Multi-level Optimization Algorithms for PDE-constrained Problems Arising in the Design of Nanoporous Materials

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Outline

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Collaborators

- David Gay (AMPL Corp.)
- Stewart Griffiths (Sandia National Labs)
- R. Michael Lewis (College of William and Mary)
- Kevin Long (Texas Tech University)
- Stephen Nash (George Mason University)
- Robert Nilson (Sandia National Labs)

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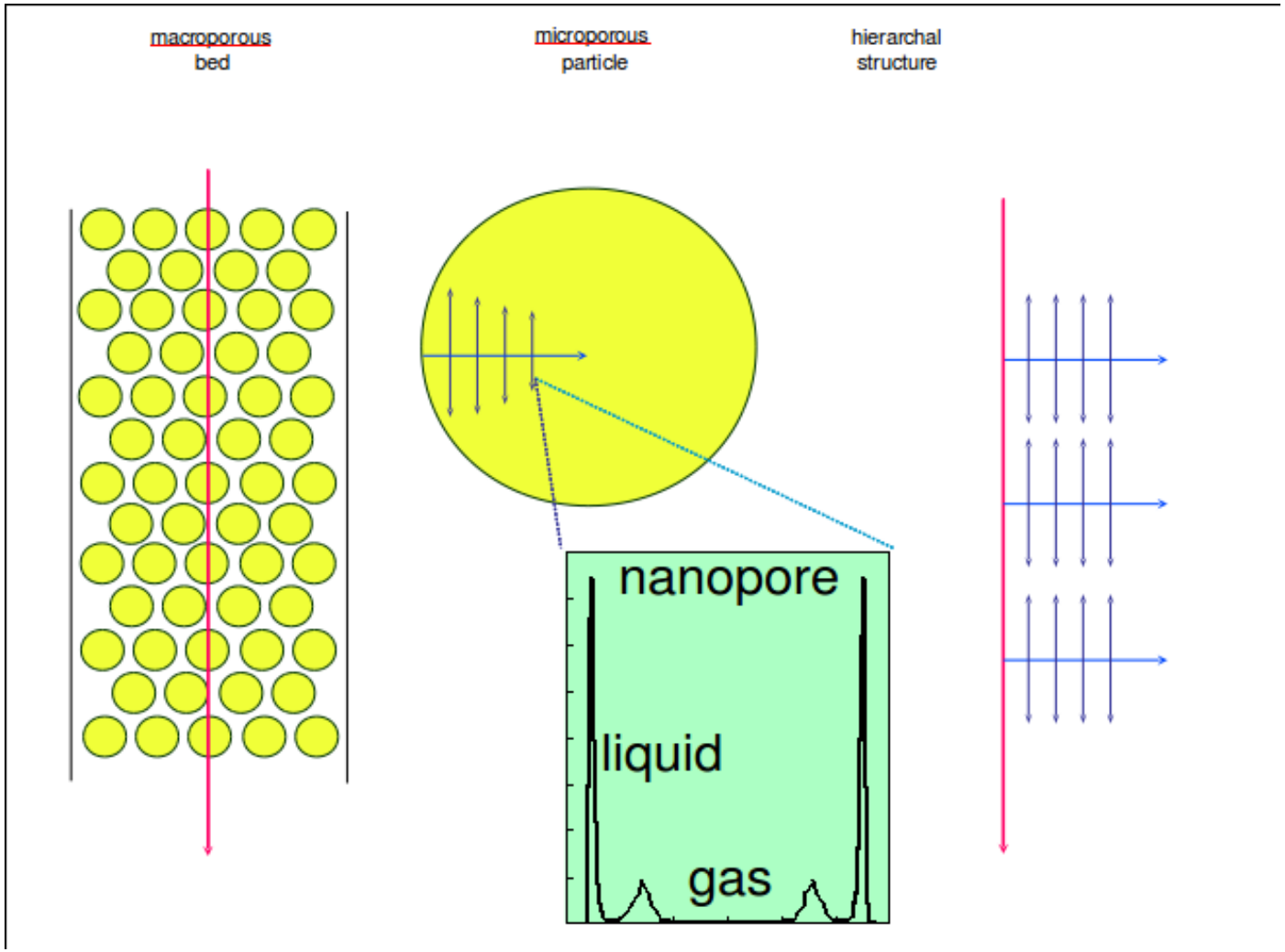
Nanoporous Materials



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Nanoporous Materials Promise

