# UNCERTAINTY QUANTIFICATION IN COMPUTATIONAL SOLID AND STRUCTURAL MATERIALS MODELING

AUTHORS: MICHAEL D. SHIELDS AND B.S. AAKASH

ORGANIZING COMMITTEE: MICHAEL D. SHIELDS, LORI GRAHAM-BRADY, SOMNATH GHOSH, MICHAEL FALK

The Uncertainty Quantification Technical Thrust Area (UQ-TTA) of the United States Association for Computational Mechanics (USACM) and the National Science Foundation (NSF) sponsored the Thematic Conference on Uncertainty Quantification in Computational Solid and Structural Materials Modeling. The conference was held January 17-18, 2019 on the campus of Johns Hopkins University in Baltimore, Maryland.

**GOAL:** Bring together prominent scholars in solid and structural mechanics, materials science, and applied mathematics with a shared interest in uncertainty quantification and computational material modeling to exhibit the state-of-the-art, collectively identify existing and future challenges, and promote promising new ideas in the field.

**FOCUS:** Understanding and quantifying uncertainties in material structure and behavior and propagating these uncertainties through computational material models. This theme encapsulated uncertainty in material performance at and across all length-scales (from atomistic to structural scale) with interest in performance across diverse structural materials ranging from concrete to metals, composites, ceramics, glasses and many others. Emphasis was placed on bringing together experts in UQ with experts in mechanics/materials who recognize the need for UQ and the challenges associated with its implementation.

**THEMES:**

Stochastic modeling of materials
Data-driven modeling and machine learning
Design and optimization for materials
Multiscale material modeling

**SESSION DETAILS:** Each session consisted of three or four 25-minute technical talks plus a 20-minute discussion period. The intention of this report is to briefly review the technical presentations, highlight major research themes/areas that emerged from the discussion, and shed light on future directions in the field.

**PEOPLE:** 26 invited speakers, 23 student posters, and 85 overall participants.

**MORE INFO:** Further details and links to several presentations can be found on the conference webpage: http://uq-materials2019.usacm.org.

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## Introduction

The performance of structural materials is strongly influenced by uncertainties associated with composition, constituent properties, and defects. This is especially true as materials approach failure and undergo large inelastic deformations, fracture, and fatigue. Computational modeling of these materials is further complicated by uncertainties in material model-form (e.g. incomplete physics), lack of data to quantify material structure and/or property distributions, and computational cost of uncertainty analyses among other challenges.

The USACM Thematic Conference on Uncertainty Quantification in Computational Solid and Structural Materials Modeling brought together a group of multidisciplinary experts with shared interest in the problem of uncertainty quantification (UQ) in materials modeling, and/or various aspects of it. As such, the conference was composed of leaders from academia, government/national labs, and industry with expertise varying from applied mathematics to mechanical engineering, civil engineering, materials science, data science, machine learning, and computational science. The conference featured a total of 26 invited speakers, who were carefully selected to fit the specific themes of the conference.

The sessions of the conference were dedidated to four primary themes:

1. Stochastic modeling of materials
2. Data-driven modeling and machine learning
3. Design and optimization for materials
4. Multiscale material modeling

with, of course, the emphasis being placed on uncertainty quantification within each of these themes. The conference was scheduled in seven sessions with two sessions dedicated to stochastic modeling of materials (one related to methodology and one related to material failure), one session each of data-driven modeling/machine learning, and design/optimization, and three sessions dedicated to multiscale material modeling (one each focusing on lower-scale and upper-scale modeling and one focused on bridging lengthscales). Each presenter was given 25 minutes to share their research related to the session theme and questions were held until the end of each session. At the end of the session, the floor was then opened to all speakers for a discussion, moderated by the session chair, on the primary research challenges related to the session theme, future directions for the field, and any specific questions related to the presentations. To foster this conversation, each speaker was asked to conclude their presentation by identifying a few future research directions related to the topic of the session.

The intention of this report is to provide a detailed review of the conference, the research presented, the discussions that ensued, and the primary takeaways related to the future of research in uncertainty quantification for materials modeling. The report is structured according to the conference program, with a section dedicated to each session. Within each section, a short review of each presentation is made. This is followed by a brief summary of the discussion for that session, and some insights are expressed related to future research in this area. Following the review of each session, we provide some global insights gained related to the main takeaways from the conference, emerging themes, and needs for future research.

## Session 1: Stochastic modeling of materials: Methodology

***Session Chair:*** **Vissarion Papadopoulos**, *National Technical University of Athens*

***Presenters:***

1. **Johann Guilleminot**, *Duke University*, "A Tour of Stochastic Modeling for Materials Science and Multiscale Analysis." (Presented remotely)
2. **George Deodatis**, *Columbia University*, "Reflections on the Use of Monte Carlo Simulation in Stochastic Mechanics." (Absent due to illness)
3. **Martin Ostoja-Starzewski**, *University of Illinois – Urbana Champaign*, "Tensor Random Fields in Continuum Mechanics."
4. **Michael Ortiz**, *California Institute of Technology*, "Optimal Uncertainty Quantification with Focus on Material Uncertainty."

***Overview:***

The objectives of this session were to discuss advances in methodologies for stochastic modeling of materials. This includes methodology related to simulation of random fields (scalar, vector, and tensor-valued and often on complex geometries) as applied to generating microstructure and parametric material properties such as those defining a constitutive model. Particular emphasis was placed on ensuring these synthetically generated quantitites satisfy mathematical constraints related to the solution of stochastic partial differential equations (SPDEs), physical constraints related to continuum balance laws and constitutive models, as well as constraints related to identifiability (i.e. from small data) and stochastic dimension.

Further objectives related to presenting methodology for uncertainty propagation in materials modeling. This include the propagation of parametric uncertainty through models of materials systems at various scales (and across scales) as well as the propagation of uncertain information in order to establish bounds on probabilistic quantities of interest (e.g. for design purposes).

Talks in this session presented an overview of some recent advances and challenges in stochastic modeling of materials, and rigorous UQ accounting for uncertainty in material parameters. The talks touched upon issues such as modeling non-Gaussian quantities on complex geometries, modeling tensor-valued coefficients in stochastic partial differential equations for materials systems, incorporating physical consistency in the generated random fields, and randomness introduced by lack of separation of scales. The talks also discussed propagation of uncertainties in materials in order to establish optimal upper bounds on the probability of failure using estimated function means and diameters.

Wide-ranging materials applications were given and included quantification of tensor elastic quantities from multiscale simulations (micro-to-meso-to-macro), quantifying non-Gaussian tensor quantities from molecular dynamics simulations, crack propagation using phase field modeling, multiscale structural modeling, human artery modeling, data-driven modeling of hyperelastic laminated composites, and ballistic impact in ductile metal plates.

***Review of Presentations:***

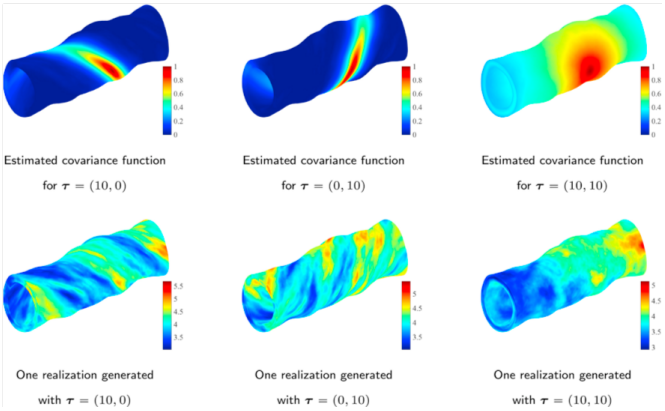



Figure 1: Estimated covariance functions and realizations of non-Gaussian random fields on an artery wall.

**Presentation 1: Johann Guilleminot** "A Tour of Stochastic Modeling for Materials Science and Multiscale Analysis."

*Problem setting/ motivation:* Uncertainty quantification in computational mechanics requires development of approaches for modeling, simulation, identification, and validation of stochastic constitutive models, on complex geometries, with spatially varying coefficients in stochastic partial differential equations (SPDEs), and non-Gaussian models for probabilistic parameters.

*Background theory:* Models are admissible if they satisfy all mathematical requirements of the problem, imposed by the relevant mechanics principles.

Within a class of admissible models, it is necessary to choose a model while accounting for physical consistency, subject to identification constraints. After a model is chosen, it is also necessary to validate it for the intended purpose. Random material parameters which need to be generated could be non-Gaussian, vector- or tensor-valued, statistically dependent, in addition to being spatially dependent.

*Methodology:* To generate non-Gaussian random fields, one approach is to use a translation process. The Gaussian germ for the translation process is obtained as the solution of a spatial SPDE solved by a Galerkin numerical method. Since the precision matrix for Gaussian fields generated in such a way is full, computing its Cholesky decomposition during calculations is expensive. To overcome this problem, a suitable approximation is made of the Gaussian fields by a Gaussian random Markov field, which has a sparse precision matrix. The methodology for sampling these Gaussian fields on manifolds was extended to sample on complex geometries. The methodology also allows generation of locally anisotropic fields. The non-Gaussian fields obtained by translation also inherit these properties.

*Examples & results:* Several examples were presented showing methodology for use in multiscale simulations. One example dealt with probabilistic multiscale modeling of a nanocomposite. Another example concerned probabilistic multiscale modeling of crack propagation. The objective was to model crack propagation with a mesoscale phase field approach. A third example considered coupling structural analysis with a multiscale solver to enable multiscale-informed structural analysis. Polynomial chaos expansion (PCE) based nonlinear upscaling was performed to achieve consistency in propagating the uncertainty.

Another example concerned modeling of human arteries, with patient-specific geometries. Non-Gaussian fields of elastic properties with anisotropy and specific signatures were able to be generated on complex geometries. Uncertainty in the random fields was propagated through finite element simulations which showed that there was large fluctuation in the von Mises stress caused by fluctuations in the elastic fields. The last example related to stochastic modeling of a laminated composite and identification of a hyperelastic constitutive model for the material.

*Conclusions:* Recent development of probabilistic methodologies were presented for non-Gaussian models for material properties, and multiscale probabilistic modeling for materials. The feature was that the methodologies presented used physics based models satisfying all mathematical requirements.

*Future Research Directions:* Prof. Guilleminot highlighted some important challenges and future research direction, such as:

- Methods to handle model uncertainties need to be adopted. He suggested that a Bayesian framework can be used for this.
- Small datasets introduce large uncertainty in identification of parameters.
- Factors such as age can change the properties of the arterial walls. Is it possible to perform Bayesian updating of the random fields to account for these changes?

**Presentation 2: George Deodatis** "Reflections on the Use of Monte Carlo Simulation in Stochastic Mechanics."

George Deodatis was absent due to illness, so the presentation was not given.

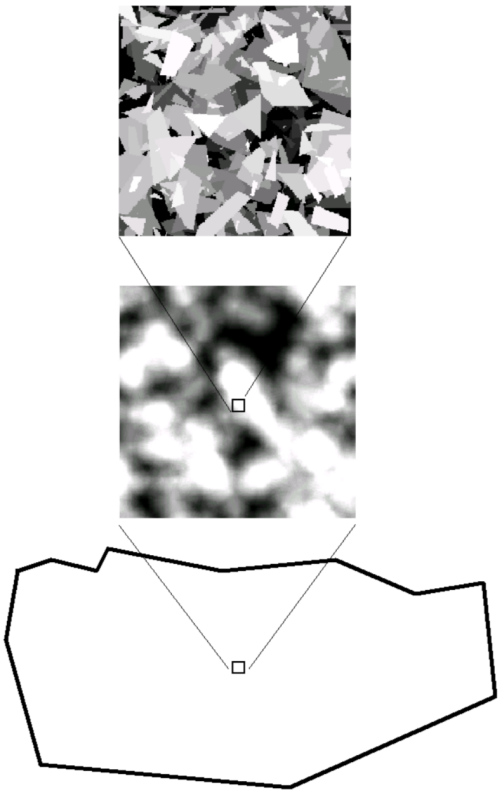


Figure 2: Three length-scale in multi-scale modeling of materials: Microscale / Microstructure (top), Mesoscale SVE (middle), Macroscale RVE (bottom).

**Presentation 3: Martin Ostoja-Starzewski** "Tensor Random Fields in Continuum Mechanics."

*Problem setting/ motivation:* In order to represent the random microstructure of materials in continuum mechanics, it is necessary to generate random fields with, for example, spatially homogeneous and ergodic statistics. For tensor-type properties of materials, it is necessary to generate tensor random fields (TRFs) with various anisotropies. TRFs are also needed as inputs into stochastic partial differential equations (SPDEs), stochastic finite elements (SFEs), etc.

*Background theory:* In continuum mechanics, it is of particular interest to infer homogenized material properties at a higher scale from random microstructure (i.e., tensor random fields). To do this, it is essential to adopt the correct variational principles and positive-definite properties. In the problem under consideration, there are 3 scales (see Figure 2): 1. microscale (at the level of the microstructure); 2. mesoscale (statistical volume element or SVE); and 3. macro scale (representative volume element or RVE). But in general, there is lack of separation of scales, so there may also be randomness in the transition between scales.

A TRF is a mapping from the material space to a vector space. As such, TRFs must satisfy certain restrictions on: 1. dependencies between quantities such as displacement, velocity, deformation, rotation, stress, etc, dictated by continuum balance laws; and 2) constitutive responses such as conductivity, stiffness, etc, dictated by microphysics/micromechanics and positive-definiteness for conservative and dissipative phenomena.

*Methodology:* Use is made of the Hill-Mandel condition, which states the equivalence of energetic and mechanical definitions of Hooke's law. The Hill-Mandel condition leads to consistent upscaling from lower to higher scales. Currently, as inputs to SPDEs or SFEs, use is made of either TRFs of locally isotropic properties, or TRFs with rather simplistic or no spatial correlations. The approach to improve on this practice was divided into two tasks: 1. Use wide range of mathematical morphology models, which might include local anisotropy, for real materials to go from microscale to mesoscale; 2. Develop statistically isotropic TRFs with local anisotropy, having the most general correlation functions. This can then be generalized to statistical anisotropy and inhomogeneity.

*Examples & results:* Representations of statistically isotropic TRFs up to rank 4 were presented. Examples included formulations of in-plane conductivity problems, anti-plane elasticity problems, and plane stress problems. Especially, TRFs for the constitutive tensor in elasticity were shown. With 29 functions, one can cross-correlate and autocorrelate between all components of the 4th rank constitutive tensor in elasticity.

*Conclusions:* The primary conclusions emphasized the need for TRFs at micro- and mesoscales. The use of the Hill-Mandel condition leads to consistent definitions of these TRFs, which are functions of the microstructure and the mesoscale.

*Future Research Directions:* Prof. Ostoja-Starzewski identified two critical questions related to TRFs in multiscale materials modeling:

- Can a unique mesoscale TRF be defined?
- How different is the solution for the mean field from the solution of a stochastic boundary value problem at the macroscale?

Addressing these two questions will provide critical insights into stochastic multiscale modeling of materials.

**Presentation 4: Michael Ortiz** "Optimal Uncertainty Quantification with Focus on Material Uncertainty."

*Problem setting/ motivation:* The overall picture is that there is a system (i.e., a black box) that has to be designed, which has random inputs and maybe some unknown unknowns (i.e., unknown inputs), has a response function $f$ which might be unknown, and has a set of outputs. Safe design of the system means to ensure, with some confidence, that the value of outputs are in some admissible set (i.e., probability of failure of the system should be below the tolerance for sure). This essentially means the upper bound on the probability of failure must be established.

*Background theory:* Exact probability of failure can, in theory, be obtained by integration. But practically this cannot be done because of several issues – namely, the priors are never known exactly and the response function of the black box system is unknown. So, it is desired to estimate an upper bound on the probability of failure (PoF) of the system and use this upper bound but not the exact computation

of the probability of failure. These bounds do not require the distribution of the inputs. Good candidate upper bounds for use are the Concentration of Measure (CoM) upper bounds, which are described to have a "Blessing of Dimensionality."

*Methodology:* There are several CoM upper bounds, and one such bound uses the "diameter". Diameters are the least possible upper bounds. Calculating the bounds needs only two quantities - function mean and function diameters. Usually these are both unknown and have to be estimated. The diameter plays the role of uncertainty and these bounds give a very clear definition of uncertainty and safety margin.

*Examples & results:* An example application of the method for the problem of simulation of ballistic impact of Magnesium plates was presented. The objective was to design the protective Mg plate against sub-ballistic threats simulated using LS DYNA. A Johnson-Cook (JC) model was used to represent the material. The design criterion was that the calculated indentation must be less than the maximum allowable indentation. It was assumed that all the uncertainty budget was consumed by the material model. Experimental data shows considerable scatter in the penetration depth. The JC model fit the data but, due to the scatter in the data, there is considerable uncertainty in the JC parameters. A range of JC model parameters was chosen such that there was a given coverage (say 95%) of the data. Bounds on the probability of failure were then computed for any given coverage of the data.

*Conclusions:* CoMs supply rigorous upper bounds on PoF of complex systems. CoM PoF bounds result in conservative designs. CoM UQ is non-intrusive. That is, it can be implemented as a wrapper around standard simulation workflows.

***Discussion:***

Questions and the subsequent discussion addressed some important issues related to stochastic modeling methodology as follows.

One question raised the difficulty of making measurements for material properties at the microscales in comparison to characterizing material microstructure by imaging. As such, what are the implications of this for multiscale modeling?

The speakers acknowledged that, while it is true that making measurements of material properties at microscale is difficult, models need to be calibrated/validated against measurements. So, the path in a multiscale approach might be to make measurement of properties at the mesoscale directly and use homogenized models at the mesoscale. It was also pointed out that while homogenization is a powerful tool in multiscale modeling, if homogenized properties from the micro- and mesoscales are used in larger scale simulations, this leads to loss of the ability to capture localization. In many materials such as quasibrittle materials, the main behavior is governed by localization. Consequently, homogenization schemes which do not allow localization to manifest must not be used for such problems. In addition, if there is no scale separation, then the homogenized properties are stochastic. Considering these facts, the relevance of the methodology and models to be used for each problem must be carefully considered.

One participant observed that, while it is rational and rigorous to employ bounds which are independent of the probability distribution of the parameters to represent uncertainty in the parameter values, it is well known that such bounds are usually quite wide. This raises the question of whether these bounds be sometimes too wide to be practical?

