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An optimization procedure for material parameter identification for masonry constitutive models

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Abstract

Constitutive models for masonry require a number of parameters to define material behaviour with sufficient accuracy. It is common practice to determine such material parameters from the results of various, relatively simple, small-scale laboratory experiments. However, the effectiveness of determining material parameters that are representative of masonry from small-scale experiments have found to be problematic. This paper investigates the material parameter identification problem for masonry constitutive models. The methodology is based on an inverse analysis containing an optimization procedure and surrogate modelling. The general framework of the non-linear estimate methodology and the parameter identification problems are discussed.

Keywords: *Numerical modelling, material parameter identification, masonry, non-linear analysis*

1 Introduction

Masonry is the oldest material used in construction and has proven to be both simple to build and durable. Although its simplicity of construction, the analysis of masonry is a challenging task. Masonry is an anisotropic, heterogeneous and composite material where mortar joints act as plane of weakens. The need to predict the in-service behaviour and load carrying capacity of masonry structures has led researchers to develop several numerical methods and computational tools which are characterized by their different levels of complexity. For a numerical model to adequately represent the behaviour of a real structure, both the constitutive model and the input material properties must be selected carefully by the modeller to take into account the variation of masonry properties and the range of stress state types that exist in masonry structures (Hendry 1998.). It is often the case that material parameters are very sensitive to the mechanical behaviour of the structure and if not selected accurately can lead to over or under estimations (Sarhosis 2015). A broad range of numerical methods is available today ranging from the classical limit analysis methods (Heyman, 1998) to the most advanced non-linear computational formulations (e.g. finite element and discrete element methods of analysis). The selection of the most appropriate method to use depends on, among other factors, the structure under analysis; the level of accuracy and simplicity desired; the knowledge of the input properties in the model and the experimental data available; the amount of financial resources; time requirements and the experience of the modeller (Lourenço, 2002). It should also be expected that different methods should lead to different results depending on the adequacy of the approach and the information available. Preferably, the approach selected to model masonry should provide the desired information in a reliable manner within an acceptable degree of accuracy and with least cost. This paper investigates the material parameter identification problem for masonry and proposes an alternative methodology for obtaining material parameters for non-linear constitutive laws.

2 Conventional methods for material parameter identification

Conventionally, material parameters for masonry constitutive models are determined directly from the results of compressive, tensile and shear strength tests on small masonry prisms. These usually consist of assemblages of masonry consisting of a small number of bricks and mortar joints. It is usually assumed that the stress and strain fields in the specimen are uniform. In some other cases, separate tests are carried out on material samples, such as masonry units and/or mortar specimens (Rots, 1997; Van der Pluijm, 1999). The testing of small specimens is simple, relatively inexpensive and involves little specialist equipment. However, the conventional approach is considered to be problematic and may not produce material parameters that are representative of masonry. As identified by Hendry (1998), brick and mortar properties are highly variable and depend primarily on the local supply of raw materials and manufacturing methods. Also, the assumption that the stress and strain in the specimen are uniform is not applicable for masonry which is an intrinsically inhomogeneous material. Moreover, the simple conditions under which the small specimens are tested in the laboratory do not usually reflect the more complex boundary conditions, the combinations of stress-state types and load spreading effects that exist in a large scale masonry structure. In addition, some of the parameters obtained from small scale tests are variable and sensitive to the method of testing. This is likely to be due to the combined effects of eccentric loading, stress concentrations and variations in the resistance to applied stress that are likely to exist in the test specimens (Hendry, 1998). According to Vermeltfoort (1997), the effects of boundary conditions such as platen restraint and the shape and size of the test specimen can have a significant influence on the magnitude of the measured parameter. For example, a mortar joint between porous and absorbent masonry units will set, harden and cure in a different way to the same mortar used to form a cube in a steel mould. Also, the restraint conditions on the mortar in the cube test will be different to those existing in the mortar joint between masonry units. Thus, the compressive strength of mortar obtained from a mortar cube test is unlikely to represent the compressive strength of the mortar in between adjacent masonry units. The situation is made more complex when workmanship is considered. Usually a much higher standard and consistency of workmanship will be achieved by constructing small scale test specimens in the laboratory compared with the construction of larger scale masonry structures. Such variations in workmanship will not be captured if the material parameters are based on the results from the testing of small scale specimens. In addition, the use of field test results presents another set of difficulties. The stress and strain levels that are found in structures in the field are likely to be very low and affected by effects such as moisture movements, shrinkage and creep. Any material parameters determined from field measurements are unlikely to represent the behaviour of masonry in the post-cracking and near-collapse conditions. Other factors such as load spreading effects, residual thermal stresses in bricks, large inclusions sometimes found in bricks, etc all contribute to the uncertainty of material parameters obtained from small scale experiments. As a result of these difficulties it is often necessary to adjust the material parameter values obtained from small scale experiments before they can be used in the numerical model.

