

Probability and Materials: from Nano- to Macro-Scale: A summary

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Abstract

The National Science Foundation funded a workshop entitled “Probability and Materials: from Nano- to Macro-Scale” at Johns Hopkins University on January 5–7, 2005. The goal of this workshop was to bring together a diverse multi-disciplinary and multi-skilled group of researchers, all of whom have an interest in the application of probabilistic models to multi-scale analysis of materials. This paper provides a summary of the workshop discussions and provides an introduction to a selected set of technical papers that were presented during the workshop and appear later in this special issue. A set of recommendations for important future research in probability and materials was proposed by the group and is provided at the end of this paper.

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1. Introduction

In recent years advanced materials have been developed that have the potential to revolutionize structural design and which require the development of new methods in applied mechanics. This revolution has been inhibited by a lack of understanding of both the fundamental behavior of these materials at multiple scales (in particular the sub-micron or nano-scale), and the links between these scales. In order to develop multi-scale models that achieve appropriate characterization of material behavior, the inherent uncertainties in materials at all scales must be treated in an accurate and systematic way. One example of this is in fracture behavior, where phenomena at the local nano- and micro-scale have a significant impact on the failure of structures at the meso- and macro-scale. Though many meetings, i.e. those of professional societies, are devoted to structural reliability, very few events focus on the field of probabilistic analysis of materials. This is most

likely due to the multi-disciplinary nature of this field, which calls for collaborations between structural engineers, applied mechanicians, and materials scientists, as well as between researchers in experimental, theoretical and computational analysis. The traditional structure of professional societies and academic departments does not make such collaborations straightforward. The recent workshop, “*Probability and Materials: from Nano- to Macro-Scale*”, was intended to be a mechanism for developing connections between researchers in all of these areas. Furthermore, the workshop discussions were used to develop recommendations regarding important future research directions in the area of probability and materials.

The workshop was held January 5–7, 2005, at Johns Hopkins University in Baltimore, Maryland (USA). 28 participants attended the workshop:

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Sanjay Arwade, Johns Hopkins University
Sarah Baxter, University of South Carolina
Denys Breysse, University of Bordeaux
Jeff Bullard, National Institute of Standards & Technology
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 Victor Li, University of Michigan
 Christian Meyer, Columbia University
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 Martin Ostoja-Starzewski, McGill University
 Sharif Rahman, University of Iowa
 Ann Marie Sastry, University of Michigan
 Gerhart Schueller, Leopold-Franzens University
 Colby Swan, University of Iowa
 Ben Thacker, Southwest Research Institute
 Sylvie Yotte, University of Bordeaux
 Nicholas Zabarar, Cornell University
 Don Zhang, University of Oklahoma

Each of these participants provided technical presentations that described recent findings and proposed new challenges to the group. Beyond the development of collaborations between these participants, the major goal of this workshop was to provide for the benefit of the engineering community the current special issue of *Probabilistic Engineering Mechanics*, which contains selected technical papers from this workshop. In order to provide the context for these contributions, the current paper provides an overview of the workshop and summaries of the discussions that took place in the workshop.

At the end of each of the three days of the workshop, a discussion took place in which participants were asked to identify best practices and new fields of particular interest, applications in which improved understanding of material randomness will have the most impact, potential cross-disciplinary collaborations, how to couple experimental work with computational/analytical models, and obstacles that have hindered progress in understanding material randomness. The themes of the three days were as follows:

- Day1: General challenges in random materials/Theoretical & experimental studies of cementitious & geo-materials
- Day2: Stochastic simulation techniques/Studies at the macro- and micro-scale
- Day3: Micro- and nano-scale models of failure and composites

Each of the discussion periods was led by a discussion leader and the comments were recorded by a scribe. After the conclusion of the workshop, the leaders and scribes were asked to summarize the day's discussion. Furthermore, after the conclusion of the workshop participants were asked to provide written comments in response to the discussions. The scribes' summaries, supplemented by the participants' written comments, are provided in Sections 2–4 of this paper. Section 5 of this paper provides a list of recommendations to funding agencies for potential future research initiatives.