- Within nanopores, can store gas at high density with low pressure
  - Gas liquefies at ambient temperatures when very close to surface
  - In nanopores all molecules are close to surface
- By similar mechanism, ions pack at higher density in nanopores
  - Nanoporous materials can be used for capacitors or batteries

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Nanoporous Materials Design: A Multi-Scale Physics Problem

- Consider gas storage
- Trade-off: get gas in and out quickly vs. maximize storage
  - Improve the flow by making channels in the material, but this lowers storage
- Physics changes as the scale is reduced
  - Make channels of smaller widths at finer scales
- Must get physics correct on all levels

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Nanoporous Materials Design: A Multi-Scale Physics Problem

- Hierarchical optimization model with multi-physics
- Can't solve problem on fine level directly (too big)
- Can we exploit the structure to create efficient algorithms?
- Issues:
  - How many levels to use
  - How to model the channels
  - How to aggregate at various levels
  - How to exploit parallelism at small scales
  - What algorithmic framework to use
  - How to construct initial guess

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The Multi-Level (Hierarchical) Optimization Problem

- The flow is described by a nonlinear, time-dependent, PDE on the coarse levels, but the parameters change as scale decreases
- It is a molecular dynamics problem on the fine level
- The physicists have shown that good steady-state approximations can be constructed

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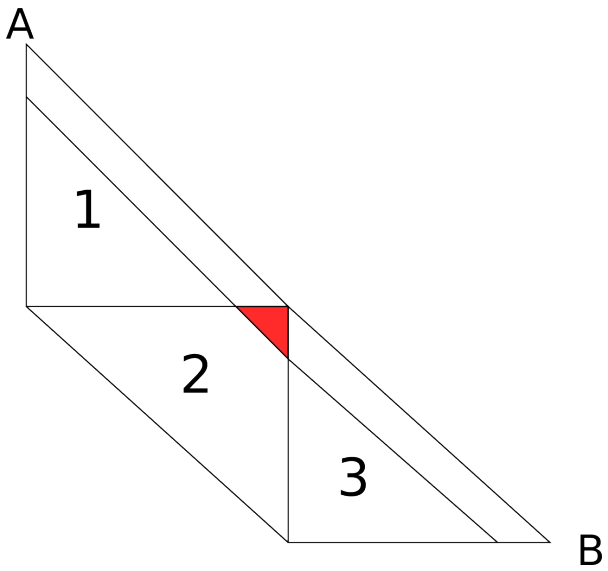
Modeling the Channels



- Allow flow along the edges of the finite element mesh
- Let w_i be the width on edge with unit tangential vector e_i
- Derive an effective mobility tensor $B = \gamma w_i^2 e_i e_i^T$ for constant γ
- Total flow is flow in channel combined with flow in the bulk

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First Problem: Steady State

- Let $\chi(x)$ be 0 in the bulk and 1 in the channels
- The net mass transfer is

$$j = -\chi(x)\rho_1 B\nabla p - (1 - \chi(x)\rho_2 \nabla p$$

- The transport equation is

$$c + \nabla \cdot j = 0$$

where c is a constant

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Finite Element Equation

- Create the weak form of the PDE with nondimensional constants Q, D, and V and test function $\bar{u}$

$$\int_\Omega \left[Q\bar{u} + D\nabla\bar{u}\cdot\nabla p\right]\xi\, dV$$
$$+\sum_{i=1}^{N}\int_e a_i\left[Vp\frac{\partial\bar{u}}{\partial l}\frac{\partial p}{\partial l}\right] dl$$
$$+\int_{\partial\Omega}\bar{u}\mathbf{j}\cdot\mathbf{n}\, dS = 0$$

- A difficulty arises because typical values for the constants are:

$$\begin{aligned} Q &= 1 \\ D &= 2 \\ V &= 10^{12} \end{aligned}$$

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The Optimization Problem

- The objective function depends on the application
- An example is to minimize mean pressure

