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To cite this article: Qian Shao, Jian Liu, Qun Huang, Jie Yang, Heng Hu, Salim Belouettar & Gaetano Giunta (2019): A data-driven analysis on bridging techniques for heterogeneous materials and structures, *Mechanics of Advanced Materials and Structures*, DOI: [10.1080/15376494.2018.1546415](https://doi.org/10.1080/15376494.2018.1546415)

To link to this article: <https://doi.org/10.1080/15376494.2018.1546415>

Published online: 18 Jan 2019.

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ORIGINAL ARTICLE

A data-driven analysis on bridging techniques for heterogeneous materials and structures

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ABSTRACT

A bridging technique based on Lagrange multipliers, namely the Arlequin method, is widely used for coupling multi-scale models. However, the definition of the following key parameters is still unclear: the energy partition functions, the characteristic length of the coupling operator and the size of the coupling zone. This work aims to investigate the influences of these factors on the coupling accuracy by conducting global sensitivity analysis on different multi-scale models. To this end, a data-driven model that approximates the input/output behavior of the numerical model is built by using the Sparse Polynomial Chaos Expansion (SPCE) methodology. Then, Sobol' indices that quantify the sensitivity of the input factors are calculated analytically from the data-driven model with a negligible additional computational cost. Interaction effects among different parameters are also captured. Using this approach, several benchmark tests, including a coarse-fine bar model, a particle-continuum model and a 2D-1D sandwich model, are considered to explore the optimal settings of the coupling factors, which hopefully help for the multi-scale analysis of heterogeneous materials and structures.

ARTICLE HISTORY

Received 4 November 2018
Accepted 5 November 2018

KEYWORDS

Arlequin method; data-driven analysis; global sensitivity analysis; sparse polynomial chaos expansion; multi-scale models; heterogeneous materials and structures

1. Introduction

Multi-scale strategies have been widely used over the past few decades to improve the accuracy and efficiency of modeling and simulation of engineering problems. In multi-scale computations, a bridging technique is necessary for connecting heterogeneous models, such as the coupling between atomistic and continuum models, or between finite element models with incompatible meshes, etc. Many efforts have been devoted to the development of coupling techniques, for instance the handshake method [1], the bridging scale decomposition [2], the bridging domain method [3], the Arlequin method [4] and so on.

Due to the flexibility and universality, the Arlequin method and its variants have been widely used [4–11]. The Arlequin method was firstly proposed by Ben Dhia [4] and it allows the superposition of various mechanical models. By means of energy partition functions and Lagrange multipliers, different models are glued in a coupling zone. Ben Dhia et al. [6] further assessed the effectiveness of the Arlequin method for coupling various finite element models in one, two and three dimensions. Hu et al. [12–15] successfully applied the Arlequin method to the multi-scale modeling of sandwich structures. He et al. [16] applied the Arlequin method to couple variable order beam elements. Whilst Biscani et al. [17] employed the Arlequin method for coupling variable kinematic plate elements. The coupling between solid and higher-order plate finite elements was

established by Biscani et al. [18]. An Arlequin-based method was also used to couple continuum and molecular dynamics systems in [19]. Kpogan et al. [20, 21] applied the Arlequin method to simulate the buckling phenomena of a rolled thin sheet. Qiao et al. [22] successfully implemented the Arlequin method into the commercial finite element software ABAQUS to couple the same type elements with different grid density or various types of elements.

As mentioned in [6], the optimal practical settings of the weighting parameter functions, the size of the superposition zone and the multiple superposition procedure are essential for a multi-scale analysis by the Arlequin method. Since then, many efforts have been devoted to explore the choices of these Arlequin parameters. In [8], Ben Dhia offered some qualitative suggestions for the choice of the weight parameter functions and the coupling operators. Considering the applications of these methods to the coupling of the particle-continuum model, the influence of coupling operators L^2 and H^1 were discussed in [9], whilst the convergence of the solution as well as the effect of the location and the size of the overlapping region were analyzed by Prudhomme et al. [10]. To avoid the drawback of mesh dependency, an improved version of the Arlequin method for blending particle and continuum models was proposed in [11]. Guidault and Belytschko [23] indicated that the H^1 coupling operator benefits from the derivatives of displacement, which allows to perfectly blend a very coarse mesh with a very fine one.

Figure 1. The Arlequin method in a general mechanical problem.

Sun and Mota [24] found that the H^1 coupling is more reliable to enforce weak compatibility than L^2 when the Lagrange multiplier and the coarse deformation mapping share the same discretization. Hu et al. [25] proposed a new coupling operator, namely H_p^1 that permits to obtain a better conditioning of the global stiffness matrix than H^1 or L^2 coupling operators when modeling sandwich structures.

Although the Arlequin method has been widely used, a quantitative guidance for setting the above mentioned parameters remains unclear. Global Sensitivity Analysis (GSA) is a reliable tool that helps quantitatively explore the respective effect of each input parameter onto the response of a physical model and further seek for regions in the space of input factors where the model output meets the optimum criterion [26]. In this work, GSA is performed to explore the quantitative influence of the parameters on multi-scale modeling accuracy. A wide range of metrics and techniques have been developed to perform GSA, such as linear regression-based methods, variance-based methods [27], etc. Among others, Sobol' indices are widely used to measure the impact of model parameters [28]. Typically, two approaches can be used to evaluate Sobol' indices, involving Monte-Carlo methods and metamodeling methods. The latter have received much attention due to their effectiveness and high-efficiency [29–31]. Following metamodeling approach, we build up a data-driven model that approximates the input/output behavior of the original numerical model. Then, Sobol' indices can be calculated analytically from the data-driven model with a negligible additional computational cost. To “train” the data-driven model, the Sparse Polynomial Chaos Expansion methodology, which uses orthogonal polynomials to approximate the response surface, has been commonly used. The idea of SPCE was first proposed by Blatman and Sudret [29–32], and further developed by Hu and Youn [33], Fajraoui et al. [34], Shao et al. [35], etc. In this work, we use the algorithm proposed by Shao et al. [35] to approximate the data-driven model with SPCE. This algorithm is based on Bayesian model averaging. The proposed algorithm uses the Kashyap information criterion (KIC) [36] to select the best SPCE model for a given input/output sample. Here, the weight functions, the characteristic length and the length of the coupling zone involving in the Arlequin method are considered as inputs for multi-scale models, whilst the relative errors between the numerical solution and the reference solution are considered as outputs. This strategy can be referred as a data-driven approach since the settings of Arlequin parameters are explored by using a large number of numerical experiments instead of intuition or personal experience.

The layout of this article is as follows. In Section 2, the Arlequin method is briefly recalled. Section 3 reviews the Sobol' decomposition and Bayesian SPCE, followed by the introduction of the framework for data-driven analysis on

the Arlequin method. In Section 4, three classical multi-scale models coupled by the Arlequin method are analyzed by the proposed procedure. Finally, conclusions on the selection of the coupling factors are drawn in Section 5.

2. The Arlequin method

In this section, the basic idea of the Arlequin method [4, 5] is recalled. As shown in Figure 1, the considered domain Ω of a mechanical system is split into two sub-domains with an overlapping zone: domain Ω_f analyzed by a fine model and domain Ω_c by a coarse model. The resulting intersecting zone is represented by Ω_s , where $\Omega_s = \Omega_f \cap \Omega_c$.

