Overall challenges in incorporating micro-mechanical models into materials design process

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Abstract. Using materials in engineering design has historically been handled using the paradigm of selecting appropriate materials from the finite set of available material databases. Recent trends, however, have moved toward the tailoring of materials that meet the overall system performance requirements, based on a process called material design. An important building block of this process is micromechanical models that relate microstructure to properties. Unfortunately, these models remain short and include a lot of uncertainties from assumptions and idealizations, which, unavoidably, impacts material design strategy. In this work, candidate methods to deal with micromechanical models uncertainties and their drawbacks in material design are investigated. Robust design methods for quantifying uncertainty and managing or mitigating its impact on design performances are reviewed first. These methods include principles for classifying uncertainty, mathematical techniques for evaluating its level degree, and design methods for performing and generating design alternatives, that are relatively insensitive to sources of uncertainty and flexible for admitting design changes or variations. The last section of this paper addresses the limits of the existing approaches from material modelling perspective and identifies the research opportunities to overcome the impediment of incorporating micromechanical models in material design process.

1. Introduction
Our innovation capabilities are tied strongly to our ability to engineer materials that meet requirements of novel product concepts. Indeed, the acceleration of material discovery is crucial for speeding up the advance of technology necessary to the design innovative products. The ultimate way to discover new materials is by the possibility of designing materials following desired functional requirement. A main goal of the field of materials design is the potential for tailoring materials from atomic scale to the system scale.

Historically, Engineering design has been taught using the paradigm of selecting materials on the basis of tabulated databases of properties [1]. Consequently, the performance of many engineering products and systems is limited fundamentally by the properties of available constituent materials. Obviously, to innovate one can no longer limit the performance of systems to available materials. Thus, the recent trends have moved toward concurrent design of material composition and microstructure together with the system level, to obtain materials with desired properties for particular applications and satisfying performance requirements on the system level. The goal is to tailor materials to meet specified ranges of performance requirements of the overall system. These...
performances are often in conflict when the microstructure is chosen. It is important to note, that these desired material properties and performance characteristics usually depend on phenomena that operate at different length and time scales. Material design is then built on a multi-scale journey from the smallest scale to the system level. One of the important multi-scale passages is the bridging of micro-scale to meso-scale through micromechanical models. These last models play a crucial role in the achievement of materials design initiative. These micromechanical models aim to predict accurately the response of a material under uniform load conditions from the properties of their constituents. The primary objective of this work is to emphasize a number of challenges related to integrating micromechanical models in material design process. These challenges are mainly associated to uncertainty due to idealization resulting from the lack of complete knowledge of microstructure and its description. In this respect, the key methods and approaches for dealing with this uncertainty were reviewed and critically evaluated from material modelling point view; first to identify their drawbacks and second to draw the research opportunities in this field.

2. Issues in integrating micromechanical model in material design process

Micromechanical models aim to predict accurately the response of a structure or device under service load conditions. Unfortunately, virtually all micromechanical models are embryonic from material design point view. It is important to emphasize that micro-mechanical models inevitably incorporate assumptions and approximations that impact the precision and accuracy of predictions. When added to the material design process, they bring their drawbacks and the uncertainty may be magnified when a model is utilized near the limits of its intended domain of applicability or when information propagates through a series of models [2]. Furthermore, microstructure itself has random character, such as sizes and distributions of grains, phases, and so forth. These sources of uncertainty give rise to the need to consider sensitivity of properties and responses of interest to variation of microstructure at various scales, as well as propagation of model uncertainty through multiscale model chains. So, one of the most important and challenging problems is the uncertainty in these models associated to various sources, including [3]:

- Insufficient knowledge about microstructure.
- Natural variability and randomness in materials (phases introduced by processing conditions) that are not taken into account.
- Ad-hoc parameters used by these models to presumably describe the microstructure.

![Figure 1. Hierarchy of levels from atomic scale to system level in concurrent materials design]({})

Uncertainty is endemic in most facets of micro-mechanical models, the uncertainty of microstructure models and model parameters impact significantly material design process. Consequently, a combined strategy of bottom-up and top-down modelling ‘figure 1’ to target
performance requirements will be very difficult [2,3]. In this respect, decreasing the uncertainty effect and partially managing its propagation through multi-scale models is of paramount importance. The only way to gain this goal is by having a good understanding of microstructure (approximations and simplifications), in order to let models be more realistic and transmit information without loss; by combining the approach with simulation tools, and finally by easing the decision design making.