The speaker replied that, while being overly conservative leads to economic losses, being overly optimistic might lead to loss of life, damage to environment, and also have economic losses. The quest is to obtain tight upper bounds which are robust. One approach is to estimate the optimal bounds that can be computed given all the information available (data, knowledge of the system, etc.) using methodologies such as "Optimal Uncertainty Quantification". This is computationally demanding and requires a global optimization problem to be solved. The effort might be justified in critical applications where having high confidence in probability of failure estimates is necessary. Using bounds results in rigorous definitions of margins and uncertainties, and establishes rigorous upper bounds on probability of failure computations. Since there can be a lot of uncertainty about probability model form and parameters, especially when there is lack of data, using bounds provides rigorous estimates with high confidence.

Another question raised the possibility of using the Weibull distribution to establish a tight upper bound. It was observed that in quasibrittle materials, the Weibull distribution generated by the weakest link model has the highest estimates of probability of failure. While the Weibull model might not

be the best in estimating the tail risk of quasibrittle materials, it always provided the highest values of the probability of failure. But since this is currently an observation, without a formal proof that this is always true, it might not be justified to make this assumption.

Another remark was that advances in other relevant fields such as statistics and mathematics must be utilized to solve challenges posed by the problem of UQ for computational mechanics and material modeling.

***Emerging Themes & Future Research:***

Several important themes emerged from the session, which motivate the need for future research into specific questions related to stochastic modeling methodology for materials. Some of these themes are summarized herein.

*Physical/Mathematical consistency of stochastic quantities in materials modeling:* A primary challenge that emerged is the ability to develop stochastic models (i.e. scalar, vector, and tensor valued random fields) that are consistent with physical conservation laws, experimental observations, and necessary mathematical principles. This poses significant challenges for modelers – especially when the relevant features are non-Gaussian, anisotropic, statistically heterogeneous, discontinuous (or discrete) and time-variant. These challenges were emphasized by both Prof. Ostoja-Starzewski and Prof. Guilleminot. In the coming years, it will be imperative to develop novel methods for simulating/generating random fields that meet these rigorous conditions.

*Model-form uncertainties, small datasets, and model uniqueness/identifiability:* While these can be viewed as three distinct themes/challenges, their relations are important and, for this reason, they are discussed together here.

In the computational modeling of materials, the form of the mathematical model used as an abstraction of the physics is governed by both theory/first principals and available data (both computational and experimental). Existing theory may be insufficient to fully describe the mechanisms of interest and data from experiments/simulations are often sparse. This poses significant research challenges that can be broadly cast as "model-form uncertainties." There are many unresolved research challenges related to model-form uncertainties, which were discussed in each of the presentations in this session. New mathematical frameworks are needed to account for model-form uncertainties that result from theoretical limitations. Small data cases pose particular challenges for model selection. Prof. Ostoja-Starzewski in particular highlighted the challenges associated with model uniqueness and identifiability – Can we even uniquely identify stochastic models from the data we have available? Prof. Guilleminot suggested that Bayesian methods are particularly well-suited to the problem of model selection and parameter identification from small datasets, but new developments along these lines are imperative. Meanwhile, Prof. Ortiz proposed a robust framework that is intended to provide rigorous theoretical bounds regardless of dataset size and suggested that future research should seek to ensure that such bounds can be attained. The overarching conclusion was that research to resolve these issues remains relatively immature and there is a strong need for methodological advances that address model-form uncertainties.

*Lack of scale-separation and localization:* Some attention was given to problems which lack a clear separation of length-scales. This issue was only touched on briefly, but poses considerable challenges for uncertainty quantification efforts. Most notably, localization effects result from this lack of scale-separation. While localization was a topic of conversation during the discussion in Session 1, it was major theme of Session 2 so discussion of future research along these lines will be reserved for that section.

*Integation of UQ methodology into design settings:* Through his proposed methodology, Prof. Ortiz raised the important general issue of incorporation of UQ methodology into a design setting. While Session 4 specifically dealt with UQ in design, the challenges posed here related to UQ methodology development. It was clear from the presentation, and the ensuing discussion, that new robust methodologies that provide rigorous bounds on performance, yet are not overly conservative are of increasing importance.

## Session 2: Stochastic modeling of materials: Material failure

***Session Chair:*** **Ernest Chin**, *US Army Research Laboratory*

***Presenters:***

1. **Jia-Liang Le**, *University of Minnesota*, "Stochastic Modeling of Damage Localization in Quasibrittle Materials."
2. **Yongming Liu**, *Arizona State University*, "Stochastic Non-local Lattice Particle Method for Voxel Level Uncertainty Quantification and Material Failure analysis."
3. **Jie Li**, *Tongji University*, "Stochastic Damage Mechanics: Developments and Recent Progress." (Presented by Prof. Xiaodan Ren.)
4. **Mircea Grigoriu**, *Cornell University*, "Estimates of Extreme Material Responses for Random Microstructures."

***Overview:***

The focus of this session was on quantification of uncertainty in material failure processes. While a considerable amount of research has been performed over the years to quantify uncertainty in elastic and other linear properties of material through, for example homogenization techniques, questions related to uncertainties in material nonlinearity, damage mechanics, localization, and other processes related to material failure remain largely unanswered. This is especially driven by the fact that micromechanical mechanisms that drive material failure processes are governed by localized phenomena the correspond to rare events, or those associated with the tails of probability distributions. These phenomena are difficult to simulate at the microscale (due to their statistical rareness and the complexity of these mechanisms) and cannot be readily modeled in larger-scale simulations due to the fact that their highly local nature suggests a lack of scale-separation.

Presentations in this session dealt with these challenges from a variety of perspectives: the challenges of simulating microstructures for material failure analysis, addressing mesh dependence in simulations of localization, macroscale stochastic modeling of materials undergoing damage growth, as well as simulations and extreme values statistics for rare events. These presentations combined provided a rich perspective on the challenges and opportunities for research in stochastic modeling of material failure.

***Review of Presentations:***

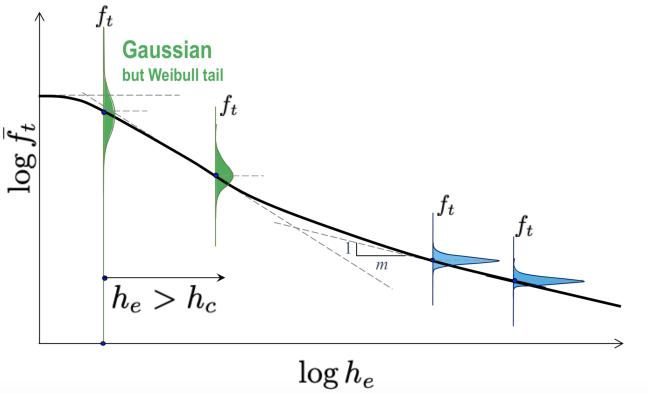



Figure 3: Depending on the localization level, the input probability distribution of tensile strength $\bar{f}_t$ varies with the mesh size $h_e$ — transitioning from a Gaussian cdf to a Weibull cdf.

**Presentation 1: Jia-Liang Le** "Stochastic Modeling of Damage Localization in Quasibrittle Materials."

*Problem setting/motivation:* The focus of the presentation was on quasibrittle materials, which often exhibit strain softening behavior. This results in loss of ellipticity of governing equations (i.e., loss of mesh objectivity in continuum FE) due to the development of a strain localization instability.

*Background theory:* Two existing methods are widely used to treat strain localization: 1. Crack band model and 2. Nonlocal continuum modeling. To date, these two methods have been only applied for deterministic simulations. In a crack band model,

there is a transition from damage initiation to damage localization. This presentation discussed the development of a probabilistic crack band model. In probabilistic finite element analyses, the mean peak value of the strength decreases as mesh element size is lowered (because there is a higher probability of extreme values of strength being sampled). This size effect seen here is not physical. So, there is a need to ensure objectivity in the developed probabilistic crack band model.

*Methodology:* In the proposed model, there is a probabilistic treatment of random onset of the localization band. Inception of localization occurs around the peak strength. The location of the localization band is determined by the material strength, which exhibits certain spatial randomness, and whose distribution depends on mesh size (see Figure 3). The number of potential crack bands is governed by the localization level.

*Examples & results:* Two examples were presented. The first example considered stochastic discrete element simulations at fine scale, with random fields for strength and fracture energy. Results at several element sizes at the micrometer scale were presented. The second example considered the probabilistic crack band model with a structure subjected to three loading conditions. The three loading cases were tension, pure bending, and three point bending. The results showed how using this method mitigated the mesh size dependence.

*Conclusions:* Stochastic FE simulation of quasibrittle fracture requires special attention on how to numerically treat the strain localization phenomenon in a smeared continuum model. Two important aspects to consider are: 1. regularization of fracture energy; and 2. mesh-dependent strength distribution. The proposed probabilistic crack band model can effectively mitigate the mesh dependence of stochastic finite element simulations, and can be potentially combined with fine-scale discrete element model to form a multiscale analysis framework that includes localization effects.

*Future Research Directions:* Prof. Le suggested some future research directions related to stochastic modeling of localization effects. In particular, he highlighted the following:

- There is a need to extend these models to dynamic fracture where the strength distribution function exhibits rate dependence.
- There is a need to relate the different length-scales in stochastic simulations. In particular, different length-scales exist, for example, for fracture and for random field correlations. These relations can be explored by incorporating random field simulations into these models.

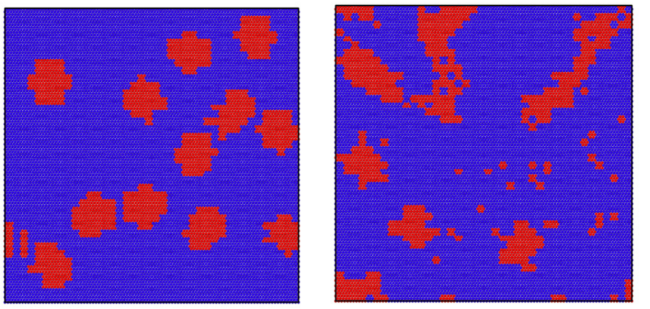


Figure 4: Pixel/voxel level probabailistic microsctructure model with different clustering parameters.

**Presentation 2: Yongming Liu** "Stochastic Nonlocal Lattice Particle Method for Voxel Level Uncertainty Quantification and Material Failure analysis."

*Problem setting/motivation:* High fidelity computational model is preferred and sometimes required in probabilistic computational material analysis. High dimensional images are available, which can be used when building high fidelity microstructure. In high fidelity models, it might also be important to capture the interface between multiple material phases. If data at each pixel/voxel is used, this leads to extremely high-dimensional probabilistic computational material analysis (curse of dimensionality).

*Background theory:* In multiphase materials, the same volume fraction with different clustering will change some mechanical behaviors of the resulting microstructure. The nonlocal lattice particle method can be employed in simulations of the high-fidelity microstructure (see Figure 4). Another possibility is to use atomic finite element method (AFEM) in computational mechanics simulations of the microstructure. Because of the extremely high dimensions, these computational methods are very expensive. Using the first order reliability methods (FORM), computational cost can be reduced with adjoint methods.

*Methodology:* Correlation-based reconstruction of microstructure using n-point correlation (specifically 2- or 3-point correlation) is performed. Simulated

annealing is employed to reconstruct the pixel level microstructure. In probabilistic simulations, it is essential to use efficient sampling methods, dimension reduction methods, surrogate model methods, and analytical methods such as FORM to deal with the challenge imposed by the extreme dimensions. Adjoint lattice particle method (ALPM) is one such method which is used here to reduce computational cost wherein the function and its gradient can be obtained by a small number of computational evaluations.

*Examples & results:* Results of validation exercises of the ALPM method using a triangular lattice were shown. The method achieved a consistent convergence behavior in the reliability index irrespective of the problem dimension when the number of problem dimensions was up to about 450, for linear and weakly nonlinear material behavior. Results were also shown for probability of failure analysis of a 2-D biphase microstructure with different values of a clustering parameter, with a dimension of 11,759.

*Conclusions:* ALPM is proposed as a probabilistic computational material analysis tool which is independent of dimensionality.

*Future Research Directions:* Prof. Liu identified several future areas of research that relate to extensions of his proposed approach as well as more general advances. These include:

- It will be important to go beyond the current linear formulation of the ALPM, which currently applies only to weakly nonlinear problems.
- For extremely high dimensional problems, it is in general necessary to leverage surrogate models and/or dimension reduction techniques.
- Physics-based learning by combining convolutional neural networks with finite element analysis has the potential to significantly reduce the number of training samples needed very extremely high dimensional problems.

**Presentation 3: Jie Li** "Stochastic Damage Mechanics: Developments and Recent Progress." (presentation given by Prof. Xiaodan Ren)

*Problem setting/motivation:* In materials such as concrete, there is both randomness and nonlinearity in the damage process. There is also damage diffusion and multi-scale stochastic fluctuation. There is a need to consider randomness in material and structure level in a unified manner.

*Background theory:* A phenomenological damage model, which is uniaxial, can be used to capture the nonlinearity in the material behavior. Principles of energy equivalence can be used to extend the uniaxial formulation to multiaxial cases.

*Methodology:* Nano-indentation testing of a three-phase concrete medium was conducted to obtain data on the strength of concrete. These test results were used to build probabilistic models of the material strength for use in computational mechanics simulations. A principle of preservation of probability, which states that the probability measure determined by the initial random source does not change in the state evolution process of the system, was used to trace the evolution of strength of the material when the concrete underwent damage.

*Examples & results:* An example of evaluating the seismic reliability of an existing concrete structure was presented. Using the method outlined in the presentation, it was possible to calculate the time evolution of the probability density function of failure during seismic loading of the structure.

*Conclusions:* The presentation showed the application of a generalized probability density evolution equation to the problem of damage evolution in a concrete structure subjected to seismic load.

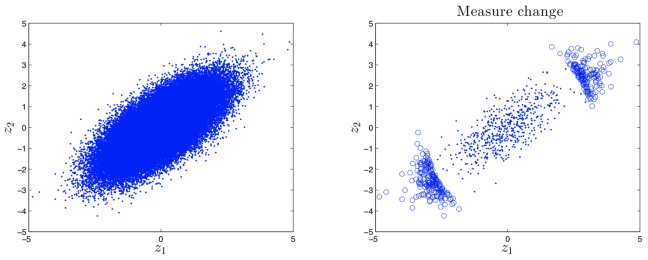



Figure 5: 100,000 samples from an original correlated Gaussian random vector (left) and 1,000 samples selected under a probability measure change emphasizing the extreme values (right).

**Presentation 4: Mircea Grigoriu** "Estimates of Extreme Material Responses for Random Microstructures."

*Problem setting/motivation:* The objective is to calculate probabilities of rare events. Standard methods may not apply in many situations arising in computational mechanics calculations because the sample size could be small.

*Background theory:* Two possible methods were out-

lined in the presentation for such cases: 1. Extreme value theory; and 2. Measure change. Extreme value theory holds for asymptotic behavior of sample extrema, analogous to the central limit theorem (CLT) for the sample mean. Measure change uses the Radon-Nikodym derivative. The idea in measure change is to use samples from a different, better measure $Q$ to estimate statistics of a random element on the desired probability space (see Figure 5).

*Methodology:* Generalized Extreme Value (GEV) distributions, based on extreme value theory are used to demonstrate their application in estimating extreme material response. GEV distributions exhibit tail sensitivity, their exact distribution is known, and they are easy to implement. Importance sampling (IS) is an example of measure change. IS estimators can theoretically achieve zero variance. A data-based approach is adopted to construct $Q$.

*Examples & results:* An example of estimating extreme stresses in a thin rectangular plate with a random microstructure subjected to uniform deterministic uniaxial tension along the $x$ direction was presented. Samples of the maximum value of the stress along the $x$ direction (i.e., the maximum principal stress) at any location were generated. A GEV distribution was fit to these samples using the method of maximum likelihood to estimate the parameters of the distribution. This distribution was used to approximate the probability that the maximum principal stress was greater than any threshold value. Another example of evaluating large seismic responses using the GEV distribution was presented. A single degree of freedom (SDOF) system is frequently used to approximate the behavior of structures, which could be complex and nonlinear. The response of the SDOF system (i.e., the intensity measure) is used to characterize the seismic demand function of the structure. It was shown that the current fragility metrics are not sensible as these do not consider the dependence between the intensity measure and the demand function, especially when both of these have high values.

*Conclusions:* GEV and measure change are methods which can be used to estimate extreme material responses. By using a carefully constructed different, better probability measure, it is possible to reduce variance in the estimates of extreme values.

***Discussion :***

A theme of the discussion was the question of length scales in the materials, and whether the methodologies presented are applicable only at certain length scales or if there are implicit length scales in the methods. The work presented using image based reconstruction was at the mesoscale, but the length scale for such methods depends on the method used for imaging - for example, whether optical or otherwise. The length scale also depends on the material. It was pointed out that for materials like steel, it is possible to achieve great control over the microstructure by methods such as laser sintering, resulting in low uncertainty. But for materials like concrete, control over the microstructure is harder to achieve.

In general, there is a length scale implicit in continuum simulations for quasibrittle materials and caution should be exercised when performing continuum simulations. There are also autocorrelation length scales which should be considered at fine scales. For materials like concrete, there are large length scales depending on the dimension of the aggregates. Also, when modeling damage and softening, there are length scales related to the size of the test specimen used to obtain the experimental data. Given the aforementioned challenges associated with lengthscale, it was expresed that caution should be used when using the term RVE because it relates to a deterministic homogenized continuum material.

It was further suggested that, for materials like concrete, probabilistic methods can be used for the purposes of understanding sensitivities of the material system. Rather than providing high confidence in the actual numbers extract from the models, these sensitivities can help gain insight into the influences of uncontrolled variability in the material.

A portion of the discussion session was related to reliability calculation. In the microstructures reconstructed from image data, material propertie at each pixel of the biphase material were modeled as a random variable having a Gaussian mixture distribution, in addition to variability in the structure of the material. Reliability analysis was conducted at the RVE scale, and not at the pixel scale. A possible improvement discussed was that the effect of hotspots in the generated microstructure could be considered in reliability analysis, rather than using only homogenized properties at RVE level. Other issues discussed were the shortcomings of using FORM for the reliability analysis, such as how it is not trivial to transform from non-Gaussian to standard Gaussian space. Also, using only one most proabable point

(MPP) for reliability calculations might not be the best method. The ALPM presented currently used FORM and a single MPP, but it is possible to extend it to SORM and multiple MPPs.

