Survey of Multigrid Applications

Paul Heckbert

20 Oct. 1998

lecture for "Hierarchical Methods for Simulation" (15-859E)

Carnegie Mellon University

We attempt a high level survey of applications of multigrid methods across science and engineering. (Articles on this are hard to find!)

- what is the state of the art?
- what are multigrid's strengths & weaknesses?
- what is current research?

Partial Differential Equations

types: elliptic, parabolic, hyperbolic

- illustrate on a simple example PDE: $au_{xx} + bu_{xy} + cu_{yy} = 0$
  - $ac-b^2>0$: *elliptic* boundary value problem
    equilibrium, e.g. Laplace's equation $u_{xx}+u_{yy}=0$
  - $ac-b^2=0$: *parabolic* initial value problem
    diffusion, e.g. the heat equation $u_{xx}-u_t=0$
  - $ac-b^2<0$: *hyperbolic* initial value problem
    e.g. wave equation $u_{xx}-u_{tt}=0$
- *steady-state* -- a boundary value problem
- *time-dependent* (unsteady) -- initial value problem
- problem can change character (elliptic/parabolic/hyperbolic) when we go from steady to unsteady, or even from point to point

Linear System Av=f

- N linear equations in N unknowns
- *symmetric positive definite* matrices
  - all eigenvalues positive, equivalently $v^T A v > 0$ for all nonzero v
  - occur for many interesting PDE's
  - level surfaces are concentric ellipsoids in N-dimensional space
- *sparse* matrices
  - PDE's tend to yield sparse matrices, only O(N) nonzeros in matrix
  - integral equations tend to yield dense matrices
- properties that often influence convergence
  - *condition number*: ratio of max to min eigenvalue
    - condition number usually increases with problem size (for finer grid)
  - *spectral radius*: largest magnitude eigenvalue

Some Iterative Methods

- Gauss-Seidel
  - converges for all symmetric positive definite A
  - converges twice as fast as Jacobi
- Conjugate Gradient (CG) Method
  - convergence rate determined by condition number
- Preconditioned Conjugate Gradient
  - instead of solving Av=f, solve $M^{-1}Av=M^{-1}f$ where M^{-1} is cheap and M is close to A
  - often much faster than CG, but conditioner M is problem-dependent
- Multigrid
  - convergence rate is independent of condition number, problem size
  - but algorithm must be tuned for a given problem; not as general as others

Critique of Multigrid 1

- works well for certain problems
  - in particular, elliptic PDE's (linear or nonlinear) with smooth boundary
  - solves a problem with N unknowns in O(N) time
    - constants usually small, e.g. 10 "work units"
    - 1 *work unit* = the work of one relaxation on the fine grid
- but multigrid methods are currently several orders of magnitude slower for non-elliptic steady-state problems
- parallelizes easily
  - (but requires more communication than some other parallel solvers)

Critique of Multigrid 2

- less theory than some other methods
  - it's a bit of a black art
- requires careful tuning to get it working on a new problem
  - not a black box, like, say, the conjugate gradient method or Gauss-Seidel
  - but when it works well, it's often the fastest
- but other fast methods often require tuning too
  - to get top performance out of the conjugate gradient method often requires an application-specific preconditioner

History of Multigrid

- 1964: first paper, Fedorenko, Russia
- 1977: Achi Brandt, Israel, made it practical, wrote seminal paper
- late 70's: Nicolaides, Hackbusch, and others proved convergence for certain PDE's
- interest took off around 1981
- but there was (and still is) much skepticism from some because there was little theory
- today used to solve PDE's in many disciplines
- current research: a drive to achieve "textbook efficiency" for general flow simulations (all Mach numbers and Reynolds numbers)

Multigrid Guidelines

- "multigridders" prefer structured grids
- grid and relaxation method are the only parts of the method that are highly problem-dependent; restriction and interpolation are generic
- on complex domains, need extra relaxation steps near boundary
  - for rough boundary conditions
  - for concave corners
- schedule parameters (how many relaxation steps and V cycles) can be:
  - fixed
  - accommodative

    e.g. software loops until residual at each step is below some tolerance
- for CFD, align the grid with the boundary and the flow

Brandt's Research Philosophy

- To do multigrid research, you should "very gradually increase the complexity of the problems" you attempt
- "we insist on obtaining for each problem the full efficiency" (e.g. 10 work units)
- strives for linear time with small constants
- "stalling numerical processes must be wrong"
- constants are particularly important when discussing algorithms that are $O(N)$; more than for algorithms that are, say, $O(N^2)$
- strives for convergence proofs with small constants: "almost all other multigrid theories give estimates which are not quantitative or very unrealistic, rendering them useless in practice"

Computational Fluid Dynamics (CFD)

- equations
  - Euler equation - linear, inviscid (no viscosity)
  - Navier-Stokes equation - nonlinear, models viscosity
- now possible to simulate flow around an airplane, with engines
  - first achieved in 1986
  - done with multigrid?
- *Reynolds Number* (Re)
  - a measure of the ratio of inertial and viscous forces
  - for an airplane, Re ~ 10^7
  - Re large => turbulence, difficult simulation

