MECHANICAL ENGINEERING

Institute for Data Sciences and Engineering
COLUMBIA UNIVERSITY

" *Uncertainty Quantification Framework for Modeling Prediction*"

Michael Frenklach

Department of Mechanical Engineering

University of California at Berkeley

MECE & IDSE joint seminar

A methodology of uncertainty quantification developed in a series of studies and termed Bound-to-Bound Data Collaboration (abbreviated to B2B-DC) will be presented. B2B-DC is framework for combining models and training data from multiple sources to explore their collective information content. It is built on an underlying physical process and associated model, a collection of experimental observations with specified uncertainties, algebraic surrogate models (response surfaces) representing parametric dependence of the physical-model predictions of the experimental observables on the uncertain parameters, and specialized constrained-optimization algorithms. The methodology makes predictions on the true feasible set, transfers the uncertainties of both model parameters and training-set experiments directly into prediction, tests and quantifies consistency among data and models, explores sources of inconsistency, discriminates among differing models, and enables analysis of global sensitivities of uncertainty in prediction to the uncertainties in data and model. Applications of the approach include combustion science and engineering, atmospheric chemistry, and system biology.

Michael Frenklach is Professor in the Department of Mechanical Engineering of the University of California at Berkeley. He received his Diploma in Chemical Technology from the Mendeleyev Russian Chemical-Technological University (Moscow, Russia) in 1969 and his Ph.D. in Physical Chemistry at Hebrew University (Jerusalem, Israel) in 1976. Professor Frenklach's faculty appointments began in 1979 in the Department of Chemical Engineering at Louisiana State University. He received the Alexander von Humboldt Research Fellowship and spent a year in the Institute of Physical Chemistry at Heidelberg University (Germany). In 1985 he joined the Materials Science Department of the Pennsylvania State University and in 1995 he accepted his current position at Berkeley. Professor Frenklach's research interests are in the areas of soot formation, diamond synthesis, interstellar dust, kinetic modeling of complex reaction networks, and currently uncertainty quantification and cyber-automation of collaborative science.

Friday, October 10th, 2014
11:00 am Seminar in 233 Mudd
Lunch served at 12:00pm
in MECE Lobby