Another question asked was whether FORM/SORM give only lower bounds on probability of failure estimates because they are based on a Gaussian distribution. The response was that it is possible to overestimate the target too, and whether these methods give lower or upper bounds depends on the limit state. This also led to the discussion that, for other applications such as in earthquake engineering, simple scalar quantities like an intensity measure are highly dependent on the probability law of the random process/random field. Hence, for material failure driven by extreme events, the use of such simplistic measures might not be rational. Most material systems are complex multi-degree of freedom nonlinear systems, and use of simplistic intensity measures or performance metrics are inadequate.

Another point of discussion was the development and use of neural networks to enable efficient uncertainty quantification and propagation. It was remarked that training neural nets based only on data required large amounts of data to achieve high accuracy whereas by using knowledge of mechanics, it is possible to significantly reduce training cost for the same accuracy levels. For example, using this physics informed approach resulted in reduction of training data to only a few hundred samples instead of requiring millions of images. Hence, as has been shown in quite a few recent works, this is a very promising direction for computational material science. The usefulness of platforms such as Tensor Flow can be greatly enhanced by using this approach.

***Emerging Themes & Future Research:***

*Lack of scale-separation and localization:* A dominant theme of this session was the challenge of addressing problems that do not exhibit a clean separation of length-scales. It was observed that there is significant randomness in damage processes and diffusion of damage and these effects manifest in localization. Several frameworks were presented to numerically treat localization – including the crack band model, nonlocal continuum modeling, and nonlocal and adjoint lattice particle methods. But, the key issues related to the fact that probability distributions of material strength and constitutive response exhibit significant non-physical length-scale dependence in numerical simulations. Consequently, there is a need to address these variations both through theoretical exploration of the extreme material properties as well as through regularization of numerical models (e.g. by regularizing fracture energy).

*Modeling interfaces:* It was highlighted that failure often initiates at material interfaces. Data-driven stochastic approaches are needed to better resolve and model these interfaces to accurately model material failure.

*Rare event simulation considering small data:* Another major theme of the sessions was related to the fact that failure occurs in the tails of the distribution where observations are rare. Future research needs to address the challenges of assessing material performance in a way that accounts for the high dimensionality and nonlinearity of the models and their strong sensitivity to the tails of the distribution. This was especially evident when considering reliability of materials which exhibit localization, where it will be important to go beyond methods like FORM that rely on linearity and Gaussian assumptions that are likely to break down for complex materials.

*Machine learning:* It was highlighted that physics-informed machine learning methods can greatly reduce the training set size needed for materials failure models. This was an observation and will be revisited in Session 3, which has machine learning as a primary theme.

## Session 3: Data-driven modeling and machine learning

***Session Chair:*** **Fariba Fahroo**, US Air Force Office of Scientific Research

***Presenters:***

1. **Charbel Farhat**, *Stanford University*, "Data-Driven Model Reduction and Probabilistic Learning for Digital Twins."
2. **Youssef Marzouk**, *Massachusetts Institute of Technology*, "Optimal Bayesian Experimental Design: Methodologies and Materials Applications."
3. **Clayton Webster**, *Oak Ridge National Laboratory*, "Learning high-dimensional systems from data by nonlinear reconstruction of polynomial approximations."
4. **George Karniadakis**, *Brown University*, "Endowing Deep Neural Networks with Uncertainty Quantification."

***Overview:***

With the need to develop, inform, and validate computational models of materials with experimental data, pass information between models (as in a multi-scale setting), and construct inexpensive surrogates and reduced order models for expensive physics-based models, there is a growing need to leverage recent advances in machine learning, data science, data mining and data fusion for UQ in materials. The aim of this session was to explore the state-of-the-art and the future of this modeling paradigm for UQ in materials.

Talks in this session focused on several different aspects of machine learning for materials applications. The talks focused heavily on the use of artificial neural networks, their training as surrogate approximators of solutions to physics-based equations (PDEs more generally), their construction, and the integration of physics into the network itself. Talks in the session also adressed model-order reduction and Bayesian methods as machine learning algorithms. Model-order reduction is cast as a specific machine learning algorithm that is inherently built from a physics-based model. Their use for digital twin construction is specifically addressed. With regard to Bayesian methods, the question of learning for optimal experimental design is addressed. Learning schemes are employed to inform experimental designs that maximize expected information gain while accounting for model uncertainty.

***Review of Presentations:***

**Presentation 1: Charbel Farhat** "Data-Driven Model Reduction and Probabilistic Learning for Digital Twins."

*Problem setting/ motivation:* A digital twin is a digital replica of a physical asset/product. A predictive model is typically built to assist the design of a product. Once the product is ready, this model is generally left unused unless something bad happens to the product. The idea of a digital twin is to keep this model current and use it for prediction throughout the life of the product.

*Background theory:* A digital twin must be updated based on data and must change as the physical counterparts age, to be a good representation of the actual product. Ideally, the digital twin is supposed to be such a good representation of the product that once the product is in service, discrepancies between the digital twin predictions and measurements from sensors on the product should indicate the necessity for maintenance of the product i.e., the philosophy is to believe the model more than the measurements. In many cases, it is not possible to only rely on data to identify the underlying model as data is sparse. Hence, physics-based models must be used in the learning process, with data informing these models.

*Methodology:* The main idea is to perform machine learning with models informed by data, rather than learning with data. This is done by learning on a parameterized Stieffel manifold. Nonlinear parameterized model order reduction is used with a physics based model of the dynamical system. A reduced order basis is constructed to represent the model of the high dimensional dynamical system approximately. Due to the large number of decisions involved in building the model, much of the uncertainty is due to ignorance about the model, and not due to the uncertainty in the model parameters. To account for this ignorance, rather than randomizing the parameters of the model, the subspace in which the solution lies is randomized - a stochastic reduced order basis is employed and information is extracted from the data.

*Examples & results:* One example presented showcased the difficulty in identifying the quantity of interest as that is often not trivial. Another example showed the results of using the approach presented in the talk to build a reduced order model of an army truck – which led to speedup on the or-

der of millions with the required accuracy. Another example showed the results of both a deterministic and a stochastic reduced order model for the wing of an aircraft. Both models performed well when compared to measurements with the measurements being within the 98% coverage region of the stochastic reduced order model.

*Conclusions:* Model reduction is machine learning with models. Applications of machine learning to the development of digital twins was demonstrated.

*Future Research Directions:* Prof. Farhat identified two critical questions related to development of digital twins:

- Often the data coming from measurements corresponds to only a very small number of degrees of freedom of the system. Prof. Farhat suggested that such a small number of quantities of interest are not sufficient for the construction of digital twins. These need to be enhanced by physics-based models and corresponding reduced order models.
- Prof. Farhat noted that it is especially challenging to build digital twins that represent nonlinear behavior, encompassing multiple scales, that also show real-time performance, with quantified uncertainty. This is a considerable challenge for the future.

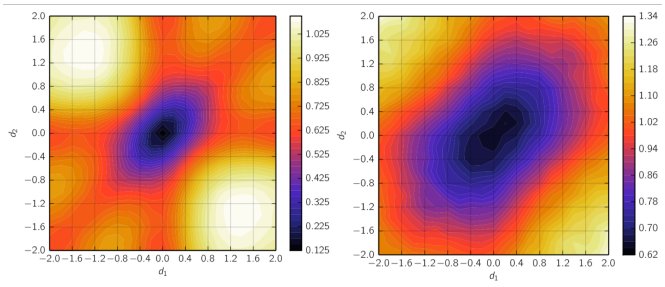


Figure 6: Expected utility for 'center' parameter (left) and 'offset' parameter (right) of model for Mossbauer spectroscopy.

**Presentation 2: Youssef Marzouk** "Optimal Bayesian Experimental Design: Methodologies and Materials Applications."

*Problem setting/ motivation:* Experimental design tries to answer the question – Given limited experimental resources, how do we find the most informative data? The approach is to develop and optimize design criteria that employ a model of the experiment, that account for uncertainties in the model, and that adapt to experimental goals.

*Background theory:* The Bayesian approach to optimal experimental design (OED) was outlined in the presentation. Experimental conditions were chosen to maximize an expected utility based on Kullback-Liebler divergence or to improve predictions of some quantities of interest. The approach can also be used for model discrimination where it is desired to concentrate the posterior onto fewer models.

*Methodology:* The methodology used a computational model to describe the experiment and needs to compute the expected information gain. Since there are no closed-form expressions for expected information gain, and there are additional challenges imposed by nonlinear computational models, nontrivial priors and noise models, and we want to avoid making large approximations, Monte Carlo simulation is employed to estimate the expected information gain. Another possibility is to use importance sampling to estimate the expected information gain. Both of these approaches are computationally expensive as there is a need to use nested Monte Carlo sampling. To overcome this problem, a layered multiple importance sampling (LMIS) approach is adopted.

*Examples & results:* The first example addressed OED for parameter inference of a model of a thin film evolving on a heterogenous substrate with the goal of learning about substrate properties from behavior of the film. The second example showed OED for model discrimination considering competing models for He trapping at Cu-Nb interfaces. Another example showed results of OED using the LMIS approach for the two parameters of a nonlinear model for Mossbauer spectroscopy (Figure 6).

*Conclusions:* The presented approach of focused design is a natural framework for incorporating models of model inadequacy. LMIS framework provides "hooks" which are convenient for large-scale computation.

*Future Research Directions:* Prof. Marzouk identified the following critical questions related to OED:

- Treatment of model error or mis-specification in Bayesian inference (broadly) and OED (specifically) is currently insufficient. Enhanced robustness to these uncertainties is necessary.
- Richer or goal-oriented design criteria are needed. For example, OED linked to downstream optimization under uncertainty or OED to better characterize material failure or rare events (from

indirect data) need further developments.
- Three is a need to develop new methods for fast approximate inference – especially in evaluating design criteria.
- Optimal sequential experimental design, particularly in dynamic environments such as dynamic programming, poses massive computational challenges.

**Presentation 3: Clayton Webster** "Learning high-dimensional systems from data by nonlinear reconstruction of polynomial approximations."

*Problem setting/ motivation:* High dimensional parameterized PDE models with deterministic and stochastic coefficients are commonly used in computational mechanics. A major research question is how to handle all these parameters and the associated plentiful data? This necessitates the use of larger computers and better data compression methods.

*Background theory:* Nonlinear approximations with multivariate polynomials makes use of the sparsity and smoothness structure of the approximate solutions and can lead to faster convergence than using Monte Carlo or quasi Monte Carlo methods. Taking advantage of sparsity induced norms and compressed sensing leads to recovery of best $s$-term approximations. Uniform recovery of the best approximations is guaranteed by the Restricted Isometry Property (RIP).

*Methodology:* Machine learning with deep neural networks is employed in several recent successful applications of function approximation. Using shallow neural networks for function approximation has been shown to have poorer performance compared to deep neural nets.

*Examples & results:* An example of using nonlinear polynomial approximations in high dimensions was presented. This example was based on machine learning methods and showed how to construct a quasi optimal neural network.

*Conclusions:* First sharp estimates of the complexity i.e., the total number of weights and computational units as well as the depth of a generalized artificial neural network required to recover the best approximation in high dimensions have been recently obtained.

**Presentation 4: George Karniadakis** "Endowing Deep Neural Networks with Uncertainty Quantification."

*Problem setting/ motivation:* There is a strong interest in UQ for physics informed learning machines i.e., neural networks to solve PDEs.

*Background theory:* Frequently, deep neural networks in practice are becoming narrow. But, neural networks should ideally be deep and wide, which is analogous to mesh refinement in FEM, and will lead to good approximations of functions. Powerful tools such as TensorFlow are available, which enable training neural networks with few lines of code. Several physics informed neural nets (PINNs) have been developed, some of which were discussed in the presentation.

*Methodology:* One of the methodologies presented for physics-informed neural nets was neural networks with arbitrary polynomial chaos expansion (NN-aPC). Another methodology presented was dropout neural networks (DNNs) used in regression. This method addresses uncertainty in data and issues of approximability of the network. In this method, units from the DNN are dropped independently and randomly with a pre-selected probability. Using DNN helps to reduce overfitting and to estimate approximation uncertainty. The mechanism of generative adversarial networks (GANs) was presented. GANs learn the entire distribution itself and not just moments. A GAN is a game between a generator neural net and a discriminator neural net. One of the aspects of using GANs is to identify criteria to know when to stop the game between the generator and the discriminator.

*Examples & results:* Intelligent Towing Tank developed at MIT was discussed, which uses machine learning and enabled a leap from 500 experiments per PhD to 80,000 experiments in just the 9 months prior. Examples using GANs to approximate stochastic processes and using PI-GANs to solve stochastic differential equations were presented.

*Conclusions:* PI-GANs can be used to solve SDEs, and scale well. In scaling up from 30 to 120 dimensions, the cost only increased by about 8-10 times, including training. The approaches have also been used for a problem in 10,000 dimensions.

*Future Research Directions:* Prof. Karniadakis outlined the following future directions for physics-informed learning machines:

- There is a need to continue developing physics-informed neural networks which encode physical laws and prior knowledge of physics

- There is a need to demonstrate the effectiveness of physics-informed neural nets in designing functional materials with tunable properties, and for other multiscale problems such as combustion, etc.
- Establishing probabilistic scientific computing as a discipline will incorporate relevant aspects of computational mathematics, information fusion, multifidelity data, etc. Pedagogically, this will better prepare future students to work at the interface of machine learning, probabilistic modeling, and physics-based modeling with high-performance computing.
- Faster tuning of neural networks and developing neural networks for high dimensions which utilize memory efficiently are essential.

***Discussion:***
The discussion session for this session was canceled due to the session falling behind schedule.

***Emerging Themes & Future Research:***
*Machine learning:* Perhaps the most common theme through the session was the various uses of artificial neural networks, and particularly deep neural networks for learning from/with physics-based calculations. Arguments have been made that discuss their advantages and disadvantages as a tool for computational modelers. It is clear that continued research is needed to establish their strengths, weaknesses, applications, and limitations as a tool for the computational materials and UQ communities. It was also emphasized that fundamental research to establish their mathematical underpinnings is also needed. Some specific research themes that arose related to neural networks were the following. There was considerable discussion on the optimal architecture for neural networks (i.e. deep vs. shallow NNs, number of layers, nodes, etc.) for solution approximation from physics-based calculations / PDEs. It was pointed out that neural networks should ideally be deep and wide. Another important question relates to the quantification of uncertainty in neural network approximations. Dropout neural networks were presented as an architecture that allows for quantification of uncertainty, but there remains considerable research need in this regard. Finally, it was emphasized that, particularly for materials applications, neural networks should be physics-informed. Different interpretations of this were presented in which the neural network serves as an approximation of a physics-based problem and where the physics are encoded into the network. Their application to materials design has not been studied in depth.

*Model-form uncertainty:* A theme that re-emerged in this session was related to accounting for model-form uncertainty in machine learning algorithms. It was argued that, due to the large number of decisions made in developing a model, much of the uncertainty is due to ignorance about the model. Prof. Farhat proposed a way to randomize the subspace of the solution to account for this uncertainty. Future research along these lines to build stochasticity directly into the models is needed. The treatment of model-uncertainty in Bayesian inference was discussed. Prof. Marzouk noted that there are significant limitations existing Bayesian methods to incorportate model uncertainties and specifically for problems that involve optimal experimenal design. The question of quantifying uncertainties in artificial neural networks was also explored, as discussed in the previous paragraph.

*Model-order reduction:* Model-order reduction is posed as a form of machine learning with models. Linking reduced order models to measurements poses significant challenges due to the difference in fidelity of measurements and models where measurements only correspond to a small number of degrees of freedom of the model. Modeal-order reduction is viewed as an important research direction for learning from higher-fidelity models and there is considerable need to improve out understanding of uncertainties in induced by both the assumptions made in the high-fidely model as well as the model-reduction.

*Experimental Design:* There remain many open questions related to experimental design. The need for future research related to incorporation of model-form uncertainties was discussed, see above. It was also mentioned that there is a need to develop experimental designs with enhanced objectives (for example, materials design optimization and/or material reliability). Several questions relate to reduce the computational expense of these methods, specifically as they relate to computing information gain and sequential sampling methods.

*Digital Twins:* The presentation of digital twins suggested a connection to materials in which multiple scales, manufacturing processes, and real-time material performance are modeled with uncertainty as a twin to the corresponding physical material. Research along these lines is needed.

## Session 4: Design and optimization for materials

***Session Chair:*** **James Warner**, National Aeronautics and Space Administration (Dr. Warner was unable to attend due to the US Government shutdown. Session chaired by Lori Graham-Brady, Johns Hopkins University)

***Presenters:***

1. **Zdenek Bazant**, *Northwestern University*, "Design of New Materials and Structures to Maximize Strength at Probability Tail: A Neglected Challenge for Quasibrittle and Biomimetic Materials."
2. **Simon Phillpot**, *University of Florida*, "Rational Design of Interatomic Potentials through Multi-Objective Optimization."
3. **Wilkins Aquino**, *Duke University*, "An Adaptive Reduced Basis Approach for PDE Constrained Optimization under Uncertainty."
4. **Jim Stewart**, *Sandia National Laboratory*, "Optimization Under Uncertainty for Predicting Properties and Performance."

***Overview:***

The goals of this session were to address questions in uncertainty quantification related to the materials-by-design paradigm. The session addresses areas of design and the optimization of materials from the perspective of probability-based design of materials (i.e. setting probabilistic design objectives informed by, for example, failure probability or risk measures) and the various roles of optimization in the analysis and design of materials. The latter includes problems related to parameter optimization for materials models, risk-based optimization of stochastic systems, multi-objective optimization, and topology optimization..

The talks proposed that design of materials should be based on reliability and/or risk with a focus on the tail of the distribution, not on low-order statistical descriptors such as mean strength. In one example, a recent model based on fishnet statistics for bio-mimetic quasi-brittle materials which allows analytical calculation of failure probabilities was presented. Another talk focused on rational design of classical inter-atomic potentials using multi-objective optimization. The rational approach when there are multiple conflicting objectives is to develop an ensemble of inter-atomic potentials on the Pareto-front and select the best-performing potential for a given application. Another talk discussed how reduced-order models can be tailored to suit optimization to guarantee convergence of optimization algorithms, using an adaptive sample-based reduced basis approach for approximating the PDE solution and an inexact trust-region framework for objective and gradient evaluation. The final talk discussed optimization under uncertainty using new risk measures utilizing buffered probabilities, and discussed issues such as spatial heterogeneity and higher variability which arise when optimizing additively manufactured materials. Approaches to address these issues using synthetic models of the microstructure evolution during additive manufacturing were presented.

