrix} 1 \\ x_2 \\ \vdots \\ x_2{}^q \end{bmatrix} \tag{10}$$

In this emulator, x_1 and x_2 represent control parameters, while α represents non-physical coefficients, that should be evaluated to properly fit the available experimental data. Here, p and q are the orders of the polynomial emulator in x_1 and x_2 directions, respectively. Note that when predicting in a higher dimensional domain with multiple control parameters (i.e. x_1, x_2, x_3, …), polynomial functions with higher number of variables must be implemented (Chan *et al.*, 2001). To avoid over fitting, it is recommended that the maximum polynomial order in each dimension (for instance, p and q) is limited to one less than the number of available experiments in the corresponding dimension. Selection of the polynomial orders for a given number of available experiments is discussed in detail in Farajpour and Atamturktur (2013). Note that the training of MFE needs to repeated for both constituent models and the coupled model.

Herein, we identify two distinct objectives, henceforth collectively referred to as model calibration:

(1) training the MFEs for each constituent model and the coupled model by determining α in Equation (10); and

(2) reducing the uncertainty in the imprecise parameter values by inferring θ values in Equations (8) and (9).

Thus, the objective function of model calibration can be defined as follows:

$$\begin{aligned} Z_{uq}(\alpha, \theta) = & \sum_{j=1}^{s_{Int}} \sum_{i=1}^{r_{Int}} \left(y_{Int}^{obs}\left((x_1)_i, (x_2)_j\right) - y_{Coupled}^{sim}\left((x_1)_i, (x_2)_j, \theta\right) - \psi_{Coupled}\left((x_1)_i, (x_2)_j, \alpha\right) \right)^2 \\ & + \sum_{j=1}^{s_A} \sum_{i=1}^{r_A} \left(y_A^{obs}\left((x_1)_i, (x_2)_j\right) - y_A^{sim}\left((x_1)_i, (x_2)_j, \theta\right) - \psi_A\left((x_1)_i, (x_2)_j, \alpha\right) \right)^2 \\ & + \sum_{j=1}^{s_B} \sum_{i=1}^{r_B} \left(y_B^{obs}\left((x_1)_i, (x_2)_j\right) - y_B^{sim}\left((x_1)_i, (x_2)_j, \theta\right) - \psi_B\left((x_1)_i, (x_2)_j, \alpha\right) \right)^2. \end{aligned} \tag{11}$$

In Equation (11), r_* and S_*(*$\in$ {*Int*, *A*, *B*}) are the number of the experiments in the control parameter dimensions x_1 and x_2, respectively, where the total number of experiments is $r_* \times s_*$. θ and α indicate the decision variables of the objective function. By minimizing $Z_{uq}(\alpha, \theta)$, we can simultaneously infer both MFEs and imprecise parameter values (Farajpour and Atamturktur, 2013). By solving Equations (6) and (11) simultaneously, we can both couple the constituent models and calibrate them against experimental measurements (Farajpour and Atamturktur, 2014).

3. Attributes of code prioritization

Utilizing the methodology discussed in the previous section, this paper presents a decision-making framework and its associated metric to prioritize constituent models for allocating resources for further code development. First, MFEs of both constituent and coupled models are inferred by exploiting separate and integral-effect experiments. Next, sensitivity of the coupled model predictions to each constituent model prediction is investigated. Finally, constituents are ranked according to their need for improvement; effect on the coupled model predictions; and demands on resources. Therefore, three factors are considered: first, relative constituent model MFE, second, sensitivity of coupled model MFE to the constituent model MFE, and third, cost of improving each constituent model predictive capability.

4. Relative MFE of constituent models

We define the relative MFE of a constituent model, $\overline{\psi}^{Rlt}$, as the ratio of the singular values of the MFE, $\overline{\psi}$ to the singular values of the model response within the entire domain of applicability as follows:

$$\overline{\psi}_{*}^{Rlt} = \frac{S\left(\psi_{*}(x_{*}, \alpha_{*})\right)}{S\left(Y_{*}^{sim}\right)}; \quad * \in \{A, B\}, \tag{12}$$

where $\overline{\psi}^{Rlt}$ is a unitless value representing the relative inexactness of a constituent model and S represents the first singular value of the MFE arrays obtained through Singular Value Decomposition (SVD) (Eckart and Young, 1936). SVD is selected herein as a means to condense the high dimensional MFE data sets as it compresses the important information within a data set into a few singular values. However, practically any suitable norm could be used in the calculation of Equation (12).

In an ideal case, constituent models would perfectly represent the reality (i.e $\psi(x, \alpha) = 0$) and $\overline{\psi}^{Rlt}$ would be 0. Higher values of $\overline{\psi}^{Rlt}$ indicate greater MFE with respect to the constituent model predictions. Without losing generality, the relative MFE of each constituent is normalized as follows:

$$MI_{*}^{N} = \frac{\overline{\psi}_{*}^{Rlt}}{\max\left(\overline{\psi}_{A}^{Rlt}, \overline{\psi}_{B}^{Rlt}\right)}; \quad * \in \{A, B\} \tag{13}$$

This normalized index is a value between 0 and 1, where 0 represents a higher predictive capability and 1 represents a lower predictive capability of the constituent model. Of course, a constituent with a higher relative MFE would have a higher priority compared to a constituent with a lower relative MFE.