2. Day 1—General challenges in random materials/Theoretical & experimental studies of cementitious & geo-materials (Leader: M. Grigoriu; Scribe: D. Corr)

There were five important themes that emerged from this discussion, and a summary of the major points discussed for each theme are outlined in the following five sections.

2.1. Analysis of scales

Essentially all engineered and natural materials display variability on some length scale that affects the material's performance. Many materials, including concrete and other cement-based materials, exhibit variability across many length scales from the nano-scale to the macro-scale.

Although multi-scale modeling of materials is a challenge even in a deterministic context, it is more so when uncertainty is to be included. The discussion brought up several points related to length scales, their challenges, and how to incorporate them into stochastic models:

- A. For a given material, is there a length scale below which structural variability no longer plays a measurable or significant role in the performance of the material on the macro-scale? If so, how is this scale identified? Also, how can the relative importance of variability along length scales be determined? Wavelets have been proposed as a solution to this area; are there other possibilities?
- B. How should information be transferred across length scales? How can we quantify the information lost in this transfer? Mean values are important for average behavior, but outliers often have important effects on extreme event behavior such as fracture. How can we ensure the important peaks and valleys in material properties are maintained through the translation across length scales?
- C. How can the effect of small length scale variability on macro-scale properties be determined *experimentally*? It is extremely difficult to conduct tests that isolate nano-scale properties while monitoring macro-scale behavior.
- D. How can data be collected on small length scales? For experimental measurements, there is always a gauge length, and very small-scale processes cannot always be measured experimentally. A systematic method is required for accounting for the error, or approximation, introduced by the introduction of probabilistic models for material properties.
- E. Can models be developed that automatically change length scales to focus on large gradient areas? Such models could alleviate some of the data storage and computational power requirements for full descriptions of small-scale properties.

2.2. Relationship between mathematical models, experiments, and theory

The consensus among the discussion group is that the link between mathematical and stochastic models, experimental studies, and theoretical analysis is crucial to the progress of advanced material engineering. It is clear that there must be an interaction, where findings in one area confirm or provide data for the other. There is also consensus that we should strive to merge theory, models, and experiments into a more unified approach to science and engineering.

Significant discussion centered on the role of imaging technologies and their benefits and drawbacks. With the 2D and 3D imaging technologies available, we have the ability

to measure geometry on essentially any length scale. The limitation is that beyond geometry, imaging technologies are less useful. Image correlation and deformation mapping techniques can measure displacements and strains with good accuracy in certain conditions with proper images, but direct measurement of stress is not possible. It was also pointed out that imaging technologies are limited to measurement of the response to a mechanism, not the mechanism itself.

An interesting perspective offered by one participant was to question whether experiments could be used in a different way. Usually the results of an experiment are used to validate a computational model, or to provide input parameters for use in the model. It was suggested that analysis with a computational model should be the first step, and the model output should be used to suggest an experiment. In this paradigm, the model would identify the pertinent information and the experiment would collect it.

In summary, numerous participants urged a correct balance between mechanics and stochastic modeling. The two areas of study can be complementary, but with a lack of information we cannot use one as a substitute for the other.

2.3. Designing for performance—robustness

An important theme throughout the session was designing materials for specific performance criteria. This category includes the research areas of materials by design and reverse engineering of materials, with the theme of first defining which properties are required, and then designing a material to meet these criteria as efficiently as possible. In the area of engineered cement-based composites, a combination of micromechanics and random microstructures are used to predict properties of the fiber reinforced material. The resulting analytical model is then used for systematic tailoring of fiber, matrix and interface so that composite tensile ductility is achieved optimally (with minimum amount of fibers).