***Review of Presentations:***

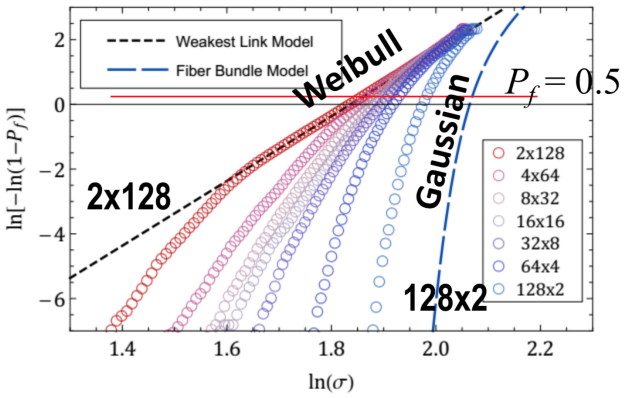



Figure 7: Weibull to Gaussian tranisition upon changing aspect ratio of the fishnet.

**Presentation 1: Zdenek Bazant** "Design of New Materials and Structures to Maximize Strength at Probability Tail: A Neglected Challenge for Quasibrittle and Biomimetic Materials."

*Problem setting/ motivation:* Reliability based design is focused on structural design but overlooks material design. $10^{-6}$ is the sited as a common tolerable probability of failure (PoF) in engineering. As such, it is necessary to optimize not the mean material strength but the strength at the tail for $10^{-6}$ PoF; in other words, it is necessary to adopt tail-risk based approach to design of materials.

*Background theory:* Controlling material architecture can profoundly alter the strength probability distribution. In quasibrittle materials, for the same coefficient of variation (CoV), superior mean strength can lead to inferior strength at the $10^{-6}$ tail.

There are only a few analytically tractable strength models for failure probability, which are the weakest-link models and the fiber bundle models. Quasibrittle materials are made of brittle constituents, but inhomogeneity size and the RVE are not negligible compared to the structure size. At increasing structure size, they transition from ductile to brittle behavior. Probability of failure can only be determined at the nano-scale for such materials. Scale transitions up from nanoscale to macroscale are governed by microcrack interactions in the fracture process zone (FPZ).

*Methodology:* The focus is on quasibrittle tensile (Type 1) failures. A fishnet structure is used to model biomimetic architected nacreous materials. This is only the third kind of model for which it is possible to obtain the probability of failure analytically. Order statistics can handle probability of failure calculations for fishnet architecture with gradually softening links.

*Examples & results:* One example highlighted the huge difference between Gaussian (normal) and Weibull cumulative distribution functions in the tails. Results showing the size effect on strength of quasibrittle materials such as concrete were presented. Results demonstrating the significant gain of safety at the tail by adopting fishnet architecture were shown (see Figure 7). Results of the strengthening effect of increased CoV in the strength of the fishnet links was shown. Results of damage evolution using gradually softening links instead of quasibrittle links were also presented.

*Conclusions:* Using the variance and the mean is not good enough, tail-risk design is necessary for quasibrittle materials. The factor of safety is size-dependent and reliability indices have been modified to account for this.

*Future Research Directions:* Prof. Bazant highlighted the following important research needs:

- There is a need to work towards fusion of advanced probabilistic methods and advanced mechanics.
- Design of quasi-brittle materials based on evaluating tail-risk is more accurate. There is a need to break from the normal approximation for strength using only the mean and standard deviation.
- There is a need to quantify uncertainty in the transition from nano-scale to micro-scale for quasi-brittle materials.

**Presentation 2: Simon Phillpot** "Rational Design of Interatomic Potentials through Multi-Objective Optimization."

*Problem setting/ motivation:* Atomic-level simulations – for example, molecular dynamics (MD) simulations, involve solving Newton's equations for a large number of particles. The potentials which exist between atoms can not currently be measured accurately and some model forms have to be assumed for the interatomic potentials. This talk presented a rational approach to selecting/designing the interatomic potentials.

*Background theory:* Different values of the parameters of interatomic potentials give rise to different properties seen in materials. Potential fitting is the inverse process of trying to fit the parameters of a given potential form to generate the targeted material properties. The traditional approach to potential fitting is to minimize a single cost function involving the error for all QoIs, typically using a gradient-based approach. Forming a single objective function requires combining all the multiple objectives into one, by taking a weighted sum of the errors in each objective. The choice of these weights is defined at the beginning of the optimization process, is not connected to the errors in the objectives, and depends on the user's preferences. This leads to subjectivity in the process.

*Methodology:* Using multi-objective optimization enables the developers to remove subjectivity in the process. Solving the multi-objective optimization entails identifying a set of solutions that are an approximation of the Pareto front, where each of these solutions is not worse than any other solution in terms of all the objectives. In the rational approach to design of interatomic potentials, the first step is to define the target properties and values. Then, an ensemble of rational potentials is developed, these potentials are assessed, and the final potential to be used is selected and tested.

*Examples & results:* Examples of applying the rational approach of interatomic potential design to selecting the Buckingham potential for MgO were presented. A database of rationally designed potentials has been developed. This database contains optimal parameter values of 7500 potentials which have been identified from multiobjective optimization.

*Conclusions:* An autonomous, machine learning approach to potential design was presented, which uses

Pareto analysis to develop an ensemble of rational potentials. User preferences are introduced towards the end of the rational process to down-select high performing potentials for their application.

**Presentation 3: Wilkins Aquino** "An Adaptive Reduced Basis Approach for PDE Constrained Optimization under Uncertainty."

*Problem setting/ motivation:* Design and control in computational mechanics require optimization under uncertainty with constraints being imposed by PDEs. This is computationally intensive to do and necessitates the use of reduced order models. The talk presented how to tailor reduced order models for such problems to suit optimization and guarantee convergence of optimization algorithms.

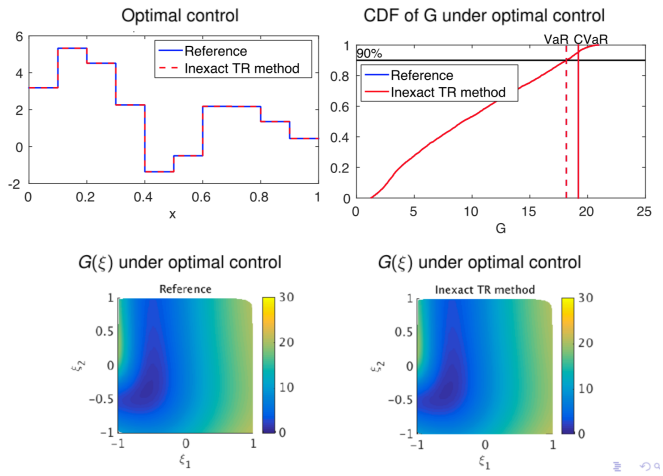



Figure 8: Results of optimal control for a 1-D advection-diffusion problem using the proposed inexact trust region framework.

*Background theory:* Stochastic formulation of the governing problem for optimization or control was first developed. It was shown that for linear PDEs with parametric uncertainty, the model is well-posed almost surely. A risk measure called conditional value at risk (CVaR) was defined and a framework for solving the risk-averse optimization problem was presented. There are computational challenges posed by this framework which requires the evaluation of the objective and its gradient, needing $N$ solutions of the state PDE and $N$ solutions of the adjoint PDE, where $N$ is the number of samples used to estimate the CVaR.

*Methodology:* A two-pronged methodology was adopted to overcome the difficulty posed by the high computational cost: 1. A provably convergent, adaptive sample-based reduced basis approach was employed for approximating the PDE solution; 2. A provably convergent, inexact trust region framework was utilized that allowed for inexact evaluations of the objective and its gradient.

*Examples & results:* The developed methodology was applied to obtain optimal control for a 1D Helmhotz problem with two stochastic dimensions. Samples generated were used to obtain Voronoi cell partitions which were used to compute local reduced basis approximation of the PDE solution. These approximate solutions were used for calculations in the inexact trust region framework to solve the optimal control problem and results are shown in Figure 8.

*Conclusions:* The three main ingredients in the presented approach were: 1. A local basis enriched with gradient information; 2. A practical and effective error indicator; and 3. An inexact trust region framework. The cost of the reduced bases solutions does not grow with the number of atoms added. Extension of this framework to nonlinear PDEs is possible.

*Future Research Directions:* Prof. Aquino identified the following future research needs as they relate to optimization under uncertainty:

- In physics-based modeling, the physical and stochastic domensions are often treated separately. Unified frameworks are needed for treatment of physical and stochastic dimensions.
- The influence of model-form uncertainty has not been adequately addressed in problems of optimization under uncertainty.
- Along a similar lines the treatment of imperfect knowledge on underlying probability laws, which induces model-form uncertainty in probability models, poses several challenges to problems of optimization under uncertainty.

**Presentation 4: Jim Stewart** "Optimization Under Uncertainty for Predicting Properties and Performance."

*Problem setting/ motivation:* Additive manufacturing has enabled new designs and materials. But, it has been observed that additively manufactured materials exhibit spatial heterogeneity and higher anisotropy. This challenges traditional design methods and new methods are necessary to handle optimization of such materials.

*Background theory:* Topology optimization leads to different designs for different performance objectives and it is important to incorporate as much relevant physics as possible. A risk measure such as the conditional value at risk (CVaR) is used when performing traditional optimization. When there is uncertainty, buffered probabilities are utilized while evaluating risk. Using buffered probabilities results in conservative designs. In additively manufactured materials, heterogeneous textures and morphologies exist across multiple scales. Microscale variations in the structure within and between components cause variations in engineering properties. Hence it is important to model microstructure and its evolution during fabrication.

*Methodology:* A microstructure simulator was utilized to model evolution of the microstructure during the additive manufacturing process. This was done using the SPPARKS stochastic simulator, developed at Sandia National Laboratories. This informs uncertainty quantification in final components fabricated, as well as allows design of the process variables. The microstructural effects are upscaled to systematically represent material properties on a larger, continuum scale. This respects length scales and microstructure morphologies and allows effective modeling of the material variability and heterogeneity. The upscaling approach utilizes simulations of multiple synthetic microstructures, which are generated via models of the additive manufacturing process, to estimate spatial statistics at quadrature points of finite element analyses. This approach enables spatial heterogeneity to be represented.

*Examples & results:* An example of simulations of a gas gun experiment were presented. A simplified model of the gas gun experiment was used in simulations. Spatial heterogeneity and variability was captured in the properties of the material subjected to impact, utilizing the developed approach. This led to estimates of the variability in the response of the material, which along with appropriate risk measures using buffered probabilities, was used in topology optimization.

*Conclusions:* An approach for upscaling the spatially heterogeneous and variable microstructure produced by additive manufacturing was presented. This materials aware approach utilized the SPPARKS simulator of microstucture evolution. The variability and heterogeneity can then be incorporated into design under uncertainty using topology optimization and analysis for predicting variability in material performance.

*Future Research Directions:* Dr. Stewart posed several important questions related to materials design under uncertainty.

- Can we "discover" new materials with desired (and revolutionary) performance properties?
- Can we reproduce such materials in a predictable and cost-effective way?
- Can we confidently "certify" that a particular material will perform as intended in a given application?
- How do we model extremely heterogeneous and variable materials at all scales?
- How do we obtain and assimilate potentially voluminous, uncertain data into models?
- How do we package our designs for human decision making?

***Discussion:***

Discussion session canceled due to the session falling behind schedule

***Emerging Themes & Future Research:***

*Probability of Failure / Risk:* A major theme that emerged from several of the presentations was the need to inform design and/or optimize for extremes associated with the tails of the probability distribution. This was posed in different ways, and different methods were applied (analytical probability of failure models, risk-measures such as conditional value at risk, and buffered probabilities) but the common task of informing design/optimization by measures of extreme performance was prominent and represents an important area for future research in materials.

*Optimization:* It was clear from the presentations that there remain many open questions in the methdology and application of optimization under uncertainty for materials applications. Different optimization paradigms were explored including model parameter optimization (where it was argued that, for design of inter-atomic potentials, a multi-objective optimization approach can reduce subjectivity, risk-based optimization with the integration of reduced-order models, and topology optimization which allows for different designs based on different performance objectives.

*Model-form Uncertainty:* Issues associated with model-form uncertainty once again arose. In the

cases presented here, the selection of appropriate inter-atomic potential models is a problem where model-form uncertainty is prominent. It was highlighted by Prof. Aquino that model-form uncertainties are particularly difficult to handle in problems of optimization under uncertainty and continued fundamental research is needed.

*Additive Manufacturing:* As an application, additivitely manufactured materials pose all new challenges to designers because they change the properties of the base material and introduce new types of uncertainties associated with, for example, anisotopies and heterogeneities that do not exist in conventionally manufactured materials. It was argued that, in additive manufacturing, there is a need to explicitly model the manufacturing process to capture stochastic morphology characteristics. The resulting microstructure morphology characteristics are then needed to inform design.

*Decision-making:* While the talks focused on specific applications and implementations of design/optimization, the more abstract question of how to use these optimization tools, measures of risk, failure probabilities etc., to inform decisions was posed as an open/unaddressed problem.

*Lack of scale-separation:* Examples in the presentations once again illustrated challenges associated with uncertainties introduced when materials do not exhibit a clear separation of length-scales. This was the case for the quasi-brittle materials of interest to Prof. Bazant as well as the additively manufactured materials of interest to Dr. Steward who expressed the need to explicitly model manufacturing processes in order to model material microstructure.

## Session 5: Multiscale material modeling – Microstructure

***Session Chair:*** **Michael Falk**, Johns Hopkins University

***Presenters:***

1. **Stephen Foiles**, *Sandia National Laboratory*, "The Fundamental Challenges to Uncertainty Quantification of Atomistic-scale Materials Simulations."
2. **James Kermode**, *University of Warwick*, "Predictive Multiscale Modelling of Materials Chemomechanics."
3. **Timothy Germann**, *Los Alamos National Laboratory*, "Role of Uncertainty Quantification in Embedded Scale-Bridging Materials Simulations."

***Overview:***

The theme of the second day of the conference was multi-scale modeling. The first of three sessions on the topic, this session focused specifically on uncertainty quantification in models of material microstructure. Given its focus on the smallest length-scales, the primary emphasis of this session was on atomistic and other nano-scale numerical models. The session addressed some of the fundamental challenges for UQ at these small length-scales including the myriad of uncertainties that exist in quantum mechanical and atomistic simulations using various microscale modeling approaches such as molecular dynamics, the embedded atom method, and density functional theory. At these length scales, many approximations are made in simulations and there is a critical need to quantitatively understand the uncertainties introduced by making these approximations. The presentations discussed various ways to account for and address these uncertainties, including the use of advanced machine learning algorithms such as Gaussian processes and artificial neural networks to learn interatomic potentials.

One of the talks proposed that while uncertainty quantification of atomic scale materials simulation is in its infancy, models are becoming sufficiently accurate to justify UQ and highlighted the need to focus on epistemic uncertainty, and using an ensemble of potentials with Bayesian methods for robust simulations. Another talk presented the Gaussian Approximation Potential (GAP) framework for modeling chemo-mechanics of silicon, with quantified uncertainties. The last talk in this session discussed scale-bridging using kriging-based surrogate models. Active learning of inter-atomic potentials, to minimize the use of expert knowledge and hence maximize the generality of the developed potentials was presented. Bayesian ensembling to reduce uncertainty in the neural networks was also discussed.

***Review of Presentations:***

**Presentation 1: Stephen Foiles** "The Fundamental Challenges to Uncertainty Quantification of Atomistic-scale Materials Simulations."

*Problem setting/ motivation:* The focus of the talk was to highlight issues related to placing error bars on atomistic simulations. Historically, the results of atomistic simulations were mainly utilized to make qualitative observations but multiscale engineering simulations require making use of atomistic simulation results in a quantitative sense. This necessitates quantification of uncertainties in atomistic simulation results.

*Background theory:* Multiscale material modeling is not a simple linear march up the length scale. Understanding the behavior of a component at multiple length scales is complex as several separate phenomena operate at overlapping length scales. Some of the challenges which arise in molecular dynamics (MD) simulations at the atomistic scale are: 1. deviations from the Born-Oppenheimer approximation; 2. inadequate interatomic potentials used in MD simulations; 3. the importance of quantum mechanical effects; 4. bifurcations in behavior; 5. the limited time scales of atomistic simulations; 6. approximations made about structure of the atoms; 7. and existence of coupling between composition and structure. Information extraction from atomistic simulations for higher scale models is not trivial as the physics is influenced by locations of millions of atoms, which is affected by the choice of interatomic potentials used in the simulations. Good practice is to chose from a repository of rationally designed interatomic potentials, those which reproduce key features of the material behavior under interest.

*Methodology:* Interatomic potentials have specific functional forms and their parameter values are estimated from data. Frequently, parameter values close to the maximum likelihood parameter estimates also fit the data almost as well. Hence, choosing an ensemble of interatomic potentials might be better in practice. A Bayesian approach can be utilized to

construct an ensemble of potentials which can be used in simulations. When multiple potentials are used, two outcomes are possible - either the system behaves more or less the same way with all the potentials (i.e., results are qualitatively similar but quantitatively different) or the results could be qualitatively different, depending on how sensitive the simulation outputs are to the parameter values of the interatomic potential. Hence, using such an approach leads to understanding the effect of uncertainty in the parameter values of the interatomic potentials. It is also possible to have an ensemble of potentials with different model forms and select the best model form for the interatomic potential.

*Examples & results:* Examples were presented of a recent study on faceting of $\Sigma = 5$ grain boundary in Fe. The objective was to study if calculations and experiments agree. Observations from this study suggest that secondary grain boundary dislocations should be considered while computing the length-scale of grain boundary facets.

Results of MD simulations of polycrystals were presented. These results showed that while initial conditions matter at the atomistic scales and resulted in different local deformation mechanisms such as grain boundary sliding occurring at different boundaries depending on the initial conditions, they do not make a huge difference for macroscopic response.

Another example presented was simulation of platinum-gold alloy. Monte Carlo simulation was performed to identify where the gold would go in this microstructure. It was observed that the gold was heterogeneously segregated in the grain boundaries of platinum.

*Conclusions:* Error estimation/uncertainty quantification for sub-continuum levels is in its infancy and is still a major challenge. More accurate models are required to justify UQ.

*Future Research Directions:* Dr. Foiles highlighted several important problems related to UQ and error estimation in atomistic modeling and in materials science more broadly as summarized in the following:

- He noted that it is increasingly necessary to make changes to material science curricula to train material scientists in the underlying mathematics and information theory required for UQ.
- He emphasized that there is a need to make UQ a regular part of the future research in sub-continuum modeling of materials by, for example, asking for uncertainty estimates during peer review of articles.
- Practically, there is a need to incorporate computational techniques such as interval computing and automatic differentiation into existing software for computational materials modeling.
- We must improve the accuracy of material models to make quantitative rather than only qualitative predictions and justify uncertainty quantification.
- There is a need to address how to evaluate the quality of simulations rationally, consistently, and objectively rather than only relying on expert opinion.

