Regularization in Variational Coarsening

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This research was performed under the auspices of the U.S. Department of Energy and is to be referenced as LA-UR-02-6659. The Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

Outline

- Modern Scientific Computing
- Multigrid Methods
- Upscaling and Homogenization
- Interpretation of Coarse Grid Operators
- Regularization Term

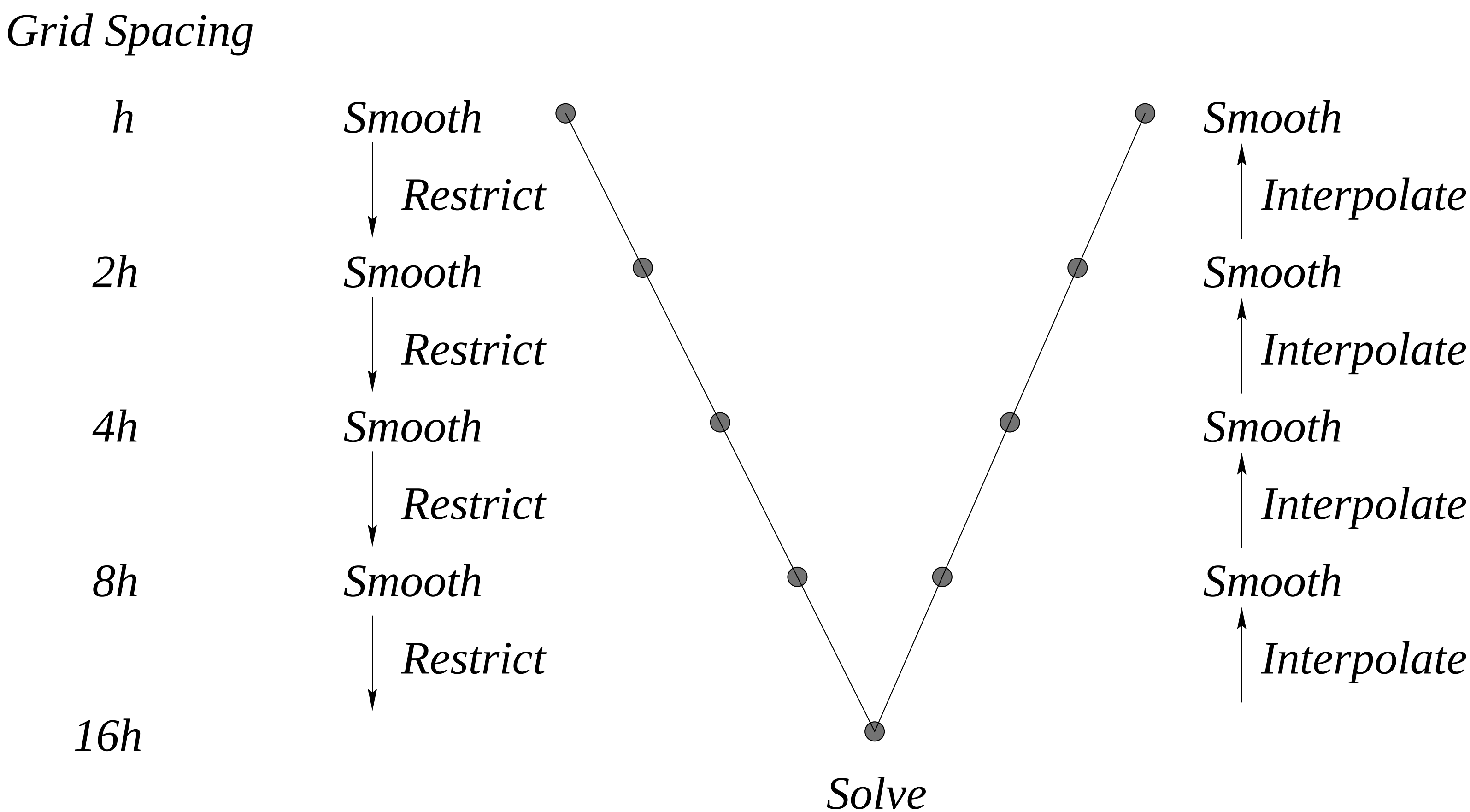
Scientific Computation

- Interested in simulating complex physical systems with parameters, and hence solutions, which vary on multiple scales
- Accuracy constraints lead to discretizations with tens of millions, or even billions, of degrees of freedom (DOFs)
- Need scalability, both algorithmic and parallel