An important issue discussed is the uniqueness of the designed material for the given performance criteria. How can we assure that we have the optimal material for a set of desired properties? It is likely that there is not simply one unique material for each set of criteria, and this notion of uniqueness needs to be addressed.

Another note of caution focused on the relationship between robust design and optimal design, often competing values. If we are designing for a given set of performance criteria, we can design a material to optimally meet them. However, if the criteria are uncertain and are realized to be different than the mean values for which we have designed the material, or if the material is not manufactured exactly as planned, then the material is no longer optimized and may perform poorly. This indicates a lack of robustness, and the discussion group urged a balance between robust and optimal designs for performance.

2.4. Specifics to cement-based materials

As the focus of this day's session was cement-based materials, a number of specific points related to these materials were

discussed. Uncertainty is prevalent throughout concrete materials science: nano- to meso-scale structural characteristics; hardened properties such as strength, permeability and durability; and “human factors” such as workmanship at job sites including processing and finishing.

Some advances in concrete technology have passively reduced the uncertainty, such as self consolidating concrete (SCC). SCC is very flowable and requires less workmanship at the job site, which removes this layer of uncertainty in the material. Also, reinforcing concrete, either through traditional steel reinforcement or with fiber reinforcing systems, reduces the influence of the uncertainty in mechanical properties of concrete (although it may increase the model uncertainty that represents the steel and concrete as a whole).

Cement-based materials science provides an important venue for the development and use of probabilistic methods. Quality control and assurance are coming to the forefront of the concrete industry, fostered by incentive programs based on first and second moment statistics of the properties of the material delivered. As these incentive programs expand, more advanced probabilistic methods will certainly help to improve the overall quality of the products.

In all materials research, and particularly in the area of cement-based materials, collaboration between materials scientists and probabilistic methods researchers could yield very fruitful results. The potential utility of probabilistic methods is often unknown in the arena of materials science and experimental mechanics. For researchers in probabilistic methods, mathematics can only take the models so far; a connection to the fundamental materials science and experimental mechanics is necessary to ensure the link between mathematical models and physical realities.

2.5. Communication

Throughout the discussion, the issue of communication with the “outside world” was a recurring theme. Ultimately the probabilistic methods community is striving for determining and improving the safety and reliability in engineered systems. This has important implications to society: a mathematical description of the risks associated with a given engineered system is an extremely valuable piece of information. However, communicating and delivering these measures of safety are areas where the research community can improve.

It was noted that there are two classifications of problems we deal with: one where uncertainty propagates through a system and becomes magnified, and another where the uncertainty diminishes. Clearly the former is more pertinent to society, so we should strive to describe problems of this nature which truly underscore the importance of probabilistic methods. Many also noted the complexity of the problems we are attempting to solve and the phenomena we are modeling. It was suggested that we look for more simple problems with clearly defined outcomes where the utility of these methods can be communicated.

Another important point with regards to communication: we need to ensure honesty in the models we are proposing, such as using a continuous random field or continuous simulation

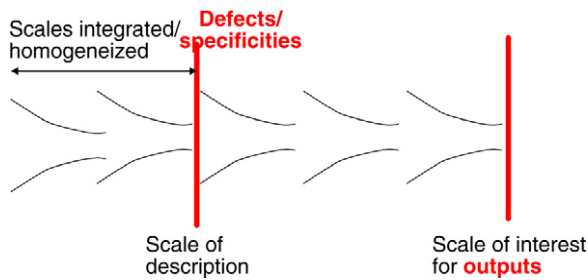


Fig. 1. Integration of information about various scales.

to describe a process that may in fact be discontinuous. An example of this is the elastic modulus in porous materials: the elastic modulus field is discontinuous, taking the value zero in the pores, so a continuous model for elastic modulus has an inherent flaw from inception. These types of approximations need to be well documented and described.