According to the Arlequin framework, the energy of the domain Ω is obtained by adding the energy of Ω_f and Ω_c . The energy E_k for each sub-domain reads:

$$E_k(\mathbf{u}_k) = \frac{1}{2} \int_{\Omega_k} \alpha_k \boldsymbol{\sigma}(\mathbf{u}_k) : \boldsymbol{\varepsilon}(\mathbf{u}_k) d\Omega_k - \int_{\Omega_k} \beta_k \mathbf{f}_k \cdot \mathbf{u}_k d\Omega_k \quad (1)$$

where $\mathbf{u}_k$ and $\mathbf{f}_k$ represent the displacement and the external force per unit volume in Ω_k with $k=f$ or c . To avoid considering twice the energy of the total system in the coupling zone, the weight functions α_k and β_k in Eq. (1) satisfy the following relations:

$$\begin{cases} \alpha_f = \beta_f = 1, & \text{in } \Omega_f \setminus \Omega_s, \\ \alpha_c = \beta_c = 1, & \text{in } \Omega_c \setminus \Omega_s, \\ \alpha_f + \alpha_c = \beta_f + \beta_c = 1, & \text{in } \Omega_s. \end{cases} \quad (2)$$

They are usually assumed to be positive piecewise continuous functions, for example, constant, linear, quadratic and so on. In this article, we limit these weight functions to be constant in the gluing zone as in Ben Dhia et al. [6] and Hu et al. [25].

To ensure the displacement continuity in the coupling zone Ω_s , the Lagrange multiplier $\boldsymbol{\lambda}$ is introduced as a fictive gluing force. Here, we consider an H^1 -type coupling operator as analyzed in [4] that possesses good mathematical and numerical properties:

$$\mathcal{C}(\boldsymbol{\lambda}, \mathbf{u}_k) = \int_{\Omega_s} \left(\boldsymbol{\lambda} \cdot \mathbf{u}_k + \ell^2 \boldsymbol{\varepsilon}(\boldsymbol{\lambda}) : \boldsymbol{\varepsilon}(\mathbf{u}_k) \right) d\Omega \quad (3)$$

The characteristic length ℓ in Eq. (3) is a positive parameter homogeneous to a length, $\boldsymbol{\varepsilon}(\boldsymbol{\lambda})$ and $\boldsymbol{\varepsilon}(\mathbf{u}_k)$ are the gradients terms. One should note that the coupling operator in Eq. (3) tends to be a L^2 -type one when the characteristic length $\ell = 0$, see [6].

For the whole problem, searching the variables $\mathbf{u}_f$ and $\mathbf{u}_c$ is equivalent to minimizing the following functional:

$$\mathcal{J}(\mathbf{u}_f, \mathbf{u}_c, \boldsymbol{\lambda}) = E_f(\mathbf{u}_f) + E_c(\mathbf{u}_c) + \mathcal{C}(\boldsymbol{\lambda}, \mathbf{u}_f - \mathbf{u}_c) \quad (4)$$

We derive the discrete formulations from the continuous one Eq. (4) by using the finite element method. The minimization of Eq. (4) leads to the following linear system:

$$\begin{bmatrix} \mathbf{K}_f & 0 & -\mathbf{C}_f \\ 0 & \mathbf{K}_c & \mathbf{C}_c \\ -\mathbf{C}_f^T & \mathbf{C}_c^T & 0 \end{bmatrix} \begin{bmatrix} \mathbf{U}_f \\ \mathbf{U}_c \\ \boldsymbol{\Lambda} \end{bmatrix} = \begin{bmatrix} \mathbf{F}_f \\ \mathbf{F}_c \\ 0 \end{bmatrix} \quad (5)$$

where $\mathbf{U}_f$, $\mathbf{U}_c$, and $\boldsymbol{\Lambda}$ represent the global displacement vector in Ω_f , Ω_c , and the global Lagrange multiplier field,

Figure 2. The process of data-driven analysis for the Arlequin method.

respectively. Solving the linear system Eq. (5) gives the displacement field of each sub-domain. The displacement field U of the multi-scale model can be then expressed as:

$$U = \alpha_f U_f + \alpha_c U_c \quad (6)$$

3. Global sensitivity analysis

In this work, GSA is performed by using a variance-based method. By Sobol' decomposition, the Sobol' indices are derived to evaluate the sensitivity of model responses to the input variables. To calculate Sobol' indices efficiently, SPCE is adopted to represent the input/output relations of the original model. The construction of SPCE is based on the theory of Bayesian model averaging. In the following, we recall briefly the Sobol' decomposition and the Bayesian SPCE. Then the procedure of data-driven analysis on the Arlequin method is introduced.

3.1. Sobol' decomposition

Let us consider a mathematical model having input vector $\mathbf{x} = (x_1, x_2, \dots, x_n)^T$ and a scalar output Y :

$$Y = M(\mathbf{x}), \quad \mathbf{x} \in \mathbb{K}^n \quad (7)$$

where the input parameters are independent random variables uniformly distributed in $[0, 1]$:

$$\mathbf{x} = \{x_1, \dots, x_n\}, \quad x_i \sim \mathcal{U}[0, 1], \quad i = 1, \dots, n \quad (8)$$

We assume that Y is square integrable, that is $Y \in \mathcal{L}^2$. The unique Sobol' decomposition of $M(\mathbf{x})$ into summands of increasing dimension reads [28]:

$$M(\mathbf{x}) = M_0 + \sum_{i_1=1}^n M_{i_1}(x_{i_1}) + \sum_{i_2>i_1}^n M_{i_1 i_2}(x_{i_1}, x_{i_2}) + \dots + M_{12\dots n}(\mathbf{x}) \quad (9)$$

where the integral of each summand $M_{i_1\dots i_s}(x_{i_1}, \dots, x_{i_s})$ over any of its independent variables is zero, that is:

$$\int_0^1 M_{i_1\dots i_s}(x_{i_1}, \dots, x_{i_s}) dx_{i_k} = 0, \quad 1 \leq k \leq s \quad (10)$$

Due to Eq. (10), the summands of the decomposition are orthogonal to each other in the following sense:

$$\int_{\mathbb{K}^n} M_{i_1\dots i_s}(x_{i_1}, \dots, x_{i_s}) M_{j_1\dots j_t}(x_{j_1}, \dots, x_{j_t}) d\mathbf{x} = 0 \quad \text{for } \{i_1\dots i_s\} \neq \{j_1\dots j_t\} \quad (11)$$

where $d\mathbf{x} = dx_1 \dots dx_n$ for the sake of simplicity.

Due to the orthogonality property in Eq. (11), the total variance of $M(\mathbf{x})$ can be decomposed as follows:

$$D = \int_{\mathbb{K}^n} M^2(\mathbf{x}) d\mathbf{x} - M_0^2 = \sum_{i_1=1}^n D_{i_1} + \sum_{i_2>i_1}^n D_{i_1 i_2} + \dots + D_{12\dots n} \quad (12)$$

where the partial variance $D_{i_1\dots i_s}$ reads:

$$D_{i_1 i_2 \dots i_s} = \int_{\mathbb{K}^s} M_{i_1 \dots i_s}^2(x_{i_1}, \dots, x_{i_s}) dx_{i_1} \dots dx_{i_s} \quad (13)$$

The Sobol' indices are defined as follows:

$$S_{i_1 \dots i_s} = \frac{D_{i_1 \dots i_s}}{D} \in [0, 1] \quad (14)$$

Obviously, they satisfy:

$$\sum_{i_1=1}^n S_{i_1} + \sum_{i_2>i_1}^n S_{i_1 i_2} + \dots + S_{12\dots n} = 1 \quad (15)$$

The first-order sensitivity index S_i represents the influence due to x_i alone. S_{ij} measures the amount of variance of Y due to the cooperative effect of x_i and x_j . Similarly, $S_{i_1 i_2 \dots i_s}$ describes the sensitivity due to the set of input parameters $\{x_{i_1}, x_{i_2}, \dots, x_{i_s}\}$. The closer the Sobol' index to 1, the more sensitive the corresponding parameters. In this work, the first-order sensitivity index S_i and the total sensitivity index S_{Ti} are used to evaluate the sensitivity of the coupling parameters. S_{Ti} evaluates the total contribution of x_i to the

Figure 3. The location of the selected points for error evaluation.

Figure 4. Sketch for a bar clamped at both ends.

Table 1. Parameters of the coarse-fine bar model.

