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Multi-scale optimization for process systems engineering☆☆

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ABSTRACT

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 study develops 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 three related NLP algorithms for RM-based optimization. The first follows the classical gradient-based trust-region method, the second avoids gradient calculations from the ODM, and the third avoids frequent recourse to ODM evaluations, using the concept of ϵ-exact RMs. We illustrate these algorithms with small examples and discuss RM-based optimization case studies that demonstrate their performance and effectiveness.

1. Introduction

Process systems engineering (PSE) faces increasing demands and opportunities for better process modeling and optimization strategies. These demands also present a number of challenges, particularly as chemical and energy processes incorporate advanced technologies that need to be modeled, integrated and optimized. To address these needs, state-of-the-art nonlinear optimization algorithms can now solve models with millions of decision variables and constraints. Correspondingly, the computational cost of solving discrete optimization problems has been reduced by *several orders of magnitude* (Biegler & Grossmann, 2004). Moreover, these algorithmic advances have been realized through software modeling frameworks that link optimization models to efficient nonlinear (NLP) and mixed-integer nonlinear programming (MINLP) solvers. On the other hand, it is important to note that these advances are enabled because these frameworks permit (indeed require) optimization models to be formulated carefully as well-posed problems with exact first and second derivatives.

Despite these advances, *multi-scale* process optimization still needs effective problem formulation and modeling environments. Current process simulation models usually consist of lumped parameter descriptions with a number of ideal assumptions (e.g., perfect mixing, plug flow, equilibrium behavior and shortcut models). These models also do not account for complex transport effects, nor do they account for phenomena that take place at broader length scales. Consequently, they cannot include detailed interactions with material design, complex fluid flow and transport effects with multiphase interactions. These effects require integration between molecular, nanoscale and distributed, continuum levels. As a result, there is a growing need for more detailed, distributed parameter, multi-scale process models.

At the process optimization level, multi-scale integration is required to model complex transport and fluid flow phenomena. For instance, optimization models for advanced power generation processes (see Lang et al., 2009; Lang, Zitney, & Biegler, 2011) comprise a heterogeneous modeling environment with lumped parameter (algebraic) models, such as heat exchangers, compressors and expanders, dynamic models (e.g. for gas separation units) and multi-phase (partial differential-algebraic) CFD models, e.g., for the gasification and combustor-turbine units. Because of the substantial complexity of the associated model solvers, the computational costs for process optimization are prohibitive. While lumped parameter flowsheet models take only a few CPU seconds to solve, a CFD combustion or gasification model alone may require many CPU hours or even days.

Moreover, one needs to consider the extension of these modeling tools to more complex multi-scale systems. This multi-scale integration requires the development and implementation of efficient and accurate model reduction strategies within the optimization framework. To capture this multi-scale, multi-fidelity model behavior one can consider a cascaded network that can potentially link models from the atomistic to enterprise-wide scales, along with optimization formulations that provide the "glue" to exploit synergies among these systems through RMs. Such

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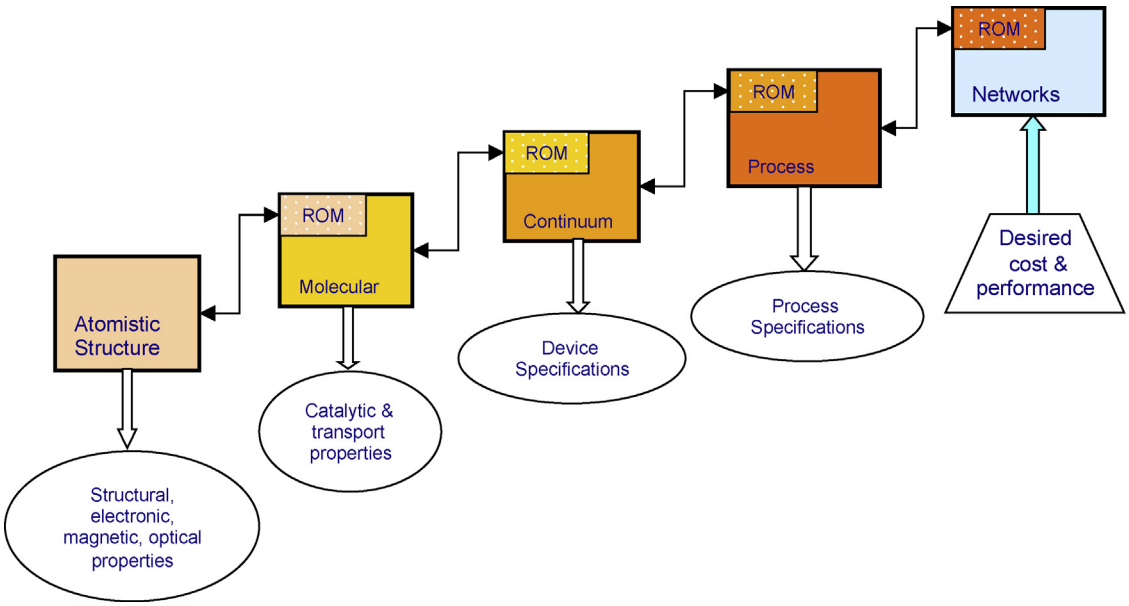