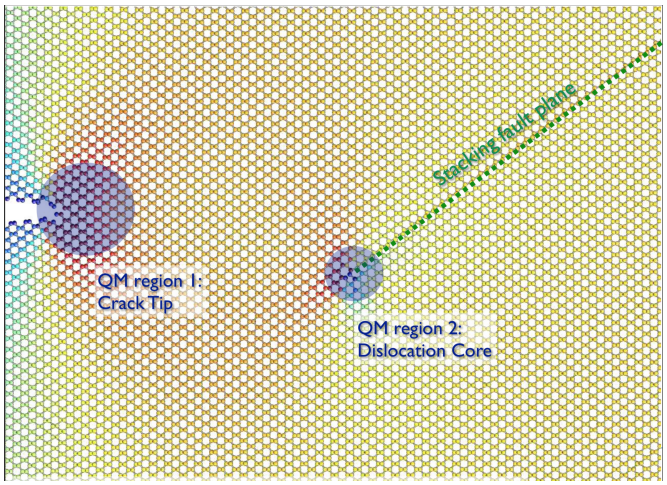



Figure 9: Hybrid QM/MM method for interaction between crack growth and dislocation.

**Presentation 2: James Kermode** "Predictive Multiscale Modelling of Materials Chemomechanics."

*Problem setting/ motivation:* Chemomechanical processes involve strong coupling between chemical bonds and mechanical strain. These processes are important especially during atomistic simulations of onset of failure in materials, and for processes such as friction, fracture, and dislocation modeling. The goal is to model complex chemistry and realistic systems such as stress corrosion cracking, dislocation/impurity interaction, and cleavage vs emission in three-dimensional systems. This requires large systems, long time-scales, and UQ.

*Background theory:* Simulation techniques at the atomistic scales range from detailed, computationally expensive quantum mechanics models at

angstrom length scales, to density functional theory and embedded atom method at nanometer length scales, to molecular dynamics simulations using interatomic potentials at length scales of about 10 nanometers. There are aleatory and epistemic uncertainties in simulations at the atomistic scale caused by uncertainties in the form and parameters of interatomic potentials used in MD simulations, random microstructure of materials, limited data to evaluate the accuracy of a chosen interatomic potential, algorithmic uncertainty in solvers, and limited transferability of interatomic potentials which causes problems in modeling chemical complexity such as that caused by impurities. In hierarchical multiscale modeling, uncertainties at atomistic scales are propagated to higher scales by stochastic coarse graining. In concurrent multiscale modeling, there is simultaneous coupling between simulations at multiple scales.

*Methodology:* To model complex chemistry in realistic systems requires the development and use of hybrid schemes which combine the advantages of detailed quantum mechanics methods and molecular dynamics simulations. These hybrid methods are typically force based and utilize quantum mechanics (QM) in regions of interest such as the crack tip or dislocation core, and molecular mechanics (MM) outside of these regions. Active learning has been used to develop interatomic potentials on the fly. A general purpose machine learning potential called Gaussian Approximation Potential (GAP) has been developed, which is a Gaussian process model trained from DFT data. By using the GAP framework, it is possible to obtain per-atom error predictions from the variance of the posterior probability distribution.

*Examples & results:* An example problem of simulation of dislocation glide in nickel based superalloys was presented to motivate the challenges in UQ at atomistic scale simulations.

Another example was a complex problem involving cleavage, partial dislocation, and stacking fault in silicon. The hybrid QM/MM method was utilized to solve this problem. This simulation can be used as a predictive model because, although crack growth was not explicitly programmed, the model was able to capture the interaction between a crack and a dislocation. It was observed in the simulation that the crack grew in the initial direction, then grew along stacking faults for some time, and then continued to grow along the initial direction (see Figure 9).

Also presented were results of simulations using the hybrid QM/MM approach of vacancy diffusion in fcc aluminum, and edge dislocation in bcc molybdenum.

Results of UQ for the silicon GAP model were shown for model vacancy migration, four-fold defect, and generalized stacking fault energy.

*Conclusions:* Methods to perform UQ at the atomistic scale using GAP framework were presented. It is especially challenging to model complex chemomechanical processes in realistic systems.

*Future Research Directions:* Prof. Kermode highlighted several important challenges for UQ in atomistic modeling of materials, including the following:

- Research is needed on methods to propagate uncertainty in GAP atomic energies through to material properties
- To date, UQ in these methods only accounts for limited training data, but there are many other sources of uncertainty — e.g. QM model error, algorithmic uncertainty, and others.
- In modeling interatomic potentials, there is significant model error. There is a need to develop a sample ensemble of "reasonable" potentials from the GP without training.
- An attractive research direction is to carry out active learning using predicted uncertainties to build models on-the-fly.
- There is a need for stochastic coarse graining methods to inform hierarchical multiscale models that address how to transfer uncertainties, both aleatory and epistemic from lower length/time scale models to higher length/time scale models, and ultimately into an engineering-scale model in a sequential scale bridging framework.
- UQ is specifically needed for concurrent QM/MM multiscale schemes

**Presentation 3: Timothy Germann** "Role of Uncertainty Quantification in Embedded Scale-Bridging Materials Simulations."

*Problem setting/ motivation:* In multiscale simulations, it is necessary to transfer information between different models at different scales, or to bridge the different scales. In scale bridging, the concept is that not just that the mesh is being refined to capture the response at lower length scales, but an entirely different physical model is being used at a different scale such as using a finite element model at continuum scale to a phase field model at a mesoscale to

molecular dynamics (MD) model at microscale and atomistic or electron structure models at finer scales.

*Background theory:* It is computationally very expensive to perform simulations at several scales and bridge the scales in sequential multiscale models. Surrogate models based on kriging can be used to emulate the expensive models at fine scales and enable scale bridging. It is also possible to identify where new simulations need to be conducted to train the emulator when kriging based surrogates are used. Kriging becomes difficult for higher dimensional response functions due to a lot of computational and numerical challenges.

Using modern machine learning approaches to obtain interatomic potentials has been promising. In order to train the machine learning models, it is necessary to generate data, and the choice of which data to generate to be used for training the models is not clear. It is essential to mitigate human bias caused by relying on expert knowledge to decide which data is used to train the models.

*Methodology:* The solution to overcome the numerical challenges in kriging is to use adaptive sampling to perform scale bridging with kriging-based surrogate models. Adaptive sampling is a technique of building the response surface on the fly, in which it is only essential to explore a low dimensional manifold in high-dimensional space, instead of the entire high dimensional space. The method of adaptive sampling uses an emulator trained from fine scale responses and the workload (i.e., the number of fine scale evaluations) can be greatly reduced by using a database of fine scale responses. This approach lets the approximation model specify where it is essential to obtain data. Choosing an acceptable error threshold is part of the process and drives the need to perform fine scale evaluations.

Interatomic potentials enable the use of force field based simulations such as MD simulations, which are computationally less expensive than the more accurate and transferable methods based on quantum mechanics such as density functional theory (DFT). Machine learning can be used to construct potentials derived from a large number of quantum mechanical simulations and it is possible to minimize use of expert knowledge for maximum generality and accuracy. Active learning (AL) enables fully automated generation of data to train machine learning potentials. AL is based on the concept of Query By Committee (QBC) which makes use of an ensemble of machine learning potentials and identifies regions where they disagree to be the regions where new data has to be generated for training. This systematic approach improves the accuracy of the ML potential and also reduces the amount of training data required.

*Examples & results:* Hierarchically interacting particle neural network (HIP-NN) is one example of a method of using a neural net to predict the total energy and properties given the configuration of a molecule.

An example of using the approach of training neural networks to generate interatomic potentials for tin was shown. Using this active learning approach, the error in the ML potential reduced with the number of training generations and enabled accurate ML potentials for tin to be developed.

*Conclusions:* Performing multiscale simulations is expensive, but applying surrogate models and databases for bridging different scales is a promising avenue. Uncertainty quantification at subcontinuum scales is still in its infancy and propagating it through multiple scales is even more challenging.

*Future Research Directions:* Dr. Germann highlighted several important research questions related to UQ in multi-scale modeling, including the following:

- How do we transfer uncertainties, both aleatory and epistemic, in sequential scale bridging from lower length/time scale models through higher length/time scale models into an ultimate engineering scale model?
- In the context of machine learning, even if predictions from multiple neural networks agree, what can be done if the neural network is incorrect? How do we estimate uncertainties in these machine learning tools for use in the concurrent scale-bridging approach?
- In the training of interatomic potentials, there is a need to collect and exploit expensive data cleverly so as to maximize its utility.
- When neural network potentials are derived from active learning, there is a need to develop improved neural net architectures that enable quantification of transferable (for example, covalent-to-metallic) and longer range descriptors of electronic state.

***Discussion:***
One of the main discussion topics was the necessity to use rational interatomic potentials in MD simulations. Choosing an interatomic potential is a delicate matter and only benchmarked, validated potentials must be used to obtain meaningful results. It is not good practice to choose a potential developed for some particular conditions without testing them for the desired conditions being studied.

Another question was about generating an ensemble of potentials. The ensemble could be generated by choosing parameter values of a potential functional form by Bayesian weighting based on a training set. It was pointed out that, in the Gaussian approximation potential (GAP) framework, it is possible to obtain an ensemble of potentials generated from the prior without training data.

Another issue discussed was the constraint on the fit due to the choice of a particular functional form for the potentials, and how to identify the right functional form. This is an especially difficult problem because it is hard to quantify the model error. Most of the approaches presented only deal with parametric uncertainty and leave out model form uncertainty. One possible approach suggested to deal with this issue was to conduct multiobjective optimization to obtain a Pareto front for a particular functional form, and repeating this with different choices of the functional form. By doing this, it is possible to test which volume of predictions cannot be reached by a particular choice of functional form for the interatomic potentials. Another approach is to perform a Bayesian analysis to pick the form of the model which maximizes the fit. It was suggested that dealing with model form uncertainty is more difficult than the parametric uncertainty and, because it might be nonparametric it was not clear which distribution form to use for model form uncertainty.

There is a lack of smoothness in the response functions from atomistic models and crystal plasticity models. This led to the question of whether this indicates there is some missing physics in the model. If so, is there a way to inject some knowledge into the model which can alleviate the lack of smoothness in the response. It was pointed out that there are structural approximations and other approximations and assumptions made in atomistic simulations. For example, while DFT is a very good approximation, it is still not the ground truth but an approximation. It is also not known how some seemingly innocuous assumptions, for example on the boundary conditions, might lead to changes in the response. There is currently no way of guarding against making such assumptions.

Another question surmised that there are 2 main challenges: 1. picking the model form for the interatomic potentials; and 2. how to identify and propagate uncertainty. The question was whether there are existing tools which allow us to solve these problems. The answer was that while there are some good avenues to overcome model form uncertainty, by for example, using active learning approaches, it is not clear how to upscale the uncertainty in the model forms. It was suggested it is possible to independently work on developing approaches to upscaling uncertainty in a multiscale framework. Another opinion was that the challenges in propagating uncertainty depends on what is the quantity of interest. For some quantities of interest, there are approaches which allow bounds to be placed.

Another question asked whether it was possible to understand the physical aspects of the sampled energy – i.e., is there some connection between the saddle points in the energy and the ground states in the system? It was thought that it could be possible to explore the connections between the energy and the states by using a combination of active learning and Monte Carlo simulation.

***Emerging Themes & Future Research:***
*Atomistic modeling:* The focus of the session was almost entirely on atomistic modeling. We saw that, as the accuracy of atomistic simulations using different theories are improving, there is a move from qualitative simulation objectives (e.g. understanding phenomenology/mechanisms) to quantitative objectives for atomistic modeling (e.g. upscaling to higher-level models). This poses enormous challenges because it requires a careful accounting of the many errors/approximations made in atomistic modeling. Atomistic methods currently rely heavily on approximations and simplifications (many of which are listed in the presentation summaries above). The approximation that was discussed universally was the rational selection and parameterization of interatomic potential models. The conclusion was that atomistic simulations are in dire need of UQ to address these approximations and that UQ can be particularly impactful in the selection of interatomic potential model forms and parameter calibration.

*Model-form uncertainty:* Again, a dominant theme

was the selection of inter-atomic potentials. It was discussed by all of the presenters and various approaches were proposed for selection of model form and for model calibration including approaches based on an ensemble of potentials and exploiting machine learning methods to learn potentials.

*Machine learning:* It was argued that machine learning methods show promise as a means to identify interatomic potentials and build surrogate models for up-scaling. But, they present a number of challenges such as training data/simulation selection and a need for rigorous frameworks through which to quantify uncertainty in machine learning algorithms.

*Curriculum and Pedagogical Changes:* It was argued that, in materials science in particular, there is a need to expand curricula to include the mathematical fundamentals of probability, information theory, etc. needed for UQ. This improved training will aid in the process of pushing atomistic level material modeling in a more quantitative, error/uncertainty-aware direction.

## Session 6: Multiscale material modeling – Multi-scaling

***Session Chair:*** **Somnath Ghosh**, Johns Hopkins University

***Presenters:***

- **Wei Chen**, *Northwestern University*, "Multiscale and Multidimensional Uncertainty Quantification in Integrated Computational Materials Engineering."
- **Jaroslaw Knap**, *US Army Research Laboratory* "Accelerating Scale Bridging via Surrogate Modeling."
- **David McDowell**, *Georgia Institute of Technology*, "Uncertainty in the Definition and Calibration of Multiscale Material Models."
- **Pedro Ponte Castañeda**, *University of Pennsylvania*, "Homogenization Estimates for the Macroscopic Response and Field Statistics in Viscoplastic Polycrystals."

***Overview:***

The second session on multiscale material modeling focused on the process/methodology of scale-briding. With this in mind, the session aimed to explore different methodologies for scale-bridging and identifying the necessary information to be passed between scales for various applications and for different multiscale approaches (i.e. hierarchical vs. concurrent). A major major topic of interest was how to model relevant information at each scale and extract it for subsequent scales, or – in the inverse case – how to calibrate lower scale models from data at upper scales. The presenters propose a variety of multiscale modeling approaches including those that leverage machine learning at individual scales (e.g. for material microstructure reconstruction) and at the interface of scales, methods that leverage surrogate models for lower-scale models that enable fast approximation of lower-scale performance, hybrid top-down/bottom-up scale-bridging to ensure physical consistency in scale-bridging, and statistical homogenization strategies.

Overall, the talks highlighted the challenges in various approaches for multiscale modeling of material response. One of the modeling approaches presented was to represent the variation in material properties at several scales with spatial random processes (SRPs), adopt top-down sampling to couple the SRPs across scales, and train surrogate models to represent the homogenized constitutive relations at scale. In another approach, Gaussian processes were used as surrogate models over subsets of the domain to emulate the at-scale responses and hierarchical Cholesky decomposition was employed to bring down the cost of surrogate model construction. In another approach, the individual models at scale were assumed to be valid and the uncertainty in the linkages was reconciled through Bayesian calibration. The uncertainty was further reduced by defining a physically meaningful inter-scale discrepancy function as part of the calibration process. The final talk focused on homogenization methods for nonlinear behavior of heterogeneous materials by making use of an optimally designed linear comparison composite, and using this method to establish bounds and statistical estimates for the macroscopic response.

***Review of Presentations:***

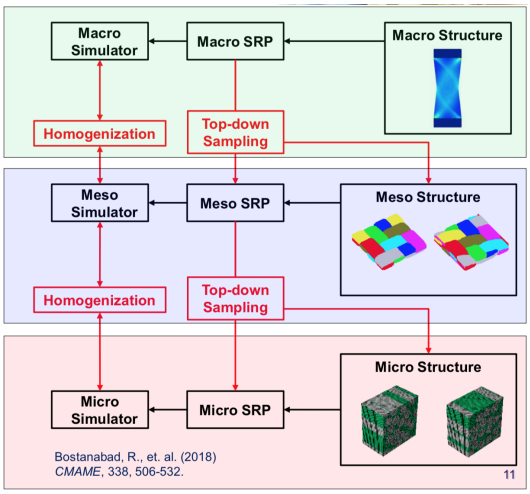



Figure 10: Approach for uncertainty quantification and uncertainty propagation in multiscale simulations.

**Presentation 1: Wei Chen** "Multiscale and Multidimensional Uncertainty Quantification in Integrated Computational Materials Engineering."

*Problem setting/ motivation:* Some challenges in the Integrated Computational Materials Engineering (ICME) framework were discussed in the presentation. These were relating to microstructure characterization and reconstruction (MCR), uncertainty quantification and propagation in multiscale materials, and Bayesian validation and calibration of multiscale simulators.

*Background theory:* In MCR, the objective is to

stochastically characterize and subsequently reconstruct the microstructure to enable automation in material design. Physical descriptors of the material microstructure are used to characterize the material structure and its spatial correlation. Reconstruction can be done via hierarchical optimization. Spatial random processes (SRPs) can be used to represent spatial variations of uncertainty sources, with coupling across length scales achieved by top-down sampling. This involves creation and use of metamodels of homogenized constitutive relations with microstructure variations. A Bayesian approach, which also accounts for potential model bias, can be used for calibration and validation of these material models.

*Methodology:* A model based approach was adopted to do MCR for complex morphology and to enable dimension reduction in the process. The phase values were modeled as functions of surrounding pixels, and a decision tree was used as a supervised learner.

The approach used for uncertainty quantification and propagation in multiscale simulations is shown in Figure 10. Model complexity is managed by adopting on-the-fly machine learning. Multi-response Gaussian processes (MRGPs) were used for quantifying correlated sources of uncertainty.

A Bayesian framework for calibration enables considering various uncertainty sources and considering potential model discrepancy. Using a modular approach for Bayesian calibration enabled better identifiability, better stability, and lower computational costs.

*Examples & results:* An example of MCR for unidimensional CFRP composites was presented. Images of the microstructure of the composite in the cross section and the longitudinal direction were analyzed to characterize the microstructure. Results of sensitivity analysis on moduli at the mesoscale, and for dimension reduction of homogenized response of woven RVE were shown. MRGP metamodels are trained at the micro and meso scales and their impact on the uncertainty at the macro scale was presented.

Another example presented the results of Bayesian calibration of MRGP metamodel to represent the response of the CFRP. Calibration was performed using the uniaxial tension test and validation was performed via the bias extension test. As a final validation example, macroscale simulations of the CFRP subjected to punch test was performed. Overall, the calibrated multiscale model matched the experiments better than the previously used models where tension and shear was decoupled at the mesoscales.