$E(\text{Pa})$	$L(\text{m})$	$l_c(10^{-1}\text{m})$	$l_f(10^{-2}\text{m})$
100	3	1.25	2.5

Table 2. The range of parameters considered for GSA.

	α_c	β_c	ℓ	L_s
case 1	[0, 1]	[0, 1]	[0, L]	[2l_c, 20l_c]
case 2	[0, 0.5]	[0, 0.5]	[0, L]	[2l_c, 20l_c]

variance of Y in the following form:

$$S_{Ti} = \sum_{r:i \in r} S_r = 1 - S_{\sim i} \quad (16)$$

where the symbol “ $\sim$ ” means “complementary of” in the sequel.

In order to calculate the Sobol’ indices in a feasible and effective way, the SPCE of the model response is introduced in the next subsection.

3.2. Bayesian sparse polynomial chaos expansion of the model response

The model response can be expanded in terms of a polynomial basis as follows:

$$Y = M(\mathbf{x}) \equiv \sum_{\mathbf{b} \in \mathbb{N}^n} a_{\mathbf{b}} \psi_{\mathbf{b}}(\mathbf{x}), \text{ with } \psi_{\mathbf{b}}(\mathbf{x}) = \psi_{b_1 \dots b_n}(\mathbf{x}) = \prod_{i=1}^n \psi_{b_i}(x_i) \quad (17)$$

where $\mathbf{b} = b_1 \dots b_n$ ($b_i \in \mathbb{N}, 1 \leq i \leq n$) is an n -dimensional index, and the $a_{\mathbf{b}}$ ’s are the polynomial coefficients.

Equation (17) is usually referred to as the polynomial chaos expansion (PCE) of Y . A polynomial basis function is a cumulative product of n univariate standardized shifted-Legendre polynomials, where b_i the i -th element of $\mathbf{b}$ denotes the order of the Legendre polynomial in x_i . For instance, the first three Legendre polynomials are: $\psi_0(x) = 1$, $\psi_1(x) = \sqrt{3}(2x-1)$, $\psi_2(x) = \frac{3\sqrt{5}}{2}(2x-1)^2 - \frac{\sqrt{5}}{2}$.

For computational purposes, the PCE is usually truncated to retain a finite number of terms. A truncated PCE whose total degree $|\mathbf{b}| \equiv \sum_{i=1}^n b_i$ does not exceed a given order p reads:

$$Y \simeq M_p(\mathbf{x}) \equiv \sum_{\mathbf{b} \in A^{p,n}} a_{\mathbf{b}} \psi_{\mathbf{b}}(\mathbf{x}), \quad A^{p,n} \equiv \{\mathbf{b} \in \mathbb{N}^n : |\mathbf{b}| \leq p\} \quad (18)$$

To reduce the number of model evaluations and to prevent overfitting, a SPCE is usually adopted. A SPCE retains a small number of terms to capture the main feature of the model response:

$$Y \simeq M_A(\mathbf{x}) \equiv \sum_{\mathbf{b} \in A} a_{\mathbf{b}} \psi_{\mathbf{b}}(\mathbf{x}), \quad A \subseteq A^{p,n} \text{ and } \frac{\text{card}(A)}{\text{card}(A^{p,n})} \ll 1 \quad (19)$$

where operator card provides the cardinality of a set.

In this work, the construction of SPCE is based on Bayesian model averaging. Suppose there are N_m plausible competing SPCE models M_{A_k} :

$$M_{A_k} \equiv \sum_{\mathbf{b} \in A_k} a_{\mathbf{b}} \psi_{\mathbf{b}}(\mathbf{x}) = \mathbf{a}_k \boldsymbol{\psi}_k, \quad k = 1, \dots, N_m \quad (20)$$

where $\mathbf{a}_k$ and $\boldsymbol{\psi}_k$ denote the vector of polynomial coefficients and polynomial terms.

Let $\mathcal{X}, \mathcal{Y}$ represent the input and output data sets respectively. By estimating each model’s posterior probability which represents the model’s ability to reproduce the data set $(\mathcal{X}, \mathcal{Y})$, the best SPCE representation among the set $\{M_{A_k}, k = 1, \dots, N_m\}$ can be selected. The posterior probabilities $P(M_{A_k}|\mathcal{Y})$ are given by Bayes’ theorem:

$$P(M_{A_k}|\mathcal{Y}) = \frac{P(\mathcal{Y}|M_{A_k})P(M_{A_k})}{\sum_{i=1}^{N_m} P(\mathcal{Y}|M_{A_i})P(M_{A_i})} \quad (21)$$

where $P(M_{A_k})$ is the prior probability. Usually, let $P(M_{A_k}) = 1/N_m$ when the prior information is vague. The denominator in Eq. (21) is the normalization constant. $P(\mathcal{Y}|M_{A_k})$ is the likelihood of the observed data, expressing the preference shown by the data for different models. Therefore, $P(\mathcal{Y}|M_{A_k})$ is used as the Bayesian model evidence. By Taylor series expansion and Laplace approximation, we can finally deduce the Kashyap information criterion (KIC) [35]:

$$-2 \ln P(\mathcal{Y}|M_{A_k}) \simeq -2 \ln P(\mathcal{Y}|M_{A_k}, \tilde{\mathbf{a}}_k) - 2 \ln P(\tilde{\mathbf{a}}_k|M_{A_k}) - P_k \ln(2\pi) + \ln(|C_{\tilde{\mathbf{a}}\tilde{\mathbf{a}}}|) = KIC_k \quad (22)$$

where the mean of the posterior $\tilde{\mathbf{a}}_k$ is referred to as the maximum a posteriori estimate (MAP), which represents the most likely parameter set for model M_{A_k} . The covariance matrix $C_{\tilde{\mathbf{a}}\tilde{\mathbf{a}}}$ is estimated at the MAP solution (i.e. $\mathbf{a}_k = \tilde{\mathbf{a}}_k$).

By introducing some assumptions about the prior probability, the parameters $\tilde{\mathbf{a}}_k$ and $C_{\tilde{\mathbf{a}}\tilde{\mathbf{a}}}$ can be calculated in an iterative way. Then, KIC_k of the competing model M_{A_k} can also be calculated. Apparently, the best SPCE is the one with the smallest KIC . In the following, we write the best SPCE as $M_{A^{opt}}$. The details of the algorithm are presented in [35].

Now let us calculate Sobol’ indices from the constructed SPCE $M_{A^{opt}}$. Write $M_{A^{opt}}$ in the form of the Sobol’ decomposition with a symbol $I_{i_1 \dots i_s}$ defined as follows:

Figure 5. The Sobol' indices of (a) case 1 and (b) case 2 for the coarse-fine bar model.

$$I_{i_1 \dots i_s} = \left\{ \mathbf{b} \in A^{opt} : \begin{array}{ll} b_k > 0, & k \in (i_1 \dots i_s), \quad \forall k = 1, \dots, n \\ b_k = 0, & k \notin (i_1 \dots i_s), \quad \forall k = 1, \dots, n \end{array} \right\} \quad (23)$$

Then, the SPCE reads:

$$\begin{aligned} M_{A^{opt}} = & a_0 + \sum_{i_1=1}^n \sum_{\mathbf{b} \in I_{i_1}} a_{\mathbf{b}} \psi_{\mathbf{b}}(x_{i_1}) + \sum_{i_2 > i_1}^n \sum_{\mathbf{b} \in I_{i_1 i_2}} a_{\mathbf{b}} \psi_{\mathbf{b}}(x_{i_1}, x_{i_2}) \\ & + \dots + \sum_{i_s > \dots > i_1}^n \sum_{\mathbf{b} \in I_{i_1 \dots i_s}} a_{\mathbf{b}} \psi_{\mathbf{b}}(x_{i_1}, \dots, x_{i_s}) \\ & + \dots + \sum_{\mathbf{b} \in I_{1, \dots, n}} a_{\mathbf{b}} \psi_{\mathbf{b}}(\mathbf{x}) \end{aligned} \quad (24)$$

where each summand in Eq. (9) can be identified in the above equation as follows: $M_{i_1 \dots i_s}(x_{i_1}, \dots, x_{i_s}) = \sum_{\mathbf{b} \in I_{i_1 \dots i_s}} a_{\mathbf{b}} \psi_{\mathbf{b}}(x_{i_1}, \dots, x_{i_s})$.