$$f(w) = \int_{\Omega} p(w)$$

- Subject to the PDE

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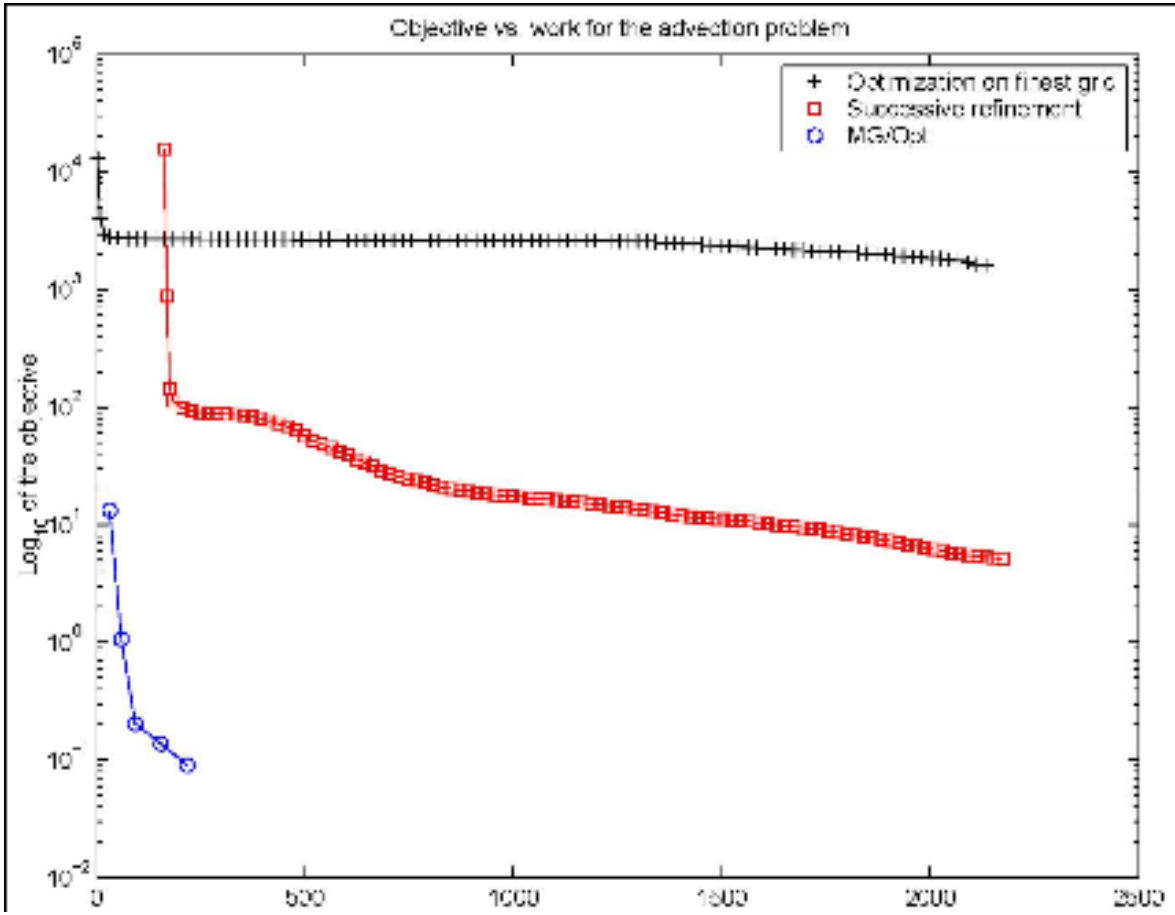
Why Multi-Grid Optimization Methods



Three different ways to apply the *same* optimization algorithm:

- straightforward
- successive refinement
- multilevel

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The Multi-Grid Optimization Algorithm

- Notation (Consider only two levels and unconstrained optimization)
  - Let x_h be the variables on fine level h
  - Let x_H be the variables on coarse level H
  - Let I_h^H be the "downdate" operator and I_H^h be the "update" operator to transform between levels
  - Let x_h^0 be the initial guess on the fine level
  - Let f_h and f_H denote the function to be minimized at each level

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The Multi-Grid Optimization Algorithm: MgOpt

- Pre-smooth
  - If on the coarsest grid, solve completely and return
  - If not, perform $k_1 > 0$ iterations to obtain x_h
- Recursion
  - Compute $\bar{x}_H = I_h^H \bar{x}_h$ and $\bar{v}_H = \nabla f_H(\bar{x}_H) - I_h^H \nabla f_h(\bar{x}_h)$
  - Call MgOpt on the "surrogate" model

$$f_s \equiv f_H(x_H) - \bar{v}_H^T x_H$$

    to obtain x_H^+
  - Compute the search directions $e_H = x_H^+ - \bar{x}_H$ and $e_h = I_H^h e_H$
  - Do linesearch to obtain α such that $f_h(\bar{x}_h + \alpha e_h) \leq f(\bar{x}_h)$
- Post-smooth
  - Apply k_2 iterations to obtain x_h^{j+1}

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Algorithm (Software) Design

- We want a general form of the MgOpt algorithm
  - Algorithm should be independent of the specifics, i.e., it shouldn't care about constraints, optimization strategies on each level, etc.
- Thus we created a "Level" object that knows
  - Objective function
  - Constraints (if any)
  - Merit function
  - Update and downdate operators
  - Computation of the search direction
  - Optimizer, including linesearch and convergence
- We construct a set of these to describe all the levels
- We allow various forms of the algorithm:
  - Can start at fine level or coarse level, use "full multi-grid" etc.