*Conclusions:* Stochasticity plays a critical role in materials behavior prediction. Dimensionality reduction can provide significant computational speedups in stochastic modeling. Big data and lack of data co-exist in materials informatics. Various sources of spatiotemporally varying uncertainty should be considered in multiscale materials.

*Future Research Directions:* Prof. Chen identified many key research challenges/questions related to multiscale materials modeling, including the following:

- How do we properly characterize location dependent and scale-coupled heterogeneous material micro-/meso-/nano-structures?
- When is (microstructural) uncertainty important to consider in multiscale systems?
- Dimension reduction and active subspaces need further development for vector valued, time-dependent, and space-dependent quantities of interest and for surrogate input-output relations.
- How do we conduct UQ when inferring 3D microstructures with 2D images?
- There is a need to build physics-aware machine learning for processing-structure relations.
- New methods are need to build time-dependent and path dependent surrogates.
- Surrogate models are needed that maintain conservation properties.
- Data fusion from multi-fidelity simulations poses significant challenges.
- There is a need to develop spatially varying calibration parameters in the presence of model bias.
- It is not clear how to define the form of the discrepancy function for many applications.
- Can "calibrated" material parameters be extrapolative?
- There is a need to develop strategies for improving model "identifiability."
- Greater thought needs to be given to design of multi-scale data collection.
- There is a need to develop methods for concurrent design of experiments and computer simulations.

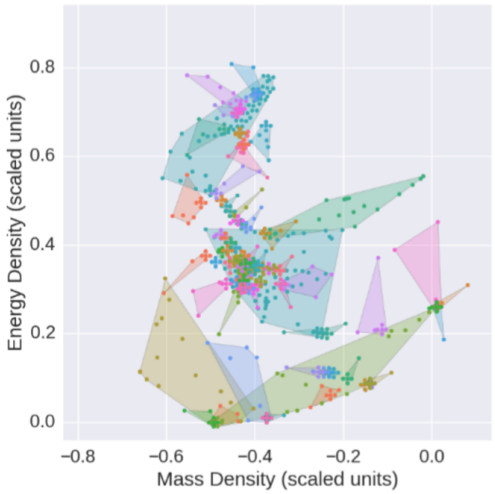



Figure 11: Surrogate models over subsets of domain.

**Presentation 2: Jaroslaw Knap** "Accelerating Scale Bridging via Surrogate Modeling."

*Problem setting/ motivation:* Multiscale modeling is a systematic approach to development of high-fidelity material models. The objective is to combine physics associated with relevant scales by bridging the models between different scales. Scale bridging is essential, but can be difficult and computationally challenging.

*Background theory:* In a hierarchical multiscale model, a higher scale model acquires missing data by querying a lower scale model. Running simulations at multiple scales can be very expensive and surrogate models can be used to alleviate this difficulty. A surrogate model is an approximation of a model, constructed from direct observations of the model. Gaussian process regression (GPR) can serve as a surrogate which is also capable of predicting the error in addition to the function values. The error prediction enables the possibility of running adaptive calculations based on a target error. But there is a bottleneck caused by the $O(N^3)$ complexity for inverting the sample covariance matrix. One possible avenue to reducing the computational cost is to build surrogate models over subsets of the domain.

*Methodology:* Constructing a two scale model of RDX with tight coupling between chemistry and deformation is notoriously hard due to difficulty in capturing the coupling. However, atomistic models can capture the coupling quite accurately. An adaptive online GPR model was used as a surrogate to significantly reduce the cost of lower-scale models. Multiple surrogate models were built over subsets of the domain of the lower scale model. These subsets are selected along trajectories induced by the higher scale model and hence the surrogate models have to cover only a portion of the domain of the lower scale model. The procedure for adaptive online GPR requires an upper bound to be imposed on the number of data points in a surrogate model. Then, surrogate models are continuously constructed from nearby data points. The covariance is employed to adaptively refine and construct new surrogate models given a target error of surrogate models. The result is that the individual surrogate models are continuous/smooth but global continuity/smoothness is lost. To regain global smoothness and reduce the cost of constructing the GPR, a method based on hierarchical Cholesky decomposition was adopted in the study.

*Examples & results:* The example presented had the goal of developing a high-fidelity model of RDX. A two scale model was developed for this. The upper-scale model was a finite element model. At each integration point for each time step, a lower scale model simulation was performed to obtain the equation of state. The lower-scale model was in LAMMPS based on dissipative particle dynamics. A single crystal of RDX with no defects was modeled at the lower scale, without modeling the chemistry.

The specific application being modeled was a 2D axisymmetric model of a cylinder of RDX impacting a rigid anvil. The model was computationally very expensive and running a high fidelity concurrent multiscale simulation was computationally intractable. Results of using the adaptive sparse grid GPR approach based on hierarchical Cholesky decomposition were shown. Figure 11 shows the spatial subsets obtained by adaptive online GPR in the domain of the lower scale model. Plots of the simulation accuracy and results of the simulation efficiency were shown for different number of grid levels, different values of the sparsity parameters, and different values of error tolerances in the adaptive sampling approach.

*Conclusions:* The total cost of repeated evaluations of the lower scale model can be often staggering, rendering the overall method impractical. Surrogate modeling can substantially reduce the cost. Gaussian process regression (GPR) is well-suited for construction of surrogate models. Using GPR enables prediction of function values accompanied by prediction of error. Hierarchical Cholesky decomposition

can bring down the cost of constructing GPR surrogate considerably.

*Future Research Directions:* Dr. Knap identified several areas where research is needed in hierarchical multiscale materials modeling, including the following:

- There is a need for improved methods for surrogate modeling in high-dimensional spaces, space-time surrogate models, and adaptive multi-fidelity surrogate models.
- Surrogate modeling in the presence of discontinuities poses many challenges.
- Spatial scale-bridging is necessary for materials with evolving internal state/microstructure and requires a stochastic treatment.
- Temporal-scale bridging has not been adequately addressed.
- Methods capable of exploiting hierarchical multiscale models for design under uncertainty for complex materials are needed.

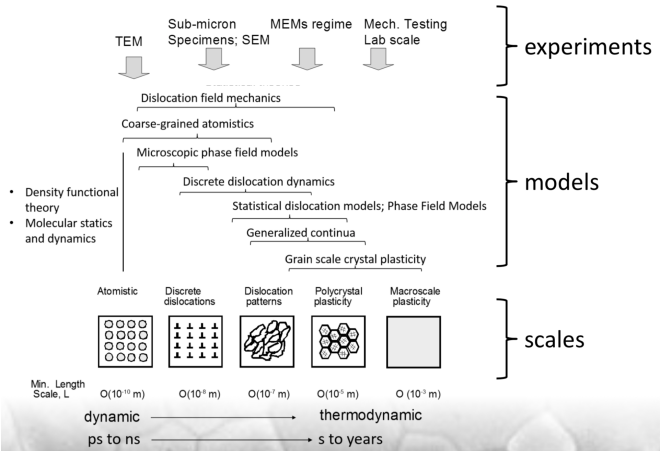



Figure 12: Challenges in hierarchical multiscale modeling.

**Presentation 3: David McDowell** "Uncertainty in the Definition and Calibration of Multiscale Material Models."

*Problem setting/ motivation:* The historical focus of verification, validation, and uncertainty quantification (VVUQ) efforts has been on individual models focusing on a single length and/or time scale. An area which needs attention is VVUQ for multiscale models comprising a simulation operating over multiple length/time scales in a concurrent or hierarchical manner. Further, VVUQ for mathematically and physically consistent multiphysics models is in its infancy.

*Background theory:* There are two approaches to multiscale modeling, using either hierarchical multiscale models (HMM) or concurrent multiscale models (CMM). In a HMM, there is one-way coupling of physics at multiple scales, and there are uncertainties in model form, initial values, parameters, and the choice of scales to bridge. In HMMs, single scale modeling is not enough, and it is also essential to address uncertainty in connections. Figure 12 shows a summary of the challenges in HMM.

Uncertainty quantification can be thought of as being applied in two cases, depending on the amount of data available - either there is 'plentiful' data or 'small' data. When there is plentiful data, uncertainty quantification and propagation is applicable and useful, and statistical learning algorithms that track uncertainty can be used. The case of having small data is the more common scenario in materials design and development. In this case, uncertainty quantification can provide algorithmic decision support to guide the choice of next experiment or simulation.

*Methodology:* Materials Knowledge System (MKS) is a localization technique based on data science, used to determine local response given macroscopic applied conditions. This enables high throughput multiscale simulations with sufficient accuracy.

The Inductive design exploration method (IDEM) is a method in which feasible ranged sets of specifications are found in a step-by-step, top-down (inductive) manner. In this method, a designer identifies feasible ranges for the interconnecting variables between two models in a model chain.

In crystal plasticity (CP) modeling, bottom-up (BU) and top-down (TD) pathways have been shown to lead to model parameter estimates that are different. A combined TDBU strategy to inform the CP model seeks reconciliation of these contrasting estimates. Individual models in the HMM hierarchy are assumed to be validated and the uncertainty of the linkage between models is at issue. The calibration method for combining TD and BU data uses a constrained maximum likelihood function. To reduce discrepancy in the calibrated model, the constrained likelihood functions are augmented with a physics-based inter-scale discrepancy layer.

*Examples & results:* Results of using MKS to predict the strain tensor for basal textured $\alpha$-titanium were shown. The strain fields were sufficiently accurate (1% to 3.5% mean error in comparison to

CPFEM results for the same material). Another example showed the application of MKS to high cycle fatigue (HCF) in $\alpha$-titanium polycrystals.

Another example presented was the application of IDEM to designing the texture of $\alpha$-titanium polycrystals.

Another example showed coordinated kink-pair formation and the Kocks-Argon-Ashby flow rule for bcc-Fe. The mesoscale flow rule had 5 calibration parameters in addition to 3 alignment variables. Normalized calibration variance was reduced significantly by introducing the inter-scale discrepancy layer.

*Conclusions:* Scale bridging at the mesoscale is especially challenging because, at lower scales behavior is governed by dynamics, while at higher scales behavior is governed by thermodynamics. There is a need to ensure consistency between these scales. To be consistent in both a TD and BU sense, models have to be reconciled at the middle.

*Future Research Directions:* Prof. McDowell identified several areas where future research is needed in multiscale modeling, including the following:

- In CMM, there is a need to address model-form uncertainty to facilitate concurrency.
- With these multiscale modeling approaches, there is a need to address complex, configuration/environment dependent phenomena.
- There is a need to advance intrusive/embedded methods for high-performance computing.
- In HMM, there is a need to shift more attention to the identification of the appropriate number of models/scales.
- There is a need to quantify uncertainty in linking algorithms and model calibration procedures. In particular, linking strategies are considered as part of the model form and require UQ in the configuration of the multiscale system and information flow.
- Further study is needed on the utility and consistency of bottom-up vs top down information.

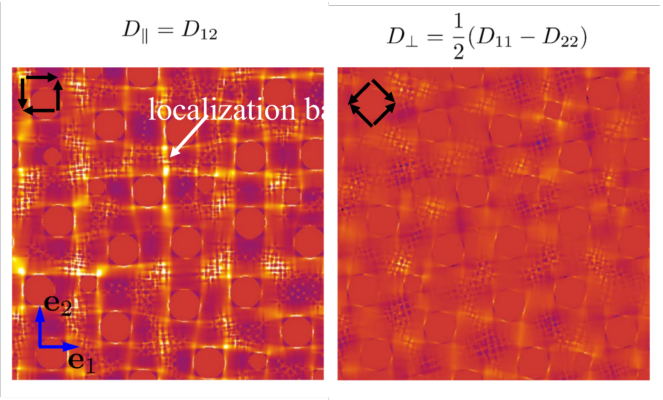



Figure 13: Map of intraphase strain rate fluctuations from full field simulations of fiber reinforced composite.

**Presentation 4: Pedro Ponte Castañeda** "Homogenization Estimates for the Macroscopic Response and Field Statistics in Viscoplastic Polycrystals."

*Problem setting/ motivation:* Homogenization is able to provide effective properties and field statistics such as phase averages and covariance tensors for stresses and strains. The presentation addresses how homogenization helps to quantify uncertainty in these fields.

*Background theory:* If there is a wide separation of length scales and the boundary conditions vary "slowly" relative to the micro-scale, then an RVE of the composite behaves like a homogeneous material with effective properties depending on the properties and distribution of the constituent phases (i.e., microstructure) but not on the specific boundary conditions. The microstructure is described using grain shape, grain orientation, and crystallographic texture. For solid polycrytalline materials, a suitably defined linear comparison composite (LCC) is homogenized to obtain effective properties to estimate the nonlinear behavior. The average response of the polycrystal has to match the average in the LCC.

In fiber reinforced composites, hard aggregates are embedded in a softer matrix. A unit cell with periodic boundary conditions is modeled and simulated making use of fast-Fourier transform (FFT).

*Methodology:* The polycrystalline material was treated as having random "ellipsoidal" granular microstructure. The instantaneous response was obtained by using fully optimized second-order (FOSO) variational method. Self-consistent estimates of the effective properties for the LCC and field statistics

in the LCC were calculated. The macroscopic response and the statistics of the nonlinear material were given by the response and statistics of the LCC.

For fiber-reinforced composites, the distribution of fibers in the plane was assumed random and isotropic. Plane strain conditions were assumed to exist, the phases were incompressible, and their behavior was governed by a power law. The material was also assumed to be strain-rate sensitive. In order to obtain statistical homogeneity and isotropy, an ensemble average was taken over 20 configurations. Second-order estimates made use of the Hashin-Shtrikman linear estimates and required the solution of three nonlinear equations.

*Examples & results:* Results for nonlinear homogenization of ice polycrystals were presented. Power-law behavior with exponent equal to 3 was used for the grains. Plots of the effective flow stress computed for the polycrystals with different levels of grain anisotropy were shown. Also shown were plots of standard deviation of equivalent strain-rate and standard deviation of equivalent stress as a function of grain anisotropy.

Results for simulations of fiber reinforced composites were shown. Fluctuations of the local stress and strain fields in the matrix phase were plotted. Results of full-field simulations showing the intraphase fluctuations of strain rate were presented for linear as well as nonlinear phases. For linear phases, the strain rate fluctuations were isotropic whereas for nonlinear phases, strain-rate fluctuations increased and became anisotropic. Fiber-reinforced composites showed strong localization of the parallel strain-rate in simple shear with nonlinear phase material properties (see Figure 13). Plots of the distribution of strain-rate components were also shown for the linear as well as for the nonlinear material and it was shown that it is possible to estimate the low-order moments using homogenization.

*Conclusions:* Homogenization methods have been developed for heterogeneous materials with nonlinear material behaviour making use of optimally designed linear comparison composite. The methods can be used to generate bounds and estimates of different types for the macroscopic (average) response. By means of appropriate perturbations, the methods can be used to generate estimates for the mean and covariance of the stress and strain fields in the phases. The methods can account for complex, multiscale microstructures including porosity (damage) as well as crystallographic and morphological texture, thus capturing the complex coupled effect of crystallographic and morphological anisotropy.

***Discussion:***
An important discussion centered about the transition of UQ in multiscale material modeling to engineering practice. It was remarked that the area of uncertainty quantification and propagation in multiscale modeling and simulation appears to be in its early stages of research/development. There are many disparate pieces and methodologies and little consensus on how to bridge scales. The question was posed as to whether integrated multiscale modeling approaches with UQ will be adopted in practice in next 5-10 years, and whether such approaches are becoming part of commercial software.

In response, it was noted that, while some of these multiscale modeling capabilities have been embedded in existing codes (e.g. LSDYNA), these are all without uncertainty quantification. It was noted that select companies have access to code for multiscale approaches and they are starting to be used in a practical industry application. But other commercial codes such as ABAQUS do not yet have the multiscale approaches embedded in them. However, integration of UQ to the process has not taken place. It was noted that handling parametic aleatory uncertainty appears to be relatively low-hanging fruit for software such as ABAQUS due to integration with Python, and that similar situations might exist for other software. Commercial software are not likely to deal with model form uncertainties and other epistemic uncertainties, on the other hand, because methodologies are still being developed. It was also pointed out that there is also software such as Dakota from Sandia National Lab, which facilitates the integration of UQ into simulations.

When asked to highlight the most important issues to be addressee for multiscaling in simulations, the general response was that there are several important issues in going from microstructures/below to higher scales, and it is very difficult to say which is the most important/most critical. However, it was also opined that model form uncertainty is an especially important topic requiring further study. It was further remarked while machine learning and surrogate models provide potentially powerful tools, but incorporating knowledge of physics must be used to improves the capability and usefulness of these machine learning tools.

Several discussions focused around questions specifically related to the topics of presentation. One such point of considerable discussion was about whether it is possible to extend homogenization estimates to higher order moments, tail statistics and extreme values beyond just moments. It was remarked that with 2-point statistics, it is possible to calculate low order moments, but 3-point statistics of microstructure are necessary to get higher moments. It was noted that specifying input moments does not specify the output moments because there is no one-to-one mapping. Therefore, even with higher order statistics of the input microstructure, it would not be possible to calculate higher order moments of the output quantities such as local stresses and strains. It was further remarked that if you know the form of the distribution of the output quantities, then it is possible to analytically compute the moments, but the form of the distribution remains unknown. It was therefore concluded that considerable advances in methods for computational homogenization are needed that can incorporate tail-dependencies, extreme values, and other higher-order properties to capture material failure.

This led to some discussion about the general practice of fitting probability models to test data for materials. For example, for concrete, 21 types of material tests can be done but most articles just fit models to results from 2-3 types of tests, and this practice needs to change.

Another aspect discussed was that epistemic uncertainty (caused by lack of samples, numerical error etc.) cannot be captured by homogenization of physical properties alone.

***Emerging Themes & Future Research:***

*Different frameworks for multiscale modeling:* As the session progressed, it became increasingly clear that several different frameworks have arisen for uncertainty quantification in multiscale modeling. At present, there is no universally accepted and unified framework for UQ in multiscale modeling. Prof. McDowell presented two potential frameworks in the hierarchical and concurrent multiscale methods, and it could be argued that many of the other methodologies presented could fit into these categories. However, it is not universally accepted that these methods are sufficiently general to capture the entire multiscale modeling paradigm. Moreover, within these multiscale methods, approaches for UQ in scale-bridging vary considerably. Presented approaches included spatial random processes, surrogate-based scale bridging, and homogenization. However, these approaches are not necessary general, have their strengths and weaknesses, and considerably more research is needed to advance these methods to a stage where general standard can be established for UQ in materials modeling.