5. Sensitivity of constituent model MFE

A constituent with negligible sensitivity would have a small influence on the MFE of the coupled system in that dedicating resources for development of this constituent may be ineffective. Therefore, the relative effect of the MFEs of the constituent models on the MFEs of the coupled model must be considered during code prioritization. Such effects can be deciphered through a sensitivity analysis, which can be studied through a statistical concept known as coefficient of determination or R^2 (Casella and Berger, 2002; Janke and Tinsley, 2005). The R^2 value determines the proportion of the

variance of one variable that is predictable from the another variable (Dvore and Berk, 2012). The R^2 values for MFE of constituents A and B can be calculated considering the first singular value of the MFEs as follows:

$$R^2_* = \frac{\left(n\sum_{i=1}^{n} S(\psi_*)_i S(\psi_{Coupled})_i - \left(\sum_{i=1}^{n} S(\psi_*)_i\right)\left(\sum_{i=1}^{n} S(\psi_{Coupled})_i\right)\right)^2}{\left(n\sum_{i=1}^{n} S(\psi_*)_i^2 - \left(\sum_{i=1}^{n} S(\psi_*)_i\right)^2\right)\left(n\left(\sum_{i=1}^{n} S(\psi_{Coupled})_i^2\right) - \left(\sum_{i=1}^{n} S(\psi_{Coupled})_i\right)^2\right)};$$

$$* \in \{A, B\}, \tag{14}$$

where n is the number of design of experiments that are used in sensitivity analysis. The coefficient of determination, R^2 assumes a value between 0 and 1. R^2 should be computed considering all possible values of MFEs in all constituents (reflecting the potential reduction in constituent model MFEs that can be achieved by modeling the missing physics and/or engineering principles). Therefore, the constituent MFEs are varied between 0 and 100 percent through a four-level full-factorial design. The analysis is performed considering four equally distributed values within the range of minimum and maximum values for each parameter of interest evaluating a sample set of $4^2 = 16$ data pairs. Note that as constituent models are dependent on each other, varying MFE of one constituent model causes variation in the MFE of the other constituents and of the coupled model. Such variations can be quantified[2] through the use of separate and integral-effect experiments. This process is repeated for all constituents to obtain the data for the four-level full factorial design. A constituent with larger values of coefficient of determination, obtained via Equation (14), influences the MFE of the coupled system more than those with smaller values, and thus has a higher priority in code improvement activities.

6. Cost analysis

In code development, the widespread use of cost estimation in budgeting and project planning has resulted in the development of several estimation techniques (Zia *et al.*, 2011; Magazinius *et al.*, 2012; Jørgensen and Shepperd, 2007; Leung and Fan, 2002). A common approach used in cost estimation, particularly in software engineering, involves the determination of the effort (usually in person-months), the duration of the project (in time), and the cost (in dollars or other currency) (Leung and Fan, 2002; Zia *et al.*, 2011). Effort is typically approximated by number of lines in the source code, delivered sets of instructions, function points and required experience levels (Zia *et al.*, 2011). Limited information about these factors in early phases of the project (Malik and Boehm, 2011) and the effect of human and organizational factors (Magazinius *et al.*, 2012; Zia *et al.*, 2011) make cost estimation challenging (Lederer and Prasad, 1991).

In this study, the amount of effort that should be dedicated for implementing missing physics or engineering principles in the constituents is used as a criterion for estimating the required cost per constituent. Note that constituents may share some of the physics or engineering principles, reducing demands on resources. In Table I, the required effort for development of the "Physics N" in the constituent U is represented by H_{UN} with the unit of person-months. Considering the missing physics and/or

engineering principles that will be addressed through code development, the development cost can be calculated for each constituent using the following equation:

$$C_* = H_* \times W; \quad * \in \{A, B\}, \tag{15}$$

where C_A and C_B are development costs and H_A and H_B are overall person-months required for improvement of constituents A and B, respectively, and W is the wage per month of the experts. Based on these values, a cost index for each constituent can be defined as follows:

$$CI_*^N = \frac{C_*}{\max(C_A, C_B)}; \quad * \in \{A, B\}, \tag{16}$$

where CI^N represents normalized cost index, which is a positive value less than or equal to 1. A lower cost index leads to a higher priority for the constituent model as a lower amount of resources are sufficient to achieve improvement. The overall goal of the code prioritization then entails achieving the most improvement in the predictive capability of the coupled system with a minimum cost.

7. Code prioritization metric and algorithm

Combining the three previously presented parameters, a Code Prioritization Metrics (CPM) metric is defined to rank the constituents for future code development activities as follows:

$$CPM_* = \frac{MI_*^N \times R_*^2}{CI_*^N}; * \in \{A, B\}, \tag{17}$$

where CPM^N represents the normalized code prioritization metric for each constituent. CPM ranges between $0 < CPM < +\infty$. Higher relative MFE and sensitivity of the constituents and lower cost index increases the value of the CPM. A higher CPM value in turn reflects a higher priority constituent model.

The algorithm for ranking the constituents of the coupled model is shown in Figure 2. Here, three components of the CPM, inferring the constituent MFEs; computing the sensitivity of constituent MFEs; and estimating the cost of constituent model improvement, proceed in a parallel manner. Figure 3 shows a detailed flowchart of the algorithm that can be executed sequentially. In this flowchart, ε_c and ε_{uq} represent the threshold values for termination of the coupling and validation processes, respectively. In this study, both of these values are considered to be 10^{-7}.

8. Case study application

The proposed resource allocation methodology is demonstrated on a portal frame used as a benchmark in several earlier studies (Figure 4) (Vadde *et al.*, 1991; Allen and Mistree, 1993;

Table I. Person-months estimation in the constituents

	Person-months required for development for each type of physics				
	Physics 1	Physics 2	Physics 3	Physics 4	Total person-months
Constituent A	H_{A1}	H_{A2}	–	H_{A4}	$H_A = \sum_{j=1,2,4} H_{Aj}$
Constituent B	–	–	H_{B3}	H_{B4}	$H_B = \sum_{j=3,4} H_{Bj}$

