Multigrid Methods and Applications

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Overview

1. What is the multigrid method?

2. 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?

Inspiration for Multigrid Method

- Typical problem:
  - Solving a PDE over simple domain (e.g. square)
  - Get sparse system Av=f
- If we solve iteratively with Gauss-Seidel
  - initial iterations reduce residual a lot
  - later iterations yield less benefit
  - why? Iterations reduce high frequencies in residual
- **Idea:**
  - **iterate on coarser grids to reduce lower frequencies**

Example: Poisson's Equation

$$-\nabla^2 u = f(x, y), \text{ solve for } u(x, y)$$

$$\text{discretize } v_{i,j} \approx u(ih, jh)$$

$$[-v_{i-1,j} - v_{i,j-1} + 4v_{i,j} - v_{i,j+1} - v_{i+1,j}]/h^2 = f_{i,j}$$

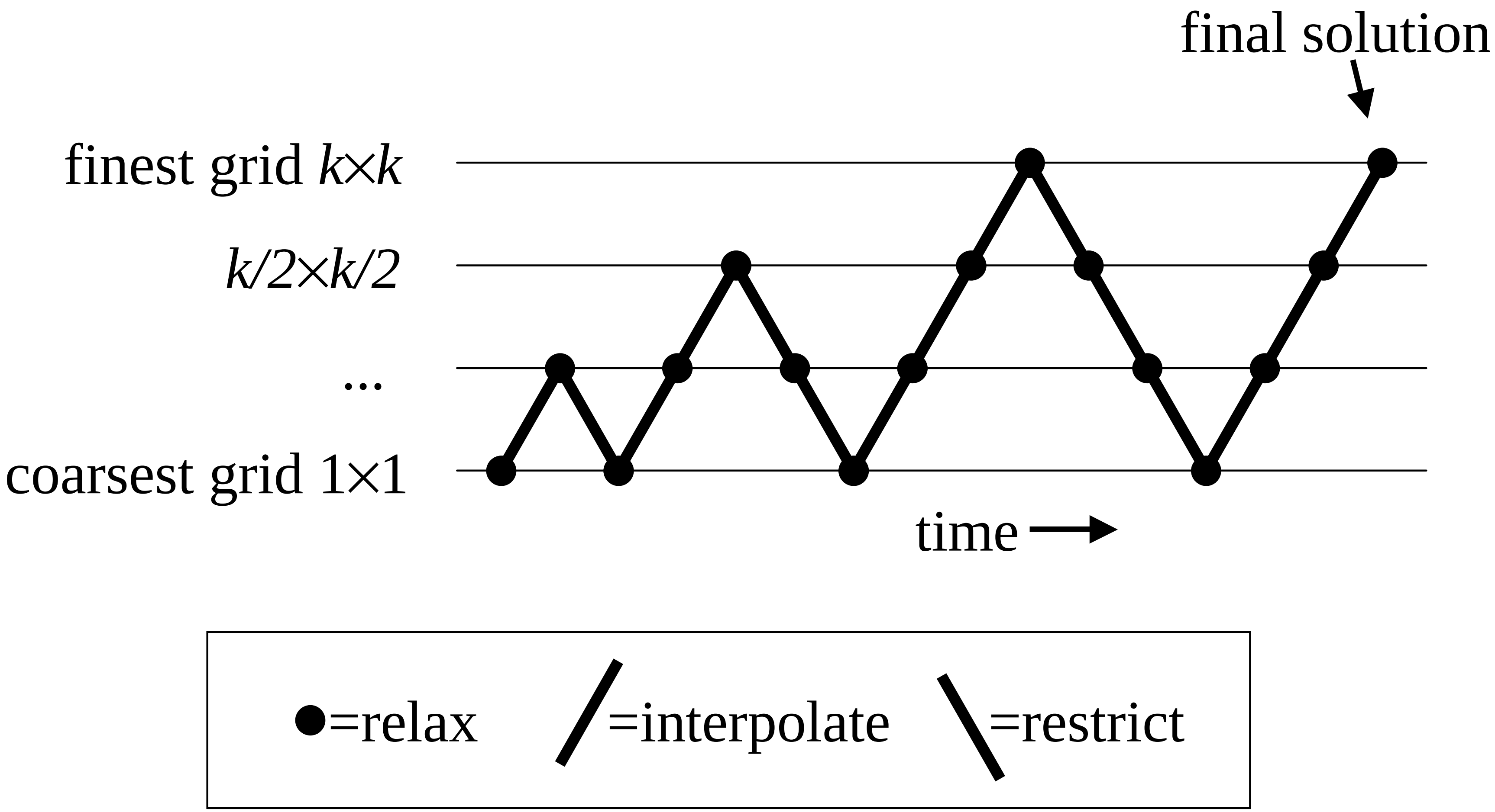
- Sweep of Gauss-Seidel "relaxes" each grid value to be the average of its four neighbors plus an *f* offset
- *Many* relaxations required to solve this on a fixed grid.
- Multigrid solves it on a hierarchy of grids.

Elements of Multigrid Method

- relax on a given grid a few times
- coarsen (restrict) a grid
- refine (interpolate) a grid

A Common Multigrid Schedule

Full Multigrid V Cycle:



Some Iterative Methods

- Gauss-Seidel
  - converges for all symmetric positive definite A
- Conjugate Gradient (CG) Method
  - convergence rate determined by condition number
  - note that condition number typically larger for finer grids
- 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

note: don't need matrix A in memory – can compute it on the fly!

Cost Comparison

on 2-D Poisson Equation, $k \times k$ grid, $n = k^2$ unknowns

METHOD	COST	
Gaussian Elimination	$O(k^6)$	$= O(n^3)$
Gauss-Seidel	$O(k^4 \log k)$	$= O(n^2 \log n)$
Conjugate Gradient	$O(k^3)$	$= O(n^{1.5})$
FFT/cyclic reduction	$O(k^2 \log k)$	$= O(n \log n)$
multigrid	$\mathbf{O(k^2)}$	$\mathbf{= O(n)}$

optimal!

Memory Requirements of Multigrid

2-D:

finest grid: k^2 (v & f arrays)

$k^2/4$

$k^2/16$

...

coarsest grid: 1

total: $k^2(1+1/4+1/16+1/64+...) = 4/3 \times k^2$

Costs only 33% more memory than storing the solution

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 (time-independent BV) problems
- low memory requirements: need mem for v & f on finest grid, plus coarser grids; don't need A
- 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
  - large constants: ~40,000 work units, no implementation?
- 1977: Achi Brandt, Israel, made it practical, wrote seminal paper
- late 70's: Nicolaides, Hackbusch, and others proved convergence for certain PDE's; Brandt proved fast convergence
- 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)
- somewhat superseded by wavelet methods?

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
- grid can be adaptive: can restrict processing at finer levels to subdomains
- 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
  - Re large => turbulence, difficult simulation
  - for an airplane, Re ~ 10^7

CFD 2

- transonic flow
  - flow is both below and above speed of sound (Mach no. <1 or >1)
  - => PDE is elliptic where subsonic and hyperbolic where supersonic
- 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 kxk pixel image in O(k log k) 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
  - Fast Multipole Method 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

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State of the art in unstructured multigrid and domain decomposition.

Shlomo Ta'asan, CMU Math (conversation)

Gary Miller, CMU CS (conversation)

Omar Ghattas, CMU CE (conversation)