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Progress and Results: Initial Guess

- We used a network approximation based on the finite element grid
  - Source of 1 at each vertex
  - Each edge is an allowable channel
  - Used a greedy algorithm to get initial set of edges with non-zero flow
  - Used a Metropolis-Hastings algorithm to improve flow

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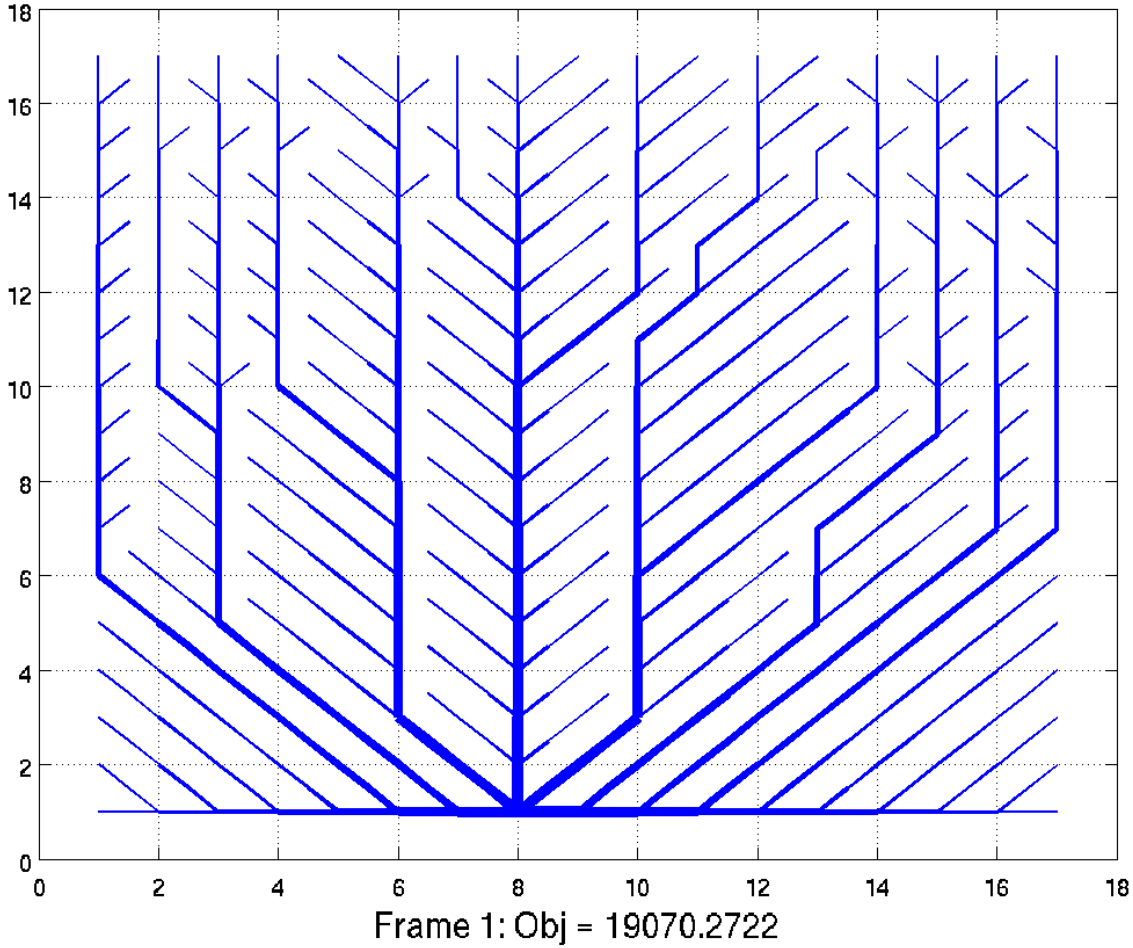
Progress and Results: Initial Guess with Greedy Algorithm



