Key computational modeling issues in Integrated Computational Materials Engineering

Jitesh H. Panchal\textsuperscript{a}, Surya R. Kalidindi\textsuperscript{b}, David L. McDowell\textsuperscript{c,*}

\textsuperscript{a} School of Mechanical and Materials Engineering, Washington State University, Pullman, WA 99164-2920, USA
\textsuperscript{b} Department of Materials Science and Engineering, Department of Mechanical Engineering and Mechanics, Drexel University, Philadelphia, PA 19104, USA
\textsuperscript{c} School of Materials Science and Engineering, Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA 30332-0405, USA

\textbf{A R T I C L E I N F O}

Keywords:
Materials design
Multiscale modeling
ICME
Databases
Uncertainty

\textbf{A B S T R A C T}

Designing materials for targeted performance requirements as required in Integrated Computational Materials Engineering (ICME) demands a combined strategy of bottom–up and top–down modeling and simulation which treats various levels of hierarchical material structure as a mathematical representation, with infusion of systems engineering and informatics to deal with differing model degrees of freedom and uncertainty. Moreover, with time, the classical materials selection approach is becoming generalized to address concurrent design of microstructure or mesostructure to satisfy product-level performance requirements. Computational materials science and multiscale mechanics models play key roles in evaluating performance metrics necessary to support materials design. The interplay of systems-based design of materials with multiscale modeling methodologies is at the core of materials design. In high performance alloys and composite materials, maximum performance is often achieved within a relatively narrow window of process path and resulting microstructures.

Much of the attention to ICME in the materials community has focused on the role of generating and representing data, including methods for characterization and digital representation of microstructure, as well as databases and model integration. On the other hand, the computational mechanics of materials and multidisciplinary design optimization communities are grappling with many fundamental issues related to stochasticity of processes and uncertainty of data, models, and multiscale modeling chains in decision-based design. This paper explores computational and information aspects of design of materials with hierarchical microstructures and identifies key underdeveloped elements essential to supporting ICME. One of the messages of this overview paper is that ICME is not simply an assemblage of existing tools, for such tools do not have natural interfaces to material structure nor are they framed in a way that quantifies sources of uncertainty and manages uncertainty in representing physical phenomena to support decision-based design.

\textsuperscript{*} Corresponding author. Tel.: +1 404 894 5128; fax: +1 404 894 0186.
E-mail address: david.mcdowell@me.gatech.edu (D.L. McDowell).

© 2012 Elsevier Ltd. All rights reserved.

1. The path to Integrated Computational Materials Engineering (ICME)

Within the past decade, several prominent streams of research and development have emerged regarding integrated design of materials and products. One involves selection of materials, emphasizing population of databases and efficient search algorithms for properties or responses that best suit a set of specified performance indices [1], often using combinatorial search methods [2], pattern recognition, and so on. In such materials informatics approaches, attention is focused on data mining, visualization, and providing convenient and powerful interfaces for the designer to support materials selection. Another class of approaches advocates simulation-based design to exploit computational materials science and physics in accelerating the discovery of new materials, computing structure and properties using a bottom–up approach. This can be combined with materials informatics. For example, the vision for Materials Cyber-Models for Engineering is a computational materials physics and chemistry perspective [3] on using quantum and molecular modeling tools to explore for new materials and compounds, making the link to properties. Examples include the computational estimate of stable structure and properties of multicomponent phases using first principles approaches (e.g., Refs. [4–6]). These approaches have been developed and popularized largely within the context of the materials chemistry, physics and science communities.

A third approach, involving more the integration of databases with tools for modeling and simulation, as well as design...
optimization and concurrent design for manufacture, is that of Integrated Computational Materials Engineering (ICME). It is concerned with multiple levels of structure hierarchy typical of materials with microstructure. ICME aims to reduce the time to market of innovative products by exploiting concurrent design and development of material, product, and process/manufacturing path, as described in the National Research Council report by a National Materials Advisory Board (NMAB) committee [7]. It is “an approach to design products, the materials that comprise them, and their associated materials processing methods by linking materials models at multiple length scales”.

ICME was preceded by another major Defense Advanced Research Projects Agency (DARPA)-funded initiative, Accelerated Insertion of Materials (AIM), from 2001–2003, which sought to build systems approaches to accelerate the insertion of new and/or improved materials into products. An NMAB study [8] discussed the DARPA-AIM program, highlighting the role of small technology startup companies in enabling this technology, and summarizing the commercial computational tools and supporting currently available databases. The impact of AIM on framing of ICME is discussed further in Ref. [9].

The significant distinction of ICME from the first two approaches (materials informatics and combinatorial searches for atomic/molecular structures) is its embrace of the engineering perspective of a top–down, goal–means strategy elucidated by Olson [10]. This perspective was embraced and refined for the academic and industry/government research communities at a 1997 National Science Foundation (NSF)-sponsored workshop hosted by the Georgia Institute of Technology and Morehouse College [11] on Materials Design Science and Engineering (MDS&E). Effectively, ICME incorporates informatics and combinatorics, as well as multiscale modeling and experiments. As mentioned, ICME is fully cognizant of the important role that microstructure plays in tailoring material properties/responses in most engineering applications, well beyond the atomic or molecular scale. This is a key concept in materials science, as typically distinct from materials physics or chemistry. For example, mechanical properties depend not only on atomic bonding and atomic/molecular structure, but are strongly influenced by morphology of multiple phases, phase and interface strengthening, etc. Fig. 1 shows a hierarchy of material length scales of atomic structure and microstructure that can be considered in design of advanced metallic alloys for aircraft gas turbine engine components in commercial aircraft. The diagram inset in the upper-left in Fig. 1 shows the Venn diagram from Olson [10] of overlapping process–structure–property–performance relations that are foundational to design of materials to the left of the vertical bar; conventional engineering design methods and multidisciplinary design optimization (MDO) are rather well established. Extending systems design methods down to address the concurrent design of material structure at various levels of hierarchy is a substantial challenge [12–15]. The process of tailoring the material to deliver application-dependent performance requirements is quite distinct from that of traditional materials selection (relating properties to performance requirements) or from combinatorial searching for atomic/molecular structure–property relations at the level of individual phases; such combinatorial searches typically do not consider the role of microstructure, which is typically central to meeting multifunctional performance requirements. The conventional approach in science-based modeling of hierarchical systems is a bottom–up, deductive methodology of modeling the material’s process path, microstructure, and resulting properties, with properties then related to performance requirements, as shown in Fig. 1. Design is a top–down process in which systems level requirements drive properties, structure and process routes.

The pervasive difficulty in inverting process–structure and structure–property relations in modeling and simulation greatly complicates this top–down enterprise, and owes to certain unavoidable realities of material systems:

- Nonlinear, nonequilibrium path dependent behavior that requires intensive simulation effort, limiting parametric study and imparting dependence upon initial conditions.
- Transitions from dynamic (lower length and time scales) to thermodynamic (higher length and time scales) models for cooperative phenomena in multiscale modeling, with non-uniqueness due to reduction of model degrees of freedom during scale-up.
- Potential for a wide range of suboptimal solutions that complicate design search and optimization.
of the bold dashed line to microstructure issues. Clearly, microstructure is solidly at this interface, the result of process–structure relations. Hence, framing ICME in terms of microstructure-mediated design facilitates enhanced concurrency of material suppliers and OEM activities. Another important goal of ICME should be to effectively remove the bold dashed line to the right in Fig. 2 that serves as a “fence” between materials development and materials selection.

- Approximations made in digital microstructure representation of material structure.
- Dependence of certain properties such as true fracture ductility, fracture toughness, fatigue strength, etc., on extreme value distributions of microstructure attributes that affect damage/degradation.
- Microstructure metastability and long term evolution in service.
- Lack and variability of experimental data for validation purposes or to support methods based on pattern recognition.
- Uncertainty of microstructure, models, and model parameters.

Since uncertainty is endemic in most facets of ICME, managing uncertainty and its propagation through model/experiment chains is of paramount importance. Materials design is complicated by the complexity of nonlinear phenomena and pervasive uncertainty in materials processing, related models and model parameters, for example. This motivates the notion of robust design and other means to address the role of uncertainty. The materials design challenge is to develop methods that employ bottom-up modeling and simulation, calibrated and validated by characterization and measurement to the extent possible, combined with top–down, requirements-driven exploration of the hierarchy of material length scales shown in Fig. 1. It is a multi-level engineering systems design problem, characterized by top–down design of systems with successive embedded sub-systems, such as the aircraft shown in Fig. 1. Multiscale modeling pertains more to the bottom–up consideration of scales of materials hierarchy.

Another critical aspect of materials design identified in the NMAICME report [7] is the key role played by quantitative representation of microstructure. The notion of microstructure-mediated design is predicated on the use of mathematical/digital representation of microstructure, rather than properties, as the taxonomic basis for describing material structure hierarchy in materials design. This is not merely semantics, but has quite practical implications in terms of actual pathways of material and product development. Specifically, process–structure relations tend to be quite dissociated from structure–property relations, with different model developers, organizations involved, degree of empiricism, etc. The timeframe for process–structure relations in materials development often do not match those of structure–property relations. Process–structure relations tend to be more highly empirical, complex, and less developed than structure–property relations. The light dashed line on the left in Fig. 2 effectively represents a “fence” between organizations/groups pursuing process–structure and structure–property relations, reflecting the common decomposition of activities between material suppliers and OEMs. One goal of an integrated systems strategy for materials design and development is to more closely couple these activities. Clearly, microstructure is solidly at this interface, the result of process–structure relations. Hence, framing ICME in terms of microstructure-mediated design facilitates enhanced concurrency of material suppliers and OEM activities. Another important goal of ICME should be to effectively remove the bold dashed line to the right in Fig. 2 that serves as a “fence” between materials development and materials selection. Conventionally, design engineers have worked with databases of existing materials to select, rather than design, materials in the process of designing components (systems, sub-systems). Tools for materials selection [1] are reasonably well-developed, supporting the materials selection problem. However, as discussed by McDowell et al. [12–15], materials selection supports the property–performance linkage to the right in Fig. 2 and is just one component of the overall integration of materials and product design. Integration of design engineering into the overall process requires a coupling back to material suppliers, for example. This is one of the great challenges to realizing ICME in terms of concurrent computational materials design and manufacturing. As stated in the report of the 1998 MDS&E workshop [11], “The field of materials design is entrepreneurial in nature, similar to such areas as microelectronic devices or software. MDS&E may very well spawn a “cottage industry” specializing in tailoring materials for function, depending on how responsive large supplier industries can be to this demand. In fact, this is already underway”.