A practical approach for accounting uncertainty involves many aspects [2,4]: quantify uncertainty to the extent possible and then mitigate uncertainty by seeking the robust solutions that are less sensitive to variation of microstructure and various other sources of uncertainty. Uncertainty quantification, propagation and management will be addressed in later sections of this paper.

3. Overview of the incumbent uncertainty managing approaches

In this section, a review of existing methods and approaches of the design process under uncertainty is presented; these methods comprise uncertainty quantification in engineering systems and uncertainty management methods.

3.1. Uncertainty quantification
3.1.1. Uncertainty classification.

The strategy and methods for quantifying uncertainty in engineering systems depend on the types of uncertainty, for that, it is necessary to categorize the types of uncertainty in a model. An understanding of these classifications is necessary to properly position the methods for design under uncertainty. There are two approaches to classify the types of uncertainty. One is classification according to the nature of uncertainty by Ayyub and Klir [5, 6], and the other is by the source of uncertainty by Der Kirurregian and others [7, 8, 9, 10]. The classification by source of uncertainty is the most widely adopted and in this case the uncertainty is split as either Aleatory (irreducible) or Epistemic (reducible) based on the causes of the uncertainty. Aleatory uncertainty is inherent in the physical system and can only be quantified in a statistical sense. Epistemic uncertainty, on the other hand, due to the lack of knowledge, which may results from idealizations (simplified relationships between inputs and outputs), approximations, or numerical errors. Examples include size of the representative volume element (RVE) of microstructure used to predict properties or responses. It can be diminished by improvements in measurements and model formulation or by increasing the accuracy or sample size of data.

3.1.2. Quantification of uncertainty.

In this section, several approaches for quantifying uncertainty will be reviewed; the uncertainty quantification is the process of identifying different sources of uncertainty and developing corresponding mathematical representations, by estimating output uncertainty (probability distribution of system response) with variability in input parameters [2]. One must mentioned that quantification of aleatory uncertainty is relatively easier than quantification of epistemic uncertainty if measuring system behaviour is feasible.

Depending on the types of uncertainty analysis methods, the types have been classified as non-probabilistic and probabilistic methods. The probabilistic methods are further devised on statistical and non-statistical approaches. Non-probabilistic methods include Interval Analysis and Fuzzy Logic methods, which are particularly useful when a system model is deterministic (there are no random errors in a system response) and input parameters are uncertain (without probability density functions due to lack of information). If a system model (computational model) is deterministic and input parameters are known as probabilistic density functions, then there are lots of techniques available in literature. If a system model is non-deterministic and input parameters are known as probability density functions then statistical methods for uncertainty analysis are also useful for uncertainty quantification. However, if a system model is non-deterministic and input parameters are uncertain, and then no existing method is applicable to uncertainty analysis. Existing uncertainty analysis methods depending on the characteristics of a system are presented in Table 1.
As discussed above, there are many available uncertainty analysis methods for deterministic system models; however, as shown in Table 1 uncertainty analysis methods for non-deterministic system models have not been developed in literature. Monte Carlo simulation is the only method for quantifying non-deterministic system response variation with the probability distributions of input parameters. If system behaviour is non-deterministic due to non-parametric input variation, it is impossible to quantify uncertainty by using statistical or non-statistical efficient uncertainty analysis methods. Uncertainty analysis for nondeterministic simulation is indispensable for multiscale materials design since the simulation models for heterogeneous material behaviour tend to be stochastic [4].