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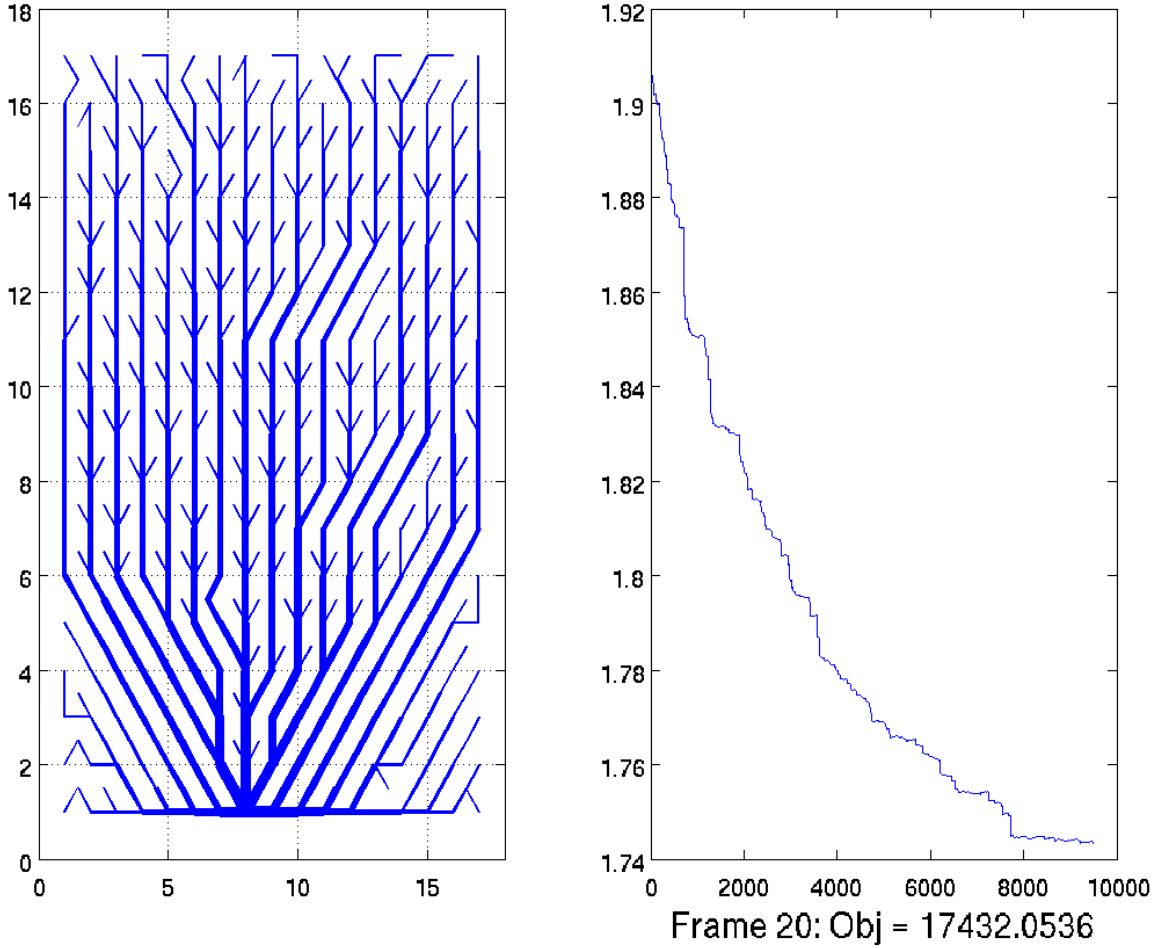
Progress and Results: Initial Guess Improved by MH



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Progress and Results: Problem Analysis

- Created accurate steady-state approximations
- Created a simple problem on simple grid to test procedures
  - Can check with both finite difference and finite element methods
  - In some cases we can get analytic solutions
- Developed specific update procedures: if 2 edges become one on the coarser level, compute the harmonic average to preserve flow

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Progress and Results: Algorithm and Software

- We have derived a basic convergence analysis of MgOpt with constraints (Nash)
- We have a basic version of the software running
  - Uses Sundance to handle the PDEs
  - Have run a 1-d Laplacian on 4 levels to debug
  - Have run the basic nanoporous problem on one level to debug the PDE implementation

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Future Work

- We developed a strategy for grid refinement; we want to do it automatically, not by hand (Kevin Long is working on this)
- Continue creating test problems with added features
- Investigate strategies for handling constraints, especially inequality constraints
- Model "real" applications

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¡Gracias!

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