The ICME report [7] focused mainly on advances in modeling and simulation, the role of experiments in validation, databases and microstructure representation, and design integration tools. In addition, cultural barriers to ICME in industry, government and academia were discussed. Elements of ICME broadly encompass:

- Modeling and simulation across multiple levels of hierarchy of structure, including both process–structure and structure–property relations
- Experiments and prototyping
- Distributed collaborative networks
- Materials databases
- Microstructure representation as the focus of the materials design problem
- Knowledge framework that integrates databases with experiments and modeling simulation to pursue inverse design
- Uncertainty quantification and management
- Integration with OEMs and materials suppliers.

The Materials Genome Initiative aspires to build on the preceding AIM and ICME initiatives to develop an infrastructure to accelerate advanced materials discovery and deployment, including all phases of development, property optimization, systems design and integration, certification and manufacturing [16]. As outlined in Refs. [7,15], this goal and the premise of ICME is more comprehensive in addressing the connection with product design and manufacturing than combinatorial searching algorithms applied using first principles calculations to discover new materials or multicomponent phases, for example. The notion of genomics as predictive exploration of crystal structures, single phases, or molecules for desirable phase properties is a valuable part of the overall concept of ICME to more broadly scope design exploration, but the “connective tissue” of multiscale modeling and multi-level decision-based design in ICME are essential aspects of its integrative character that links microstructure to performance and considers integrated systems design, certification, manufacturing, and
product scale-up. Moreover, the analogy of ICME to bioinformatics, DNA sequencing and so forth is therefore limited and not fully descriptive of scope and challenges of ICME. In our view, the notion of integrating manufacturing processes with concurrent design of materials and products is at the core of ICME, considering the inescapable role of the hierarchy of material structure (i.e., microstructure) on properties and performance. Of course, one can conceive of important application domains in which discovery of new material phases, perhaps addresses the majority of the accelerated deployment problem; it may be entirely sufficient for purposes of searching for specific molecular or atomic structures for nanoscale application such as quantum dots, semiconductors, etc. But even in many applications where certain key performance indicators are dictated by atomic structure (e.g., piezoelectrics, battery and fuel cell electrodes, etc.), material durability and utility in service is often dictated by mesoscopic heterogeneity of structure and its lack of reversibility under cycling or in extreme environments. Therefore, materials informatics is a key technology for nanoscale design problems but only one toolset in the solution strategy for multi-level material design that must consider scale-up and long term product performance. This paper will focus on several critical path issues in realizing ICME, namely materials databases, the role of multiscale modeling, materials knowledge systems and strategies that support inverse design (top–down in Fig. 1), and uncertainty quantification and management considerations that undergird plausible approaches.

2. Materials databases and the need for a structure-based taxonomy

The NMAE report [7] has emphasized the key role of materials databases in capturing, curating, and archiving the critical information needed to facilitate ICME. While the report does not elaborate on how these databases should be structured or what specifically they should include, it discusses how these new databases will produce substantial savings by accelerating the development of advanced high performance materials, while eliminating the unintended repetition of effort from multiple groups of researchers possibly over multiple generations.

Before we contemplate on the ideal structure and content of such novel databases, it would be beneficial to get a historic perspective on the successes and failures of the prior efforts on building materials databases. In a recent summary, Freiman et al. [17] discuss the lessons learned from building and maintaining the National Materials Property Data Network that was operated commercially until 1995. Although this network contained numerous databases on many different materials, it proved too costly to maintain because of (i) a lack of a common standard for information on the very broad range of materials included in the database, (ii) enhancements/modifications to testing procedures used for evaluating properties of interest that sometimes invalidated previous measurements, and (iii) the placement of onus on a single entity as opposed to being jointly developed by multiple entities that possess the broad range of requisite sophisticated skill sets. Notwithstanding these shortcomings, a major deficiency in these, as well as other similar, databases is that they did not aim to capture the attributes of the microstructure. It is well-known in the materials science and engineering discipline that the microstructure–property connections are not unique, and that composition alone is inadequate to correlate to the many physical properties of the material. Indeed, the spatial arrangement of local features or “states” in the internal structure (e.g., morphological attributes) at various constituent length scales play an influential role in determining the overall properties of the material [18–20].

The key materials databases needed to facilitate ICME have to be built around microstructure information. There is therefore a critical need to establish a comprehensive framework for a rigorous quantification of microstructure in a large number of disparate material systems. Furthermore, the framework has to be sufficiently versatile to allow compact representation and visualization of the salient microstructure–property–processing correlations, which populate the core knowledge bases used by materials designers. It is important to recognize here that only the microstructure space can serve as the common higher dimensional space in which the much needed knowledge of the process–microstructure–property correlations can be stored and communicated reliably without appreciable loss of information. Any attempt to represent this core knowledge by circumventing microstructure using lower dimensional spaces (e.g., processing–property correlations or composition–property correlations) should be expected to result in substantial loss of fidelity and utility in the generated knowledge bases.

In arriving at a rigorous framework for microstructure quantification, it is extremely important to recognize and understand the difference between a micrograph (or a microstructure dataset) and the microstructure function [21]. Microstructure function is best interpreted as a stochastic process, in essence a response to applied stimuli, whose experimental outcome is a micrograph (a two or three dimension microstructure dataset). As such, the microstructure function cannot be observed directly and is expected to capture the ensemble-averaged structure information from a multitude of micrographs extracted from multiple samples processed by nominally the same manufacturing history. Since individual micrographs have no natural origin, the only meaningful information one can extract from each micrograph has to be concerned with the relative spatial arrangement or spatial correlations of local material states (e.g., phases, orientations) in the structure. A number of different measures of the spatial correlations in the microstructure have been proposed and utilized in literature [19,20]. Of these, only the n-point spatial correlations (or n-point statistics) provides the most complete set of measures that are naturally organized according to increasing degree of microstructure information. For example, the most basic of the n-point statistics are the 1-point statistics, and they reflect the probability density associated with finding a specific local state of interest at any randomly selected single point (or voxel) in the microstructure. In other words, they essentially capture the information on volume fractions of the various distinct local states present in the material system. The next higher level of microstructure information is contained in the 2-point statistics, denoted \( c_{hh'} \), which capture the probability density associated with finding local states \( h \) and \( h' \) at the tail and head, respectively, of a prescribed vector, \( r \), randomly placed into the microstructure. There is a tremendous increase in the amount of microstructure information contained in the 2-point statistics compared to the 1-point statistics. Higher-order correlations (3-point and higher) are defined in a completely analogous manner. Another benefit of treating the microstructure function as a stochastic process is the associated rigorous quantification of the variance associated with the microstructure [21]. The variance in structure can then be combined appropriately with the other uncertainties in the process (for example, those associated with the measurements and those associated with the models used to predict overall properties or performance characteristics of interest in an engineering application) to arrive at the overall variance in the performance characteristics or responses of interest.

Materials Informatics has recently emerged as a new field of study that focuses on the development of new toolkits for efficient synthesis of the core knowledge in large materials datasets (generated by both experiments and models). The NMAE report [7] has specifically highlighted the important role to be played by Materials Informatics in the realization of the potential of ICME. The standardization and adoption of a rigorous framework, such as the
n-point statistics, in enabling the quantification of the microstructure is a critical and essential step in the emergence of Materials Informatics. In recent work, it was demonstrated that the use of concepts borrowed from informatics can produce a new toolkit [22] with the following unprecedented capabilities: (i) archival, real-time searches, and direct quantitative comparisons of different microstructure datasets within a large microstructure database, (ii) automatic identification and extraction of microstructure features or other metrics of interest from very large datasets, (iii) establishment of reliable microstructure–property correlations using objective measures of the microstructure, and (iv) reliable extraction of precise quantitative insights on how the local neighborhood influences the localization of macroscale loading and/or the local evolution of microstructure leading to development of robust, scale-bridging, microstructure–property–processing linkages. The new field of Materials Informatics is still very much in its embryonic stage of development. The customization and adoption of modern information technology tools such as image-based search engines, data-mining, machine learning and crowd-sourcing can potentially identify completely new research directions for addressing successfully some of the most difficult computational challenges in the implementation of the ICME paradigm.

3. Multiscale modeling and materials design

Multiscale modeling involves seeking solutions to physical problems that have important features at multiple spatial and/or temporal scales. Multiscale models are necessary to address the relative contributions of various levels of material structure hierarchy shown in Fig. 1 to responses at higher scales [12–15, 23–25]. However, multiscale models are subervient to the overall design integration strategy in materials design. In other words, they offer utility in various specific ways to materials design, including, but not limited to:

- relating polycrystalline and/or polyphase microstructures to properties involving cooperative behavior at higher scales (e.g., yield strength, ductility, ductile fracture, etc.),
- quantifying sensitivity of higher scale responses to different mechanisms and levels of structure/microstructure hierarchy,
- supporting microstructure-sensitive prediction of material failure or degradation,
- quantifying the influence of environment or complicating contributions of impurities, manufacturing induced variability or defects,
- considering competition of distinct mechanical, chemical and transport phenomena without relying too heavily on intuition to guide solutions in the case of highly nonlinear interactions, and
- bridging domains of quantum physics and chemistry with engineering for problems that span vast ranges of length and time scales.

Olson’s Venn diagram structure in Fig. 1 should not be confused with multiscale modeling strategies; the former is much more comprehensive in scope, embedding multiscale modeling as part of the suite of modeling and simulation tools that provide decision-support in design. For example, structure–property relations can involve the full gamut of length and time scales, as can process—structure relations. In other words, the levels in Olson’s linear design strategy of Fig. 1 do not map uniquely to levels of material hierarchy. Even concurrent multiscale models which attempt to simultaneously execute models at different levels of resolution or fidelity do not serve the full purpose of top–down materials design. Materials design and multiscale modeling are not equivalent pursuits. This distinction is important because it means that notions of cyberdiscovery of new or improved materials must emphasize not only modeling and simulation tools but also systems design strategies for using simulations to support decision-based concurrent design of materials and products.

