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Optimization Program WISO Workshop
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Lecture: ***Model Discrimination and Parameter Estimation for Complex Reactive Systems***

Speaker: Larry Biegler

Abstract:

Parameter estimation and model discrimination of reaction kinetics with limited (informative) measurement data remains an important and challenging problem. To address this problem we propose a strategy based on maximum likelihood principles, non-linear optimization techniques, as well as collocation methods that discretize the differential-algebraic model. Within this approach we estimate variances of the noise in system variables (e.g. concentrations) from measurements, assess the sensitivity of model parameters, determine state profiles and model parameters, and discriminate among physics-based candidate models. Key components of this strategy are large-scale nonlinear programming (NLP) and post-optimality analysis. The resulting approach is presented on two case studies drawn from real-world processes for the manufacture of specialty chemicals.