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Using Discrete and Continuous Models to Solve Nanoporous Flow Optimization Problems

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Abstract. We consider using a discrete network model in combination with continuous nonlinear optimization models to solve the problem of optimizing channels in nanoporous materials. The problem and the hierarchical optimization algorithm are described in [2]. A key feature of the model is the fact that we use the edges of the finite element grid as the locations of the channels. The focus here is on the use of the discrete model within that algorithm. We develop several approximations to the relevant flow and a greedy algorithm for quickly generating a "good" tree connecting all of the nodes in the finite-element mesh to a designated root node. We also consider Metropolis-Hastings (MH) improvements to the greedy result. We consider both a regular triangulation and a Delaunay triangulation of the region, and present some numerical results.

AMS subject classifications: 49M37, 65K04, 90C08

Key words: Multigrid Optimization, Multilevel Optimization, Nonlinear Optimization, Complex Hierarchical Optimization.

1. Introduction

We consider using a discrete network model in combination with continuous nonlinear optimization models to solve the problem of optimizing channels in nanoporous materials. The problem and the hierarchical optimization algorithm are described in [2]. The focus here is on the use of the discrete model within that algorithm. We begin by summarizing the physics problem and our hierarchical approach, thus providing the necessary context for the ensuing discussion.

Nanoporous materials have the desirable property that within the nanopores a gas can be stored at much higher density than, say, in a tank with comparable pressure.

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Many important applications, including the storage of electric charge, are noted in [2]. The problem is that it is difficult to charge, i.e., fill, these materials rapidly. It has been suggested that a series of channels be constructed in the material to act like a vascular system that facilitates the charge and discharge of the gas. Thus there are tradeoffs among the storage capacity, the volume of the channels, and the time needed to charge or discharge the materials. One version of the design problem is to choose the channel structure, including the topology and the widths of the channels, to minimize some property of the system, e.g., the average pressure, subject to the condition that the total volume of the channels divided by the total volume of the material (called the porosity) be bounded and that the rates of charge and discharge dictated by the particular application be achieved. Other versions are clearly possible.

As noted above, our approach to solving these problems is described in [2]. Briefly, we specify a PDE on the flow's domain and allow channels to be built along the edges of the finite element grid. Building the channels in this way restricts the channels somewhat, but is much more efficient than solving a general topology optimization problem. We comment more on this below. One node on the boundary of the domain is designated as the outlet node. The optimization problem is to determine the widths of the channels to solve the optimization problem described above. In a typical vascular system, wide channels split into successively narrower channels to cover the domain sufficiently to achieve the design criteria. It is thus natural think about formulating the problem on different scales, starting with a coarse scale to get the general shape of the channel system, followed by refinements of the scale to achieve better coverage. The problem on the finest scale captures all of the variables of the optimization problem and is where the ultimate problem is formulated. This problem, however, can be huge; exploiting this hierarchical structure, as shown in [2], can lead to significant computational savings.

The resulting optimization problems are challenging to solve. There are many design variables (the widths of the numerous channels within the material) and many more state variables (from the finite-element discretizations of the PDEs for the flows in the channel and bulk material). The dramatic difference in flow rates between the channels and bulk gives rise to significant ill conditioning. In addition, because the numerous small channels individually have only a small and subtle effect on the objective, the solution to the optimization problem is nearly degenerate. Finally, it is not at all clear how to obtain quality initial approximations that lead to reasonable solution times.

The hierarchical optimization algorithm developed in [2] is a multilevel method based on the multigrid optimization (MG/Opt) framework from [14]. The implementation is called χOpt and is described below in more detail. The MG/Opt framework is designed for solving continuous nonlinear optimization problems in cases where a hierarchy of optimization models is available. The hierarchy consists of a high-fidelity (fine) model that is typically expensive to evaluate, along with lower-fidelity (coarser) models that are used to update the estimate of the solution to the fine model. Typically the coarser models will be cheaper to evaluate, leading to computational savings. It