As long as a SPCE of a model response is built, it is easy to calculate the Sobol' indices analytically by the SPCE's coefficients. Due to the orthonormal property of the polynomial basis, the first-order and total Sobol' indices of input variables x_i can be derived analytically according to Eqs. (13), (14), and (16) as follows:

Table 3. The Sobol' indices of *case 1* and *case 2* for the coarse-fine bar model.

		Err_w		Err_f		Err_s		Err_c	
		S_i	S_{Ti}	S_i	S_{Ti}	S_i	S_{Ti}	S_i	S_{Ti}
<i>case 1</i>	α_c	0.7126	0.9318	0.9508	0.9938	0.9428	0.9843	0.9508	0.9938
	β_c	0	0	0	0	0	0	0	0
	ℓ	0.0304	0.0947	0.0062	0.0492	0.0157	0.0572	0.0062	0.0492
	L_s	0.0258	0.2270	0	0	0	0	0	0
<i>case 2</i>	α_c	0.0027	0.0027	0.0080	0.2966	0.0044	0.0134	0.0080	0.2966
	β_c	0	0	0	0	0	0	0	0
	ℓ	0.3053	0.6554	0.4361	0.9920	0.7114	0.9796	0.4361	0.9920
	L_s	0.3419	0.6920	0	0.3376	0.0160	0.2761	0	0.3376

$$S_i^{A^{opt}} = \frac{D_i^{A^{opt}}}{D^{A^{opt}}} = \frac{\sum_{b \in I_i} a_b^2}{\sum_{b \in A^{opt} \setminus \{0\}} a_b^2} \quad (25)$$

$$S_{Ti}^{A^{opt}} = \sum_{b: b_i > 0} S_b^{A^{opt}} \quad (26)$$

3.3. The proposed approach of data-driven analysis

Here we propose a data-driven approach based on the Bayesian SPCE to analyze the settings of the Arlequin parameters. Suppose that we have “ m ” Arlequin parameters to analyze, and “ n ” model responses of interest. The computing process is sketched in [Figure 2](#) and outlined as follows:

Step 1: Generate samples for the analyzed parameters in given probability distributions with N_d realizations, e.g. $\mathcal{X} = \{\mathcal{X}_1, \mathcal{X}_2, \dots, \mathcal{X}_m\}$ where $\mathcal{X}_i = \{\mathcal{X}_i^{(1)}, \mathcal{X}_i^{(2)}, \dots, \mathcal{X}_i^{(N_d)}\}^T$ with $1 \leq i \leq m$. There are several sampling methods, such as Latin Hypercube sampling, quasi-random low discrepancy sequences and quasi-Monte Carlo (QMC) method, etc. In this work, the input data set is generated by QMC method for its excellent property in space filling.

Step 2: Evaluate the multi-scale model at each group of design points using numerical methods. The corresponding model responses of interest are gathered into the vectors, say $\mathcal{Y}_j = \{\mathcal{Y}_j^{(1)}, \mathcal{Y}_j^{(2)}, \dots, \mathcal{Y}_j^{(N_d)}\}^T$ with $1 \leq j \leq n$. To assess the effectiveness of the coupling, the relative errors between the coupling solution and the reference solution are chosen as the model responses.

Step 3: Transform the data $(\mathcal{X}, \mathcal{Y}_j)$ ($1 \leq j \leq n$) into standardized form $(\mathbf{x}, \mathbf{y}_j)$ ($1 \leq j \leq n$). And construct the data-driven model for each model response Y_j from the data set $(\mathbf{x}, \mathbf{y}_j)$. The SPCE based on the theory of Bayesian model averaging is used to approximate the input/output relations of the multi-scale model. Thus, the optimal SPCE for each model response is written as $Y_j = M_j^{opt}(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_m)$ ($1 \leq j \leq n$).

Step 4: Perform GSA on the data-driven model instead of the multi-scale model. Sobol' decomposition is easily conducted on the SPCE model. And subsequently the Sobol' indices for each Arlequin parameter are computed analytically. For every model response Y_j , we calculate both the first-order sensitivity indices $S_i^{(j)}$ and the total sensitivity indices $S_{Ti}^{(j)}$ to account for interactions between parameters.

4. Numerical examples

In this section, three typical examples using the Arlequin method are analyzed by the proposed approach: a coarse-fine bar model, a particle-continuum model and a 2D-1D sandwich model. The coarse-fine bar model is a widely studied benchmark for the Arlequin method, see Ben Dhia et al. [6, 8], Guidault and Belytschko [37], Sun and Alejandro [24], etc. This benchmark test is firstly considered to verify the effectiveness of the approach. Then a more complex example, the particle-continuum model is studied. This is also a popular benchmark for the Arlequin method which has been studied by Bauman and Ben Dhia et al. [9], Prudhomme et al. [10], Chamoin et al. [38] when considering heterogeneous materials. At last, an example accounting a heterogeneous structure [25] is investigated.

In all cases, the coupling zone is always located at the center of the whole domain, which implies that the sub-domains of the multi-scale model possess the same size. Suppose L is the size of the whole domain. For the sake of simplicity, we define the element length of the coarse model l_c as:

$$l_c = \frac{L}{n}, \quad n \in \mathbb{N}^* \quad (27)$$

and the size of the coupling zone L_s is defined as:

$$L_s = 2n_s l_c, \quad n_s \in \mathbb{N}^* \text{ and } 2n_s \leq n-4 \quad (28)$$

In this work, we set $n = 24$. Thus, the maximum range of $2n_s$ is $[2, 20]$.

For each model, the energy partition functions α_c and β_c , the characteristic length of the coupling operator $\mathcal{L}$ and the size of the coupling zone L_s are collected in the input variables $\mathbf{X} = \{\alpha_c, \beta_c, \ell, L_s\}$, whilst the model responses $\mathbf{Y} = \{Err_w, Err_f, Err_s, Err_c\}$ denote the relative errors of displacements at specific points and can be calculated as follows:

$$Err_j = \left| \frac{\mathbf{U} - \mathbf{U}_{ref}}{\mathbf{U}_{ref}} \right|_j, \quad j = w, f, s, c \quad (29)$$

where $\mathbf{U}_{ref}$ denotes the reference solution of displacement. Err_w is the maximum relative error of the whole domain. Err_f , Err_s , Err_c are respectively the relative errors at l_c near the left end, in the middle, and at l_c near the right end of the domain (see [Figure 3](#)). Since the maximum range of the coupling zone is $[2l_c, 20l_c]$, it is obvious that with the change of coupling zone, point f and point c always locate at Ω_f and Ω_c , respectively, while point s is always in the coupling

Figure 6. The marginal effect of Arlequin parameters in (a) case 1 and (b) case 2 for the coarse-fine bar model.

Figure 7. The Arlequin method in a particle model.

zone. The relative errors at selected points together with the maximum relative error in the whole domain can represent the responses of the whole model.

The maximum range of the coupling parameters α_c , β_c , ℓ , and L_s are respectively $[0, 1]$, $[0, 1]$, $[0, L]$, and $[2l_c, 20l_c]$. The parameters are assumed to be statistically independent and uniformly distributed. Among others, L_s is a discrete variable with values equal to $2l_c, 4l_c, 6l_c, \dots, 20l_c$, where each value is equally likely. The sample size for each case is denoted by N_d . The convergence of Sobol' indices with respect to the sample sizes is presented in [Appendix A](#).