Table 1. Uncertainty analysis methods versus the characteristics of a system.

| System model | Deterministic | Non-deterministic |
|--------------|---------------|-------------------|
| Input        | Uncertain     | Probability       |
| Available    | Non-probabilistic | methods        |
| uncertainty  | Interval       | Statistical       |
| analysis     | analysis       | methods           |
| methods      | Fuzzy logic    | Monte Carlo       |
|              | Probabilistic  | simulation        |
|              | methods        | Latin Hypercube   |
|              |                | sampling          |
|              |                | -Non- statistical |
|              | methods        | First and second  |
|              |                | order moment      |
|              | methods        | methods           |
|              |                | Polynomial chaos  |
|              | methods        | expansion          |
|              |                | Stochastic response|
|              | methods        | surface methods   |

As mentioned the Aleatory system uncertainty is quantifiable; however, epistemic uncertainty that arises from incomplete knowledge of a system is virtually impossible to quantify [2]. Therefore, reducing uncertainty (instead of being quantified) is feasible when designer has large amounts of data and by increasing the knowledge or getting more information about system. Instead, researchers [11, 12, 13, 14] have focused on procedures to reduce uncertainty and validate a model’s accuracy. However, the restriction of these methods is that designers must have some true results. In some cases, we cannot obtain any better data than current data due to severe uncertainty in a system or restrictions of computational or experimental expenses, which is the case of multiscale materials design specially micromechanical model.

3.2. Uncertainty management
3.2.1. Robust Design.

Uncertainty management refers to reducing the uncertainty effect on systems design. Several techniques have been performed to achieve target system performance in the presence of uncertainty such as robust design and reliability based design and optimization (RBDO). Robust design techniques aimed to minimize the effects of uncertainty on system performance [15], while reliability-based design optimization techniques are based on finding optimized designs characterized by low probability of failure [16]. The robust design is approach for managing uncertainties; it’s allowed to design a system to be insensitive to uncertainty without eliminating or reducing its sources in the system.

There are several categories of robust design that deal with different types of uncertainty. Type I robust design, originally proposed by Taguchi [17], focuses on achieving insensitivity of performance
with respect to noise factors—parameters that designers cannot control in a system. Type II robust design [18] relates to insensitivity of a design to variability or uncertainty associated with design variables—parameters that a designer can control in a system. A method for types I and II has been proposed, namely the Robust Concept Exploration Method [19]. These types of robust design have been extended to include Type III [4], which considers sensitivity to uncertainty embedded within a model (model parameter/structure uncertainty).

As illustrated in ‘Figure 2’, type III Robust Design Considers not only the objective function but also the two uncertainty limits due to the non-parametric variability, un-configured variability, and model parameter uncertainty, the optimal and Type I and II robust solution have larger performance deviations than the Type I, II, and III robust solution. The most accurate way to incorporate the embedded uncertainties as well as the uncertainty in control and noise factors during design exploration is to perform actual simulation using statistical techniques. Monte Carlo Simulation is a popular method to measure variations of performance by simulating input variations (uncertainty analysis). Even though this approach could produce accurate results in design exploration; it requires a large number of experiments for uncertainty analysis even in a single evaluation during a design exploration process. It is nearly impossible to employ this approach in materials design exploration even if a sampling technique have been applied, such as Latin Hypercube sampling, to reduce number of experiments. So the computationally inexpensive uncertainty analysis method is necessary to solve this problem.

3.2.2. Robust design of multidisciplinary systems

There are many techniques for multi-level deterministic optimization which taken account the uncertainty. An example; the Analytical Target Cascading (ATC) approach [20]. ATC is an approach for cascading overall system design targets to sub-system specifications based on an hierarchical multi-level decomposition [20]. The subsystem design problems are formulated as minimum deviation optimization problems and the outputs of the subsystem problems are used as inputs to the system-level problem. This approach eliminates bottom-up uncertainty propagation though a multi-level chain since the problem is decomposed and design exploration is executed only at each level, also the super-level iteration must wait for the results of sub-level optimization; therefore, multi-level optimizations are highly interdependent and cannot be parallelized.

To have the possibility to parallelize the bottom-up simulations and to identify candidate ranged solutions that must be selected in the context of a top-down strategy in the design system, an iterative approach is essential for bottom-up information flow (simulations, experiments), combined with top down guidance from applications performance requirements. Choi et al. [21, 22] have developed an
approach called the Inductive Design Exploration Method (IDEM), schematically shown in Figure 3. IDEM [22,23] has two major objectives: (1) to explore top–down, requirements driven design, guiding bottom–up modeling and simulation, and (2) to manage uncertainty in model chains. It’s based on three steps:

- **Step 1:** It is necessary to define the rough design space (x space in ‘Figure 3’), the interdependent space (y space), and the performance space (z spaces). Discrete points are generated in each of these spaces (Discretizing).