Materials with long range order, such as crystalline materials or oriented fibrous composites or thermoplastic polymer chains, offer a particular challenge and motivate sophisticated multiscale modeling methods. Characteristic scale transitions achieved by multiscale modeling do not follow a single mathematical or algorithm structure, owing both to the consideration of long range order and to the fact that as models are coarse grained, the models shift from those concerning nonequilibrium, dynamic particle systems to continuously distributed mass systems that often invoke statistical equilibrium arguments and radically reduce degrees of freedom. A distinction is made between so-called hierarchical and concurrent multiscale modeling schemes. The former apply scale-appropriate models to different levels of hierarchy to generate responses or properties at that scale. In contrast, the latter attempt to cast the problem over common spatial and temporal domains by virtue of boundary conditions and introduction of consistent variable order descriptions of kinematics to achieve a variable resolution/fidelity description. Clearly, concurrent schemes are more costly but are argued to provide high value in cases in which localization of responses within a microstructure cannot be located or anticipated a priori, as well as the propagation of such localization events across a broad range of scales shown in Fig. 1. Information is lost in either way — in the case of hierarchical multiscale models, information is lost (i.e., increase of information entropy) by disposing of model degrees of freedom, while in the case of concurrent multiscale modeling information is lost by virtue of the idealization necessary to frame the models with consistent structure to pass information back and forth across length and time scales.

It is a daunting task to briefly summarize a range of multiscale modeling approaches for all relevant process—structure or structure–property relations for all material classes, beyond the scope of any single work. We accordingly limit discussion here to multiscale dislocation plasticity of metals to illustrate the range of considerations involved. Dislocation plasticity is a multiscale, multi-mechanism process [24–27] that focuses on evolving irreversible microstructure rearrangement [28] associated with line defects crystals. Existing approaches address mechanisms over a wide range of length and time scales, as summarized below.

(a) Discrete to continuous modeling approaches based on contiguous (domain decomposition) or overlapping (coarse graining) domains:
- Domain decomposition, with an atomistic domain abutted to an overlapping continuum domain to atomistically resolve crack tips and interfaces [29–35] to model fracture and defect interactions.
- Quasi-continuum approaches with the continuum elastic energy function informed by nonlocal atomistic interatomic potentials, suitable for long range fields without defects [36–39], with adaptivity to selectively model regions with full atomic resolution [40].
- Dynamically equivalent continuum or quasi-continuum, consistent with fully dynamic atomistic simulations over same overlapping domain [41–46].
- Coarse-grained molecular dynamics [47–51] for somewhat longer ranged spatial interactions of microstructure and defects such as dislocation pile-ups.
- Continuum phase field modeling (PFM) [52,53] to simulate microstructure morphology, and evolution, including microscopic PFM [54] informed by ab initio or atomistic simulations in terms of energy functions, with kinetics (mobilities) established by matching overlapping MD or experiments [55].
Table 1
Examples of dominant material length scales (in each row) for design with regard to bulk mechanical properties of metallic systems.

<table>
<thead>
<tr>
<th>Strength</th>
<th>Bulk polycrystals</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Inelastic flow and hardening, uniform ductility</td>
</tr>
<tr>
<td>2 nm — unit processes of nucleation (low defect density single crystals, nanoscale multilayers)</td>
<td>2 nm — bond breaking (cleavage)</td>
</tr>
<tr>
<td>20 nm — source activation (nanocrystalline metals with prior cold work)</td>
<td>200 nm — dislocation multiplication, junctions</td>
</tr>
<tr>
<td>200 nm — source controlled (NEMS, MEMS)</td>
<td>200 nm — dislocation multiplications, junctions</td>
</tr>
<tr>
<td>2 µm — free surfaces and starvation (micropillars, unconstrained layers)</td>
<td>20 µm — statistical field of junctions, forests</td>
</tr>
<tr>
<td></td>
<td>20 µm — intergranular interactions</td>
</tr>
<tr>
<td></td>
<td>20 µm — intergranular interactions</td>
</tr>
<tr>
<td></td>
<td>20 µm — intergranular interactions</td>
</tr>
</tbody>
</table>

(b) Concurrent multiscale continuum modeling schemes for plastic deformation and failure processes based on imposition of consistent multiscale boundary conditions and/or higher order continua accounting for heterogeneous deformation at fine scales over the same physical domain [56–61].

(c) Multiscale modeling schemes of hierarchical nature for inelastic deformation and damage in the presence of microstructure:
- Multilevel models for plasticity and fracture based on handshaking [62–65].
- Self-consistent micromechanics schemes [66–68].
- Internal state variable models informed by atomistic/continuum simulations and coupled with micromechanics or FE methods [69,70].
- Weak form variational principle of virtual velocities (PVV) with addition of enhanced kinematics based on microstructure degrees of freedom [71–73].
- Extended weak form variational approaches of generalized continua or second gradient theory with conjugate micromodules to represent gradient effects [74–79].

(d) Statistical continuum theories that directly incorporate discrete dislocation dynamics [80–89] and dislocation substructure evolution [24,25].

(e) Field dislocation mechanics based on incompatibility with dislocation flux and Nye transport [90–93].

(f) Dislocation substructure formation and evolution models based on fragmentation and blocky single slip or laminated flow characteristics, including non-convex energy functions [94–98].

(g) Transition state theory, based on use of atomistic unit process models [99–101] to inform event probabilities in kinetic Monte Carlo models of mesoscopic body behavior [102] and other coarse graining approaches [103].

Clearly, even in the focused application area of multiscale dislocation plasticity, no single multiscale modeling strategy exists or suffices to wrap together the various scale transitions. Each material class and response of interest is influenced by a finite, characteristic set of length and time scales associated with key controlling microstructure attributes. For this reason, materials design can be (and often is) pursued using sets of models that are scale appropriate to the length scales and microstructure attributes deemed most influential on the target response(s) at the scale of the application. So if the scale of the application is on the order of tens of microns, as in MEMS devices, both the atomic scale structure and mesostructure of defect distributions (dislocations, grain boundaries, etc.) can be important. For nanostructures, however, atomic scale arrangement and its evolution is dominant. In many systems, the hierarchy includes strong heterogeneity or phase contrast (e.g., weldments in structures, fiber-reinforced polymer composites) and these scales may dominate responses of interest. Even interfacial-dominated phenomena, such as fracture of heterogeneous materials (cf. [104–107]), is complicated according to whether the fracture occurs via brittle or ductile separation, with the latter involving interface structure only as a gating mechanism for inelastic deformation modes [108].

For illustrative purposes, at the risk of oversimplifying the wide range of phenomena and scales over a wide range of metallic systems, Table 1 attempts to identify dominant material length scales to address in design for various target mechanical properties of metallic systems. Although phenomena occur over a full spectrum of scales, the role of defects and microstructure is largely manifested at various discrete levels of structure. One important point is that certain properties are sensitive to material structure at only one or two levels of hierarchy. These observations suggest that distinct models or scale transition methods that bridge several scales can supply first order information for materials design. Clearly, no single multiscale modeling strategy exists or suffices to link the various scale transitions. Table 2 offers a partial glimpse into the complexities of models at various length and time scales for metallic systems, distinguishing scale transition methods from models appropriate to each scale.

It is emphasized that there is considerable uncertainty in any kind of multiscale modeling scheme, including the selection of specific length scales to model, approximations made in separating length and time scales in models used, model structure and parameter uncertainty at each scale, approximations made in various scale transition methods as well as boundary conditions, and lack of complete characterization of initial conditions. 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. Uncertainty will be addressed in a later section of this paper.
dramatically reducing the design space by focusing on the most nonlinear and time-dependent processes are considered. The use of explicit, rather than implicit, simulation of a large parametric range of microstructures via finite element or finite difference methods is extremely time-consuming, particularly if parametric range of microstructures via finite element methods are used to solve the governing field equations. The design problem is set up as an optimization problem, where the objective is the maximization of a selected macroscale property (or a performance criterion) and the design space enumerates all of the possible assignments of one of the available choices of material phases (e.g., a solid or a pore phase) to each of the spatial bins in the numerical model [110,111]. Although the method has been successfully applied to a limited class of problems [111–116], its main drawback is that it is likely to explore only a very small region of the vast design space. As an example, consider a relatively small problem with about 100 elements covering the space and assume that there are two choices for the selection of a material phase in each element. For this simple problem, the design space constitutes $2^{100}$ discrete choices of microstructures. It is therefore very unlikely that an optimization process can explore the complete design space unless constraints (perhaps ad hoc or limited in nature) are imposed. Moreover, explicit simulation of a large parametric range of microstructures via finite element or finite difference methods is extremely time-consuming, particularly if nonlinear and time-dependent processes are considered.

A number of modern approaches to material design start by dramatically reducing the design space by focusing on the most important measures of the microstructure deemed relevant to the problem. However, this reduction of the design space is attained by rational consideration of the governing physics of the problem and/or taking into account the constraints on the availability of microstructures (i.e., recognizing that only a very small fraction of all theoretically possible microstructures are accessible by currently employed manufacturing options). In other words, in these approaches, the design space in the simple problem illustrated above will be drastically reduced first by consideration of suitably selected subset of microstructure measures deemed relevant to the selected physical phenomenon of interest, and then optimal solutions will be explored in this reduced space. It is anticipated that the approach described above will produce better solutions compared to conventional approaches that rely exclusively on the optimization algorithms. We next discuss examples of approaches that attempt to reduce complexity of top–down design as an illustration.