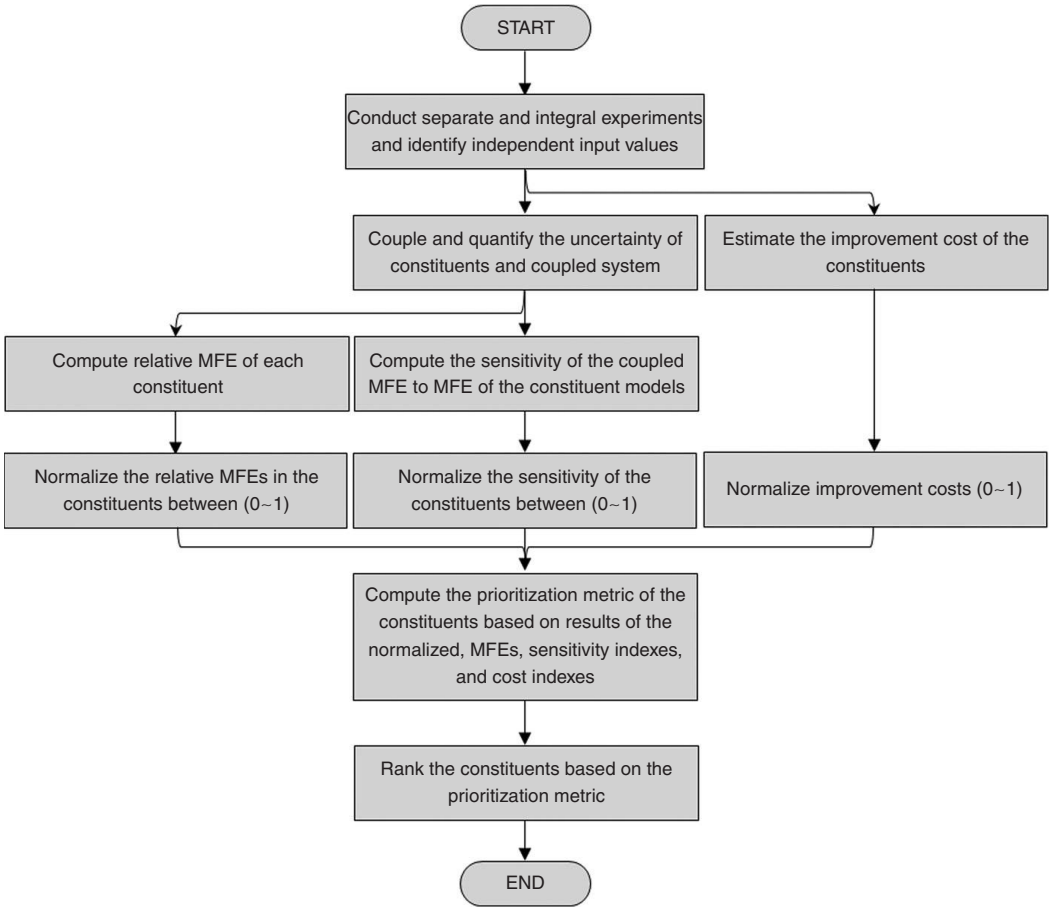

Figure 2.
Code prioritization procedure

Sobieszczanski-Sobieski *et al.*, 1985). Experimental data used for uncertainty inference are synthesized using the hypothetical exact model.

By removing the shear deformation capabilities from the exact model, an inexact numerical model is obtained. The inexact model for the portal frame (i.e. coupled system) is decomposed into three substructures (i.e. constituents) (Vadde *et al.*, 1991), and the outputs of each constituent model are transferred to adjacent constituents through the coupling procedure. Dependent parameters that are exchanged between the constituent models include the displacements and internal forces calculated for the end nodes in each member (Figure 4).

9. Exact model

The portal frame consists of two vertical steel members that are fixed at the base and a beam member that is rigidly connected to the vertical members. The vertical members have uniform square tube cross-sections with outer dimensions of 10.0×10.0 cm and 1.0 cm wall thickness, and the beam is constructed of aluminum with the same cross-section as the vertical members. Material properties and geometrical data for the model frame used to generate the synthetic experimental data are given in Table II. A lateral force is applied to the frame below the force levels that would cause structural members to yield under bending and/or shear stresses. Therefore, the material non-linearity is expected to be negligible.