3. Day 2: Stochastic simulation techniques/Studies at the macro- and micro-scale (Leader: D. Breysse, Scribe: M. Gutierrez)

For this workshop, multi-scale modeling was a main topic of interest. The understanding of behavior at different scales is a key point for modeling as well as for experiments or data gathering. When looking at the multi-scale problem in materials (Fig. 1) it appears that the engineer is interested in outputs at a given macro-scale, that is relevant for engineering decisions (e.g. mechanical or physical properties), and s/he is ready/able to give specifications about the material properties at another (lower) scale, that of defects whose influence upon many scales will induce the macro-properties.

The materials scientist/researcher generally focuses on some aspects of multi-scale approaches, depending on his/her main concerns and fields of expertise. The focus area can be:

- data gathering and data analysis at micro-scale, in relation to observation at this scale,
- modeling and rebuilding of the material, i.e. development of numerical tools, algorithms and simulation schemes,
- simulation practice, with various purposes like the simple understanding and description of response (simulation being regarded as a way to improve the knowledge or to assist the experimental work, see Section 2.2), or more ambitious purposes like the prediction of response, for instance in reliability analysis or material design using optimization, robust design, etc., as discussed in Section 2.3.

In relation to the various ways to undertake research in multi-scale analysis of materials, some questions must be addressed, a non-exhaustive list being:

1. What is the scale of interest? What are the outputs of interest?
2. What is (are) the dominant scale(s)?
3. What are the dominant features for the dominant scale(s)?
4. What is the more efficient use of (validated) models?

5. Facing even more complexity, how to deal with time scales (as well for very short time scales, like in biological materials or chemistry, as seen in hydration modeling in cement pastes, as for very long time scales, like in aging problems).

It seems useful to highlight the arguments and proposals which have been given during the discussion, highlighting those which appear as of collective concern, or as tracks towards promising research developments.

3.1. Regarding the scale of interest

When it exists, this scale can be defined as that for which the phenomena have a major influence on the macro-scale response. Thus, one can consider that all phenomena/properties at lower scales are averaged over many scales and have therefore only little influence. The choice of the dominant scale is, of course, important, since it enables a good description/prediction of macro-response, allowing simplifications and efficiency of simulations. One main question is the choice of the scale and of the relevant data to describe, which obviously depend on what phenomena are considered. In many cases, this is a very complex question, either because one can have some interplay between scales and statistics of these scales, or because several scales can be dominant, like in geomechanics.

The main challenge is then the proper selection of the relevant scale, which often results from expertise, but lacks any formal criterion to validate/justify the choice. How can one be sure s/he has chosen the appropriate scale to capture all the consequences s/he wants to describe/predict? It seems we lack any “universal law” to give a simple answer, even if some tools, like wavelet analysis, can provide, in some situations, useful information about the contribution each scale has on the overall macro-response. The fact that we cannot rely on trial and error methods remains and that *there are insufficient mathematical tools to decide what is the dominant scale* leads to real questions that remain to be answered.

3.2. How can we (as experts of disordered/stochastic materials) prove that what we are doing is essential?

This question deepens the discussion from Day 1 regarding communication (see Section 2.5). This boils down to the identification of *problems for which the probabilistic/disordered description cannot be replaced by the usual deterministic description*. Fracture is one phenomenon for which probabilistic models are critical, and the consequences of fracture on structural reliability are large enough to justify the development of such questions. But other complex phenomena, in which the disorder plays an important role, can be quoted:

- *disorder can have positive effects*, for instance helping in avoiding resonance,
- *some interaction problems* (e.g., in soil–structure interaction) can be handled only through disorder descriptions,

- sound *reliability analysis* not only requires the development of an efficient algorithm but also the quality of inputs on the material variability. This is of major concern in civil engineering.