**4. Methods for requirements-driven, top–down design**

As mentioned earlier, many of the currently available materials databases are better suited for material selection [109] instead of rigorous materials design. This is because materials design requires knowledge of a validated set of process–microstructure–property linkages that are amenable to information flow in both forward and reverse directions, as essential to facilitate solutions to top–down, requirements-driven (inverse) design problems. For example, sophisticated analytical theories and computational models already exist for predicting several macroscale (effective or homogenized) properties associated with a given microstructure. However, most of these theories are not well suited for identifying the complete set of microstructures that are theoretically predicted to meet or exceed a set of designer-specified macroscale properties or performance criteria. Topology optimization is one of the early approaches developed for materials design. In this method, the region to be occupied by the material is tessellated into spatial bins and numerical approaches such as finite element methods are used to solve the governing field equations. The design problem is set up as an optimization problem, where the objective is the maximization of a selected macroscale property (or a performance criterion) and the design space enumerates all of the possible assignments of one of the available choices of material phases (e.g., a solid or a pore phase) to each of the spatial bins in the numerical model [110,111]. Although the method has been successfully applied to a limited class of problems [111–116], its main drawback is that it is likely to explore only a very small region of the vast design space. As an example, consider a relatively small problem with about 100 elements covering the space and assume that there are two choices for the selection of a material phase in each element. For this simple problem, the design space constitutes $2^{100}$ discrete choices of microstructures. It is therefore very unlikely that an optimization process can explore the complete design space unless constraints (perhaps ad hoc or limited in nature) are imposed. Moreover, explicit simulation of a large parametric range of microstructures via finite element or finite difference methods is extremely time-consuming, particularly if nonlinear and time-dependent processes are considered.

A number of modern approaches to material design start by dramatically reducing the design space by focusing on the most important measures of the microstructure deemed relevant to the problem. However, this reduction of the design space is attained by rational consideration of the governing physics of the problem and/or taking into account the constraints on the availability of microstructures (i.e., recognizing that only a very small fraction of all theoretically possible microstructures are accessible by currently employed manufacturing options). In other words, in these approaches, the design space in the simple problem illustrated above will be drastically reduced first by consideration of suitably selected subset of microstructure measures deemed relevant to the selected physical phenomenon of interest, and then optimal solutions will be explored in this reduced space. It is anticipated that the approach described above will produce better solutions compared to conventional approaches that rely exclusively on the optimization algorithms. We next discuss examples of approaches that attempt to reduce complexity of top–down design as an illustration.

Microstructure Sensitive Design (MSD) was formulated using spectral representations across the process, microstructure, and property design spaces in order to drastically reduce the computational requirements for bi-directional linkages between the spaces that can enable inverse design [20,117–125]. Much of the focus in MSD was placed on anisotropic, polycrystalline materials, where the local material state is defined using a proper orthogonal tensor that captures the local orientation of the crystal lattice in each spatial bin in the microstructure with respect to a fixed sample (or global) reference frame. The corresponding local state space is identified as the fundamental zone of $SO_3$ (the set of all distinct proper orthogonal tensors in 3-D) that takes into account the inherent symmetries of the crystal lattice. The distinguishing feature of MSD is its use of spectral representations (e.g., generalized spherical harmonics [126]) of functions defined over the orientation space. This leads to compact representations of process–structure–property relationships that can be executed at minimal computational cost. Most of the MSD success stories have focused on 1-point statistics of microstructure (also called Orientation Distribution Function [126]). At its core, the MSD effort involved the development of very large and highly efficient databases organized in the form of microstructure hulls and anisotropic property closures. Microstructure hulls delineate the complete set of theoretically feasible statistical distributions that
quantitatively capture the important details of the microstructure. Property closures identify the complete set of theoretically feasible combinations of macroscale effective properties for a selected homogenization (composite) theory. The primary advantages of the MSD approach are its (a) consideration of anisotropy of the properties at the local length scales, (b) exploration of the complete set of relevant microstructures (captured in the microstructure hull and property closures) leading to global optima, and (c) invertibility of the process-microstructure-property relations (due to the use of spectral methods in representing these linkages).

Extension of the MSD framework to include 2-point statistics of orientation has proved to be computationally expensive because of the very large number of statistical variables and terms involved. It is important to recognize that 1-point statistics are defined exclusively over the local state space, whereas the higher-order statistics are defined over the product spaces of the orientation space (for the local state variables) and the real three-dimensional physical space (for the vectors defining the spatial correlations). While the use of generalized spherical harmonics provides substantial compaction for functions over the orientation space, the analogous compact representations for functions over the real three-dimensional physical space are yet to be developed.

In an effort to address the need to establish high fidelity microstructure-property-process relations that include higher-order descriptors of the microstructure, a new mathematically rigorous approach for scale-bridging called Microstructure Knowledge Systems (MKS) was recently developed. MKS facilitates bi-directional exchange of information between multiple length (and possibly time) scales. In the MKS approach [127–131], the focus is on the localization (the opposite of homogenization), which describes the spatial distribution of the response field of interest (e.g., stress or strain fields) at the microscale for an imposed loading condition at the macroscale. Localization is critically important in correlating various failure-related properties of the material with appropriate microstructure conformations that produce the hot spots associated with damage initiation in the material. Moreover, if one can successfully establish accurate approximation for localization (referred to as localization linkages), it automatically leads to highly accurate homogenization and computationally efficient multiscale modeling and simulation.

The MKS approach is built on the statistical continuum theories developed by Kröner [132,133]. However, the MKS approach dramatically improves the accuracy of these expressions by calibrating the convolution kernels in these expressions to results from previously validated physics-based models. In recent work [131], the MKS approach was demonstrated to successfully capture the tails of the microscale stress and strain distributions in composite material systems with relatively high phase contrast, using the higher-order terms in the localization relationships. The approach has its analogue in the use of Volterra kernels [134,135] for modeling the dynamic response of nonlinear systems.

In the MKS framework, the localization relationships of interest are expressed as calibrated meta-models that take the form of a simple algebraic series whose terms capture the individual contributions from a hierarchy of microstructure descriptors. Each term in this series expansion is expressed as a convolution of the appropriate local microstructure descriptor and its corresponding local influence at the microscale. The microstructure is defined as a digital signal using the discrete approximation of the microstructure function, $m_h$, reflecting the volume fraction of local state $h$ in the spatial bin (or voxel) $s$. Let $p_s$ be the averaged local response in spatial cell $s$ defined on the same spatial grid as the microstructure function; it reflects a thoughtfully selected local physical response central to the phenomenon being studied, and may include stress, strain or microstructure evolution rate variables [127–130]. In the MKS framework, the localization relationship captures the local response field using a set of kernels and their convolution with higher-order descriptions of the local microstructure [132,133,136–142].

The localization relationship can be expressed as

$$
p_s = \left( \sum_{h_1 \ldots h_S} \sum_{t_1 \ldots t_H} \lambda_{h_1 t_1} \frac{m_{h_1 t_1}}{p_{s}}, \ldots, \sum_{h_1 \ldots h_S} \sum_{t_1 \ldots t_H} \lambda_{h_S t_H} \frac{m_{h_S t_H}}{p_{s}} \right). \tag{1}
$$

where $H$ and $S$ denote the number of distinct local states and the number of spatial bins used to defined the microstructure signal ($m_h$), and all the $t_i$ enumerate the different vectors used to define the spatial correlations. The kernels, or influence coefficients, are defined by the set $\{ \lambda_{h_1 t_1}, \lambda_{h_2 t_1}, \lambda_{h_3 t_2}, \ldots, \lambda_{h_1 t_1}, \lambda_{h_2 t_2}, \ldots, \lambda_{h_1 t_1}, \lambda_{h_2 t_2}, \lambda_{h_3 t_3}, \ldots \}$, and $\lambda_{h_1 h_2 h_3}$ are the first, second, and third-order influence coefficients, respectively. The higher-order descriptions of the local microstructure are expressed by the products $m_{h_1 t_1} m_{h_2 t_2} m_{h_3 t_3}$, and $N$ denotes the order.

The higher-order localization relationship shown in Eq. (1) is a particular form of Volterra series [134,135,143–146] and implicitly assumes that the system is spatially-invariant, causal, and has finite memory. The influence coefficients in Eq. (1) are analogous to Volterra kernels. The higher-order terms in the series are designed to capture systematically the nonlinearity in the system. The influence coefficients are expected to be independent of the microstructure, since the system is assumed to be spatially invariant. Application of the concepts of Volterra series directly to materials phenomena poses major challenges. Materials phenomena require an extremely large number of input channels (because of the complexities associated with microstructure representation) and an extremely large number of output channels (because of the broad range of response fields of interest). However, the microstructure representation described above allows a reformulation of the localization relationship into a form that is amenable for calibration to results from previously validated numerical models (e.g. finite element models, phase-field models) by linear regression in the Discrete Fourier transform space [127–131], which is one of the distinctive features of the MKS framework.

A major challenge in the MKS framework is the calibration of the selected higher-order influence coefficients via linear regression. Although other approaches have been used in literature to approximate the higher-order Volterra kernels (e.g. cross-correlation methods [145,146], artificial neural networks [144], and Bayesian methods [147,148]), the solutions obtained using ordinary least squares fit [131] generally provide the best solutions for the MKS case studies conducted to date. Fig. 3 demonstrates the accuracy of the MKS approach for predicting the local elastic response in an example microstructure with a contrast of 10 in the values of the Young's moduli of the local states. The MKS methodology has thus far been successfully applied to capturing thermo-elastic stress (or strain) distributions in composite materials, rigid-viscoplastic deformation fields in composite materials, and the evolution of the composition fields in spinodal decomposition of binary alloys [127–131]. The latter two phenomena (rigid-viscoplastic deformations and...
Fig. 3. Demonstration of the accuracy of the MKS approach in predicting the local elastic fields in a two-phase composite system with a contrast of 10 in the elastic moduli of the constituent phases. The strain contours on a mid-section through the 3-D composite microstructure are shown along with the strain distributions in each phase in the entire 3-D volume element. It is seen that the MKS approach produced excellent predictions at a fraction of the computational cost associated with the finite element method (FEM).

spinodal decomposition) involve highly nonlinear governing field equations. However, MKS framework has not yet been applied to highly complex microstructures such as those seen in polycrystalline material systems. For the compact inclusion of lattice orientation in the higher-order localization relationships, it would be necessary to introduce the spectral representations over the orientation space (used in the MSD framework) into the MKS framework described above.

MSD and MKS approaches described in the preceding address the compact representation of high fidelity microstructure–property–processing linkages at a selected length scale. In order to obtain viable materials design solutions, one needs to link relevant models from different length and time scales, quantify uncertainty in each model, and communicate the uncertainty throughout the model chain in a robust multi-level design framework.