Table 4. Parameters of the particle-continuum model.

k_1 (N/m)	k_2 (N/m)	l_1 (10^{-4} m)	l_2 (10^{-4} m)	l_c (10^{-1} m)	L (m)
100	1	1.5625	1.5625	1.25	3

4.1. The coarse-fine bar model

A both-ends clamped bar with uniform axial force $q = 1$ N/m is presented in [Figure 4](#). The domain Ω is split into

Table 5. The Sobol' indices of *case 1* and *case 2* for the particle-continuum model.

		Err_w		Err_f		Err_s		Err_c	
		S_i	S_{Ti}	S_i	S_{Ti}	S_i	S_{Ti}	S_i	S_{Ti}
<i>case 1</i>	α_c	0.7109	0.9321	0.9497	0.9935	0.9413	0.9836	0.9497	0.9936
	β_c	0	0	0	0	0	0	0	0
	ℓ	0.0305	0.0958	0.0065	0.0503	0.0164	0.0587	0.0064	0.0503
	L_s	0.0254	0.2280	0	0	0	0	0	0
<i>case 2</i>	α_c	0.0031	0.0031	0.0065	0.2872	0	0.0089	0.0084	0.3044
	β_c	0	0	0	0	0	0	0	0
	ℓ	0.3496	0.6716	0.4524	0.9876	0.7212	0.9794	0.4196	0.9916
	L_s	0.3253	0.6474	0.0059	0.3272	0.0206	0.2707	0	0.3496

(a)

(b)

Figure 8. The Sobol' indices of (a) *case-1* and (b) *case-2* for the particle-continuum model.

two sub-domains, where Ω_f is discretized by using a fine mesh, whilst a coarse mesh is considered for Ω_c . The coupling between these two models is achieved in the overlapping zone by the Arlequin method with the H^1 -type coupling operator.

The geometrical and material parameters are illustrated in Table 1, where E and q represent the Young's modulus and the uniform axial force respectively, l_c and l_f stands for the element length of the coarse model and the fine model, respectively. The cross-sectional area is set to unity for simplicity.

A linear Lagrange interpolation is used for the discretization of the displacement fields and the Lagrange multipliers:

$$\langle N \rangle = \left\langle \frac{1-\xi}{2} \quad \frac{1+\xi}{2} \right\rangle \quad (30)$$

where ξ represents the natural local coordinate. The bar is isotropic and meets Hook's law. The axial strain and stress can be expressed as follows:

$$\sigma_x = E\varepsilon_x \quad \text{and} \quad \varepsilon_x = \langle N_{,x} \rangle \{q_e\} \quad (31)$$

where q_e denotes the elementary displacement vector.

Lagrange multipliers share the same mesh with the displacement in the coarse model. Considering Eqs. (1), (3), (4), (31), and (30), a linear system is obtained as shown in Eq. (5). For a given set of input parameters, solving this linear system results in the solution of each sub-domain. And then the displacement field U of the multi-scale model are calculated via Eq. (6). For this example, the analytic solution can be obtained easily, which will be used as the reference U_{ref} . For brevity, here we do not present the details on how to obtain the analytic solution.

Now we draw a sample of size $N_d = 2^{10}$ in the maximum ranges of the coupling parameters $\langle \alpha_c, \beta_c, \ell, L_s \rangle$ (see Table 2 case 1). Note that $N_d = 2^{10}$ is sufficient to guarantee the convergence of GSA for this example. After building the SPCE model between the coupling parameters and the relative errors, Sobol' indices are calculated. The resulting first-order and total Sobol' indices are displayed in Figure 5(a) and Table 3 case 1. We recall that, in GSA, the first-order sensitivity index S_i evaluates the sensitivity due to the input variable x_i alone, while the total sensitivity index S_{Ti} measures the total effect caused by x_i including the interactions. The higher the sensitivity index is, the more important x_i is for the model response. Apparently, $1 \geq S_{Ti} \geq S_i \geq 0$. We can notice that the most influential parameter is the internal energy partition function α_c , whose total sensitivity indices

Figure 9. The marginal effect of Arlequin parameters in (a) case 1 and (b) case 2 for the particle-continuum model.

for the four model responses Err_j ($j = w, f, s, c$) are all higher than 0.93 (very close to 1). In Figure 6(a), we plot all the obtained data of Err_j ($j = w, f, s, c$) versus the coupling parameters $\langle \alpha_c, \beta_c, \ell, L_s \rangle$. The curves in Figure 6(a) represent the marginal effect of each parameter on different model responses. It is worth noting that when α_c approaches 1, the relative errors raise sharply. Especially the maximum relative error of the whole domain Err_w can increase to about 50%, which indicates that the effectiveness of the coupling drops drastically. Therefore the value of α_c should be far from 1, that is to say, the internal energy distribution should be always partially shared with fine model. This is consistent with the results in Ben Dhia et al. [8]. It is reasonable since the fine model describes the energy of the domain more accurately and it deserves a higher weight.

From Figure 6(a) and Table 3 case 1, we notice that the Sobol' indices of the external energy partition function β_c are equal to 0, which means that β_c does not influence the accuracy of the coupled model. The state-of-the-art about the Arlequin method mainly discuss the choice of α_c , while the value of β_c is set equal to α_c by default, such as in Ben Dhia et al. [6] and Guidault and Belytschko [37].

The Sobol' indices of the characteristic length ℓ and the size of the coupling zone L_s are very low for this example. The total Sobol' index of L_s on Err_w ($S_{Ti} = 0.2270$) is higher than the corresponding first-order Sobol' index ($S_i = 0.0258$), which means the effect of L_s on the coupling is mainly reflected in interactions. Besides, in Figure 6(a), the marginal effect curves of model responses versus the two coupling parameters $\langle \ell, L_s \rangle$ show very slight changes. The

Figure 10. The total Sobol' indices of α_c and β_c at different points in the domain of the particle-continuum model.

Figure 11. Sketch of a cantilever sandwich beam.

results above indicate that the sensitivity of the coupling due to ℓ and L_s is very low compared to α_c ; these two parameters slightly affect the coupling in this case.

To further investigate the influence of ℓ and L_s , we narrow the sampling range of energy partition functions α_c , β_c from $[0, 1]$ to $[0, 0.5]$, while the sampling range of ℓ and L_s stay the same (see Table 2 case 2). We draw samples of size $N_d = 2^{10}$ from the new prior distribution of case 2 followed by numerical computations to obtain the relative errors. Subsequently, a GSA is performed based on the Bayesian SPCE. The obtained Sobol' indices are presented by Figure 5(b) and Table 3 case 2. The sensitivity indices of α_c on the maximum relative error Err_w decrease drastically from a high level in case 1 ($S_i = 0.7126$, $S_{Ti} = 0.9318$) to almost 0 ($S_i = S_{Ti} = 0.0027$). Besides, the value of the maximum relative error Err_w also decreases significantly. Here the maximum relative error is less than 5%, which is much less than about 50% in case 1. This implies that when the sampling range of energy partition functions reduce to $[0, 0.5]$, the coupling is slightly sensitive to α_c and the accuracy of the coupled model is significantly improved. The total Sobol' indices of α_c on Err_f and Err_c are obviously higher than the corresponding first-order Sobol' indices, while all the Sobol' indices of α_c on Err_s are very low. That means, in this case, the effect of the choice of α_c mainly appears in the whole domain except Ω_s in the form of interactions and are very small in the coupling zone Ω_s . The marginal effect of α_c on model responses is negligible as illustrated in Figure 6(b). In particular, the maximum relative error of the displacement in the whole domain has been reduced to an acceptable level. We can also

Table 6. Parameters of the 2D-1D sandwich FE models.

E_1 (MPa)	E_2 (MPa)	L (m)	H_3 (m)	H_1/H_2	μ_1	μ_2
6.9	6.9×10^4	0.2	0.01	1	0.3	0.3

Table 7. The Sobol' indices of case 1 and case 2 for the 2D-1D sandwich model.

