Complex Hierarchical Optimization Algorithms for the Design of Nanoporous Materials

Optimization Algorithms for Hierarchical Problems, with Application to Nanoporous Materials

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Abstract

We present a class of optimization strategies that can be applied to a variety of complex engineering design problems that have an exploitable hierarchical structure. In addition, we demonstrate the power of these strategies by applying them to the design of nanoporous materials, which hold promise in many applications, including those in energy production and storage.

In the hierarchical systems that we consider, the physics changes as the scale of the problem is reduced and it is important to account for physics at the fine level to obtain accurate approximations at coarser levels. The hierarchical optimization strategies can greatly accelerate the computation by exploiting the coarse model levels to produce high-quality search directions on the fine levels. By working explicitly in an optimization framework, it is possible to extend traditional multigrid techniques to a rich class of optimization models, including those with inequality constraints. It is also possible to provide strong guarantees of convergence. We have implemented our algorithm strategy in a flexible code called ChiOpt, or χOpt, for Complex HIerarchical OPTimization, that we have used to obtain promising results.

This is joint work with Paul Boggs, Stewart Griffiths, and Paul Boggs (Sandia National Labs.); David Gay (AMPL Corp.); R. Michael Lewis (College of William and Mary); and Kevin Long (Texas Tech University).