In a later section, the Inductive Design Exploration Method (IDEM), will be introduced as a means of mitigating or managing uncertainty while facilitating top–down searches for candidate microstructures based on mappings compiled from bottom–up simulations. In general, the utility of IDEM might be greatest for applications involving highly heterogeneous datasets and/or material models for which the inverse design strategy afforded by MSD or MKS approaches might be less clearly related to microstructure representation. Such cases may be typical of multiphysics phenomena with weak coupling to each other or to radically different length scales of microstructure, or to problems for which the microstructure–property/response relations run through a sequence of hierarchical models, with each transition characterized by a reduction of model order.

5. Characterization for model validation and process–structure models

Verification and validation (V&V) is a core component of ICME [7]. Model verification and validation is an underdeveloped aspect of simulation-supported design of materials and products within the ICME vision. Within systems engineering, verification refers to the process of ensuring that the “system is built right” (i.e., the system meets its requirements) whereas validation refers to building the “right system” (i.e., the system satisfies the users’ needs) [149]. These are general definitions that apply to verification and validation of individual and multiscale models, design processes and design outcomes. Within the context of simulation model development [150], verification and validation have specific definitions, which are consistent with the systems engineering definitions above:

- Verification: The process of determining that a model implementation accurately represents the developer’s conceptual description of the model and the solution to the model.
- Validation: The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model.

One of the most difficult tasks in validating models is the documentation of the material microstructure and its evolution in any selected process. As noted earlier, it is essential to address stochasticity of microstructure. Consequently, there is a critical need to establish rigorous protocols for documenting in a statistically meaningful way the rich three-dimensional (3-D) topological details of the microstructure that might span multiple length scales. These protocols need to establish reliable statistical measures to assess if a sufficient number of datasets have been
acquired, and if the spatial extent and spatial resolution in the acquired datasets are adequate. The protocols should also address reconstructions of representative volume elements (RVEs) from the measured datasets. Since the microstructure has a stochastic character, it is unlikely that a single sample or statistical volume element of microstructure [24,25] can accurately represent the microstructure. Therefore, one aim is to establish protocols for extracting a set of such samples that accurately reflect the natural variance in the microstructure such that the statistics of the ensemble can be statistically representative (i.e., statistically homogeneous).

Obtaining 3-D microstructure datasets from samples continues to be a major challenge for most advanced material systems. Impressive advances have been made in generating 3-D microstructure datasets [151–162]. Despite these advances, the acquisition of such datasets remains effort intensive, highly expensive, very slow, and inaccessible to the broader scientific community. Moreover, the volumes of materials studied using these approaches are often limited, which raises critical questions regarding their adequacy for reliably extracting desired microstructure measures and their variances.

If we restrict attention to 2-point and 3-point statistics of the microstructure (these constitute the most important spatial correlations), it should be possible to acquire and assemble 3-D descriptions of these statistics from large 2-D microstructure scans on multiple oblique sections into the sample [138,163]. This is because all of the vectors used to define the 2-point and 3-point statistics can be populated on carefully selected oblique sections into the sample. Since it is significantly less expensive to obtain large 2-D microstructure scans in most materials, this approach is much more practical for statistically meaningful characterization of the microstructure in a given sample set.

It is important to emphasize that the complete set of 2-point statistics is an extremely large set. Compact and meaningful grouping of the dominant 2-point statistics in a given material system is an area of active current research. It has long been known that the complete set of 2-point statistics exhibits many interdependencies. Gokhale et al. [164] showed that at most \( N (N - 1) / 2 \) 2-point correlations are independent for a material system comprised of \( N \) distinct local states. Niezgoda et al. [165] recently showed that only \((N - 1)\) of the 2-point correlations are actually independent by exploiting known properties of the Discrete Fourier transform representation of the correlations. However, for a material system comprising a very large number of local states (e.g., a polycrystalline material system), even tracking \((N - 1)\) spatial correlations is an arduous task. It was recently demonstrated that techniques such as principal component analysis (PCA), commonly used in face recognition and pattern recognition, can be used to obtain objective low dimensional representations of the 2-point statistics [21,22], as shown in Fig. 4. Since the \( n \)-point statistics are smooth analytic functions with a well defined origin, PCA decomposition is quite effective in establishing an uncorrelated orthogonal basis for any ensemble of microstructure datasets. The PCA decomposition allows one to represent each microstructure as a linear combination of the eigenvectors of a correlation matrix, with the weights interpreted in the same manner as Fourier coefficients. The weights now form an objective low dimensional representation of the much larger set of independent 2-point statistics. The PCA representations allow simple visualization of an ensemble of microstructures, and a rigorous quantification of the microstructural variance within the ensemble [120] (see Fig. 4). The same concepts can also be used effectively to define weighted sets of statistical volume elements (WSVEs) as an alternative to identifying RVEs for a given ensemble of microstructure datasets [22,166,167].

Successful pursuit of the ICME vision requires integration of all of the different components described earlier. The NMAB report on ICME [7] specifically identifies three main tasks for integration tools: (i) linking information from different sources and different knowledge domains, (ii) networking and collaborative development, and (iii) optimization. Certainly, collaborative multidisciplinary design optimization presents challenges due to the geographically distributed nature of the materials supply and product design enterprises, often undertaken in different corporations and in different divisions, as well as in consulting and university laboratories [15]. Major emphasis to date on design integration has been placed on use of commercial software [13,14] that includes capabilities to manage databases and pursue various optimization strategies. With regard to optimization, materials design suffers substantially from conventional problems in design optimization owing to the complexity, nonlinearity, and uncertainty [168,169] of material process–structure and structure–property models. It is not merely the case where existing tools can be identified and deployed, but rather basic research issues at the intersection of computational materials science and engineering, experimental mechanics and processing, and multidisciplinary design optimization must be identified and addressed.

As mentioned earlier, one of the most difficult challenges in the integration is the visualization of microstructure–property–processing linkages in a common space. This is exacerbated by the fact that a comprehensive description of the microstructure requires a very large number of statistics or spatial correlations. Therefore, reduced-order representations of the microstructure are essential. The PCA decompositions of the \( n \)-point statistics discussed earlier offer new exciting opportunities to build new integrations tools. As an example, consider the process design problem where the objective is to identify hybrid processing routes comprising an arbitrary sequence of available manufacturing routes aimed at transforming a given initial microstructure into a desired one. Fig. 5 shows schematically how one might address the process design problem by representing the microstructure–property–processing linkages in a common (microstructure) space. The green volume in Fig. 5 depicts a microstructure hull corresponding to an ensemble of digitally created porous solids [22]. Each point in this space represents a microstructure (an example is depicted in the top right in Fig. 5) through the PCA weights of its 2-point correlations. The elastic moduli for all microstructure members in the selected
ensemble were evaluated using finite element models (FEM), and were correlated to the first two PCA weights using artificial neural networks. The correlation and its validation are depicted in the contour plot on the bottom right in Fig. 5. It is seen that the microstructure–modulus correlation provides excellent predictions for various members of the ensemble (with less than 5% error) [22]. It is noted that the PCA weights of the microstructure can also be related to properties of interest using various regression methods.

Fig. 5 illustrates schematically the superposition of processing information on the microstructure hull in the form of process pathlines. In any selected processing option, the salient features of the microstructure are expected to change, which can be visualized as a pathline in the multi-dimensional microstructure space. Different processing operations are expected to change the microstructure in different ways, and therefore there are likely to be different processing pathlines intersecting at each microstructure. Identification (either experimentally or by modeling) of all the processing pathlines in the microstructure hull corresponding to all available processing options that may be exercised results in a large database (or a process network). Once such a database is established, it should be possible to identify the ideal hybrid process route (based on cost or other criterion such as sustainability) that will transform any selected initial microstructure into one that has been predicted to exhibit superior properties or performance characteristics. The basic concept was evaluated recently in a simple case study that aimed at transforming the given initial crystallographic texture in a sample into a desired one [123]. In all examples considered, the process network identified solutions that could not be arrived at by pure intuition or by brute-force methods (including constant performance maximization or repeated trials). There is a critical need to further develop this framework to include higher-order descriptions of microstructure (possibly based on n-point statistics) and higher-order homogenization theories (e.g. MKS framework). This linkage of models that explicitly consider microstructure to process path design is a key underdeveloped technology within the ICME paradigm, as discussed earlier in reference to Fig. 2.

6. Uncertainty in ICME

One of the key enablers of the ICME paradigm is the ability to account for different aspects of uncertainty within models, experiments, and the design process. Uncertainty is a first order concern in the process of simulation-supported, decision-based materials design. It is often overlooked in discussion of ICME and materials design, possibly because it is assumed that approaches exist within systems design and uncertainty management methods that are suitable. This is generally not the case in addressing nuances and complexity of multi-level materials design. Only two paragraphs were devoted to the uncertainty section in the NMAB ICME report [7], and little discussion was devoted to MDO aspects and the richness of required verification and validation approaches; however, these are perhaps among the most critical scientific obstacles to realizing ICME owing to its nascent stages of formulation. The ICME report focused more on model integration/communication, i.e., assembling and networking modeling and simulation tools along with accompanying supportive experimental methods. There are various sources of uncertainty in addressing ICME, inexhaustively listed without classification as [15]:

- Variability induced by processing, operating conditions, etc. and due to randomness of microstructure.
-Incomplete knowledge of model parameters due to insufficient or inaccurate data, including initial and boundary conditions.
- Uncertain structure of a model due to insufficient knowledge (necessitating approximations and simplifications) about a physical process such as process–structure or structure–property relations.
Uncertainty in meshing and numerical solution methods.

- Propagation of uncertainty through a chain of models (amplification or attenuation).
- Experimental idealizations and measurement error.
- Lack of direct connection of measured quantities to model degrees of freedom.