		Err_w		Err_f		Err_s		Err_c	
		S_i	S_{Ti}	S_i	S_{Ti}	S_i	S_{Ti}	S_i	S_{Ti}
case 1	α_c	0.4621	0.9221	0.6572	0.9598	0.5417	0.9510	0.6828	0.9674
	β_c	0	0	0	0	0	0	0	0
	ℓ	0.0067	0.1215	0.0111	0.0926	0.0056	0.0494	0.0088	0.0771
	L_s	0.0713	0.4468	0.0291	0.2564	0.0434	0.4341	0.0238	0.2452
case 2	α_c	0.0090	0.5852	0.3018	0.6475	0.1622	0.6051	0.2180	0.7003
	β_c	0	0	0	0	0	0	0	0
	ℓ	0	0	0.0710	0.2413	0.0987	0.3313	0.0952	0.6043
	L_s	0.4148	0.9910	0.2411	0.5636	0.2185	0.6717	0.0367	0.5669

note that the influence of β_c still seems to be negligible as the Sobol' indices of β_c are still equal to 0. Hence, choosing the value of energy partition functions in the range of $[0, 0.5]$ is feasible when using the Arlequin method.

In case 2, the Sobol' indices shown in Figure 5(b) and Table 3 case 2 demonstrate that the coupling accuracy is mainly affected by the characteristic length ℓ and the size of the coupling zone L_s , as the Sobol' indices rise significantly compared to case 1. The interactions of these factors are evident as $S_{Ti} > S_i$. From the curves displayed in Figure 6(b), we can see that, the closer the value of ℓ to 0, the greater the model responses. When $\ell = 0$, H^1 coupling operator is converted to L^2 coupling operator. The increase of relative errors at $\ell = 0$ implies that H^1 coupling operator is more reliable than L^2 coupling operator. The same conclusion has been reported in Ben Dhia et al. [8] and Guidault and Belytschko [37]. Considering Eq. (3), the existence of gradients coupling terms can reduce the condition number of stiffness matrix which leads to better accuracy and stability of the coupling. The characteristic length ℓ is used to balance the two kinds of coupling conditions. Therefore, according to the marginal effect of ℓ in Figure 6(b), $\ell > 2l_c$ is suggested for the coupling.

From Figure 6(b), we can notice that as the size of the coupling zone L_s increases, the model responses change slowly. In particular, there is a slightly positive correlation between maximum relative error Err_w and L_s . Besides, considering the lower degrees of freedom, it is suggested that a relatively smaller coupling size should be adopted. We suggest that L_s in $[2l_c, 6l_c]$ is appropriate.

4.2. The particle-continuum model

A particle model with uniform axial force $q = 1$ N/m is illustrated in Figure 7, where the connections between these particles are represented by periodically distributed springs with stiffness k_1 , k_2 and equilibrium length l_1 , l_2 .

To reduce the size of the particle model, a particle-continuum model that involves the particle model in Ω_f and a continuum model in Ω_c is considered. The Arlequin method is used to couple the two different models. As suggested in [9], a linear elastic bar model is employed as the continuum model, whose modulus E can be calculated as:

Figure 12. The Sobol' indices of (a) case 1 and (b) case 2 for the 2D-1D sandwich model.

$$E = \frac{k_1 k_2}{k_1 + k_2} (l_1 + l_2) \quad (32)$$

Note that the cross-sectional area of the bar is set to be unity for simplicity.

The parameters of the particle-continuum model are listed in Table 4, where l_c represents the elementary length of the continuum model.

The linear Lagrange interpolation is used for the discretization of the displacement fields and the Lagrange

Figure 13. The marginal effect of Arlequin parameters in (a) case 1 and (b) case 2 for the 2D-1D sandwich model.

multipliers. Based on the formulations in Section 2, one can easily obtain a linear system Eq. (5) and consequently the global displacement field via Eq. (6). The solution of a full particle model is adopted as the reference U_{ref} .

Same as the previous example, we investigate the sensitivity of the coupling parameters in their maximum sampling range (see Table 2 case 1). Note that the sample size N_d for this example is set to 2^{10} which can ensure the convergence of GSA. The Sobol' indices and the marginal effect shown in Table 5 case 1, Figures 8(a) and 9(a) illustrate a similar trend as that in the coarse-fine bar model. The internal energy partition α_c is the most influential parameter. More weight should be attached to the particle model than the continuum model. According to the Sobol' indices, the external energy partition β_c has no effect on the coupling accuracy. For further investigation, we select a series of uniformly distributed points in the whole domain with interval equal to l_c and study the effects of the energy partition functions on the relative error at these points. The total Sobol' indices of each point are illustrated in Figure 10. The results show that the Sobol' indices of α_c are very high in the whole domain, which indicates the huge impact of α_c on the coupling. The Sobol' indices of β_c are equal to 0 in the whole

domain, which means that β_c does not influence the coupling accuracy in this case.

Then a narrower sampling range $[0, 0.5]$ is considered to reduce the influence of α_c and to further investigate the influence of ℓ and L_s (see Table 2 case 2). In Figures 8(b) and 9(b), the same phenomenon has been observed as in the previous example: the sensitivity indices of α_c and the maximum relative error Err_w both decrease significantly and all the model responses are reduced to an acceptable level (the maximum relative error is less than 5%). The results show that the suitable range of the energy partition functions lies in $[0, 0.5]$.

In case 2 with optimal choice of energy partition functions, the Sobol' indices in Figure 8(b) and Table 5 case 2 show that ℓ and L_s are the main influencing factors for the coupling. In Figure 9(b), the marginal effect curves show that a smaller ℓ close to 0 leads to a higher relative error. Similar results have been reported by Guidault and Belytschko [23], which indicate that the H^1 coupling may be beneficial to couple a very coarse mesh with an atomistic model than L^2 coupling where $\ell = 0$. To achieve a good coupling, the characteristic length ℓ is suggested to be larger than $2l_c$.

According to the marginal effect of L_s in Figure 9(b), the maximum relative error increases with the increase of L_s . Thus, a small coupling zone L_s in the range $[2l_c, 6l_c]$ is recommended.

4.3. The 2D-1D sandwich model

In this part, a cantilever sandwich beam subjected to a uniformly distributed load $q = 100 \text{ N/m}$ is considered, as shown in Figure 11. The geometric and material parameters of the sandwich beam are listed in Table 6, where E , μ , and H stand for Young's modulus, Poisson's ratio, and thickness, respectively. The top and bottom layers of the beam have the same geometric and material parameters. The subscript 1 and 2 in Table 6 represent the parameters related to the middle layer and top layers, respectively. The thickness of the whole beam is H_3 .

The 2D-1D sandwich multi-scale model developed in [25] is used to model this beam, in which the 2D model is used near the boundary to accurately capture the boundary effects and the 1D sandwich model in the rest region to reduce the computational cost. The detailed formulations of the 2D-1D coupling model are presented in Appendix B. In the thickness direction, six 2D elements are sufficient. In the longitudinal direction, the elementary length of the 2D FE model and 1D beam model are, respectively, $l_f = 1.67 \times 10^{-3} \text{ m}$ and $l_c = 8.33 \times 10^{-3} \text{ m}$. The mesh scheme considered here is sufficient to yield convergent results. Reference solution U_{ref} is the middle plane displacement fields obtained by using the 2D model in the whole structure.

