

# Agenda: Workshop on Quantification of Uncertainties in Material Science

	Thursday 14-Jan-16	Friday 15-Jan-16
8:00-8:45am	<b>Registration, breakfast</b>	<b>Breakfast</b>
8:45-9:00am	<b>Opening remarks, introductions</b>	
9:00 - 9:15am	<b>Jim Warren (NIST)</b>	<b>Opening remarks</b>
	<b>Session A (Chair: TBA)</b>	<b>Session C (Chair: TBA)</b>
9:15-9:40am	<b>Antonio Possolo (NIST)</b> "Evaluating and Quantifying Uncertainty"	<b>Vince Hackley (NIST)</b> "Uncertainties in nanoparticle size measurements: Dealing with challenges of method dependent values"
9:50-10:15am	<b>Bill David (ISIS/Oxford)</b> "Statistical uncertainties, model selection and managing model incompleteness in the analysis of powder diffraction data"	<b>John Villarubia (NIST)</b> "Uncertainties in Nanometer-Scale Dimensional Metrology"
10:25-10:50am	<b>Nicholas Ritchie (NIST)</b> "Calculating the uncertainty due to matrix corrections in electron probe microanalysis"	<b>Max Gunzburger (FSU)</b> "Uncertainty quantification and multiscale nonlocal modeling for material mechanics"
11:00-11:25am	<b>Jean-Pierre Fleurial (NASA)</b> "The Challenge of Measuring Thermoelectric Materials and Devices Electrical and Thermal Performance"	<b>WK Liu (Northwestern)</b> "Linking Process, Structure, Property, and Performance for Metal-based Additive Manufacturing: Computational Approaches with Experimental Support"
11:35am - 1:00pm	<b>LUNCH</b>	<b>LUNCH</b>
	<b>Session B (Chair: TBA)</b>	<b>Session D (Chair: TBA)</b>
1:00-1:25pm	<b>Richard Lesar (Iowa)</b> "A Perspective on Uncertainty Quantification in the Multiscale Simulation of Materials"	<b>Ursula Kattner (NIST)</b> "The CALPHAD method and its uncertainty quantification challenge"
1:35-2:00pm	<b>Francesca Tavazza (NIST)</b> "A NIST effort towards the quantification and benchmarking of Density Functional Theory (DFT) uncertainty"	<b>Marius Stan (Argonne)</b> "Certainty and Uncertainty at Multiple Scales"
2:10-2:35pm	<b>Nicholas Zabaras (Warwick)</b> "A Data-Driven Approach to Predictive Multiscale Materials Modelling"	<b>Nathan Gibson (Oregon State)</b> "Electromagnetic wave propagation in complex dispersive media"
2:45-3:10pm	<b>Ralph Smith (NCSU)</b> "Bayesian Inference and Sensitivity Analysis for Multi-Scale Materials"	<b>Markos Katsoulakis (UMass Amherst)</b> "Path-space information metrics for uncertainty quantification and coarse-graining of molecular systems"

3:10 - 3:30pm	<b>Coffee break</b>	<b>Coffee break</b>
3:30 - 4:30pm	<b>Panel discussion: “ UQ Issues in Measurements vs Modeling: Commonalities and Differences“. Moderators: Levin (NIST), Lesar (Iowa)</b>	<b>Panel discussion: “Directions for UQ Research in Materials Science“. Moderators: Boettinger (NIST), Du (Columbia)</b>
5pm	<b>GROUP DINNER</b>	<b>CONCLUDING REMARKS</b>