Accounting for uncertainty involves four aspects: uncertainty quantification, uncertainty propagation, uncertainty mitigation, and uncertainty management. Uncertainty quantification is the process of identifying different sources of uncertainty and developing corresponding mathematical representations. There are perhaps several unique aspects of materials with regard to uncertainty quantification [168]:

- The long range character of defect/structure interactions in materials necessitates complex nonlocal formulations of continuum field equations or corresponding coarse grain internal variables. An economics analogy might be consumer reaction to market instabilities abroad.
- Use of 2D images to reconstruct 3-D microstructures to estimate properties/responses is often necessitated by lack of expensive and time-consuming 3-D quantitative microstructure information; moreover, measured microstructures of new materials of interest to materials design do not yet exist, and predicted microstructures may not be thermodynamically feasible or metastable.
- Extreme value (rare event) problems are common in failure of materials, such as localization of damage within the microstructure in fracture or high cycle fatigue. An analogy might be insurance company estimation of probabilities of rare events such as 1000 year floods, tsunamis, and so forth.
- The large range of equations used in solving field equations of nonlinear, time-dependent, multi-physics behavior of materials, including constraints, side conditions, jump conditions, thresholds, etc., which may vary from group to group (i.e., little standardization).

Uncertainty propagation involves determining the effect of input uncertainties on the output uncertainties, both for individual models and chains of models. The combination of uncertainty representation and propagation is sometimes referred to as uncertainty analysis. Uncertainty mitigation utilizes techniques for reducing the impact of input uncertainties on the performance of the material system. Finally, uncertainty management involves deciding the levels of uncertainty that are appropriate for making design decisions and prioritizing uncertainty reduction alternatives based on the tradeoff between efforts and benefits. While uncertainty quantification and propagation activities are carried out by analysts or model developers, uncertainty mitigation and management are activities performed by system designers during the design process. These four aspects and corresponding techniques are discussed in a fairly general way in Sections 6.1 through 6.4, followed by a brief discussion of some of the unique aspects associated with multiscale modeling and design of materials.

### 6.1. Uncertainty quantification

During the past few decades, a number of different classifications of uncertainty have been proposed. Different classifications have emerged within diverse fields such as economics and finance, systems engineering, management science, product development, and computational modeling and simulation. Uncertainty classification has also evolved over time, e.g., within economics the classification has evolved from (a) risk and uncertainty in early 20th century to (b) environmental and behavioral uncertainty in the mid 20th century, to the recent classification of fundamental uncertainty and ambiguity [169]. Uncertainty is also related to the concept of risk which can be defined as a triplet of scenarios, likelihood of scenarios, and possible consequences [170]. Uncertainty gives rise to risk. While risk is always associated with undesirable consequences, uncertainty may have desirable consequences [171]. An understanding of these classifications is necessary to properly position the methods for design under uncertainty.

Within computational modeling and simulation, uncertainty has been classified from different standpoints. Chen et al. [172] classify uncertainty into three types — Type 1 uncertainty associated with inherent variation in the physical system, Type 2 uncertainty associated with lack of knowledge, and Type 3 uncertainty associated with known limitations of simulation models. With specific goal of materials design, Choi et al. [173] classify uncertainty associated with different aspects of simulation models into model parameter uncertainty, model structural uncertainty, and propagated uncertainty.

The most widely adopted classification splits uncertainty into aleatory uncertainty and epistemic uncertainty. Aleatory uncertainty is due to the inherent randomness in material systems, such as nearest neighbor distributions of grain size, orientation, and shape in metallic polycrystals. This uncertainty is also referred to as irreducible uncertainty, statistical variability, inherent uncertainty, or stochastic uncertainty. Aleatory uncertainty associated with parameters is commonly represented in terms of probability distributions. Probability theory is very well developed and hence has served as a language and mathematics for uncertainty quantification. This is one of the reasons that aleatory uncertainty has received significant attention both in engineering design and computational materials science.

Epistemic uncertainty, on the other hand, refers to the lack of knowledge which may be due to the use of idealizations (simplified relationships between inputs and outputs), approximations, unanticipated interactions, or numerical errors. Examples include size of the representative volume element (RVE) of microstructure used to predict properties or responses, simplified material constitutive models, including the form and/or structure of such models, and approximate model parameters. Epistemic uncertainty is also referred to as reducible uncertainty, subjective uncertainty, and/or model-form uncertainty. Attempts have been made to use a Bayesian approach to quantify epistemic uncertainty using probability functions. Under the Bayesian framework for epistemic uncertainty, the subjective interpretation of probability functions is used [174]. Subjective interpretation of probability is different from the frequentist interpretation in the sense that subjective probabilities refer to degree of belief rather than the frequency of occurrence. The subjective interpretation allows for modeling all types of uncertainty (epistemic and aleatory) into a common framework, which is convenient for uncertainty analysis. The Bayesian approach involves determining prior probability distributions of uncertain parameters that represent modeler’s initial belief about uncertainty and using Bayes’ theorem to update the probability functions based on new pieces of information (e.g., from experiments).

However, by the very nature of epistemic uncertainty, it is inherently difficult or impossible to characterize probability functions associated with limited knowledge such as model idealization. An incorrect representation of uncertainty may result in wrong decisions. Hence, different types of mathematical techniques are needed for representing epistemic uncertainty. Alternative approaches for representing epistemic uncertainty include fuzzy set theory, evidence theory, possibility theory, and interval analysis [175]. Different representations are suitable under different situations.
While there has been significant progress in accounting for aleatory uncertainty using probability theory, little progress has been made on (a) holistic quantification of epistemic uncertainty within multiscale material models, and (b) simultaneous consideration of different mathematical constructs for representing both aleatory and epistemic uncertainty in an integrated manner. We regard this as one of the primary challenges facing ICME.

6.2. Uncertainty propagation

Within statistics, uncertainty propagation refers to the effect of uncertainties in independent variables on the dependent variables. In the context of simulation-supported design (decisions based at least in part on modeling and simulation), this translates to the effect of input uncertainty on the output uncertainty. Of course, the same general logic applies to input–output relations in experiments, which assert certain models in their own right and have error and approximation. In addition to the uncertainty at individual scales, materials design is associated with propagation of uncertainties in networks of interconnected models, which may either cause amplification or reduction of uncertainties in serial application of models. Hence, for the realization of ICME, techniques are required for (a) propagating uncertainty from the inputs of one model to its outputs, (b) propagating uncertainty from lower level models to upper level models within a model chain, (c) propagating uncertainty from material composition to structure through process route, material microstructure to material properties or responses, and from material properties to product performance.

A number of techniques such as Monte Carlo techniques and global sensitivity analysis are available for propagating uncertainty in the inputs (represented as random variables) to the outputs. Probability-based techniques have also been developed for propagating uncertainty across models. Lee and Chen [176] discuss five categories of methods for (typically aleatory) uncertainty propagation: Monte-Carlo methods, local expansion based methods (e.g., Taylor's series expansion), most probable point (MPP) based methods (e.g., first order reliability method and second order reliability method), functional expansion based methods (e.g., polynomial chaos expansion), and numerical integration based methods. A comparison of full factorial numerical integration, univariate dimensional reduction method, and polynomial chaos expansion is presented in Ref. [176].

The primary challenge with Monte Carlo techniques is that they are computationally intensive in nature. Repeated execution of simulation models may be computationally expensive and generally infeasible when using multiscale models with a number of sources of uncertainty. Hence, efficient techniques for uncertainty propagation are necessary. Chen and co-authors [172] have developed techniques for efficient uncertainty propagation using metamodels, but the use of metamodels in multiscale modeling where sound physical basis must exist for models at fine scales has not been fully acknowledged or pursued. There is strong suspicion that metamodels are too limited for this task, in general. Yin et al. [177] use random fields to model uncertainty within material microstructure and use dimension reduction techniques for efficient uncertainty propagation. Methods for propagation of uncertainties represented as intervals are also available [178]. However, approaches for propagating different types of uncertainty in a single framework are in early stages.

A related issue is whether to engage description of stochasticity at each level of simulation in terms of parameter distribution (e.g., variation of microstructure, model parameters) or to use many deterministic realizations of microstructure and corresponding models/parameters extracted from assigned probabilistic distributions at some “primal” scale to propagate uncertainty to higher levels of predicted response(s). The latter approach is straightforward and tractable, but requires identification of some scale as a starting point at which finer scale response can be treated as deterministic, which of course does not fully accord with physics. From a practical perspective, Table 1 suggests that each property or response may have a dominant minimal scale which can serve as a starting point for applying deterministic models with probability distributions of inputs to propagate through a multiscale modeling framework. On the other hand, the temptation with a fully stochastic approach is to avoid the hard but fruitful work of assessing the viability of such a scale, perhaps leading to an early concession to Bayesian approaches to provide answers where the physics is complex or microstructure-sensitive models are limited or avoided. In this regard, there are some recent works that merge the two approaches in multiscale modeling in a manner that may provide promising avenues for future applications [179].

6.3. Uncertainty mitigation

Uncertainty mitigation refers to reducing the effect of uncertainty on systems design. Techniques such as robust design and reliability based design and optimization (RBDO) have been developed in the systems design community to achieve desired system performance in the presence of uncertainty. Robust design techniques are based on the principle of minimizing the effects of uncertainty on system performance [180] whereas reliability-based design optimization techniques are based on finding optimized designs characterized by low probability of failure [181]. Note that reducing the effect of uncertainty on design using these approaches is different from reducing the (epistemic) uncertainty itself. In robust design and RBDO approaches, the levels of uncertainty are generally assumed to be fixed (or given). The goal is to determine the best design that is insensitive to the given uncertainty or has low probability of failure.

Robust design techniques are rooted in Taguchi’s quality engineering methodology [182]. One of the earliest robust design approaches for systems design include the Robust Concept Exploration Method (RCEM) [183] which combines statistical techniques of surrogate modeling and compromise decision support problems [184] to perform robust design. RCEM has been extended to account for other sources of uncertainty (e.g., uncertainty in input variables) [185], and to develop product platforms [186]. The multi-disciplinary design optimization (MDO) community has developed techniques for optimizing systems in the presence of uncertainty [187–190].

Existing techniques for multi-level deterministic optimization have also been extended to account for uncertainty. An example is the extension of the Analytical Target Cascading (ATC) approach to Probabilistic Analytical Target Cascading (PATC) [191]. ATC is an approach for cascading overall system design targets to sub-system specifications based on an hierarchical multi-level decomposition [192], similar to the concurrent material and product design problem shown in Fig. 1, when layered with the understanding of Olson’s Venn diagram. 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. Within PATC, uncertainty is modeled in terms of random variables and uncertainty propagation techniques are used to determine the impact of uncertainties at the bottom level on parameters at the top level.