*Surrogate Modeling:* An important theme of this session was use of surrogate models for scale-bridging. Surrogate models can be powerful tools for multiscale simulations, but continued advances are needed in their design and implementation for this purpose.

*Model consistency:* An important topic that was raised was the issue of model-consistency. It was emphasized that scale-bridging models must be physically consistent at both upper- and lower- length scales, they must also be consistent whether being approach through a top-down or bottom-up framework. It is not clear that many multiscale methodologies have worked to ensure this level of consistency, and it has been suggested that this should be a standard for scale-bridging.

*Machine Learning:* As in previous sessions, machine learning was a popular topic of discussion. It was highlighted that machine learning frameworks can be useful for scale-bridging but additional work is needed to investigate their applicability for different problems, e.g. having different data structures and constraints, and their limitations.

*Homogenization:* Considerable effort is needed to overcome the low-order moment limitations associated with existing homogenization methods. It was argued that future efforts should focus on homogenization techniques that are capable of reproducing extremes and material response to be consistent with the true, potentially non-Gaussian probability distribution of material performance.

## Session 7: Multiscale material modeling – Macroscale

***Session Chair:*** **Sanjay Govindjee**, University of California at Berkeley

***Presenters:***

- **Sankaran Mahadevan**, *Vanderbilt University* "Multi-scale Multi-physics Uncertainty Quantification of Manufacturing Effects on Material Performance."
- **John McFarland**, *Southwest Research Institute*, "Calibration and Uncertainty Analysis for a Temperature-dependent Yield Strength Model of Additively Manufactured Alloy 718Plus."
- **Stephanie TerMaath**, *University of Tennessee*, "Sensitivity Analysis for Multi-Scale Modeling to Inform Design Optimization."

***Overview:***

The final session of three on multiscale modeling focused on integration of uncertainty in modeling of materials at the macroscale (i.e. from millimeter up to structural length scales). In particular, the goal was to discuss how information from lower scale simulations and experimental data can be fused to inform material models at length scales of interest for practical engineering applications.

One of the talks focused on multi-scale uncertainty quantification for additive manufacturing during multi-physics analyses. Approaches to perform sensitivity analysis while incorporating epistemic uncertainty were outlined. Another talk presented a Bayesian approach for quantifying confidence in models accounting for epistemic uncertainty, with application to a physics-based constitutive model for yield strength of Ni based superalloys. Discrepancy between the model and experiments was accounted for in a post-processing step by adding a bias-correction term to the model. In the final talk of the session, damage modeling of composite patches used for repairing aluminum superstructure of ships was presented.

***Review of Presentations:***

**Presentation 1: Sankaran Mahadevan** "Multi-scale Multi-physics Uncertainty Quantification of Manufacturing Effects on Material Performance."

*Problem setting/ motivation:* Due to low volume production of parts from additive manufacturing (AM), there is limited data on part-to-part variability and hence variability reduction efforts have to be model-based, instead of being only based on test data. Uncertainties in the manufacturing process parameters must be propagated to bulk material properties through multiscale modeling. The focus of the talk was on uncertainty quantification and propagation for multiscale and multiphysics modeling of additive manufacturing.

*Background theory:* There are several challenges in modeling the AM process, due to the models involving multiple scales, multiple physical phenomena, high-dimensions, and coupling. There are also multiple aleatory and epistemic uncertainty sources which need to be accounted for. A Bayesian network with Markov chain Monte Carlo simulation can be used for multiscale uncertainty quantification. Model errors are introduced by choice of the model form, discretization in numerical solution, and surrogate model error, if a surrogate model is used. If model parameters are uncertain, then this leads to an even larger set of variables , i.e. hyper-parameters, used to represent the parameter uncertainty, in addition to the model parameters. All of these uncertainties must be accounted for systematically to perform sensitivity analyses.

*Methodology:* The methodology adopted for multiscale UQ was a structural equation modeling (SEM) framework which made use of lower level data to validate the higher level model under uncertainty. Using Bayesian hierarchical modeling and Markov chain Monte Carlo (MCMC) simulation techniques it was feasible to estimate the posterior distributions of SEM parameters.

It was also necessary to perform sensitivity analysis considering epistemic uncertainty due to model uncertainty and data uncertainty. However, it is not possible to use traditional variance-based sensitivity indices for cases where the uncertainties are epistemic. The approach adopted used an auxiliary variable for each stochastic variable which enabled computation of several global sensitivity indices accounting for the contributions of epistemic and aleatory uncertainty sources to the overall uncertainty in the model output.

Since the multiscale and multiphysics model was very computationally intensive, it was necessary to use a surrogate model in the UQ approach. Since the inputs and outputs are field quantities, even surrogate models from methods such as co-kriging or

GPR are very severely affected by the high dimensionality. Hence, dimension reduction methods are important. It was essential to perform singular value decomposition (SVD) or principal component analysis (PCA) first to reduce the dimensionality of the input/output and then build a surrogate model.

*Examples & results:* Multiscale modeling and simulation was used to obtain the bulk material properties such as Young's modulus of an additively manufactured material. Results of the sensitivity of the variance of the Young's modulus at the macroscale to manufacturing process parameters were presented.

A multiscale multiphysics model of the AM process was built to predict microstructure evolution during solidification of the material. The forward problem involved uncertainty aggregation from the various sources, including the surrogate model error, and sensitivity analysis, using the approach presented. Sensitivity analysis showed the important first order and interactive effects. Then the surface roughness sensitivity to different process parameters was studied. PCA was used to reduce the dimension of the output. Active subspace discovery was used to reduce the dimension of the inputs. A surrogate model was then built and this model was verified and validated. This enabled the entire AM process to be simulated.

*Conclusions:* Epistemic and aleatory uncertainty from several sources were aggregated and propagated through a multiscale multiphysics model using a Bayesian network. Sensitivity analysis was performed accounting for the effects of epistemic and aleatory uncertainties separately. Surrogate models were developed after dimension reduction of the input and outputs to make multiscale multiphysics simulation of an AM material tractable.

*Future Research Directions:* Prof. Mahadevan identified several important challenges that require further research, including the following:

- It is necessary to develop methods for online monitoring of the manufacturing process for multiple quantities of interest.
- Model calibration, model validation, model error estimation, and uncertainty reduction are difficult for any model, but are especially challenging for multi-scale, multi-physics models.
- There is a need to enable process parameter optimization to reduce variability in additively manufactured parts.
- Methods for process control under uncertainty that include fusion of model prediction and monitoring data are needed to improve AM processes.

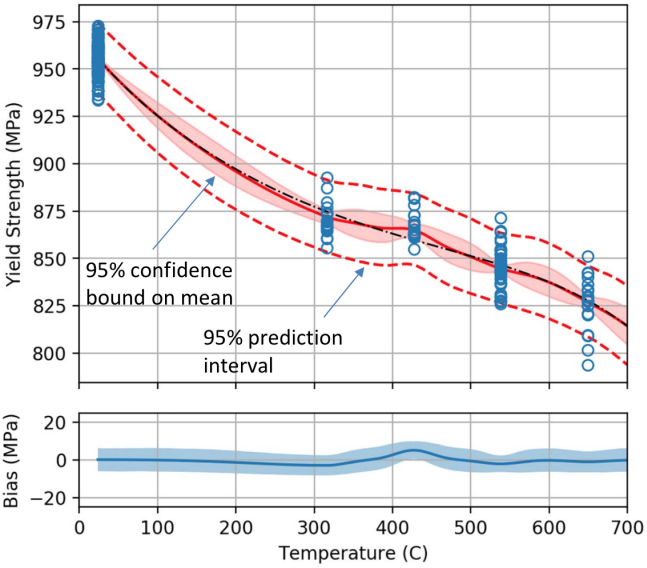



Figure 14: Calibrated yield strength prediction with bias correction.

**Presentation 2: John McFarland** "Calibration and Uncertainty Analysis for a Temperature-dependent Yield Strength Model of Additively Manufactured Alloy 718Plus."

*Problem setting/ motivation:* Models are necessary to accelerate qualification of new processes and materials. Epistemic uncertainty is a key element which must be accounted for during decision making about qualification. Demonstrating and quantifying confidence in models is a significant barrier to adoption of model-based qualification approaches.

*Background theory:* The qualification process requires deciding whether enough evidence is available to qualify the process/material, and if not, determining what new information must be collected to obtain the necessary evidence. This needs a framework for quantifying confidence in model predictions, which should be based on what is known about the physics (i.e., the model) and available data. Epistemic uncertainties exist due to inability to fully characterize unobservable model parameters. Inherent variations (i.e., aleatory uncertainties) also exist in the available test data. It is necessary to quantify both uncertainty types and understand how they impact predictions. A Bayesian approach can be used for quantifying confidence in model predic-

tions. Once the uncertainties in the material properties such as yield strength are quantified, they can be propagated through structure-scale models.

*Methodology:* A physics-based constitutive model is used to represent the yield strength and subsequent plastic response of a Ni-based superalloy. The constitutive model has six yield strength components, due to contributions from various microstructural properties. Bayesian calibration with a discrepancy function is performed using test data available for the material. In a standard Bayesian calibration framework, the data is modeled as the sum of the material model prediction and an error term which represents random variation. In Bayesian calibration with a discrepancy function, the test data is modeled as a sum of the material model prediction, a bias/discrepancy function, and an error term.

*Examples & results:* The framework was applied for a Ni based superalloy. The specimens were additively manufactured using direct metal laser sintering (DMLS), with a fixed set of process parameters. After the specimens were manufactured, they were subjected to post-processing operations such as stress relief, hot isostatic pressing (HIP), solution treatment, and ageing. The microstructure of the manufactured material was then characterized by measuring the grain size and the $\gamma$' precipitate size and volume fraction. Mechanical characterization was performed using several tensile test specimens, from 2 powder lots, tested at 6 different temperatures. The test data for the yield strength of these specimens was shown. This data was used to quantify variability and calibrate the yield strength model. It was observed that there was a small discrepancy at some temperatures, which can be corrected with a modified formulation which accounts for bias in the model predictions. After analysis using this modified Bayesian framework, parameter samples were post-processed to quantify model discrepancy and prediction uncertainty. Posterior predictions utilize calibrated parameter values and temperature- dependent bias correction. The results obtained were as shown in Figure 14.

*Conclusions:* The presentation demonstrated a framework for quantifying epistemic and aleatory uncertainty for qualification of additively manufactured materials. The Bayesian framework provides flexibility and allows accounting for discrepancy between model and tests. Using the Bayesian framework, it was possible to obtain probabilistic material model parameters with quantified confidence and identify the relative contribution of epistemic uncertainties.

*Future Research Directions:* Dr. McFarland identified many important research challenges related to UQ for additively manufactured materials, including the following:

- We are only beginning to understand the sources of variability in additively-manufactured parts. These may include lot-to-lot powder variability, machine-to-machine variability (even when the same architecture is used), variability due to differing machine architecture, machine settings (power, speed, hatch, etc.), and specimen geometry/orientation, location-specific properties within part which could be caused by, for example, difference in thermal history near surface.
- UQ can be a critical tool to establish when experimental "re-characterization" of the AM process is needed.

**Presentation 3: Stephanie TerMaath** "Sensitivity Analysis for Multi-Scale Modeling to Inform Design Optimization."

*Problem setting/ motivation:* Prototype composite patches (GRP laminates) are installed for temporary repair of aluminum superstructure cracks on US Navy ships. It is not feasible to test a large number of potential configurations and material combination of the patches. Therefore, a rapid, physics-based approach is desired to evaluate structural reliability with these patches installed.

*Background theory:* The patches were applied on a thick metallic substrate, and hence bending effects were important to be modeled. The substrate was made of aluminum 5000 series alloys, which are susceptible to sensitization caused by magnesium precipitates which increases brittleness and causes cracking, leading to corrosion by seawater. The patches were in an environment where they could be subjected to low-velocity impact. The manufacturing tolerances were not tightly controlled, and this had to be factored into the analysis. There was also a lack of sufficient data for strength assessment; hence A or B basis values were not available for use in design. After application of the repair patch, the hybrid structure suffers damage, which can be minor but can substantially degrade performance. Multiple damaged regions may exist internally in the

hybrid structure. There are multiple possible damage mechanisms and these may interact, leading to failure of the patch. It was therefore necessary to develop models and methodology at multiple scales to predict damage tolerance in a patched structure. It was also necessary to identify the design and installation parameters which had the most influence on structural performance.

*Methodology:* A sequential multiscale methodology was adopted for modeling the material. The approach combined first-principles calculations based on density functional theory at the atomistic/electronic scales, peridynamics simulations at the microscale and finite element modeling at the macroscale. A hybrid model was developed which accounted for varying mechanisms of damage in the metal, in the GRP, or in the bondline. This led to a very complex damage behavior that varies with load, configuration, boundary conditions, and materials. Tests were conducted on the composite material for calibration and validation of the models. Macroscale testing was also performed to obtain data at different boundary conditions and configurations. The tests conducted were 3-point and 4-point bending tests, low velocity impact test, crack growth test. All damage mechanisms such as fiber breakage, matrix cracking, delamintaion, disbond, were initiated in the test specimens.

*Examples & results:* Results of the 4 point bending tests with 4 different configurations of the material were shown. Different damage mechanisms caused failure depending on the material configuration. The different damage mechanisms were quantified by energy absorption. Simulation results were able to replicate the test results for all the 4 configurations. A surrogate model was constructed for interpolation between the data points but this surrogate model did not give accurate predictions due to the need to include hundreds of input parameters. Instead, an approach was applied to build a surrogate model at each analysis scale and only include sensitive parameters from scale i in the surrogate model for scale i+1. Results were also shown for low-velocity impact simulations and stress corrosion cracking simulations.

*Conclusions:* It was observed in the study that all potential damage mechanisms do not appear at the same time, and their contributions can vary depending on loading conditions and input parameter values. As a result, it is necessary to study parameter interactions and to map contributions of damage mechanisms throughout the parameter space. Many highly sensitive parameter values were based on low quality data and it is necessary to fully characterize these parameters through experimental testing to improve the models.

*Future Research Directions:* Prof. Termaath identified the following research challenges associated with multiscale material modeling:

- Many multiscale materials problems are very high dimensional. Methods are needed to build accurate surrogate models for large dimensional problem, with $\sim 50 - 200$ input parameters, for 5-10 design objectives and a highly nonlinear space.
- Along a similar lines, methods to limit the parameter space for complex models a priori could be used to simplify the challenges associated with high dimension.

***Discussion:***

The discussion revolved largely around the treatment of model form uncertainty and, overall, treatment of epistemic uncertainty was one of the emerging themes from the workshop. A question was posed asking what is the best approach to handle model form uncertainty. The presenters responded that a Bayesian approach is attractive, but cautioned that since they work mostly with Bayesian methods, their opinion might be biased. Within the Bayesian context, model error is included through a discrepancy term. But this is only accounting for discrepancy of that model at the level of the measurements, and using this approach does not allow characterization of model error outside of the range of measurements. Another approach currently being developed by the presenters is trying to use the governing equation (i.e., a physics-based approach) instead of a discrepancy term for the model error. This enables discrepancy estimation in coupled multiphysics models using Bayesian state estimation methods and allows identification of the sources of the discrepancy.

In the treatment total uncertainty, a further point of discussion was whether information is being discarted if all the uncertainty (aleatory and epistemic) is rolled up into a single metric. The presenters response was that it depends on the scenario and what the decision-maker needs from the uncertainty analysis. If the decision-maker wants/needs one value of the uncertainty, then it makes sense to compute one uncertainty values by pooling together

all the sources of uncertainty. But, if the objective of the uncertainty is different, for example if it is desired to find out whether to budget for reduction is epistemic uncertainty (which is possible by collecting more information) then it is necessary to keep the aleatory and epistemic uncertainties from all sources separate.

***Emerging Themes & Future Research:***
*Additive Manufacturing:* Models of AM processes are multiscale, multiphysics models that have a very large number of uncertainties associated with the process parameters, collected data and measurements, and models of different physics at different scales. Robust modeling approaches are needed that can fuse these disparate uncertainties in a unified framework and further enable the influences of individual uncertainties to be assessed (i.e. enable sensitivity analysis). These frameworks will be essential to develop manufacturing process controls that incorporate model uncertainties as well as monitoring data collected during the manufacturing process.

Limited experimental/manufacturing data requires that materials studies and qualifiction of additivitly manufactured materials be model-based. However, it was clear from the presentations that we are only beginning to understand the many uncertainties that come into these models. It will be necessary to quantify the many uncertainties in AM processes needed to build model-based material qualification standard that we can trust.

*Sensitivity Analysis:* A major theme of the session was the ability to assess the sensitivity of material performance to various parameters and uncertainties that arise in manufacturing and modeling. This was shown for additively manufactured materials where is necessary to know how various process parameters influence material performance and to assess the importance of modeling uncertainties in process modeling. For composite patches, it was necessary to understand the influence of the many material parameters across many lengthscales on patch performance and reliability.

*Aggregation of Aleatory and Epistemic Uncertainties:* Both the presentations and the discussions highlighted the need for consistent unified frameworks that can adequately track both aleatory and epistemic uncertainty.

## Closing Session

***Session Chair:*** **Michael D. Shields**, Johns Hopkins University

***Presenters:***

- **Sanjay Govindjee**, *University of California at Berkeley* "NSF NHERI SimCenter."

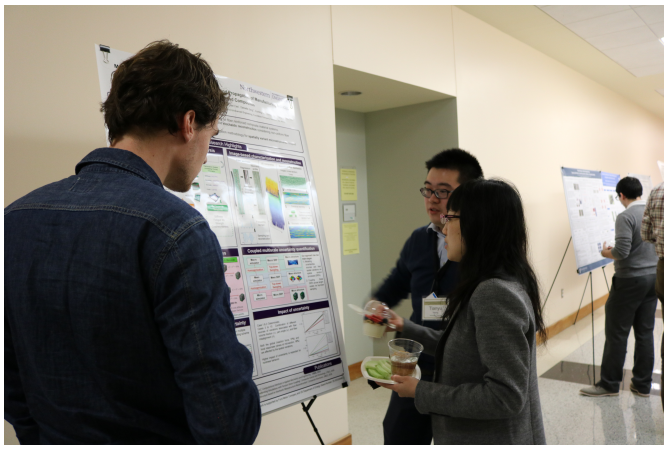
***Overview:***

The intention of this session was to provide a forum for discussion of the common themes and challenges identified through the conference. One presentation was scheduled to be given on the NSF Natural Hazards Engineering Research Infrastructure SimCenter, which provides a software infrastructure for uncertainty analysis. This was to be followed immediately by the discussion. Due to time constraints, the closing session was merged with Session 7. Both Prof. Govindjee's presentation and the discussion were held during Session 7.

