



**MUMS Agent-Based Modeling and
Uncertainty Quantification Workshop
March 11-12, 2019**

SPEAKER TITLES/ABSTRACTS

Bobby Gramacy
Virginia Tech

“Replication or Exploration? Sequential Design for Stochastic Simulation Experiments”

We investigate the merits of replication, and provide methods that search for optimal designs (including replicates), in the context of noisy computer simulation experiments. We first show that replication offers the potential to be beneficial from both design and computational perspectives, in the context of Gaussian process surrogate modeling. We then develop a look ahead based sequential design scheme that can determine if a new run should be at an existing input location (i.e., replicate) or at a new one (explore). When paired with a newly developed heteroskedastic Gaussian process model, our dynamic design scheme facilitates learning of signal and noise relationships which can vary throughout the input space. We show that it does so efficiently, on both computational and statistical grounds. In addition to illustrative synthetic examples, we demonstrate performance on three challenging real-data simulation experiments from Bayes factor hyperprior sensitivity to inventory management and epidemiology.