Fig. 1. Multi-scale optimization linked through RMs.

a holistic strategy is described in Chung, Jhon, and Biegler (2011) and depicted in Fig. 1.

This study is an extended and substantially enhanced version of Biegler and Lang (2012). In this extension we derive, develop and analyze an optimization framework that addresses the above multi-scale modeling challenges. Our overall strategy replaces the original detailed models (ODMs), comprising complex differential-algebraic equations (DAEs) and partial differential-algebraic equations (PDAEs), by reduced models (RMs) consisting of algebraic equations, and it applies large-scale equation-based optimization strategies to the RMs. Nevertheless, because the RM-based optimization strategy is allowed to evaluate and compare information from the ODMs the framework will capture relevant multi-scale phenomena such as complex fluid flow, particle mechanics, and dynamic operation within the process optimization. Moreover, we consider a general strategy for the construction of RMs that applies to a broad variety of physics-based or data-driven model reductions. This is enabled through advances over the past decade in trust region concepts and derivative-free optimization (DFO).

To develop this strategy, we consider the following basic questions:

- What properties are needed for the RM-based optimization framework to converge to the optimum of the original system models?
- What properties govern the (re)construction of RMs in order to balance model accuracy with computational cost during the optimization?
- Can RM-based optimization be performed efficiently without frequent recourse to the original models?

The next section briefly reviews developments in model reduction with a particular focus toward our RM-based optimization framework. The challenges of RM-based optimization are then illustrated with a toy problem. We then present a natural progression of three related trust region algorithms based on reduced models. The third and fourth sections describe Algorithms I and II, respectively. The first algorithm requires gradients directly from the ODM while Algorithm II does not. Two literature case studies are used to briefly describe the performance of these methods. More importantly, both methods work directly with the RM, but they also guarantee convergence to the optimum of the ODM. Moreover, Algorithms I and II provide the supporting concepts for our third algorithm, which is developed in the fifth section. Here we consider the special case of ϵ-exact models, which avoid frequent recourse to the original models and lead to greater efficiency of Algorithm III, the new optimization strategy. In addition, two small examples are presented that describe this approach, along with a comprehensive polymer process optimization case study that demonstrates the efficiency of this method. Finally, conclusions and future work are discussed in the sixth section.

2. Development of reduced models

Model reduction is a widespread practice that extends over many engineering disciplines, and over several decades. Early work on nonlinear model reduction for PSE includes the use of reduced models for physical properties embedded within detailed flowsheeting models (see Barrett & Walsh, 1979; Boston & Britt, 1978; Leesley & Heyen, 1977). These early strategies provide a vision for reduced models that extends beyond physical property models to a wide range of process engineering tasks. More recently, Caballero and Grossmann (2008) developed and applied a trust region RM-based strategy for distillation models in flowsheet optimization. Moreover, a derivative-free optimization framework with enhanced reduced models for flowsheet optimization of energy systems has been developed in Cozad and Sahinidis (2011).

Because model reduction strategies are widely applied over a broad range of engineering disciplines, our survey of such strategies is necessarily limited and we will cover two general approaches: model order reduction and data-driven model reduction.

2.1. Model order reduction

The first approach is based on an order reduction of the model that retains most of the structure of original equations but leads to a much simpler and smaller model. The PSE literature abounds with examples that include shortcut models based on physical phenomena, and simplifying assumptions associated with model development. Similarly, in the PDE modeling community, reduced order modeling (ROM) strategies have been developed that include