3 Proposed method for material parameter identification

From the above discussion it is evident that an alternative method of determining material parameters that better reflects the complex nature of masonry and the range of stress state types that exist in practice is worthy of further investigation. According to the proposed method, a numerical analysis for each large scale “non-trivial” experiment is carried out using an initial estimate of the material parameters. These initial values are “tuned” to minimise the difference between the responses measured from the large scale laboratory experiments and those obtained from the numerical simulation. It was envisaged that such tests would be carried out in the laboratory and the large scale structures selected for this purpose would be subjected to loading that would create a variety of different stress states. The responses measured in the laboratory would normally be deflections or distortions. An assumed range of material parameters is initially used in the model for the simulation of the large scale experiments. These initial material parameters could be based on the results obtained from conventional small-scale experiments, on values provided in codes of practice or from experience and engineering judgement. It should also be mentioned that the range of the selected material parameters should produce similar mechanical behaviour to that obtained from the large scale experiment. The selection of the range of material parameters is very important and will depend on the experience of the modeller. The material parameter identification problem can then be considered as an optimization problem in which the function to be minimized is an error function that expresses the difference between the responses measured from the large scale experiments and those obtained from the numerical analysis. Responses are based on the mechanical response of the masonry to be analyzed and can include: failure load, load at initial cracking, load-deflection characteristics, etc. The use of optimization software is essential for the evaluation of the approximation of responses as well as for the implementation of the optimization process. Once should be aware that the optimization procedure should provide a single set of material parameters (e.g. global minimum) that are representative for the case under investigation. The use of graphical illustrations of the solution in the form of response surface analysis is highly recommended.

The proposed method of material parameter identification is illustrated in Figure 1. The method was initially proposed by Toropov and Garrity (1998) and later expanded and validated for low strength masonry by Sarhosis & Sheng (2014).

The aim of the identification problem is to obtain the optimum estimate of the unknown model parameters taking into account uncertainties which may exist in the problem, such as the inherent variation of material properties, experimental errors and errors in the model estimation method. The estimates of the material parameters obtained from this approach could be referred to as the *"maximum likelihood estimates"* and can be used to *"inform"* the computational model. Sarhosis (2014) suggested that in order to account for the inherent variations in the materials and unavoidable variations in workmanship, for each of the large scale experiments at least three specimens should be tested. Also, it is important to note that the above method can be used for any constitutive model describing masonry as long as the constitutive model describes the mechanical behaviour of masonry with sufficient accuracy. It is anticipated that after undertaking a series of studies, an extensive library of material parameters can be obtained where one can download and use for the numerical simulation.