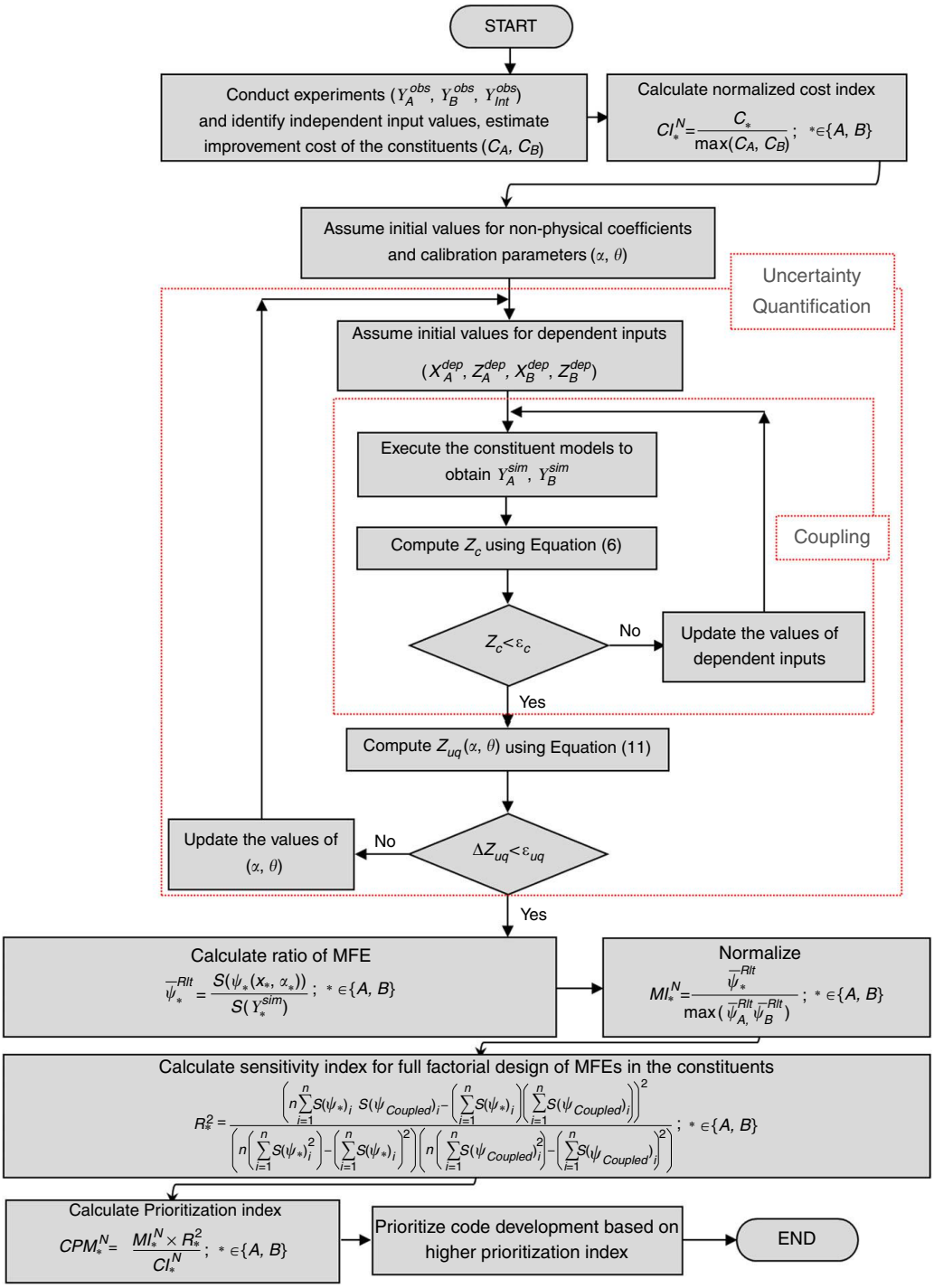

Figure 3.
Flowchart for the calculation of code prioritization metric

The nodal coordinates of the members measured from the member end is treated as one of the control parameters (as indicated by the arrows in Figure 5). For constituent 2, the rotation imposed on the right end of the beam is treated as a control parameter, while the applied force is treated as a control parameter for constituents 1 and 3, and for the coupled system.

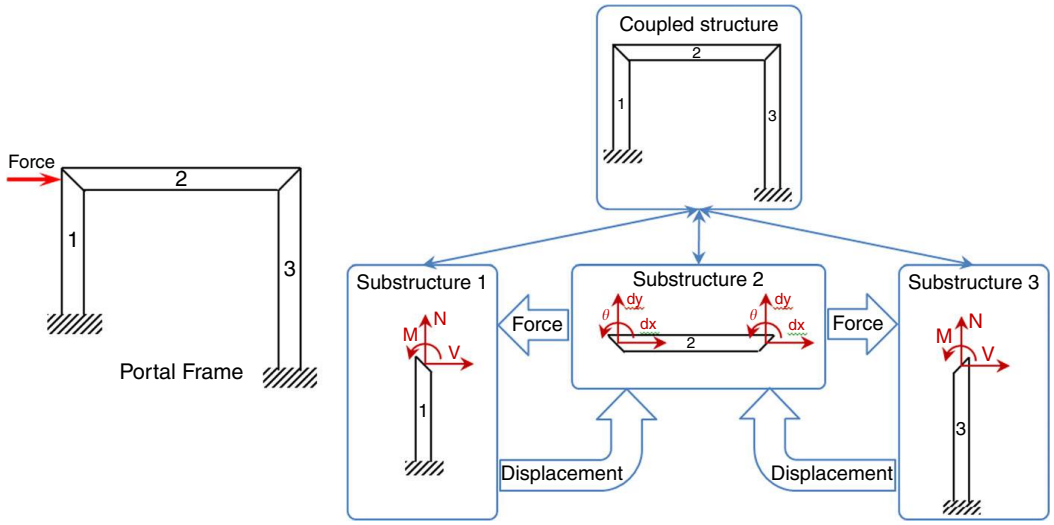

Figure 4.
Constituents of the portal frame in partitioned analysis

Description (unit)	Substructure 1	Substructure 2	Substructure 3
Material	Steel	Aluminum	Steel
Length of the member (cm)	300.0	300.0	360.0
Thickness of the tube (cm)	1.0	1.0	1.0
Outer dimensions of the tube (cm)	10.0	10.0	10.0
Area moment of inertia (cm^4)	492	492	492
Young's modulus (Pa)	200×10^9	69×10^9	200×10^9
Shear modulus (Pa) [$E/(2 \times (1 + v))$]	7.6746×10^{10}	2.5862×10^{10}	7.6746×10^{10}
Poisson's ratio	0.303	0.334	0.303
Shear area coefficient	0.667	0.667	0.667

Table II.
Input data of the portal frame

Here, the authors used the Timoshenko beam theory (Hartmann and Katz, 2007) to consider the axial, shear, and flexural deformations of frame elements. The output of the finite element (FE) models of the entire portal frame and each of the constituents are used as synthetic integral-effect and separate-effect experiments, respectively.

10. Synthetic experimental data

In synthesizing the integral-effect and separate-effect experiments, three gauges are assumed to be mounted on each vertical member measuring horizontal displacements, and two gauges are assumed for the horizontal beam measuring vertical displacements, as shown in Figure 5. The control parameters of the vertical members are the imposed lateral forces at the top of the members, while the control parameter of the horizontal member is the rotation at the right end of the beam.