3.3. Validation of models

When micro–macro models are developed, one has to question the effect of additional (or more accurate) data on the quality of the output, or conversely, to address the effect of lack of knowledge. The sensitivity analysis often brings interesting information about the quality of models. Consistency of the data across the scales must be looked for, in relation with the question of dominant scales and with the objectives which are pursued. *The lack of collaborative research in the field of model validation is identified as a major challenge.*

In conclusion, the questions which are more frequently asked are very similar to those asked in the field of materials science (e.g. see books by Ashby & Jones): they consider data collection and analysis, modeling, validation and use of models. In the field of disordered media, independent of the kind of material (organic, mineral, metallic) or of the kind of properties, one can however identify some specific collective challenges to address in future work:

- the development of the theoretical framework and tools to answer the question of relevance of dominant scales, with consequences on the cost of data collection and validity of simulations,
- the undertaking of collaborative research programs facing the validation of models: a wide variety of models are developed and used in parallel, but little effort is devoted to comparing their merits,
- the identification of some specific practical fields (like interaction problems, or analysis of the influence of disorder on reliability) as the basis of collective developments, since for such problems, the description of the microstructural disorder can be bypassed and the added value of micro–macro models will be real.

4. Day 3: Micro- and nano-scale models of failure and composites (Leader: N. Zabar, Scribe: S. Arwade)

The theme of the third day of the workshop was modeling of failure in materials across the full range of length scales. Six presentations were made, covering topics ranging from the nano-scale to the macro-, or component scale. At the small (nano-) end of the spectrum, molecular dynamics simulations illustrated the importance of nano-scale stress concentrators such as inclusions, voids, or cracks in determining the overall strength and failure properties of macroscopic material samples. New material design results showed how the inclusion of nano-scale grains in polycrystalline microstructures with otherwise micron-scale grains, can dramatically improve both the strength and ductility of such materials. A series of three presentations addressed, at the micro- or meso-scale, the particular phenomenon of fracture initiation in spatially

heterogeneous and random materials. Finally, at the macro-scale, enhanced finite element simulations showed that the modeling of material properties (for example the elastic modulus) as random fields can successfully recreate known, random failure modes in ductile tension members.

Closing the day's session and the workshop as a whole was an open discussion period that proved wide ranging, yet delved deeply into many of the issues presented during the day. Discussion proceeded along two lines: issues in deterministic multi-scale analysis of materials, and issues in stochastic multi-scale analysis.

4.1. Multi-scale deterministic analysis

Several discussants emphasized that the need for better tools for multi-scale analysis exists even before the complication of uncertainty is added to the problem. This need for improved deterministic multi-scale techniques can be placed in the context of the overall societal need for materials with improved performance. One specific application, relevant particularly to civil engineers, is the need for highly durable, high-performance, infrastructure materials. A main direction of research in this area is that of high performance fiber reinforced cementitious composites (HPFRCC). In such materials, where traditional reinforcement is completely or partially replaced by small diameter, relatively short fibers, the material microstructure is of utmost importance in determining the overall properties, and, most importantly, the failure characteristics of the material. Whereas in traditional reinforced or prestressed concrete the zone of interaction between the steel and concrete is relatively confined, in HPFRCC these regions permeate the entire material. To allow the implementation of HFRCC in even standard structural engineering applications requires the modeling of mechanics ranging from microns (fiber diameter) to meters (structural length scales). An important adjunct to this observation is that it is critical in all multi-scale analyses to identify the scale at which no further information is being gained (cf Section 3.1). For example, in the case of HPFRCC, it is unlikely that the introduction of molecular dynamics simulations for the fiber material would add significant fidelity to any model for the behavior of the HPFRCC. On the other hand, in applications such as polycrystal plasticity, it is useful to include physics down to at least the scale of dislocations. Experimental techniques exist that can resolve material structure and behavior down to the nano-scale, and these tools must be used to guide the simulation community in limiting multi-scale modeling only to the scales of relevance to the particular problem.