Examples showing studies for material parameter identification for large deformation plasticity models include: a) test data of a solid bar in torsion (Toropov et al., 1993) and b) test data for the cyclic bending of thin sheets (Yoshida et al., 1998). Later, Morbiducci (2003) applied the method to two different masonry problems in order to: a) identify the parameters of a non-linear interface model (Gambarotta et al., 1997a) to describe the shear behaviour of masonry joints under monotonic loading, where shear tests were chosen as the experimental tests; b) to evaluate the parameters of a continuum model for brick masonry walls under cyclic loading (Gambarotta et al., 1997b); and c) to evaluate the parameters of low bond strength masonry (Sarhosis 2014; Giamoundo et al. 2014). From the above studies, the following points have been observed and should be taken into consideration when using such method:

a) When modelling masonry, different material parameters influence different stages of mechanical behaviour;
b) large number of full scale experiments may be required; and
c) a significant amount of computational time is required to carry out parameter sensitivity studies.

4 Formulation of the material parameter identification problem

4.1 Formulation of the optimization problem

Consider an experimental test performed on $\mathcal{M} = 1,2,\dots,m$ specimens. Also, the design variables or unknown parameters to be estimated are $\mathcal{P} = 1,2,..,\mathrm{p}$ which form part of the constitutive model for the masonry material. Let's assume that $\mathcal{N} = 1,2,\dots n$ represents the number of responses that are recorded from the experimental data and are going to be compared with the numerical simulation. Also, let's consider the variable $\mathrm{R}_{n}^{\mathrm{exp}}$ to be the value of the n^{th} measured response which corresponds to the large scale experiment carried out in the laboratory. Consider $\mathrm{R}_{n}^{\mathrm{comp}}$ as the value of the n^{th} measured response quantity corresponding to the computational simulation. The model takes the general function form $x = \mathcal{R}(\mathcal{P})$. To calculate this function for the specific set of parameters, x, once has to use a non-linear numerical simulation, usually based on a discrete or finite element method of analysis. The intention is to simulate the mechanical behaviour of the experimental test under consideration. In this way, the difference between the experimental and the numerical responses can be obtained. This form an error function that can be expressed by the difference D=$\mathcal{R}_{\mathrm{M,N}}^{\mathrm{exp}} - \mathcal{R}_{\mathrm{M,N}}^{\mathrm{comp}}$.

The optimization problem can then be formulated as follows:-

$$\mathrm{F}_{(x)}^{1} = \sum\left[\left(\mathcal{R}_{1,1}^{\mathrm{exp}} - \mathcal{R}_{1,1}^{\mathrm{comp}}\right)^2 + \left(\mathcal{R}_{1,2}^{\mathrm{exp}} - \mathcal{R}_{1,2}^{\mathrm{comp}}\right)^2 \dots\dots + \left(\mathcal{R}_{1,\mathrm{n}}^{\mathrm{exp}} - \mathcal{R}_{1,\mathrm{n}}^{\mathrm{comp}}\right)^2\right] \tag{1}$$

$$\mathrm{F}_{(x)}^{2} = \sum\left[\left(\mathcal{R}_{2,1}^{\mathrm{exp}} - \mathcal{R}_{2,1}^{\mathrm{comp}}\right)^2 + \left(\mathcal{R}_{2,2}^{\mathrm{exp}} - \mathcal{R}_{2,2}^{\mathrm{comp}}\right)^2 \dots\dots + \left(\mathcal{R}_{2,\mathrm{n}}^{\mathrm{exp}} - \mathcal{R}_{2,\mathrm{n}}^{\mathrm{comp}}\right)^2\right] \tag{2}$$

$$\vdots$$

$$\mathrm{F}_{(x)}^{m} = \sum\left[\left(\mathcal{R}_{m,1}^{\mathrm{exp}} - \mathcal{R}_{m,1}^{\mathrm{comp}}\right)^2 + \left(\mathcal{R}_{m,2}^{\mathrm{exp}} - \mathcal{R}_{m,2}^{\mathrm{comp}}\right)^2 \dots\dots + \left(\mathcal{R}_{m,\mathrm{n}}^{\mathrm{exp}} - \mathcal{R}_{m,\mathrm{n}}^{\mathrm{comp}}\right)^2\right] \tag{3}$$