Similar to the previous two examples, we analyze two cases as shown in Table 2. The difference consists in using two different ranges of weight functions α_c and β_c . The sample size N_d for this example is set to 2^9 which can ensure

Figure 14. Transverse displacement along the beam axis.

the convergence of GSA. The Sobol' indices are presented in Table 7 and plotted in Figure 12 for clarity. The marginal effect of each parameter on different model responses is shown in Figure 13. The following conclusions could be found based on the obtained results:

- Similar to the previous two examples, α_c is still the most important parameter, that is, the model responses increase sharply when α_c approaches to 1 as shown in Figure 13(a). When α_c is in the range $[0, 0.5]$, the effect of α_c is significantly reduced compared to case 1. In case 2, with the increase of α_c , the maximum relative error Err_w remains stable, but the relative errors of the three representative points Err_f , Err_s , and Err_c increase slowly. It means that the coupling effects of the whole domain may become worse. This further verifies that the coarse model should be associated with less weight in this heterogeneous structure. Considering Err_w has been reduced to an acceptable range ($Err_w < 3.4\%$) in case 2, the range of $[0, 0.5]$ is desirable for the energy weight functions.
- The Sobol' indices of β_c are still equal to 0 in both cases, which indicates that β_c still has negligible effect.
- In case 1, the characteristic length ℓ slightly affects the coupling solution. The effect of ℓ mainly appears in the form of interactions as $S_{Ti} > S_i \approx 0$. For case 2, $\mathcal{L}$ has no effect on the maximum relative error Err_w as $S_{Ti} = S_i = 0$, but affects the coupling of the selected points in the domain. This result can also be observed from the marginal effect curves in Figure 13(b), where Err_w does not change with the increase of ℓ , while Err_f , Err_s , and Err_c increase when ℓ is approaching 0. One could also note that $\ell = 0$ would lower the coupling accuracy, which coincides with the conclusion drawn by Hu et al. [25]. Here, we suggest that $\mathcal{L}$ should be greater than $2l_c$ to achieve a good coupling solution.
- The size of the coupling zone L_s is the second most influential factor in this example. For both cases, with the increase of L_s , Err_w decreases slightly and then increases significantly, while Err_f , Err_s , and Err_c increase slowly. This indicates that a large coupling zone may deteriorate the precision of coupling and cause unsatisfactory solution in the whole domain. Like the previous

two examples in Sections 4.1 and 4.2, we can see that taking the value of L_s in the range of $[2l_c, 6l_c]$ is still reasonable.

To verify the above findings, we select two sets of coupling parameters: (a) set 1: $\alpha_c = 0.01$, $\beta_c = 0.5$, $\ell = 3l_c$, $L_s = 2l_c$, (b) set 2: $\alpha_c = 0.99$, $\beta_c = 0.5$, $\ell = l_c$, $L_s = 16l_c$. In set 1, all coupling parameters are within the suggested ranges, while in set 2, values of α_c , ℓ , and L_s are beyond the suggested ranges. We present the transversal displacements of the middle plane of the sandwich structure in Figure 14 by using these two sets of parameters. The reference solution of displacement obtained by using the full 2D model is also plotted and compared to the coupled results. One can easily find that the results in set 1 agree well with the reference solution, whereas results obtained by set 2 deflect far from the reference. This proves that the suggested ranges of the coupling parameters are reliable. It also verifies that the Arlequin method, with reasonable coupling parameters, can yield accurate solutions. On the other hand, if the coupling parameters are not well set, the model errors can be relatively large, leading to inaccurate solutions.

5. Conclusions

In this article, a data-driven approach based on SPCE is used to quantitatively and qualitatively investigate the influence of Arlequin parameters, namely the energy partition functions α_c and β_c , the characteristic length ℓ of the coupling operator and the size of the coupling zone L_s , on the accuracy of multi-scale models. Three typical benchmark tests are considered, which are a coarse-fine bar model, a particle-continuum model and a 2D-1D sandwich model. The influence of each parameter and their interactions are carefully discussed and the optional settings of these factors can be drawn as follows:

1. The internal energy partition function is the most important factor in the coupling and should be put on the refined model. The optimal range of α_c is $[0, 0.5]$.
2. According to the results, the external energy partition function β_c hardly affects the coupling accuracy and the influence of β_c can be almost ignored compared to that of α_c . For simplicity, we suggest that the value of β_c is set equal to α_c .
3. The characteristic length ℓ of the coupling operator is not supposed to be small. We suggest $\ell > 2l_c$.
4. The size of the coupling zone L_s should not be large. The recommended range of L_s is $[2l_c, 6l_c]$.

The multi-scale models analyzed in this work are all linear models. The Arlequin parameters in cases of non-linear multi-scale models [12, 15, 39] will be analyzed by the proposed approach in subsequent work. Besides, the location of the coupling region is intentionally arranged in the middle of the entire domain, which deserves further investigation. The data-driven strategy presented in this work shows huge potential for analyzing complicated mechanical problems.

Funding

This work has been supported by the National Natural Science Foundation of China (Grant Nos.: 11702199 and 11772238) and the Natural Science Foundation of Hubei Province (Grant No: 2017CFB147). The authors would like to acknowledge the support of EU H2020 COMPOSELECTOR project (Grant No: 721105).

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Appendix A: Convergence analysis of the sample sizes

The algorithm that we adopt to "train" the metamodel is efficient and accurate, and can get precise results at low sample sizes [35]. However, a relative larger data basically yields a more accurate estimation. In this part, we take the 2D-1D sandwich model as an example to investigate the effect of the sample size N_d on results. The samples are drawn from the uniform distributions shown in Table 2 case 1. And the model response Err_f is considered as output data. A SPCE model is constructed to approximate the input/output relations.

According to Shao et al. [35], a relative training error δ^2 could be relied on to evaluate the quality of the constructed SPCE model. The relative training errors for different sample sizes are listed in Table 8. We can note that choosing the sample size as 2^6 leads to a quite large relative error $\delta^2 = 0.117$, while increasing the model evaluations, the relative training error decreases. When N_d equals 2^9 , the relative training error has been reduced to $\delta^2 = 0.046 < 0.05$, which is an acceptable level as suggested in [35].

Table 8. The relative training errors for different sample sizes in the 2D-1D sandwich model.

N_d	2^6	2^7	2^8	2^9
δ^2	0.117	0.144	0.065	0.046

Figure 15. 95% confidence intervals of the Sobol' indices with different sample sizes.

Besides, the 95% credible intervals of both the first-order and total Sobol' indices estimates with different sample sizes are plotted in Figure 15. One clearly notes that with the sample size increases, the credible intervals become narrow and the maximum a posteriori estimates of the Sobol' indices converge. So choosing the sample size as 2^9 for this case is reasonable.

Appendix B: Formulations for the 2D-1D sandwich model

The 2D FE model is discretized by 2D-Q8 elements, thus the displacement fields are described by

$$\begin{cases} u_{2D}(x, z) = \langle \mathbf{N}_u \rangle \{ \mathbf{q}_e \} = \langle N_1 \ 0 \ \dots \ N_8 \ 0 \rangle \langle u_1 \ v_1 \ \dots \ u_8 \ v_8 \rangle^T, \\ v_{2D}(x, z) = \langle \mathbf{N}_v \rangle \{ \mathbf{q}_e \} = \langle 0 \ N_1 \ \dots \ 0 \ N_8 \rangle \langle u_1 \ v_1 \ \dots \ u_8 \ v_8 \rangle^T, \end{cases} \quad (33)$$

where u_i and v_i ($i = 1, \dots, 8$) are respectively the longitudinal and the transversal nodal displacements of the 2D element. The shape functions N_i can be found in [25], they are not presented here for brevity.