In synthesizing the integral-effect experiments for the coupled model, the portal frame is subjected to two different levels of lateral static loads (50 kN, 100 kN). Deformations of the unloaded portal frame are assumed to be 0. In synthesizing the separate-effect experiments for the constituent models, the three members of the frame are analyzed separately, where the bases of the vertical members are fixed (constituents 1 and 3 in Figure 5), and the aluminum beam is fixed at the left end and pinned at the right end (constituent 2 in Figure 5). The separate-effect experimental data are obtained

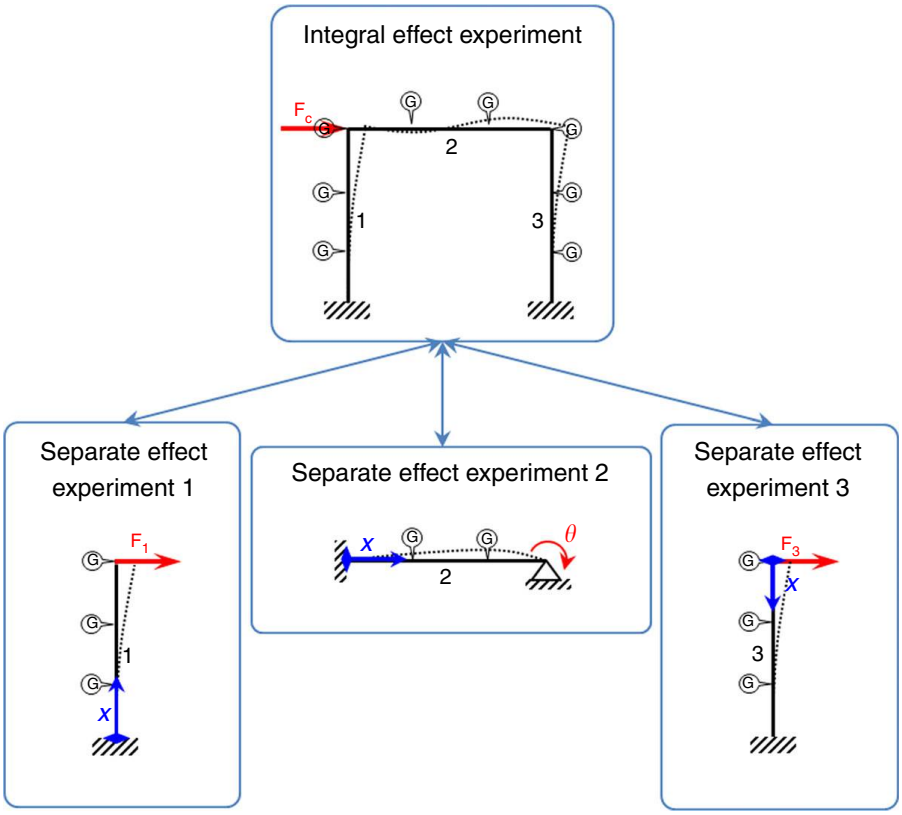

Figure 5.
Location of the gauges in the portal frame and constituents used to acquire integral-effect and separate-effect experimental data

by evaluating displacements for two levels of lateral force (50 kN, 100 kN) for the vertical members, and for two levels of rotations at the pinned support (0.02 Rad, 0.04 Rad) for the beam member. For all members, deformations of the unloaded members are assumed to be 0. In all cases, a 2 percent experimental error is considered as the zero-mean Gaussian random variable.

The synthetic experimental data will be used later on to establish the MFEs of the constituents and coupled system and also to conduct sensitivity analysis of the constituents.

11. Inexact and imprecise computer model

A FE model is developed according to the Euler-Bernoulli beam theory (Hartmann and Katz, 2007) to analyze the constituents and the coupled system. This model is inexact as shear deformations are missing in the formulation of the stiffness matrix. This missing mechanics principle, the source of inexactness of the model, causes MFE in model predictions. Moreover, uncertainties in material properties introduce imprecision to the model output and cause further deviation between the model predictions and synthetic experimental data. In this proof-of-concept application, Young's moduli of the three members are considered uncertain and thus, treated as calibration parameters.

The inexact constituents (vertical and horizontal members) are coupled together to obtain the response of the coupled system (portal frame) with the horizontal point load applied at the connection of constituents 1 and 2, shown in Figure 5. In the analysis of the coupled model, the lateral load is applied to constituent 1, and the resulting deformation of constituent 1 is imposed on constituent 2. Next, the difference between

the reaction force of constituent 2 for the imposed deformations (shown in Figure 4 by dx, dy and θ) and the internal forces of constituents 1 and 3 are computed for the imposed forces (shown in Figure 4 by M, N, V). This process is repeated until this difference falls below the selected threshold value, 10^{-7}. Hence, in the coupled frame, the internal forces and node deformations at the interfaces between all three constituents converge below the threshold value.

The MFEs of the constituents and coupled system are trained using a polynomial function with two control parameters (nodal coordinates and applied force/deformation) as shown in Equation (10). There is one polynomial function for each of the constituents and three polynomial functions for the coupled system; thus a total of six functions must be trained. Note that with two control parameters, the trained MFE is a surface function.

A third order polynomial is trained in the dimension of the first control parameter (i.e. the coordinate of the nodes), while a second order polynomial is trained for the second control parameter (i.e. imposed forces or rotations). The order of the first control parameter is selected to be one less than the number of experiments, i.e., number of nodes with known displacements (three sensor locations and one boundary condition thus, four nodes for each member), and the order of the second control parameter is selected to be one less than number of force/rotation levels imposed on the structure (three levels by considering the unloaded/undeformed conditions). Thus, recalling Equation (10), when $p = 3$ and $q = 2$, the number of non-physical coefficients of the trained MFE is $(p+1)\times(q+1) = (3+1)\times(2+1) = 12$ for each member. Since the total number of functions is six, the total number of non-physical coefficients for this case study is $12 \times 6 = 72$. Thus, considering three additional calibration parameters, i.e. Young's modulus of the members, the total number of decision variables in the objective function for the uncertainty quantification process is 75.

Herein, to solve the uncertainty quantification problem, a gradient-based optimization is used (Nelder-Mead Simplex Method) through the *fminsearch* function available in MATLAB (Lagarias *et al.*, 1998). As the desired value of the objective function is known in advance (ideally it should be 0), the local minima is not a concern. Through optimization, the values of calibration parameters and of the non-physical coefficients of the polynomial functions that represent the trained MFEs are simultaneously inferred. The initial values of the calibration parameters (i.e. Young's modulus of the materials) are randomly selected within the range of ± 25 percent of the exact values provided in Table II, and the initial values of the non-physical coefficients are considered as 0. The threshold value of the uncertainty quantification process is set at 10^{-7}.

12. Prioritization of the constituents

The calibrated values of Young's modulus for members 1, 2, and 3 are 199.99×10^9, 69.03×10^9, and 199.75×10^9, respectively. The trained surfaces for the MFEs of the coupled frame and of each constituent are provided in Figure 6. Because model incompleteness originates from the lack of consideration for shear deformations, without imposed force or deformation, the frame would be unreformed for both exact and inexact models, therefore the MFEs would be equal to 0. Increasing the imposed forces and deformations increases the MFE.

The normalized relative MFEs of the constituents calculated according to Equation (12) are given in Table III, theresults of which show that the relative error of the second constituent, (i.e. aluminum beam) is higher than that of the steel columns. Table III also

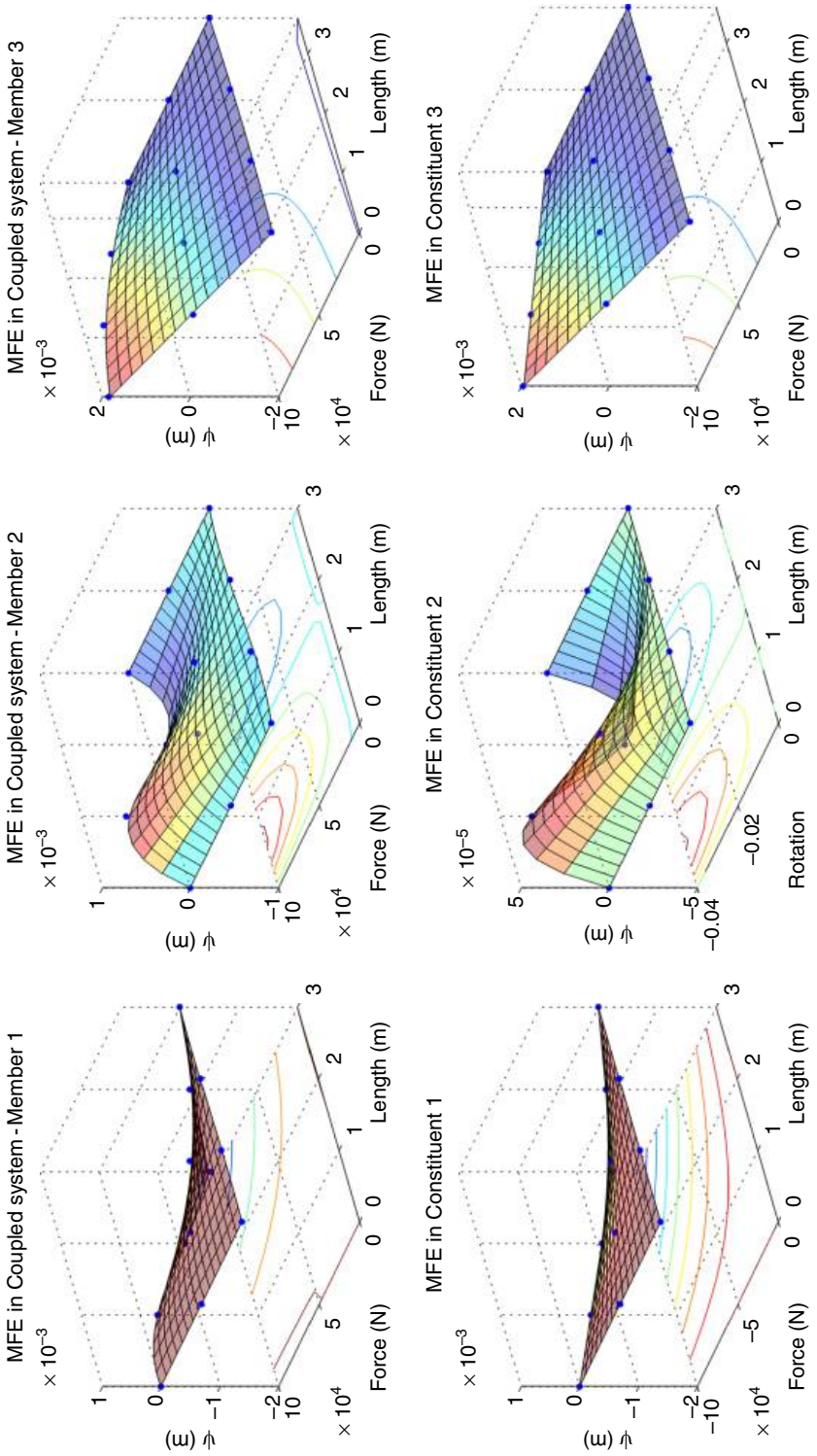

Figure 6.
Trained MFE of the coupled system and constituents

shows the coefficient of determination for the three constituents calculated via the sensitivity analysis. Here, the MFE of the coupled system is more sensitive to variation of the MFE of constituent 1 than those of constituents 2 and 3. In this case study, we assume that the development costs of all three constituents are equal leading to cost indices that are equal to one. Accordingly, the values of the CPM for three constituents are calculated according to Equation (17) (Table III). CPM metric assigns higher priority for constituent 2 compared to constituents 1 and 3 for allocating resources for future code development efforts.

13. Effect of the geometric dimensions on prioritizing the code development of constituents

Any parameter that influences the MFE of the constituents or coupled system can alter the value of the CPM and consequently, alter the prioritization order. This section demonstrates the effect of the geometric dimensions of the portal frame on the prioritization order. The values of the CPM for all three constituents are calculated based on various lengths of the members in the portal frame (recall Figure 5). In Figures 7(a)-(c), the x and y axes represent the relative values of the member lengths, where dark region signifies higher priority of the corresponding constituent for development activity. In this figure, bright regions represent a lower priority for code improvement activity. For instance, in Figure 7(a), by reducing the length of the member 1, the priority of that member for development activity increases (the same observation can be made for member 3 in Figure 7(c)). Simultaneously, increasing the lengths of members 1 and 3 increases the priority of constituent 2 (Figure 7(b)).