$F^{M}(\mathbf{x}) = \mathrm{F}_{(x)}^{1} + \mathrm{F}_{(x)}^{2} + \dots + \mathrm{F}_{(x)}^{m}$ is a dimensionless function. The problem is then to find the vector $\boldsymbol{x} = [x_1, x_2, x_3 \dots x_p]$ that minimizes the objective function:

$$\mathrm{F}_{(x)}^{\text{total}} = \sum \theta^{\mathcal{M}} (F^{M}(\mathbf{x})), \qquad A_i \leq X_i \leq B_i \qquad (i = 1 \ldots\ldots N) \tag{4}$$

where $\mathrm{F}_{(x)}^{\text{total}}$ is a function of the unknown parameters $(x_1, x_2, x_3 \ldots x_p)$, $\theta^{\mathcal{M}}$ is the weight coefficient which determines the relative contribution of information yielded by the M-th set of experimental data, and A_i, B_i are the lower and upper limits on the values of material parameters identified by physical considerations. The objective function is an implicit function of parameters x, where $x \in \mathbb{R}$. Also, once should expect that since a series of numerical simulations will be required, a considerable amount of computational time will result. Also, the optimization procedure may present some level of numerical noise. Since the computational simulations would involve an excessive amount of computational time to execute and convergence of the above method cannot be guaranteed due to the presence of noise in the objective function values, routine task analysis such as design optimization, design space exploration, sensitivity analysis and *what-if* analysis become impossible since they require thousands of simulation evaluations. One way to mitigate against such a burden is by constructing surrogate models (also referred to by some researchers as response surface models or metamodels). These mimic the behaviour of the model as closely as possible while at the same time they are time effective to evaluate (Queipo et al., 2005). Surrogate models are constructed based on modelling the response predicted from the computational model to a limited number of intelligently chosen data points. In the case that a single variable is involved, the process is known as curve fitting, see Figure 2. New combinations of parameter settings, not used in the original design, can be plugged into the approximate model to quickly estimate the response of that model without actually running it through the entire analysis. This approach can result in less computational iterations leading to substantial saving of computational resources and time.

Using this approach, the initial optimization problem, equation (4), is replaced with the succession of simpler mathematical programming sub-problems as follows:

Find the vector $\boldsymbol{x}_k^*$ that minimizes the objective function:

$$\tilde{F}_k(x) = \sum \theta^{\mathcal{M}} \tilde{F}_k^{M}(x), \quad A_i^k \leq X_i \leq B_i^k, \; A_i^k \geq A_i, B_i^k \leq B_i \quad (i = 1 \ldots\ldots N) \tag{5}$$

where k is the iteration number. The limits A_i^k and B_i^k define a sub-region of the optimization parameter space where the simplified functions $\tilde{F}_k^M(x)$ are considered as current approximations of the original implicit functions F^M(x). To estimate their accuracy, the error parameter $r_k = \left|[F(x_k^*) - \tilde{F}_k(x_k^*)]/F(x_k^*)\right|$ is evaluated. The value of the error parameter gives a measure of discrepancy between the values of the initial functions and the simplified ones. Any conventional optimization technique can be used to solve a sub-problem, equation (5), because the functions involved in its formulation are simple and noiseless.

4.2 Choice of the surrogate model

To construct the simplified noiseless expression for the function $\widetilde{F}_k^M(x)$ in equation (5), different methods of regression analysis can be used including the Least Squares Regression (LSR) method, the Moving Least Squares (MLS) method and the Hyper Kriging approach for building approximation models. The LSR and the MLS methods will be described for approximating noisy experimental results such as those obtained from the testing of masonry structures. Hyper Kriging is not considered further as it is suitable for modelling highly non-linear response data that does not contain numerical noise.

4.2.1 Least Squares Regression (LSR)

LSR is an approximation method which finds application in data fitting (Toropov et al., 2005). The best fit in the least squares sense minimizes the sum of the squared residuals i.e. the difference between an observed value and the fitted value provided by the model. Let N points located at positions x_i in $\mathbb{R}$ where $i \in [1 \dots N]$. We wish to obtain a globally defined function $f(x)$ that approximates the given scalar values f_i at points $\boldsymbol{x}_i$ in the least squares sense with the error function $r_{LS} = \sum_i \|f(\boldsymbol{x}_i) - f_i\|^2$. The following optimization problem can be obtained:

$$min \sum_i \|f(x_i) - f_i\|^2 \qquad (6)$$

, where f is taken from the polynomial basis vector and the vector of unknown coefficients to be minimized in equation (6).

4.2.2 Moving Least Squares (MLS)

MLS is an approximation building technique that is proposed for smoothing and interpolating data (Toropov et al., 2005). MLS is a generalisation of a conventional weighted least squares model building method. The main difference between MLS and LSR is that with MLS the weights associated with the individual experimental sampling points do not remain constant but are functions of the normalized distance from an experimental sampling point to a point x where the approximation model is evaluated. In the weighted least squares formulation, we use the error function $r_{WLS} = \sum_i W_i \|f(x_i) - f_i\|^2$ for a fixed point $\tilde{x} \in \mathbb{R}$, which we minimize:

$$min \sum_i W_i \|f(x_i) - f_i\|^2 \qquad (7)$$

The function is similar to equation (6) only that, now, the error is weighted by W_i. Many choices for the weighting function W_i have been proposed in the literature (Alexa et al., 2003). Equation 8 shows the Gaussian formulation:

$$W_i = e^{-\theta r_i^2} \qquad (8)$$

, where r_i are the Euclidian normalized distances from the $i - th$ sampling point to a current point. Also, the parameter θ refers to the "closeness of fit" and by varying its value we can directly influence the approximating/interpolating nature of the MLS fit function. A low value of θ leads to least squares smoothing (e.g. in the case where $\theta = 0$, then equation (7) is equivalent to the traditional least squares regression). Alternatively, when the parameter θ is large, it is possible to obtain a very close fit through the sampling points (i.e. interpolating), if desired. When the MLS method is used to approximate results obtained from experiments carried out on masonry structures, interpolation (i.e. a high value of θ) would not be appropriate, as there is a considerable amount of variation in the masonry material properties resulting in experimental noise.

4.3 Choice of the optimization method

In order to solve the sub-problem in equation (5), there are a number of available optimization methods to be used. Currently, a gradient-based method (known as Sequential Quadratic Programming) and a global search algorithm method (known as the Genetic Algorithm approach) are the two representative methods that can be used for the comparison of results (Toropov and Yoshida, 2005).

The Sequential Quadratic Programming (SQP) method is used for solving constrained optimization problems by creating linear approximations to the constraints (Toropov et al., 2010). The fundamental principle behind this method is to create a quadratic approximation of the Lagrangian function that combines the objective function with active constraints. The quadratic problem is then solved for the search direction avoiding any constraint violations. On the other hand, a Genetic Algorithm (GA) is a machine learning technique modelled after the evolutionary process theory. Genetic algorithms differ from conventional optimization techniques in that the work is based on a whole population of individual objects of finite length, typically binary strings (chromosomes), which encode candidate solutions $(x_1, x_2, x_3, \ldots, x_n)$ using a problem-specific representation scheme (Toropov et al., 2010). These strings are decoded and evaluated for their fitness, which is a measure of how good a particular solution is. Following Darwin's principle of "survival of the fittest" (or natural evolution), strings with higher fitness values have a higher probability of being selected for mating purposes to produce the next generation (i.e. new population created from current population) of candidate solutions (Toropov et al., 2010). Evolution is performed by breeding the population of individual designs over a number of generations. The advantages and the limitations of SQP and GA methods for solving optimization problems are shown in Tables 1 & 2.