- **Step 2:** The discrete points which are generated are evaluated based on the mapping models (models f and g in ‘Figure 3’) and the evaluated data sets which are composed of a discrete input point and output range are stored in a database.

- **Step 3:** Feasible regions in y and x spaces are sequentially identified, along with a given final performance range in z space. We call this step Inductive Discrete Constraints Evaluation (IDCE).

![Figure 3. A schematic of steps 1 and 2 in IDEM [1].](image)
4. Critical evaluation of uncertainty managing approaches from material modelling perspective

After presenting an overview of available methods and approaches of the design under uncertainty process, the capabilities of those methods and approaches are critically evaluated from material multiscale modelling perspective. Then, the research opportunities in this field are discussed, in order to develop new perspective for overcoming the shortness of present approaches.

The table 2 summarizes all the gaps among the management taxonomy of uncertainty including quantification and mitigation uncertainty discussed above.

Table 2. Summary of critical evaluation of the reviewed approaches and methods.

| Issues                                    | Approach                          | Limits                                                                 |
|-------------------------------------------|-----------------------------------|------------------------------------------------------------------------|
| Classification of uncertainty             | Classification by the nature of uncertainty | The classification is difficult to incorporate with mathematical modelling in systems design |
|                                           | Classification by the sources of uncertainty | There are disagreements among the researchers for defining types of uncertainty. None of the reviewed approaches studied explicitly the type of uncertainty in computational models that predict material behaviours. |
| Analysis and quantification of uncertainty| Existing methods for uncertainty analysis (Interval analysis, Monte Carlo method, etc.) | Uncertainty analysis methods for nondeterministic system models have not been developed in literature except for Monte Carlo (MC) method. The MC method is computationally intensive to apply into materials design |
|                                           | Methods for reducing uncertainty   | Designers must have some true results. In some cases, we cannot obtain any better data than current data due to severe uncertainty in a system or restrictions of computational or experimental expenses, which is the case of multiscale materials design |
| Robust design under uncertainty           | Type I robust design (Taguchi method), Suh’s Axiomatic design | Type I robust design is not valid if noise factors cannot be quantified as numeric parameters or quantitative levels. However, the types of uncertainty in materials design problem tend to be unparameterizable. |
|                                           | Type II robust design (RCEM)       | No study has been done for establishing robust design methods for designing a system to be insensitive to uncertainty and unquantifiable variability (such as morphology changes in materials) in a system model. |
|                                           | Type III robust design             | Any computationally inexpensive uncertainty analysis method have been developed for this approach |
| Robust design of multidisciplinary systems | Analytical Target Cascading (ATC)  | Eliminates bottom-up uncertainty propagation though a multi-level chain since the problem is decomposed and design exploration is executed only at each level. Multi-level optimizations are highly interdependent and cannot be parallelized (the super-level iteration must wait for the results of sub-level optimization). |
|                                           | Inductive exploration design method (IDEM) | It cannot be overcome the uncertainty in material models due to idealization associated with a lack of complete knowledge of a given microstructure and its description. May be computationally intensive if the number of design variables is large or the simulation model is |
expensive.

The problem of uncertainty in material design process has been widely studied, but the main conclusion to be drawn is that none of the outlined approaches for mitigation uncertainty had satisfactory results to deal with this endemic uncertainty in constitutive models, which are used to represent behavior especially in micromechanical modeling, that why the improvement of the accuracy of these models and facilitate their incorporating in material design process is our primary proposes. In this perspective, new approach for modeling micromechanical models has to be carried out, which will be able to gather between homogenization requirements and between material design exigencies.

5. Closure
The main issues in integrating micromechanical models in material design process were investigated. This investigation was mainly based on the uncertainty characterization and quantification in these models and the robust design under uncertainty. Each of these issues has been studied rigorously. We, also, reviewed the literature related to these issues and we critically evaluate existing methods dealing with uncertainty; first to identify their drawbacks and second to clarify the research opportunities in this field. The principal conclusion is that, up to now, there is no approach to deal with uncertainty in micromechanical models, due to idealization resulting from the lack of complete knowledge of microstructure and its description. As a perspective, we aim to develop a robust material design perspective framework for developing efficient micromechanical models.

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