Recalling that the source of MFE in this case study is shear deformation, a reduction in the length of a member enhances the incompleteness of its constituent model (Blodgett, 1966). As seen, the proposed CPM metric successfully targets the constituents with a reduced length for development activity. The results of Figure 7 are combined in Figure 8, in which the constituent to be improved is determined by the relative length of the members. Three guiding steps are provided in Figures 8(a)-(c) for the development efforts. Figure 9 is a summary of Figures 8(a)-(c), representing the order of all three constituents for code development.

If code development is to be conducted on more than one constituent and new experimental data will be gathered, the ranking of the constituents should ideally be repeated in each step of development activity. This repetition is useful in incorporating the most updated constituents in the ranking process. Thus, Figure 8 only represents the development order if new experimental data after each step of the development is unavailable.

14. Conclusion

In this paper, the authors propose an approach to prioritize code development efforts in partitioned analysis of complex systems. The resource allocation metric proposed here

Description (unit)	Constituent 1	Constituent 2	Constituent 3
Model form error index (MI^N)	0.854	1.000	0.593
Sensitivity index (R^2)	0.439	0.436	0.125
Cost index (CI^N)	1.000	1.000	1.000
Code prioritization metric (CPM)	0.375	0.436	0.074

Table III. Code prioritization metric (CPM)

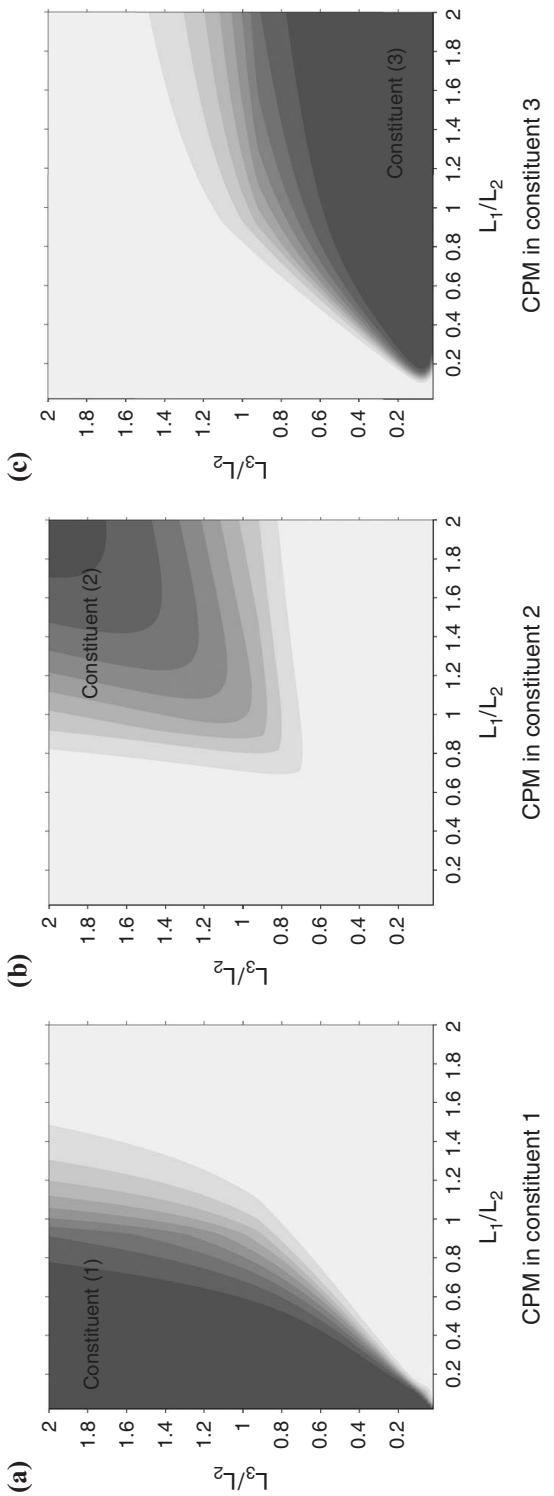

Figure 7.
Value of the CPM vs relative length of the members

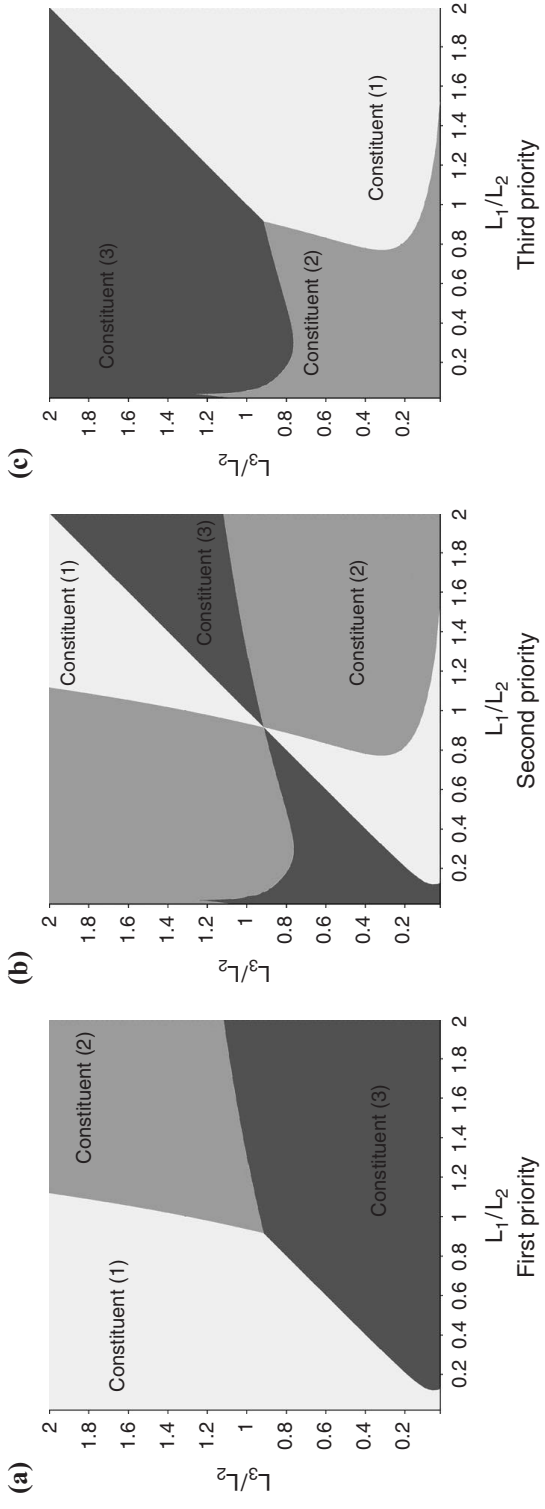

Figure 8.
Priority of code development based on member length ratio

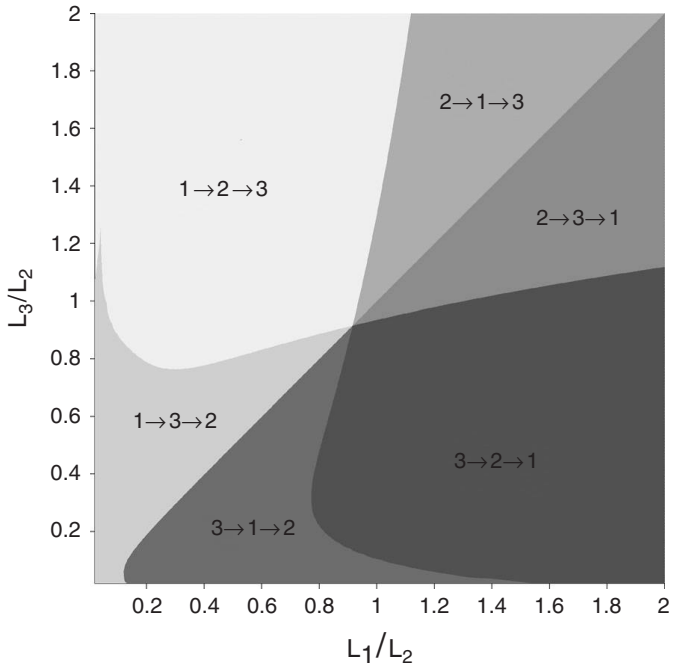

Figure 9.
Order of the code development as a function member length ratio

incorporates three major components related to the constituent model: first, the ratio of the MFE over the simulation response for each constituent in the coupled system, second, the sensitivity of the MFE of the coupled system to the MFE of the constituents, and third, the development cost of each constituent. This metric is successfully applied to a proof-of-concept example of a steel-aluminum portal frame, with optimization techniques used to determine a solution for the simultaneous coupling and uncertainty quantification problem. Analysis of the frame is achieved through coupling of the three substructures, and the CPM is used to rank the three constituents.

As both relative MFE and sensitivity index (Equations (13) and (14)) are dependent upon the value of the input parameters, the value of CPM would change for different input parameters. Therefore, although governing equations are similar for all three constituents in the portal frame studied herein, the code development priority of constituents will vary based on their input parameters. Similarly, the CPM value is dependent upon the selected response of the coupled system. Thus, prioritization of the constituents as suggested here is plausible only for a set of specific input and output parameters, changing these parameters may change the priority of the constituents.

In this study, the MFEs of the constituents are trained using polynomial surfaces exploiting the simulated experimental data synthesized at various settings of the two control parameters. The continuous surfaces representing MFEs trained by fitting the tested settings are used to predict model incompleteness at untested settings. In this case study, the number of non-physical coefficients for all the trained functions is 72. If the order of the polynomial in both control parameters is increased by 1, the number of non-physical coefficients will be $(4+1)\times(3+1)\times 6 = 120$; for an additional increase by 1, this number will increase to $(5+1)\times(4+1)\times 6 = 180$. Increasing the number of control parameters will also increase the number of independent variables in the polynomials, which will increase the number of non-physical coefficients. Therefore, one of the challenges of the proposed approach entails the computational cost for calculating MFEs in the constituents and in the coupled system, especially problematic

when conducting sensitivity analysis. As a large number of non-physical coefficients in the MFEs significantly impacts the number of decision variables in the optimization problem, limiting the number of non-physical coefficients can reduce the computational cost of the procedure. Therefore, for higher dimensional problems with MFEs of low correlation length, functional forms that can be represented with fewer parameters must be preferred.

In experiment-based validation, code development efforts and experimental campaigns are often ongoing processes in which feedback from the previous experiments and code development activities are used for future development. In such cases, to increase the efficiency of the proposed constituent ranking process, the new experimental data and most recent version of codes should be used to obtain the most updated results.

The authors did not consider the relative importance of the three major components of the defined metric, i.e. error, sensitivity and cost. For instance, in that MFE and sensitivity have an equal effect in the defined metric, a consideration of weighting factors for these parameters may be required in future studies. Furthermore, investigating the role of numerical errors in the context of partitioned analysis is left out of the scope of the present paper, however changes in the computational cost due to for instance the refinement of the mesh size, which reduces the numerical error, can also be considered in the definition of the cost.

This study addresses the efficient allocation of resources for code development. Equally important is the efficient allocation of resources for experimentation. Therefore, subsequent research must involve designing optimal experiments considering both separate and integral-effects to improve the predictive capabilities of the coupled system.

Notes

1. In reality, residual errors would never be zero but converge to a value below the predefined threshold.
2. The model form errors at the untested settings are estimated by a functional form fitted to the model form error at the tested settings.

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