Table 1 Sequential Quadratic Programming: Advantages and limitations

Advantages	**Limitations**
- Converges fast to a highly accurate solution when gradients are accurate; - There is no dramatic increase in	- As with any other gradient-based technique, SQP falls into the nearest local optimum so might need restarts from different points; - Converges poorly when gradients are

the number of iterations when the number of design variables grows.	inaccurate; - Deals with continuous problems. In the case of a discrete problem, the solution has to be discretised (e.g. rounding off); - As a sequential technique, parallelisation is only possible for getting gradients.

Table 2 Genetic Algorithm: Advantages and limitations

Advantages	**Limitations**
- More likely to find a non-local solution as it works with a population of sets of variables rather than a single set; - Can handle noise and occasional failure to compute responses; - As GA is a non-deterministic search method (it exhibits different behaviours on different runs), it makes the search highly robust; - Simplicity; - Can be easily parallelised; - Only requires the objective function and not the derivatives; - Allows both discrete and continuous (discretized) variables as it codes the variables rather than taking the variables themselves.	- High number of design iterations; - Lower accuracy compared with gradient based techniques for continuous problems; - Lack of indication as to how close the solution is to the optimum; - A few parameters need to be defined that affect the solution process.

5 Conclusion

A methodology for material parameter identification for nonlinear masonry constitutive laws has been proposed. Usually, the material parameters used for modelling masonry within computational models are based on the results of simple tests that do not reflect the more complex boundary conditions and combinations of stress-state types that exist in a real masonry structure. A method which is considered likely to determine more representative material parameters for masonry constitutive models has been proposed. This involves the computational analysis of large scale experimental tests on masonry structures. The initially assumed material parameters are tuned to minimize the difference between the responses measured from the large scale tests and those obtained from the computational simulations. The procedure has been successfully validated by (Sarhosis, 2014) when used to determine the material parameters for low bond strength masonry for a microscopic discrete element model. Both computational and experimental test data from a number of low bond strength brick masonry wall panels, each containing an opening to represent a large window, loaded at mid-span are used. Such wall panels were chosen as they contain regions of different types of stress when subjected to an externally applied load. In addition, the panels were considered to be sufficiently large to include inherent variations in the masonry materials and variations in workmanship. In the future, the effectiveness of the methodology is going to be applied to identify material parameters for macro-models.