A strong case was made that we find ourselves at a turning point in the application of simulation to problems in materials engineering and the prediction of structure property relationships. The significant advances to be made in the near future promise to transform the introduction of new materials by allowing so-called materials-by-design to come into use. An example from current research was given in which the creation of polycrystalline materials with grain sizes ranging from the nano- to the micro-scale has been guided by a combination

of experimentation and simulation, and has resulted in the creation of materials with unexpected combinations of strength, stiffness, and ductility. Because of the widely varying length scales in such materials, their design cannot be accomplished without reliable, deterministic, multi-scale analysis methods.

4.2. Multi-scale stochastic analysis

One of the main challenges even in deterministic multi-scale analysis is the passing of information between the different length scales of the problem. This issue is even more acute when the analysis becomes stochastic. Another exacerbating feature of the problems discussed in this workshop is that they often entail what can be described as uncertainty magnification. That is, the uncertainty of the response of interest—strength, fatigue lifetime, etc.—can exhibit uncertainty that is much larger than the uncertainty associated with the input or system parameters—material property fields, applied load, etc. Uncertainty magnification is particularly prevalent in problems that involve highly non-linear phenomena such as fracture. Since material failure is a fundamentally non-linear phenomenon, the effects of uncertainty magnification cannot be avoided in most limit state based design problems. Even a relatively small uncertainty in local material properties, for example, may lead to a large uncertainty in the overall component strength.

Wavelet analysis and the use of information theory are two approaches that were mentioned as possible routes to solution of the problem of information passing between length scales in stochastic multi-scale problems. Wavelets have the advantage of naturally capturing behavior at multiple length scales in a way that is amenable to implementation in a multi-scale simulation. Information theory, on the other hand, has the inherent ability to handle extremely large amounts of data in highly efficient ways. This is particularly useful in stochastic multi-scale analysis as the small-scale simulations (molecular dynamics, for example) have the tendency to generate very large data sets. Information theory may provide the tools for interpreting these data at higher scales, and thus serve to propagate this information along the path of the multi-scale analysis.

Three other points were raised with respect to the passing of information between scales of a multi-scale analysis and validation of models (see Section 3.3.). First, new mathematics must be developed that quantify, in a rigorous way, the error associated with each stage of the analysis. Second, these mathematics should lead us to provable statements regarding the convergence properties of these stochastic multi-scale analysis tools. Such proofs of convergence are substantively lacking even from many commonly used stochastic finite element (SFEM) implementations, and the lack of such convergence proofs considerably hampers the wider acceptance of these methods. Third, the focus of uncertainty modeling at this workshop has been overwhelmingly on the side of modeling physical uncertainty, for example, spatial variability of material properties. Another significant source of uncertainty is model uncertainty, the so-called epistemic uncertainty. The treatment of model uncertainty may be particularly important

in stochastic multi-scale analysis since such uncertainty can propagate across scales as error or information loss. Since the problems of interest to stochastic multi-scale analysis are often ones that exhibit uncertainty magnification, the propagation of non-physical model uncertainty can be particularly detrimental to solution accuracy.

It was lastly emphasized that the underlying assumptions of current SFEM technology are largely untested, for example, the assumption that underlying structural material properties can be represented by random fields. Since the emerging stochastic multi-scale approaches are in some sense building upon the extensive SFEM framework already in place, the lack of verification of these assumptions is troubling. Thus, there is a tremendous role for experimentalists to play in extending our understanding of the behavior of structural materials across length scales by verifying current assumptions about material modeling and identifying new properties of materials to be incorporated into numerical models.

