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[Current Events](#)[Lectures ▾](#)[Events Archive ▾](#)

Computational Mathematics Seminar Series

Model Calibration for Coarse-Grained Models**Xiu Yang, Brown University**Lockett Hall 233
November 19, 2013 - 03:30 pm**Abstract:**

We investigate the selection of parameters in coarse-grained model in mesoscopic simulations. In order to capture the desired target physical properties, e.g., viscosity, diffusivity, appropriate choice of parameters, e.g., magnitude of the forces, cut off radius, is important.

We use generalized polynomial chaos (gPC) to construct a surrogate model of the response surface. By employing compressive sensing method, we are able to compute the gPC coefficients based on relatively few simulations. Then we apply Bayesian inference with the gPC surrogate model to search the suitable sets of parameters. In many cases, this method will help to achieve model reduction as the correlation between parameters can be revealed, hence parametric compression is possible. We present an example of using dissipative particle dynamics (DPD) model to study a polymer melt system. In this example, we set six parameters originally; and our method helps to determine four of them. The correlation between the remaining two parameters are also discovered. Thus, the number of parameters can be reduced.

Speaker's Bio:

Xiu Yang is a Ph.D. candidate working Prof. George Em Karniadakis at Division of Applied Mathematics, Brown University. He received his B.S. and M.S. in applied mathematics from Peking University (China). His main interest is in uncertainty quantification.