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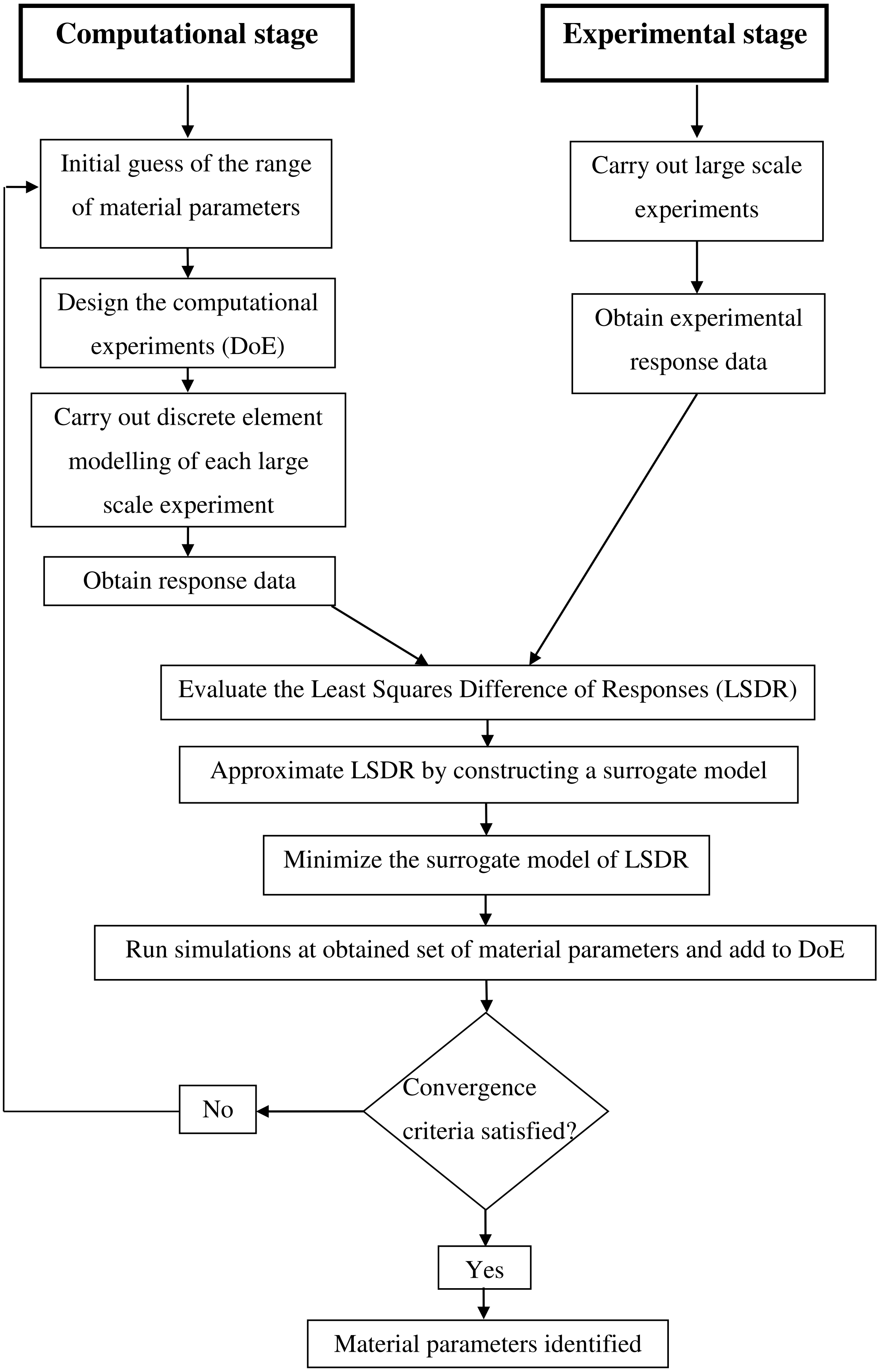

Figure 1 Proposed methodology for the identification of material parameters (Sarhosis 2014)

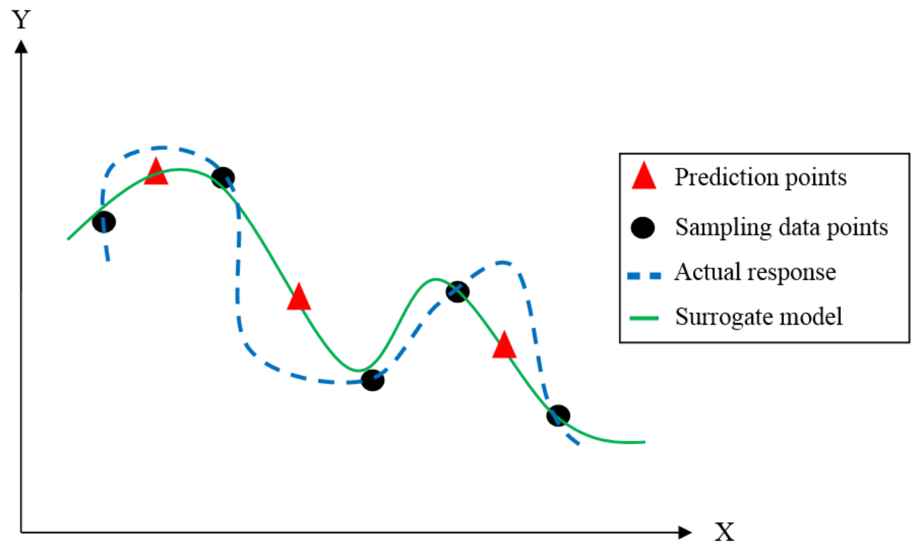

Figure 2 Curve fitting