Multigrid Basics

- Need a solver whose performance doesn't significantly degrade as your problem size increases
- Multigrid methods obtain optimal efficiency through complementarity
- Use a smoothing process (such as Gauss-Seidel) to eliminate oscillatory errors
- Use a coarse grid correction process to eliminate smooth errors
- Obtain optimal efficiency through recursion

The V-Cycle



Grid Spacing
h
2h
4h
8h
16h
Smooth
Restrict
Smooth
Restrict
Smooth
Restrict
Smooth
Restrict
Solve
Interpolate
Smooth
Interpolate
Smooth
Interpolate
Smooth
Interpolate
Smooth

Intergrid Transfer Operators

- Multigrid V-Cycle requires transfers of residuals and corrections from one grid to the next
- Accomplished through Interpolation (Prolongation) and Restriction operators (matrices!)
- Often pick a form of interpolation (P) and take restriction $R = P^T$ (theoretical benefits)
- Many choices for interpolation
  - Piecewise constant
  - Linear, bilinear, trilinear
  - $\ldots$
  - Operator Induced

Coarse Grid Operators

- Smoothing on coarse grids requires operators on those grids
- These operators must well-approximate the fine grid operator
- Many ways to create coarse grid operators (CGOs)
  - Rediscretization
  - Averaging
  - Galerkin coarsening

Variational Multigrid

- Multigrid with $R = P^T$ and $A_c = RAP$ is called a *variational formulation*
- Terminology comes from minimization form of $Lu = f$:

$$F(v) = \frac{1}{2}\langle Lv, v\rangle - \langle f, v\rangle$$
$$u = \arg\min_{v \in \mathcal{H}} F(v)$$

- Given an approximation v to the solution on the fine level, it can be shown that the optimal coarse grid correction Pw solves

$$(P^T A P)w = P^T (f - Lv)$$

BoxMG

- The Black Box Multigrid Algorithm (BoxMG) was developed by Dendy for diffusion problems with discontinuous coefficients
- Coarsening is done in a geometrically regular fashion
- BoxMG chooses interpolation in a manner which preserves the continuity of normal flux
- BoxMG uses a variational formulation, and is thus quite robust
- In 2-D, if initial operator is 5-point or 9-point, then all coarse grid operators are 9-point operators

BoxMG Wrappers

- Original BoxMG code written in Fortran 77
- We’ve written wrappers for the code in C
- Benefit from dynamic memory allocation
- Designed a simpler interface to the code
- In use for implicit time-stepping in chemical diffusion (Jelena, Yi)
- In use for solving linearized steady-state diffusion equation resulting from Kirchoff transformation of Richards’ Equation (Lilia, Daniel)

Example - Porous Media Flow

- Interested in simulating flow in a reservoir
- Modeling saturated flow via Darcy's Law:

$$u(x,y) = -D(x,y)\nabla p(x,y)$$
$$\nabla \cdot u(x,y) = Q(x,y)$$

- Simulation domain is on the order of 10^3 meters in length
- Fine scale changes in material properties on the order of 10^{-3} meters
- Range of scales is on the order of 10^6

The Curse of Dimensionality

- As we consider 2- and 3-dimensional simulations, cost of resolution increases exponentially
- For 1-D porous media flow, need $\backsim 10^6$ DOFs
- For 2-D porous media flow, need $\backsim 10^{12}$ DOFs
- For 3-D porous media flow, need $\backsim 10^{18}$ DOFs
- Fully resolved 3-D simulation is still beyond the capability of modern supercomputers (the fastest of which performs 3.5×10^{13} floating point operations per second)

The Need for Upscaling

- Naive discretizations require too many DOFs to be computationally feasible
- We must accurately account for the influence of fine-scale variation in the material properties if we hope to obtain physically meaningful solutions
- In general, we cannot directly account for the influence of fine-scale variation in material properties in a coarse-scale discretization
- The goal of upscaling and homogenization techniques is to derive effective, coarse-scale material properties to use in coarse-scale models and discretizations

Durlofsky's Approach

- Based on a two-scale asymptotic analysis, and thus strictly valid only for two-scale periodic media
- Consider pressure which is locally of the form

$$p = p_0 + G \cdot (x - x_0),$$

  then the average flow through a local cell can be shown to be

$$\langle u \rangle = -\hat{D} \cdot G.$$

- So, the local effective permeability can be recovered by choosing boundary conditions to induce particular G and then calculating the average flow for that G
- Overall upscaling technique requires solution of 2 fine-scale problems over each macro-element (in 2D)