The kinematic field of the 1D sandwich beam is defined as follows:

$$\begin{cases} u^t(x, z) = -\left(z - \frac{H_1}{2}\right) w_{,x} + \frac{H_1}{2} \beta(x) & \frac{H_1}{2} < z \leq \frac{H_3}{2}, \\ u^m(x, z) = z \beta(x) & -\frac{H_1}{2} \leq z \leq \frac{H_1}{2}, \\ u^b(x, z) = -\left(z + \frac{H_1}{2}\right) w_{,x} - \frac{H_1}{2} \beta(x) & -\frac{H_3}{2} \leq z < -\frac{H_1}{2}, \\ w(x, z) = w(x), \\ \beta(x, z) = \beta(x), \end{cases} \quad (34)$$

where the superscripts t , m and b denote respectively the top, the middle and the bottom layer. Subscript x preceded by comma stands for

1) 2D element

$$\begin{cases} C_{2D}^t = E_2 \int_{-1}^1 \int_{-1}^1 \left(\left(-\left(z - \frac{H_1}{2}\right) \{ \mathbf{N}_{w,x} \} + \frac{H_1}{2} \{ \mathbf{N}_\beta \} \right) \langle \mathbf{N}_u \rangle + \{ \mathbf{N}_w \} \langle \mathbf{N}_v \rangle + \mathcal{L}^2 \left(-\left(z - \frac{H_1}{2}\right) \{ \mathbf{N}_{w,xx} \} + \frac{H_1}{2} \{ \mathbf{N}_{\beta,x} \} \right) \langle \mathbf{N}_{u,x} \rangle \right) \mathcal{J} d\xi d\eta, \\ C_{2D}^m = E_1 \int_{-1}^1 \int_{-1}^1 \left(z^2 \{ \mathbf{N}_\beta \} \langle \mathbf{N}_u \rangle + \{ \mathbf{N}_w \} \langle \mathbf{N}_v \rangle + \mathcal{L}^2 z^2 \{ \mathbf{N}_{\beta,x} \} \langle \mathbf{N}_{u,x} \rangle \right) \mathcal{J} d\xi d\eta, \\ C_{2D}^b = E_2 \int_{-1}^1 \int_{-1}^1 \left(\left(-\left(z + \frac{H_1}{2}\right) \{ \mathbf{N}_{w,x} \} - \frac{H_1}{2} \{ \mathbf{N}_\beta \} \right) \langle \mathbf{N}_u \rangle + \{ \mathbf{N}_w \} \langle \mathbf{N}_v \rangle + \mathcal{L}^2 \left(-\left(z + \frac{H_1}{2}\right) \{ \mathbf{N}_{w,xx} \} - \frac{H_1}{2} \{ \mathbf{N}_{\beta,x} \} \right) \langle \mathbf{N}_{u,x} \rangle \right) \mathcal{J} d\xi d\eta. \end{cases} \quad (37)$$

2) 1D element

$$C_{1D} = C_{1D}^t + C_{1D}^m + C_{1D}^b \quad (38)$$

with

$$\begin{cases} C_{1D}^t = E_2 \int_{\frac{H_1}{2}}^{\frac{H_3}{2}} \int_{-1}^1 \left(\left(-\left(z - \frac{H_1}{2}\right) \{ \mathbf{N}_{w,x} \} + \frac{H_1}{2} \{ \mathbf{N}_\beta \} \right) \left(-\left(z - \frac{H_1}{2}\right) \langle \mathbf{N}_{w,x} \rangle + \frac{H_1}{2} \langle \mathbf{N}_\beta \rangle \right) + \{ \mathbf{N}_w \} \langle \mathbf{N}_v \rangle + \mathcal{L}^2 \left(-\left(z - \frac{H_1}{2}\right) \{ \mathbf{N}_{w,xx} \} + \frac{H_1}{2} \{ \mathbf{N}_{\beta,x} \} \right) \left(-\left(z - \frac{H_1}{2}\right) \langle \mathbf{N}_{w,xx} \rangle + \frac{H_1}{2} \langle \mathbf{N}_{\beta,x} \rangle \right) \right) d\xi dz, \\ C_{1D}^m = E_1 \int_{-\frac{H_1}{2}}^{\frac{H_1}{2}} \int_{-1}^1 \left(z^2 \{ \mathbf{N}_\beta \} \langle \mathbf{N}_u \rangle + \{ \mathbf{N}_w \} \langle \mathbf{N}_v \rangle + \mathcal{L}^2 z^2 \{ \mathbf{N}_{\beta,x} \} \langle \mathbf{N}_{u,x} \rangle \right) d\xi dz, \\ C_{1D}^b = E_2 \int_{-\frac{H_3}{2}}^{-\frac{H_1}{2}} \int_{-1}^1 \left(\left(-\left(z + \frac{H_1}{2}\right) \{ \mathbf{N}_{w,x} \} - \frac{H_1}{2} \{ \mathbf{N}_\beta \} \right) \left(-\left(z + \frac{H_1}{2}\right) \langle \mathbf{N}_{w,x} \rangle - \frac{H_1}{2} \langle \mathbf{N}_\beta \rangle \right) + \{ \mathbf{N}_w \} \langle \mathbf{N}_v \rangle + \mathcal{L}^2 \left(-\left(z + \frac{H_1}{2}\right) \{ \mathbf{N}_{w,xx} \} - \frac{H_1}{2} \{ \mathbf{N}_{\beta,x} \} \right) \left(-\left(z + \frac{H_1}{2}\right) \langle \mathbf{N}_{w,xx} \rangle - \frac{H_1}{2} \langle \mathbf{N}_{\beta,x} \rangle \right) \right) d\xi dz, \end{cases} \quad (39)$$

where $\mathcal{J}$ denotes the Jacobian determinant, the characteristic length $\mathcal{L} \in [0, L]$. And the summands in each integral are the longitudinal displacement, the transversal displacement and the longitudinal deformation couplings respectively.

After assembling all these elementary matrices, we can calculate the displacement field of the 2D-1D sandwich model that have the similar formulation as Eq. (5).

differentiation. The longitudinal displacement, the transverse displacement and the additional rotation of the normal to the mid-plane are respectively expressed by u , w and β . The 1D sandwich beam is discretized by the two-node 1D element, in which β is discretized by the Lagrange linear shape functions $\mathbf{N}_\beta$ and w by the Hermite shape functions $\mathbf{N}_w$. Thus, the elemental unknowns are $\langle \phi_e \rangle = \langle w_1 \ \frac{\partial w_1}{\partial x} \ \beta_1 \ w_2 \ \frac{\partial w_2}{\partial x} \ \beta_2 \rangle$.

$$\begin{cases} \langle \mathbf{N}_w \rangle = \left\langle \frac{(1-\xi)^2(2+\xi)}{4} \ \frac{L_e(1-\xi^2)(1-\xi)}{8} \ 0 \ \frac{(1+\xi)^2(2-\xi)}{4} \ \frac{L_e(-1+\xi^2)(1+\xi)}{8} \ 0 \right\rangle, \\ \langle \mathbf{N}_\beta \rangle = \left\langle 0 \ 0 \ \frac{1-\xi}{2} \ 0 \ 0 \ \frac{1+\xi}{2} \right\rangle. \end{cases} \quad (35)$$

The field of Lagrange multipliers is the same as the displacement field of 1D sandwich model:

$$\begin{cases} \lambda_u^t = \left(-\left(z - \frac{H_1}{2}\right) \langle \mathbf{N}_{w,x} \rangle + \frac{H_1}{2} \langle \mathbf{N}_\beta \rangle \right) \{ \lambda_e \}, \\ \lambda_u^m = z \langle \mathbf{N}_\beta \rangle \{ \lambda_e \}, \\ \lambda_u^b = \left(-\left(z + \frac{H_1}{2}\right) \langle \mathbf{N}_{w,x} \rangle - \frac{H_1}{2} \langle \mathbf{N}_\beta \rangle \right) \{ \lambda_e \}, \\ \lambda_w = \langle \mathbf{N}_w \rangle \{ \lambda_e \}, \end{cases} \quad (36)$$

where λ_u and λ_w are the longitudinal and transversal Lagrange multipliers, and λ_e is the element unknowns.

As only the longitudinal normal strain and stress under consideration, $\mathcal{K}_{1D}$, $\mathcal{K}_{2D}$, $\mathcal{F}_{1D}$ and $\mathcal{F}_{2D}$ which denote the element stiffness matrices and external force vectors of 1D and 2D sandwich element individually can be calculated easily by introducing the energy partition functions α_c and β_c . Besides, by introducing the coupling operator H_p^1 proposed by Hu et al. [25], the element coupling matrices can be calculated as: