χOpt – Complex HIerarchical OPTimization Algorithms for the Design of Nanoporous Materials

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Outline

Collaborators

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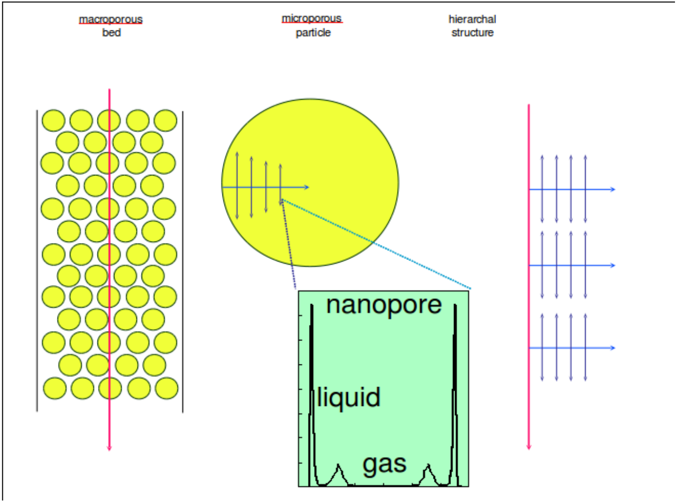
- Stewart Griffiths (Sandia National Labs)
- R. Michael Lewis (College of William and Mary)
- Kevin Long (Texas Tech University)
- Stephen Nash (George Mason University)
- Robert Nilson (Sandia National Labs)

Outline

Nanoporous Materials



Summary of Problem Set-Up

- Want to design channels to facilitate charge/discharge of the material
  - Trade-off: get gas in and out quickly vs. maximize storage
- Hierarchical optimization: nano- to macro-scale
- As channels are added at finer scales, coarse level parameters change

Nanoporous Materials Design: A Multi-Scale Physics Problem

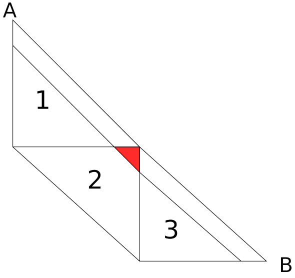
- Hierarchical optimization model with multi-physics
- Can't solve problem on fine level directly (too big)
- Can we exploit the structure to create efficient algorithms?
- Issues:
  - How many levels to use
  - How to model the channels
  - How to communicate between levels
  - What algorithmic framework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

Outline

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 the problem is being solved
- It is a molecular dynamics problem on the fine level
- Important point: The physicists have shown that good steady-state approximations can be constructed

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

First Problem: Steady State

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

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

  where p is the pressure and ρ_1 and ρ_2 are constants
- The transport equation is

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

  where c is a constant

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:

$$Q = 1$$
$$D = 2$$
$$V = 10^{12}$$

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
- Subject to other constraints, e.g., a max allowable porosity

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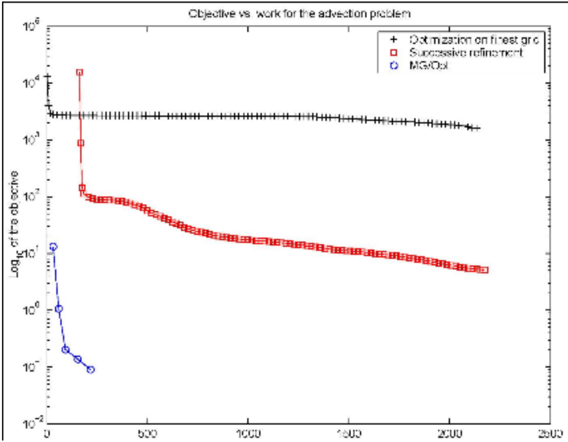
Why Multi-Grid Optimization Methods



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

- straightforward
- successive refinement
- multilevel

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

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}

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 criteria
- 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.
  - We want to use Sundance to handle the PDEs, meshes, etc.

Outline

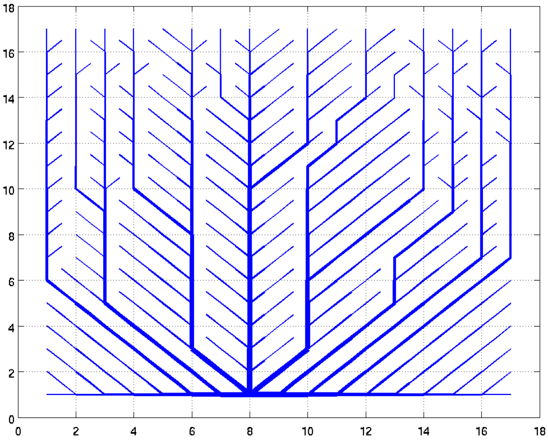
Communication Between Levels
Exploit/Preserve the Physics

- Harmonic averaging to downdate w_i
- “Reverse” process to maintain same ratio
- Modify the constraint on porosity to reflect channels not visible at coarse level
- Modify diffusivity on coarse channel to reflect channels on fine scale