While analytical target cascading approach is based on choosing a design point during each iteration and repeating the optimization loops until convergence is achieved, approaches such as the Inductive Design Exploration Method (IDEM) use ranges of parameters and design variables [15,193,194]. The primary advantage of working with ranging sets of design points is the possibility...
Fig. 6. Inductive Design Exploration Method [15,193–195]. Step 1 involves bottom–up simulations or experiments, typically conducted in parallel fashion, to map composition into structure and then into properties, with regions in blue showing the feasible ranged set of points from these mappings. Step 2 involves top–down evaluation of points from the ranged set of specified performance requirements that overlap feasible regions (red) established as subsets of bottom–up simulations in Step 1. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

IDEM facilitates design while accounting for uncertainty in models and its propagation through chains of models. IDEM [193,194] has two major objectives: (i) to explore top–down, requirements-driven design, guiding bottom–up modeling and simulation, and (ii) to manage uncertainty in model chains. Fig. 6 illustrates the concept of IDEM. We consider multiple spaces of different dimension (DOF), between which models, simulations or experiments serve as mappings that project points in a given space (e.g., composition) to the next (e.g., microstructure) and to the final (e.g., properties/responses). First we must configure the design system, including information flow between specific databases and modeling and simulation tools, and specify ranged set of performance requirements. Then, steps in IDEM, shown below in Fig. 6, are as follows:

1. Perform parallel discrete points evaluation at each level of design process (bottom–up simulations and experiments).
2. Perform inductive (top–down) feasible space exploration based on metamodels from Step 2.
3. Obtain a robust solution with respect to model uncertainty.

Projected points need not comprise simply connected regions in each space, but we plot as such for simplicity. There is also provision for reconfiguring the design system in case there is no overlap between performance requirements and feasible ranges of the bottom–up projections and/or to mitigate uncertainty. Mitigation of uncertainty is a second primary feature of IDEM. If two candidate solutions exist, say Designs 1 and 2, for which final performance is identical, then which design should we select? In general, we select solutions that lie the furthest from the constraint boundaries in each space, including the boundaries of feasible regions established in Step 1 of IDEM (blue regions in Fig. 6). Current robust design methods cannot address this issue since these methods only focus on the final performance range. The fundamental difference between IDEM and other multi-level design methods is that IDEM involves finding ranged sets of design specifications by passing feasible solution spaces from final performance requirements by way of an interdependent response space to the design space while preserving the feasible solution space to the greatest extent possible.

Choi and co-authors [195] use the IDEM framework to design a multi-functional energetic structural material (MESM) using a multiscale model consisting of a microscale discrete particle mixture (DPM) model and a continuum non-equilibrium thermodynamic mixture (NTM) model. The inputs of the DPM model are volume fractions and mean radii of the MESM constituents and the output is the weighted average temperature of local hotspots. The inputs of the NTM model include volume fractions and critical temperature for reaction initiation and the output is the accumulated reaction product. For each input–output mapping, the inputs space is discretized using experimental design techniques. The model is executed at discrete points considering various types of uncertainty (discussed in Section 6.1). Due to the uncertainties, each point maps to a subspace in the output space. Specific techniques have been developed to account for inputs shared across multiple levels. After generating the mappings between different levels, measures such as Hyperdimensional Error-Margin Index (HD-EMI) are used to determine the robustness of the design to various forms of uncertainty while satisfying the problem constraints. Using the IDEM approach, Choi and co-authors [195] determine robust combinations of design variables (volume fractions, and radii of constituents) to achieve the desired accumulation of reaction products. Other examples of the IDEM implementation are discussed in [15,193,194].

The forward mappings in Step 1 of IDEM pertain either to multiscale models, in which information from a model at one scale is projected onto inputs into higher scale models, or multi-level models, in which composition is mapped into structure and structure into properties. By remaining as far as possible from constraints, IDEM attempts to pursue solutions that are less sensitive to uncertainty, particularly in terms of solutions that avoid infeasible designs. The IDEM process accounts for the effect of aleatory uncertainty in the input parameters (such
as randomness in particle sizes and randomness in simulated microstructure) on the outputs of the multiscale model, along with the propagation of aleatory uncertainty along a design chain. Instead of using a concurrent multiscale modeling approach, an information-passing approach is used in IDEM. The primary distinction is that instead of passing information about single design points throughout the model chain, ranset solutions are passed across different levels. It allows for independent execution of models at different scales, which simplifies the uncertainty propagation within models. Since the process of uncertainty analysis is decoupled from design exploration, IDEM is flexible to be extended for other forms of uncertainty using existing uncertainty propagation techniques. Recently, IDEM has been extended to account for model parameter uncertainty [196]. Further work needs to be carried out to account for other representations of epistemic uncertainty such as intervals and fuzzy sets.

6.4. Uncertainty management

Uncertainty management is the process of deciding the levels of uncertainty that are appropriate for design decisions and prioritizing uncertainty reduction alternatives based on the tradeoff between efforts and benefits. The focus in uncertainty management is on deciding when to reduce epistemic uncertainty by gaining additional knowledge and when to reduce the complexity of the design process by using simpler models and design processes. The notion of introducing uncertainty by using simplified models during the early conceptual design phases has received little attention from the engineering design and the materials science communities.

When designing a material system, the focus is on achieving properties such as strength and ductility that address performance requirements. In contrast, when managing uncertainty in the design process, focus is placed on design-process goals such as reducing the complexity of the design process and achieving the best design in the shortest possible time. The notion of designing the design process is also important because of (a) evolving simulation models, resulting in multiple fidelities of models at different stages of a design process, and (b) significant model development and execution costs, necessitating judicious use of computational resources. Moreover, the needs for accurate information depend on whether the goal is to narrow down the alternatives to a specific class of materials (i.e., during early design phase) or to optimize the composition and structure of a specific material (i.e., during the later stages of design). In the early phases of design, models and accurate representations of uncertainty may not be available — they may also not be necessary. Uncertainty management can be applied to problems such as refinement of simulation models [197], selection of models from a set of available models [198], and reducing the complexity of the design process [199].

A potential approach to uncertainty management is to utilize concepts and mathematical constructs from information economics [200,201] such as value of information to quantify the cost/benefit tradeoff to make the best design decisions in the presence of uncertainty. Information economics is the study of costs and benefits of information in the context of decision-making. Metrics from information economics, specifically the expected value of information, are extended to account for both statistical variability and imprecision in models. The value of this added information is referred to as the improvement in a designer’s decision-making ability. Mitigation of uncertainty in simulation models is effectively analogous to the acquisition of a new source of information, and the set of results from the execution of this refined model is analogous to additional information for making a decision.

Different measures are developed for quantifying the benefit of uncertainty mitigation in individual models [197,202]. These include (a) the improvement potential, and (b) process performance indicator (PPI). The improvement potential quantifies the maximum possible improvement in a designer’s decision that can be achieved by refining a simulation model [197] (e.g., through increasing fidelity, improving the physical basis of the model, etc.). If the improvement potential is high, the design decision can possibly be improved by refining the simulation model. However, if the improvement potential is low, then the possibility of improving the design solution is low. Hence the level of refinement of the model is appropriate for decision-making. The main assumption is that the bounds on the outputs of models, which translate to the bounds on payoff, are available throughout the design space. The improvement potential measure is applied to problems involving simulation model refinement [197] and the coupling between simulation models at different scales [15,199].

The PPI is developed for scenarios where information about upper and lower bounds on the outputs of models are not available but it is possible to generate accurate information at a few points in the design space. This is generally the case when physical experiments are expensive and can only be executed at a few points in the design space. Another application of the PPI is when there are multiple models (or refinements of the same model) that a design can choose from, and one of the models is known to be the most truthful. The PPI is calculated as the difference in payoff between the outcomes of decisions made using the most truthful model and the outcomes achievable using less complex models.

The improvement potential and the process performance indicator account for the benefits of gaining additional information by reducing epistemic uncertainty but do not directly capture the effort involved in reducing uncertainty. This is due to a lack of holistic models that predict the effort involved in developing and executing simulation models. The effort models must be predictive in nature because they need to be employed before the simulation is developed or refined. An effort model for ICME would be based on the cost models from software development and systems engineering [204]. The effort model accounts for three dimensions of effort — person hours, monetary cost, and computational time. Using this effort model, measures that account for both value and effort are under development.

Constructs based on information economics can also be used to choose between a concurrent multiscale modeling approach and a hierarchical multiscale modeling approach. In the case of concurrent multiscale modeling, models at various scales are tightly coupled with each other. In contrast, hierarchical multiscale modeling approaches typically involve passing information between models in the form of ranges of values or surrogate models. Due to the tight coupling in concurrent multiscale models, it is more challenging to identify the impact of specific sources of uncertainties and specific models on the overall output uncertainty. Additionally, the impact of uncertainty propagation through individual models is difficult to evaluate. Hence, it is more challenging to determine which models within a multiscale framework should be refined to reduce the impact uncertainty or which models can be simplified to reduce the complexity of the process for initial design exploration purposes. Information economics can be used to strike the balance between the complexity of concurrent multiscale models and the loss of information in hierarchical multiscale models. These are very important practical considerations for tools for addressing uncertainty in materials design.

Efficient and effective means for uncertainty management must be integrated with the materials design strategy, and can be leveraged tremendously by incorporation of parallelized computational evaluations of process–structure and structure–property relations. Clearly, the parametric nature of the underlying modeling and simulation necessary to quantify sensitivity to variation of material structure must rely on increasing computational power to enhance feasibility and utility.
7. Verification and validation

Verification and validation were defined at the beginning of Section 5. In the context of ICME, pursuit of V&V consists of following activities:

1. Individual model V&V — single model focusing on single length and/or time scales.
2. Multiscale model V&V — single model or coupled set of models comprising a simulation operating over multiple length/time scales in concurrent or hierarchical manner.
3. Multi-physics model V&V — ensuring that the implementation of a modeling framework spanning multiple phenomena is consistent mathematically and physically.
4. Design process validation — ensuring that the configured design process will yield a solution that satisfies design requirements.
5. Design (outcome) validation — comparing design outcomes to system-level requirements.