Interpretation of Multigrid CGOs

- Consider a fine-scale discretization via finite elements

$$A_{ij} = e_j^T A e_i = \int_\Omega \langle D(x,y) \nabla \phi_i, \nabla \phi_j \rangle d\Omega$$

- Use of Galerkin coarsening means that the coarse grid operator is equivalent to a finite element discretization on that grid

$$\begin{aligned}
(A_c)_{ij} &= (P^T A P)_{ij} = (P\hat{e}_j)^T A (P\hat{e}_i) \\
&= (\sum_k p_{kj} e_k^T) A (\sum_l p_{li} e_l) \\
&= \sum_{k,l} p_{kj} p_{li} (e_k^T A e_l)
\end{aligned}$$

Interpretation . . .

- So,

$$
\begin{aligned}
(A_c)_{ij} &= \sum_{k,l} p_{kj} p_{li} \int_\Omega \langle D(x,y) \nabla \phi_l, \nabla \phi_k \rangle d\Omega \\
&= \int_\Omega \left\langle D(x,y) \nabla \left(\sum_l p_{li} \phi_l \right), \nabla \left(\sum_k p_{kj} \phi_k \right) \right\rangle d\Omega \\
&= \int_\Omega \langle D(x,y) \nabla \hat{\phi}_i, \nabla \hat{\phi}_j \rangle d\Omega
\end{aligned}
$$

- Basis functions on coarse grids come from summing the fine grid basis functions (weighted by the interpolation/restriction operators)

Reinterpretation of Multigrid CGOs

- Consider a bilinear discretization in 2-D
- Using a full-coarsening multigrid algorithm (such as BoxMG) results in 9-point operators on all coarse grids
- Any 9-point operator can be written as a linear combination of the bilinear FE operators for $I, \partial_x, \partial_y, \partial_{xx}, \partial_{yy}, \partial_{xy}, \partial_{xxy}, \partial_{xyy}, \partial_{xxyy}$
- If we start with a symmetric, zero row-sum operator, Galerkin coarsening guarantees that the coarse grid operator will also have these properties
- This forces the coarse grid operator to be a linear combination of $\partial_{xx}, \partial_{yy}, \partial_{xy}, \partial_{xxyy}$

Reinterpretation . . .

- The coarse grid operator can thus be interpreted as the coarse grid discretization of

$$-\nabla \cdot (\hat{D}\nabla u) + \partial_{xy} E(x,y) \partial_{xy} u = \hat{f}$$

- It is possible to recover piecewise constant approximations of the effective $\hat{D}$ and E based on the stencil entries
- That is, we can recover the homogenized permeability tensor directly from the coarse grid operator

Effects on Homogenization

- Accounting for the regularization term has allowed us to (in some instances) accurately recover the homogenized permeabilities for model problems
- This allows the extension of the work of Dendy, Hyman, and Moulton from periodic BCs to Neumann BCs
- Difficulties still arise
  - Coarsening of BCs appears inconsistent
  - No physical interpretation of the regularization term

Effects on Multigrid

- Accounting for the regularization term also explains the performance of multigrid on certain problems
- Consider, for example, the region $[0, 1]^2$, with

$$D(x, y) = \begin{cases} 1 & \text{if } y > \frac{1}{2} \\ 0.01 & \text{if } y < \frac{1}{2} \end{cases}$$

- Can show that the homogenized permeability is anisotropic

$$\hat{D} = \begin{bmatrix} 0.505 & 0 \\ 0 & 0.0198 \end{bmatrix}$$

Effects ...

- If we directly discretize the homogenized problem and use pointwise relaxation (such as Gauss-Seidel), we expect an inefficient algorithm
- Pointwise relaxation is inherently inefficient in anisotropic problems
- But ... we get good results!
- The regularization term makes the coarse scale problem effectively isotropic, while maintaining the coarse-scale effective permeability

End Goal

- Want an efficient, reliable numerical homogenization algorithm
- Need to accurately account for regularization term
- Currently, can account for it in some problems, but unresolved boundary effects on others

MGH Library

- Working on assembling homogenization codes into a library
- Include user-friendly wrappers
- 2D/3D, periodic/Neumann/?? BCs

Future Work

- Complete analysis of regularization term
- Complete MGH library
- Investigate use of homogenized permeabilities in Finite Volume discretizations and multigrid
- Investigate effect of regularization term in other multilevel solvers (AMG, scAMG)