Multi-scale Optimization for Chemical Processes

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Efficient Nonlinear Programming (NLP) algorithms and modeling platforms have led to powerful process optimization strategies. Nevertheless, these algorithms are challenged by recent evolution and deployment of multi-scale models (such as molecular dynamics and complex fluid flow) that apply over broad time and length scales. Integrated optimization of these models requires accurate and efficient reduced models (RMs). This talk presents a rigorous multi-scale optimization framework that substitutes RMs for complex original detailed models (ODMs) and guarantees convergence to the original optimization problem. Based on trust region concepts this framework leads to NLP algorithms for RM-based optimization that deal directly with multi-physics models. The basic approach stems from a classical gradient-based trust-region method that includes multi-physics models. This algorithm is then extended through a DFO framework so that gradient calculations from the ODM can be avoided. Finally, we consider a third approach that avoids frequent recourse to ODM evaluations, using the concept of epsilon-exact RMs. We illustrate these algorithms with small examples and discuss RM-based optimization case studies on chemical processes, in order to demonstrate their performance and effectiveness.