It is noted that this decomposition is much broader than typical notions of V&V applied either to models or design processes.

7.1. Individual model V&V

Development of a computational model involves various steps such as conceptual modeling, mathematical modeling, discretization and algorithm selection, computer programming, numerical solution, solution representation [205]. Uncertainties and errors may be introduced during each of these steps. The process of verification and validation of simulation models is illustrated in Fig. 7. It consists of the following tasks [206]:

- **Conceptual model validation** (also called theoretical validation): process of substantiating that the theories and assumptions underlying a model are correct and that the representation of the system is reasonable for the intended simulation study.
- **Model verification**: process of assuring that a computerized model is a sufficiently accurate representation of the corresponding conceptual model.
- **Operational validation**: process of determining whether the computerized model is sufficiently accurate for the needs of the simulation study.
- **Data validation**: process of ensuring that all numerical data used to support the models are accurate and consistent.

Verification and validation of models has recently received significant attention in simulation-based design community. The Bayesian framework is one of the commonly adopted frameworks for model validation [207]. Bayesian techniques for model validation have also been extended to include epistemic uncertainty regarding statistical quantities [208]. Another widely adopted technique involves concurrently validating models and exploring the design space [209]. The traditional view of validation of simulation models is that if the outputs of the models are close enough to the experimental data, the models are valid. However, this view is much too limiting in ICME, which is characterized by a hierarchy of material scales and scales on designing novel materials that may not have been previously realized or characterized. Furthermore, it is essential to recognize that experimental data also have uncertainty. This uncertainty typically increases at lower scales owing to an interplay between spatial resolution of the measurement device/method and duration of measurement signal accumulation. In fact at the molecular level, the uncertainty in experiments due to signal resolution and accumulation may exceed that of models. It may be infeasible or too expensive to run the experiments for complete model validation before using them for design. Hence, validation activities and design activities need to be carried out in an iterative manner.

Models are used to guide design, and the design process guides the validation experiments. There is another validation-related challenge in ICME due to the focus on design. When models are developed and employed to design materials that do not exist, the models cannot be experimentally validated before the system is designed. Experiments are also characterized by epistemic uncertainty such as the lack of knowledge regarding the system configuration. Hence, validation using experiments must account for both aleatory and epistemic uncertainty associated with the experiments. In that sense, the distinction between simulation models and experiments is blurred.

Due to the specialized nature of models, their reuse is currently severely limited in ICME. It is generally assumed that someone who is familiar with the complete implementation details of the model is always available to customize or adapt the models for different scenarios. The notion of using models as black boxes is generally discouraged because their validity outside the ranges for which they are developed is unknown and generally undocumented. Currently, significant attention is not given to the reuse of models within ICME. While the models capture a significant amount of domain-specific knowledge, they are fragile in nature. Their fragility is not due to a non-robust implementation but due to a lack of documentation of their capabilities, scope of application, and limitations. Hence, the models cannot be used by system designers for integration into the design process as reusable, plug-and-play, “black box” units as might be desired for a robust methodology. As ICME develops we maintain that significant efforts are needed to embed knowledge and methods regarding the validity of models [210] so that they can be used by designers who may be generally familiar with the underlying physics but not familiar with all the internal details of the model and its implementation.

Finally, the validity of a model depends on its purpose. Model validation is effectively the process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model. As discussed in the uncertainty management section above, the designers may prefer to use simpler models during the early design phases to narrow down the design space. Hence, there is a need for different levels of scope, maturity and fidelity of models within the design process. There is a need for a classification scheme to classify models based on their scope and levels of fidelity [211], perhaps relating to a combination of model scope, readiness, and material length scale level of input/output structure. The systems designers can use this classification scheme in association with information economics constructs to choose appropriate models that are valid within a given application context.
Valid models for given characteristic length and time scales may not result in valid multiscale models across scales. Hence, multiscale model V&V is an important aspect of the overall V&V strategy, and very little attention has been devoted to it. Multiscale model V&V consists of two aspects:

(a) ensuring compatibility between the domains of validity for individual models, and
(b) estimating the propagation of uncertainty through the chain of models.

Compatibility assessment is the process of determining whether the domain of inputs of an upper-level model is consistent with the domain of outputs of the lower-level model. Individual models are generally valid within a domain of inputs. The input domain can be defined as a hypercube in terms of the lower and upper bounds on input variables \([x_{\text{lb}}, x_{\text{ub}}]\). The set of inputs within this hypercube generates an output domain, which can be non-convex with disjoint sub-domains. This output domain serves as the input domain to a higher-level model. Multiscale model V&V involves ensuring that the output domain of the lower-level model is a subset of the valid input domain of the upper-level model. Otherwise, the multilevel model would result in erroneous system-level predictions. Techniques such as support vector machines have been used for mathematically quantifying the validity domains of individual models [212].

The second aspect of multiscale modeling V&V is related to the effect of uncertainty propagation across a chain of models. Uncertainty in models at lower material length scales and/or in the process–structure–property mappings may be amplified as information flows from lower-level to upper-level models. Both types of chains are relevant to materials design, the first in terms of multiscale modeling and the latter in terms of multi-level design. The goal of V&V is to ensure that the effects of uncertainty at the lower-level(s) do not amplify beyond the desired uncertainty levels at which design decisions must be made. Uncertainty propagation can be viewed from both bottom–up or top–down perspectives. From the bottom–up perspective, the effect of lower-level uncertainties on system-level prediction is determined. From a top–down view, the allowable uncertainty in system-level predictions is used to determine the allowable uncertainty in lower-scale/level models.

7.3. Design process V&V

Design processes involve decisions regarding how to search the space of alternatives so that the design targets can be achieved at a minimum cost. It involves decisions such as how to decompose the design problem, how to reduce the design space, sequencing fixation of design parameters in iterations, which models to develop, how to invest the resources in achieving the design objectives, etc. These decisions affect not only the final design outcome but also affect the amount of effort required.

Analogous to model validation, where the goal is to ensure that models accurately predict the desired response, the goal of validating design processes is to ensure that a given design process will yield a solution that satisfies the design requirements. Design process validation is important to guide the selection of appropriate design methods and to support the development and evaluation of new methods. In simulation-based multilevel design, the design processes represent the manner in which the networks of decisions and simulation models are configured. One of the approaches for validating design methods is the validation square [213,214]. The validation square, shown in Fig. 8, consists of four phases:

1. **Theoretical structural validation**: Internal consistency of design method, i.e., the logical soundness of its constructs both individually and integrated.
2. **Empirical structural validation**: The appropriateness of the chosen example problem(s) intended to test design method.
3. **Empirical performance validation**: The ability to produce useful results for the chosen example problem(s).
4. **Theoretical performance validation**: The ability to produce useful results beyond the chosen example problem(s). This requires a ‘leap of faith’ which is eased by the process (1)–(3) of building confidence in the general usefulness of the design method.

7.4. Design (outcome) validation

Li et al. [215] argue that validation should be done on the design rather than computational models used to obtain them. The goal of design validation is to gain confidence in the resulting design (of the material) rather than the simulation model(s) used for design. Validation of the design involves determining whether the system as designed will perform as expected. The design outcomes are evaluated against the system-level design requirements. This is generally carried out using experiments.

8. Closure: advancing computational modeling and simulation to pursue the ICME vision

The vision of Integrated Computational Materials Engineering is compelling in terms of value-added technology that reduces time to market for new products that exploit advanced, tailored materials. This article addresses underdeveloped concepts/tools within the portfolio, as well as some important points regarding the contribution of multiscale modeling to the overall materials design process. Effectively, the role of computational modeling and simulation is so pervasive that the probability of success of ICME is inextricably intertwined with addressing certain scientific and technological “pressure points” as follows:

- ICME extends beyond informatics and combinatorics pursued at the level of individual phases, addressing hierarchical microstructures/structures of materials and embracing the “systems” character of integrating materials design with product design and development. An engineering systems approach is essential.
- Recognition of material structure hierarchy is of first order importance in multiscale modeling and multi-level materials design. Multiscale modeling and multi-level materials design are complementary but distinct enterprises, with the former serving the needs of the latter in the context of ICME.
Novel methods for inverse design including knowledge systems and process path design are underdeveloped and require attention.

Uncertainty is a pervasive and complex issue to address, with uncertainty quantification, propagation, mitigation and management carelessly distinguished. Improvement of physically-based models provides a promising foundational technology. Approaches to uncertainty that recognize and embrace the full complexity of ICME are in their infancy.

Integration of multiscale modeling and multi-level design of materials with manufacturing and systems optimization is essential to pursuing the vision of ICME.

In advancing methodologies and tools to address ICME, it is essential to maintain a consistent long term vision among industry, academia, and government. A critical assessment of prospects for progress towards the ICME vision in this regard was recently offered by McDowell [216]. ICME is an engineering-directed activity, requiring distributed, collaborative systems based design. Clearly, one consistent thread throughout the past two decades of developing this field of integrated design of materials and products is the trend towards increasing emphasis on the role of computational materials science and mechanics across a broad range of length and time scales, depending on application. Much is to be gained by extending beyond the conventional computational materials science community to incorporate important advances in multiscale modeling and design optimization in the computational mechanics of materials and structures communities, as well as the MDO and manufacturing communities. The tools and methods that are foundational to ICME effectively constitute the elements of an expanded ‘materials innovation infrastructure’ in the Materials Genome Initiative [16], as shown in Fig. 9.

Acknowledgments

JHP acknowledges financial support from National Science Foundation awards CMMI-0954447 and CMMI-1042350. SRK acknowledges support from Office of Naval Research (ONR) award N00014-11-1-0759. DLM acknowledges the support of the Carter N. Paden, Jr. Distinguished Chair in Metals Processing, as well as the NSF Industry/University Cooperative Research Center for Computational Materials Design (CCMD), supported by CCMD members, through grants NSF IIP-0541674 (Penn State) and IIP-541678 (Georgia Tech). Any opinions, findings and conclusions or recommendations expressed in this publication are those of the author(s) and do not necessarily reflect the views of the NSF or ONR.

References


Malak RJ, Paredis CJJ. Using support vector machines to formalize the valid input domain in predictive models in systems design problems. Journal of Mechanical Design 2010;132: 101001(1–14).


