Model Reduction for the Optimisation of Large-Scale Chemical Systems

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Abstract: Efficient design of chemical processes typically results in the (computationally intensive) constrained optimisation of large-scale, often distributed parameter, nonlinear systems. For systems with relatively few degrees of freedom, reduced Hessian decomposition methods can be used, which exploit the low dimensionality of the parameter space. Such methods, however, rely on Jacobian and Hessian matrices being explicitly available.

Here, a model reduction-based optimisation methodology is presented, for the cases where these essential matrices are not available in closed form, but a dynamic representation of the problem is, e.g. the process dynamics being simulated by a commercial software package or a legacy code. This work is an extension of a class of techniques motivated by model unavailability [1].

We combine the Recursive Projection Method [2], which identifies the, typically, low dimensional slow dynamics of the (dissipative) model, with a second reduction to the low-dimensional subspace of the decision variables. This results in the solution of a low-order optimisation problem. Optimal conditions are then computed in an efficient way using only low-dimensional numerical approximations of gradients and Hessians.

The reduced model-based optimisation methodology and its potential extensions for multi-scale approaches are discussed with the aid of illustrative examples.

References:

1. C.W Gear, I.G. Kevrekidis, C. Theodoropoulos, Computers & Chem. Eng. 26 (2002) 941.
2. G.M. Shroff, H.B. Keller, SIAM J. Numer. Anal. (1993) 30, 1099.