5. Potential funding agency ideas

In addition to the above comments and questions that were raised during the discussion, many specific ideas were mentioned as topics that are deserving of support from governmental funding agencies. This list of ideas may form the basis of a discipline-wide white paper formulated to make a case for requiring increased support of research in the area of stochastic multi-scale material design and analysis. The suggestions fell into four general themes, as listed below:

1. *Joint experimental/stochastic mechanics research:* Stochastic modeling at the macro-level requires explicit knowledge of the statistical descriptors for key material parameters. As of today, most of the work in this area does not provide any systematic way for estimating such descriptors, such as correlation lengths, n th-order correlation functions, etc. Computing such information from both experimental and from the micromechanical point of view is very important to identification of critical scales. The role of experiments is central—not only as the means to verify stochastic models but to provide information when models cannot work due to either insufficient information or a high degree of complexity. A dynamic experimental/computational framework needs to be developed for analysis and design of solids. A potentially successful effort along these lines might be to formulate a research team of both theoreticians in stochastic mechanics and experimentalists, which is focused on a single material (e.g., concrete, geomaterials, composites). In this way, the investigation could be placed on a firm footing of observations and verifications.
2. *Advances in stochastic modeling at specified scales:* Issues of representation of heterogeneities in materials are important. Without the ability to model full statistics at each length scale, it will be difficult to investigate statistical information passing across length scales. How do you model microstructural variability, how do you classify microstructures

and how do you use a classification scheme for model representation and for exploring structure/property/process relations? It is important to develop techniques that would enable models of microstructure evolution to develop. It is a major challenge to develop models within a given physical scale that allow computation of solutions at various scales of resolution (e.g., in modeling dendrites in solidification, or in predicting the development of shear bands in geomaterials).

3. *Advances in stochastic multi-scale modeling:* Classical (deterministic) homogenization techniques do not always make sense for materials applications. For example, fracture of a two phase grain structure cannot be addressed by homogenizing the structure and then applying linear fracture mechanics to the homogenized material. Stochastic techniques to address such discontinuous processes need to be developed; the term “stochastic homogenization” may therefore imply something completely different from classical deterministic homogenization. A challenge to developing such techniques is that statistics generated in different length scales are not separable—e.g. one cannot make independent assumptions as to the variability of material descriptors at the macro- and meso-scales. For example, in fibrous composites a region of higher elastic modulus at the macro-scale is suggestive of a more dense distribution of fibers at the micro-scale. Issues of compatibility of data across length scales are important in particular when different physical and mathematical models are used in different scales (e.g. Boltzmann lattice methods vs. Navier–Stokes equations). Some possible frameworks for developing such models include information theory, the application to solids of stochastic variational multi-scale methods (currently under development in fluid mechanics), stochastic finite element methods, spectral stochastic methods, or moving-window/local homogenization techniques in connection with stochastic simulation. Such methods need to be developed because they provide a consistent mathematical framework connecting statistics across length scales.

4. *Expansion and validation of stochastic modeling techniques:* In general, one needs many methods for representing uncertainty. There is not one unified method applicable to all materials problems. For example, discontinuous processes, bifurcations, multiple equilibrium states, etc. cannot be modeled with spectral or other series expansions. A critical

step to implementation of any stochastic model is to provide proofs of convergence and error estimates. Issues of verification of stochastic models are unresolved (too few data are available even for simple problems). Work is needed to address these mathematical issues to allow wider but correct use of these tools in multiple applications. In addition, development of parallel solvers, domain decomposition methods, etc. constitutes an unexplored area. Synergies with other fields need to be explored: Bayesian and spatial statistics work using data across length scales; selection of Markov random fields using physical length scales is important for inverse modeling and parameter estimation (e.g. estimating permeability); sampling techniques, Markov chain Monte Carlo simulation, hypothesis testing, need to be explored.

6. Conclusions

From each of the days described above, technical papers follow in this issue. Day 1’s focus on cement-based materials came from an experimental perspective (Li & Wang), a modeling perspective (Duprat & Sellier), and efforts to link experiments and models (Corr et al.). Day 2 had an emphasis on stochastic simulation (Koutsourelakis), on macro-scale material randomness (Elachachi et al.), and micro-scale material randomness (Williams & Baxter). Day 3 moved the focus down to the micro-scale (Gutierrez, Ostoja-Starzewski & Wang) and the nano-scale (Frantziskonis & Deymier).

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