***Review of Presentations:***

**Presentation 1: Sanjay Govindjee** "NSF NHERI SimCenter."

The goals of the NSF NHERI SimCenter at Berkeley were presented. An overview of the facilities which are part of the 10 centers in the NHERI consortium as well as the SimCenter was provided. Some examples of the kind of work, such as regional level simulation of hazards with high resolution, which can be undertaken with the workflows being facilitated by SimCenter were shown. The main message was that there is an opportunity for UQ researchers to find application of their research at the NHERI SimCenter. In particular, some opportunities facilitated by SimCenter that were highlighted were: 1. algorithms for Bayesian updating of expensive models and model class selection, with access to data and models, 2. a testbed for methods for extreme events (i.e., low probability but high impact events), 3. a testbed for tools for multi-level Monte Carlo methods, 4. high impact, broader impact arena for tools and methods for supporting decision making, and 5. high impact, broader impact arena with very high dimensional random variables and random fields.



## Speed "Poster Slam"

During the final session of day one, each of the poster presenters was given one minute to promote their poster. The students/postdocs were instructed to give a brief glimpse into the topic of their poster to encourage the conference participants to visit their poster to learn more. The poster sessions were held during the coffee and lunch breaks and there was a very positive response to the short poster presentations. The students were very effective at giving a short introduction to their presentation to spark interest.

## Summary of Final Takeaways and Future Research Directions

The conference highlighted some of the most important topics of research in UQ for materials modeling and a primary objective of the conference (and this report) was to distill the vast array of research activity in this area down to identify some of the key challenges in the field. The following provides a brief, non-exhaustive list of some of these challenges identified during the conference and serves as a recap to the more detailed discussions above.

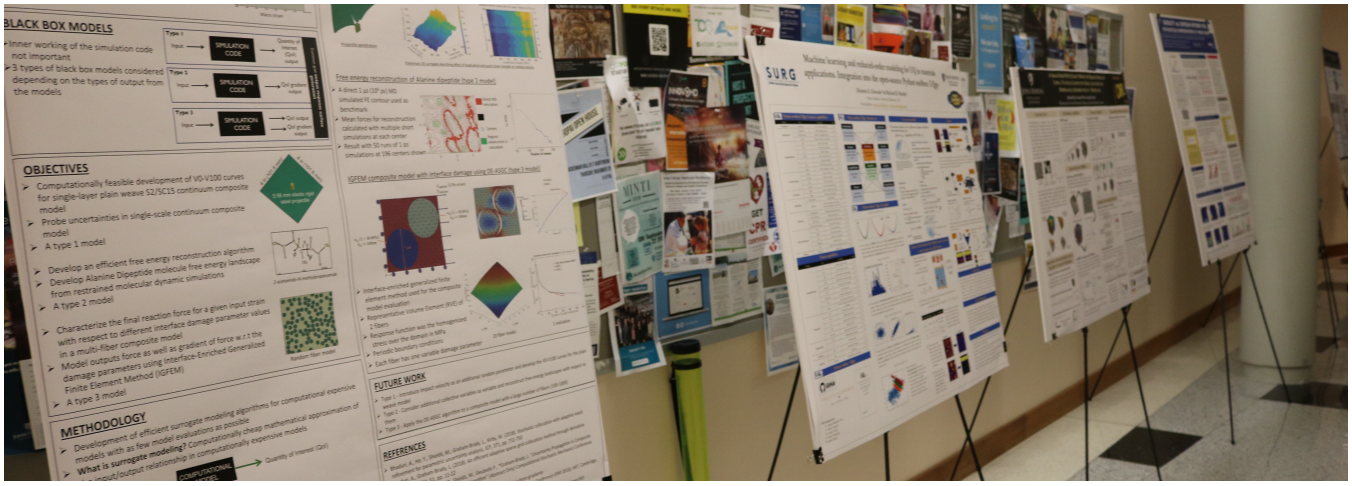
- A major challenge in material modeling, specifically as it relates to uncertainty quantification, is the assessment of model form and model selection from competing models. This is true at all length- and time-scales from the quantum to the structural scale as well as in the form of models used to pass data between scales.
- There is a significant need for research related to uncertainties associated with lack of scale-separation in a multi-scale modeling paradigm. This is especially important for material failure processes that are governed by localization or extrema at a lower scale that must be accounted for at a higher-scale. More generally, the application of UQ methods for problems related to extremes in material response are critically important.
- Machine learning, surrogate modeling, and dimension reduction techniques present new opportunities for advancements in materials modeling practice, but they need to be approached with caution, used appropriately, and rigorously mathematically developed to include estimates of the uncertainties induced by exploiting these tools.
- Methodologies that are capable of accounting for all sources of uncertainties, both aleatory and epistemic, stemming from sources as disparate as small datasets, model-form, parametric variations, and "unknown unknowns" need to be more broadly applied for material modeling problems at various length-scales.
- The field has only recently begun to contemplate how to address challenges of materials-by-design in a way that considers uncertainty. This poses numerous challenges as they relate to inverse modeling practices such as Bayesian inference, design of experiments, optimization under uncertainty, machine learning and surrogate modeling as applied to materials.

Again, these are just a few of the critical research areas in UQ for materials modeling, but overall the conference helped to shed light on some of the specific challenges faced in each of these areas, which are likely to be some of the major areas of materials research of the next 5, 10, or 20 years and beyond.

## List of speakers

A total of 26 invited presentation were given at the conference. The speakers at the workshop are listed in alphabetical order below:

- **Wilkins Aquino**, *Duke University*
- **Zdenek Bazant**, *Northwestern University*
- **Wei Chen**, *Northwestern University*
- **Charbel Farhat**, *Stanford University*
- **Stephen Foiles**, *Sandia National Laboratory*
- **Timothy Germann**, *Los Alamos National Laboratory*
- **Mircea Grigoriu**, *Cornell University*
- **Johann Guilleminot**, *Duke University*
- **George Karniadakis**, *Brown University*
- **James Kermode**, *University of Warwick*
- **Jaroslaw Knap**, *Army Research Lab*
- **Jia-Liang Le**, *University of Minnesota*
- **Jie Li**, *Tongji University*
- **Yongming Liu**, *Arizona State University*
- **Sankaran Mahadevan**, *Vanderbilt University*
- **Youssef Marzouk**, *Massachusetts Institute of Technology*
- **David McDowell**, *Georgia Institute of Technology*
- **John McFarland**, *Southwest Research Institute*
- **Michael Ortiz**, *California Institute of Technology*
- **Martin Ostoja-Starzewski**, *University of Illinois*
- **Pedro Ponte-Castaneda**, *University of Pennsylvania*
- **Simon Phillpot**, *University of Florida*
- **Jim Stewart**, *Sandia National Laboratory*
- **Stephanie TerMaath**, *University of Tennessee*
- **Clayton Webster**, *Oak Ridge National Laboratory*




## List of poster presenters

A total of 23 posters were presented at the conference. The poster presenters, along with the titles of their posters, are listed alphabetically below. Thanks to support from the National Science Foundation, a total of 13 travel awards were presented to student/postdoctoral poster presenters. The award recipients are denoted by a *.

- B.S. Aakash, *Johns Hopkins University*, "Variability in the thermo-mechanical behavior of structural aluminum."
- Bahmani Bahador*, *University of Tennessee*, "The use of statistical volume elements for homogenization and fracture analysis of quasi-brittle materials."
- Anindya Bhaduri, *Johns Hopkins University*, "Uncertainty propagation with a variety of computational models."
- Gurjot Dhaliwal*, *University of Toronto*, "Uncertainty analysis and estimation of robust interatomic potential parameters."
- Fei Ding*, *University of Notre Dame*, "Inflow and model-form uncertainty quantification in CFD using surrogate models."
- Matthias Faes, *Katholieke Universiteit Leuven*, "Inverse quantification of multivariate interval uncertainty in FE models."
- Dimitris Giovanis, *Johns Hopkins University*, "Machine learning and reduced-order modeling for UQ in materials applications. Integration into the open-source Python toolbox: UQpy."
- Eric Hall*, *RWTH Aachen University*, " Causality and Bayesian network PDEs for multiscale representation of porous media."
- Henry Herbol, *Johns Hopkins University*, "The physical analytics pipeline Bayesian accelerated materials discovery."
- Tianyu Huang*, *Northwestern University*, "Multiscale and multidimensional quantification and propagation of manufacturing induced uncertainty in fiber reinforced composites."
- Xiaoguai Li*, *University of Pennsylvania*, "How to discover dissipative PDEs from particles? Particle fluctuations determine evolution operator."
- Wen Luo*, *Northwestern University*, "Inferring the strength distribution of nacreous materials from statistical size effect."
- Xianfeng Ma*, *University of Tennessee*, "Hydrogen embrittlement in sensitized Al-Mg alloy: Peridynamic and molecular simulation."
- Deniz Ozturk, *Johns Hopkins University*, "Multi-scale modeling of deformation and fatigue crack nucleation in polycrystalline titanium alloys."

- Maxwell Pinz, *Johns Hopkins University*, "An image based finite element model for Ni-based superalloys using a two scale constitutive model accounting for morphological distributions of $\gamma\prime$ precipitates."
- George Stavroulakis, *National Technical University of Athens*
- Alberto Torres, *Johns Hopkins University*, "Robust design for additive manufacturing: Topology optimization considering geometric, material, and loading uncertainty."
- Lohit Vandanapu, *Johns Hopkins University*, "Higher-order multi-dimensional spectral representation methods: An FFT approach."
- Manav Vohra*, *Vanderbilt University*, "Efficient methods for UQ in atomistic simulations."
- Long Wang*, *Johns Hopkins University*, "Uncertainty quantification for systems with multiple systems with application to cold-formed steel shear walls."
- Ting Wang*, *Army Research Laboratory*, "Surrogate model based scale bridging with accelerated Gaussian learning."
- Mengjian Wen*, *University of Minnesota*, "Uncertainty quantification in atomistic simulations with dropout neural network potentials."
- Jiaxin Zhang*, *Oak Ridge National Laboratory*, "Online machine learning methods to accelerate Monte Carlo simulation"

## Administrative Support

The conference would not have been possible without the efforts of our outstanding administrative support.

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US Association for
Computational Mechanics

**Amanda Jackson**
Dept. of Civil Engineering
Johns Hopkins University

**Jess Ader**
Hopkins Extreme Materials
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Johns Hopkins University


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Additional administrative support was provided by the Dept. of Civil Engineering at Johns Hopkins University.

## Appendix: Conference Program & Additional Details

The conference program is provided in the following pages. Further details on the conference and links to available presentations can be found at the webpage of the workshop – http://uq-materials2019.usacm.org.

# USACM Thematic Conference:

## Uncertainty Quantification in Computational Solid and Structural Materials Modeling

Jan. 17–18, 2019
Johns Hopkins University
Baltimore, MD

USACM

Johns Hopkins Whiting School of Engineering

Sponsors:

HEMI Hopkins Extreme Materials Institute

NSF

# **Day 1**: Thursday, 17 January 2019

| | |
|---|---|
| 7:30–8:00 | Registration & Breakfast—Hodson Hall Lobby |
| 8:00–8:15 | Opening Remarks—Michael Shields, Lori Graham-Brady, Somnath Ghosh, Michael Falk<br>*HEMI Introduction—KT Ramesh* |
| Session 1: Stochastic Modeling of Materials–Methodology<br>Chair: Vissarion Papadopoulos, National Technical University of Athens<br>Room: Hodson Hall 210 | |
| 8:15–8:40 | A Tour of Stochastic Modeling for Materials Science and Multiscale Analysis<br>*Johann Guilleminot – Duke University* |
| 8:40–9:05 | Reflections on the Use of Monte Carlo Simulation in Stochastic Mechanics<br>*George Deodatis – Columbia University* |
| 9:05–9:30 | Tensor Random Fields in Continuum Mechanics<br>*Martin Ostoja-Starzewski – University of Illinois* |
| 9:30–9:55 | Optimal Uncertainty Quantification with Focus on Material Uncertainty<br>*Michael Ortiz – California Institute of Technology* |
| 9:55–10:15 | Discussion |
| **10:15–10:30** | **Coffee Break & Posters—Hodson Hall** |
| Session 2: Stochastic Modeling of Materials–Material Failure<br>Chair: Ernest Chin, Army Research Lab<br>Room: Hodson Hall 210 | |
| 10:30–10:55 | Stochastic modeling of damage localization in quasibrittle materials<br>*Jia-Liang Le – University of Minnesota* |
| 10:55–11:20 | Stochastic non-local lattice particle method for voxel level uncertainty quantification and material failure analysis<br>*Yongming Liu – Arizona State University* |
| 11:20–11:45 | Stochastic Damage Mechanics: Developments and Recent Progress<br>*Jie Li - Tongji University* |
| 11:45–12:10 | Estimates of extreme material responses for random microstructures<br>*Mircea Grigoriu – Cornell University* |
| 12:10–12:30 | Discussion |
| **12:30–1:30** | **Lunch—Hodson Hall** |
| Session 3: Data-Driven Modeling and Machine Learning<br>Chair: Fariba Fahroo, Air Force Office of Scientific Research<br>Room: Hodson Hall 210 | |
| 1:30–1:55 | Data-Driven Model Reduction and Probabilistic Learning for Digital Twins<br>*Charbel Farhat – Stanford University* |
| 1:55–2:20 | Optimal Bayesian experimental design: methodologies and materials applications<br>*Youssef Marzouk – Massachusetts Institute of Technology* |

| | |
|---|---|
| 2:20–2:45 | Learning high-dimensional systems from data by nonlinear reconstruction of polynomial approximations<br>*Clayton Webster – Oak Ridge National Laboratory* |
| 2:45–3:10 | Endowing Deep Neural Networks with Uncertainty Quantification<br>*George Karniadakis – Brown University* |
| 3:10–3:30 | Discussion |
| **3:30–3:45** | **Coffee Break & Posters—Hodson Hall** |
| Session 4: Design and Optimization for Materials<br>Chair: James Warner, National Aeronautics and Space Administration<br>Room: Hodson Hall 210 | |
| 3:45–4:10 | Design of New Materials and Structures to Maximize Strength at Probability Tail: A Neglected Challenge for Quasibrittle and Biomimetic Materials<br>*Zdenek Bazant – Northwestern University* |
| 4:10–4:35 | Rational Design of Interatomic Potentials through Multi-Objective Optimization<br>*Simon Phillpot – University of Florida* |
| 4:35–5:00 | An Adaptive Reduced Basis Approach for PDE Constrained Optimization under Uncertainty<br>*Wilkins Aquino – Duke University* |
| 5:00–5:25 | Optimization under uncertainty for predicting properties and performance<br>*Jim Stewart – Sandia National Laboratory* |
| 5:25–5:45 | Discussion |
| **5:45–6:00** | **Speed Poster Slam—Hodson Hall 210** |
| **6:00–6:30** | **Break** |
| **6:30** | **Depart for Dinner—Bus Departs from Hodson Hall**<br>**Buses Depart: Hodson Hall—6:30, Inn at Colonnade—6:45** |
| **7:00–10:00** | **Dinner – 13th Floor Belvedere**<br>**Buses Depart: 9:30/9:45 and return to Inn at Colonnade** |

## **Day 2**: Friday, 18 January 2019

| | |
|---|---|
| 8:00–8:30 | Registration & Breakfast—Hodson Hall Lobby |
| Session 5: Multiscale Material Modeling–Microstructure<br>Chair: Michael Falk, Johns Hopkins University<br>Room: Hodson Hall 210 | |
| 8:30–8:55 | The Fundamental Challenges to Uncertainty Quantification of Atomistic-scale Materials Simulations<br>*Stephen Foiles – Sandia National Laboratory* |
| 8:55–9:20 | Predictive Multiscale Modelling of Materials Chemomechanics<br>*James Kermode – University of Warwick* |
| 9:20–9:45 | Role of Uncertainty Quantification in Embedded Scale-Bridging Materials Simulations<br>*Timothy Germann – Los Alamos National Laboratory* |
| 9:45–10:00 | Discussion |
| **10:00–10:15** | **Coffee Break & Posters** |

| | |
|---|---|
| **Session 6: Multiscale Material Modeling–Multiscaling**<br>Chair: Somnath Ghosh, Johns Hopkins University<br>Room: Hodson Hall 210 | |
| 10:15–10:40 | Multiscale and Multidimensional Uncertainty Quantification in Integrated Computational Materials Engineering<br>*Wei Chen – Northwestern University* |
| 10:40–11:05 | Accelerating scale bridging via surrogate modeling<br>*Jaroslaw Knap - Army Research Laboratory* |
| 11:05–11:30 | Uncertainty in the Definition and Calibration of Multiscale Material Models<br>*David McDowell – Georgia Institute of Technology* |
| 11:30–11:55 | Homogenization estimates for the macroscopic response and field statistics in viscoplastic polycrystals<br>*Pedro Ponte Castañeda – University of Pennsylvania* |
| 11:55–12:15 | Discussion |
| **12:15–1:15** | **Lunch—Hodson Hall** |
| **Session 7: Multiscale Material Modeling–Macroscale**<br>Chair: Sanjay Govindjee, University of California at Berkeley<br>Room: Hodson Hall 210 | |
| 1:15–1:40 | Multi-scale multi-physics uncertainty quantification of manufacturing effects on material performance<br>*Sankaran Mahadevan – Vanderbilt University* |
| 1:40–2:05 | Calibration and uncertainty analysis for a temperature-dependent yield strength model of additively manufactured Alloy 718Plus<br>*John McFarland – Southwest Research Institute* |
| 2:05–2:30 | Sensitivity Analysis for Multi-Scale Modeling to Inform Design Optimization<br>*Stephanie Termaath* |
| 2:30–2:45 | Discussion |
| **2:45–3:00** | **Coffee Break & Posters—Hodson Hall** |
| **Closing Session**<br>Chair: Michael Shields, Johns Hopkins University<br>Room: Hodson Hall 210 | |
| 3:00–3:15 | NSF NHERI SimCenter<br>*Sanjay Govindjee – University of California at Berkeley* |
| 3:15–4:00 | Closing Discussion – Primary Challenges and Future Directions |

*Organizing Committee*:
Michael D. Shields, JHU
Lori Graham-Brady, JHU
Somnath Ghosh, JHU
Michael Falk, JHU

*Administrative Support*:
Ruth Hengst, USACM
Amanda Jackson, JHU
Jessica Ader, JHU