Progress and Results: Initial Guess

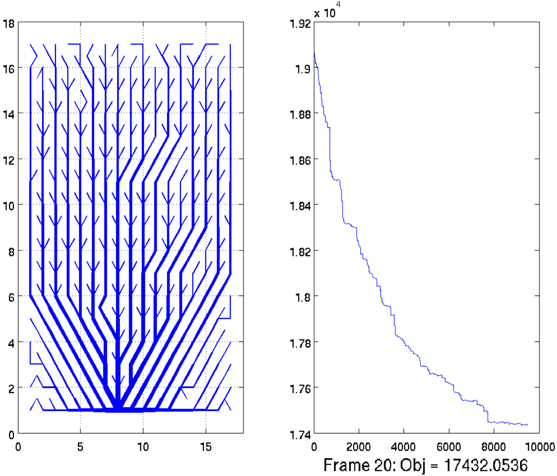
- We used a network approximation based on the finite element grid
  - Source of 1 at each vertex
  - Each edge is an allowable channel
  - Used a greedy algorithm to get initial set of edges with non-zero flow
  - Used a Metropolis-Hastings algorithm to improve flow

Progress and Results: Initial Guess with Greedy Algorithm



Frame 1: Obj = 19070.2722

Progress and Results: Initial Guess Improved by MH



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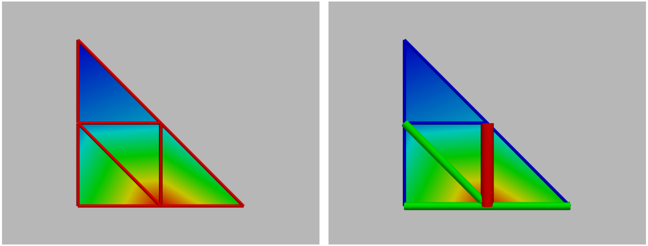
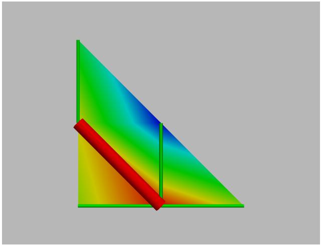
Numerical Results
Simplest Problem - Uniform Start

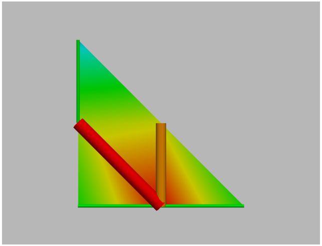


(a) Initial Guess (b) Final Solution

Numerical Results
Simplest Problem - Tree Start 1

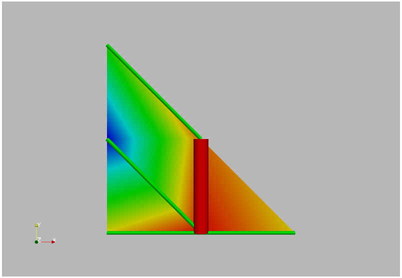


(c) Initial Guess

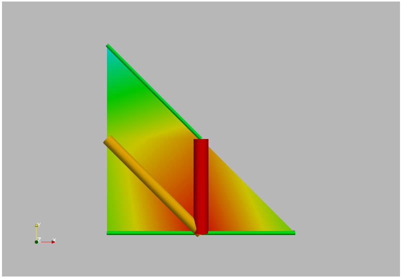


(d) Final Solution

Numerical Results
Simplest Problem - Tree Start 2



(e) Initial Guess

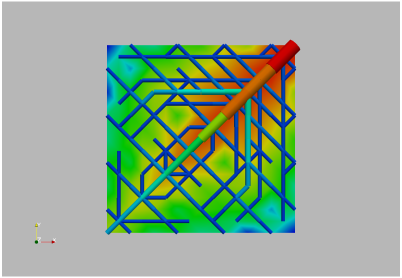


(f) Final Solution

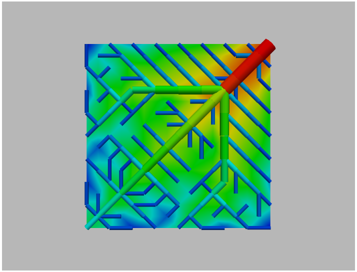
Discussion

- Differences in pressure, etc.

Numerical Results
4-Level Problem



(g) No Cut-Off



(h) With Cut-Off 1.0e-04

Discussion

- Advantage of cut-off

Numerical Results
Larger Problem

Discussion

- Can do larger problem

Progress and Results: Algorithm and Software

- We have derived a basic convergence analysis of χ*Opt* with constraints (Nash)
- We have a reasonable implementation of the software running
  - Uses Sundance to handle the PDEs
  - Have run a variety of tests
  - Have designed and implemented an automatic mesh refinement algorithm
  - Have coded the special update and downdate procedures making use of automatic refinement
  - Have added strategies to handle the "integer" nature of the problem

Outline

Future Work

- Add post-processing to maintain tree structure
- Develop convergence analysis for situation where problem changes dynamically as algorithm proceeds
- Improve aspects of the code
- Continue creating test problems with added features
- Investigate strategies for handling constraints, especially inequality constraints
- Develop aggregation strategies for very fine level grids based on domain decomposition

Thanks!

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