CFD 2

- transonic flow
  - flow is both below and above speed of sound (Mach no. <1 or >1)
  - => PDE is both elliptic and hyperbolic
- high Reynolds number steady state flows

  => non-elliptic
- use boundary-fitted structured grids
- boundary layer tricky
  - in viscous simulation, flow near surface (of e.g. wing) has high gradient, since flow speed at surface is zero, but speed inches away could be high
  - you often want the elements (grid quadrilaterals) to be highly stretched (e.g. "*aspect ratio*" of 4000:1) in boundary layer to get accurate simulations
  - high aspect ratio slows convergence or complicates the relaxation method

Multigrid Applications 1

- computational fluid dynamics (CFD)
  - application for which multigrid has been most used
  - weather prediction (whole earth simulations)
- structured grid generation
  - use elliptic PDE to define geometry of grid nodes, create grid using multigrid!
- ill-posed (underdetermined) problems
  - edge detection in noisy image
    - can find all straight features (lines, edges) in NxN pixel image in O(N log N) time
  - image segmentation
  - tomography (i.e. CAT scan)
  - approximating noisy data with a piecewise smooth function with known or unknown discontinuities

Multigrid Applications 2

- integral operators
  - multiplication by a dense NxN matrix in O(N) time
  - easy if matrix (or kernel) is smooth; slower if not
  - n-body force computations
    - gravity
    - molecular interactions
    - thermal radiation
  - FMM is faster than $O(N^2)$ alg. only for n>1000, they say
    - is Brandt's method faster? (unpublished)

Multigrid Applications 3

- global optimization
  - works even if many local minima
  - "each step can be interpreted as an optimization over a certain subspace"
  - protein folding
- constrained optimization
  - optimal control, e.g. robot motion planning
- solid mechanics
  - set up using finite element methods (unstructured grid), not finite difference

Multigrid Applications 4

- quantum chemistry
  - compute eigenfunctions of Schroedinger's eqn. (the PDE governing quantum mechanics) to find electron density functions
- macroscopic from microscopic
  - statistical physics, particle physics (QCD)
    - derive macroscopic properties (e.g. nonlinear elasticity) by using multigrid on microscopic level (on atomic forces)
  - unified wave/ray methods for simulating electromagnetic radiation
    - combine wave model (to simulate diffraction, interference, when wavelength comparable to scale of objects) and
    - ray model (to simulate free flight of photons in air/vacuum)
- VLSI design
  - highly nonlinear

Related Methods

- *unstructured multigrid*
  - uses an unstructured grid (irregular topology), not structured one
  - this complicates relaxation, restriction, & interpolation, but permits solution on complex domains (e.g. around an aircraft wing with flaps)
- *algebraic multigrid*
  - multigrid without the grid
  - analyze and do clustering on graph implied by matrix A
  - input is A only -- no high level problem knowledge
- *domain decomposition*
  - divide domain into (possibly overlapping) pieces
  - solve alternately on each piece, using solution of other pieces as boundary conditions
  - useful for complex domains, parallelizes easily

References 1

my comments in italics

Brandt, 1988, The Weizmann Insitute Research in Multilevel Computation: 1988 Report, Proc. Copper Mtn. Conf. on Multigrid Methods, 1989 (53 pp.) *Survey of recent applications. I found this quite thought-provoking.*

Brandt, 1982, Guide to Multigrid Development, in Hackbusch & Trottenberg, eds., Multigrid Methods, pp. 220-312. *Guidelines for multigrid implementers. Long.*

Brandt, 1997, The Gauss Center Research in Multiscale Scientific Computation, Proc. Copper Mtn. Conf. on Multigrid Methods, on web (50 pp.) http://www.wisdom.weizmann.ac.il/research.html *More esoteric than 1988 report above.*

Brandt, 1980, Multilevel Adaptive Computations in Fluid Dynamics, AIAA J., vol. 18, pp. 1165-1172. *Short, fairly readable.*

Brandt, 1977, Multi-Level Adaptive Solutions to Boundary-Value Problems, Mathematics of Computation, pp. 333-390. *The seminal paper on multigrid.*

References 2

Wesseling, 1992, An Intro. to Multigrid Methods, chapter 8. *Good textbook*.

Parsons & Hall 1990, The Multigrid Method in Solid Mechanics, Intl. J. for Numer. Meth. in Eng., vol. 29, pp. 719-754. *Experiments applying MG to mechanical engineering*.

Chan, Go, & Zikatanov, 1997, Lecture Notes on Multilevel Methods for Elliptic Problems on Unstructured Grids, 77 pp., http://www.math.ucla.edu/~chan/mgpapers.html *State of the art in unstructured multigrid and domain decomposition.*

Gary Miller, CMU CS (conversation)

Omar Ghattas, CMU CE (conversation)