

Optimal solvers for partial differential equations

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why this talk?

- I have been thinking about what are the goals of codes which numerically solve differential equations
- there are reliable black boxes for ODE IVPs
 - `ode45` in `MATLAB`
- what properties would a good PDE black box have?

Outline

how to approximately solve a PDE

what is an “optimal solver”?

multigrid

barriers & extensions to optimality

Poisson equation

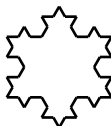
- for much of this talk I'll use two example PDE problems

1. *Poisson equation* with Dirichlet boundary conditions:

$$-\nabla^2 u = f \quad \text{on } \Omega \subset \mathbb{R}^d \text{ with } u|_{\partial\Omega} = g,$$

- a linear elliptic PDE problem in dimension $d = 2$ or $d = 3$
- recall that $\nabla^2 u = \nabla \cdot (\nabla u) = u_{xx} + u_{yy} + u_{zz}$
- source $f(x, y, z)$ given
- boundary values $g(x, y, z)$ given
- will use various domains Ω including a square, a cube, and

- a snowflake fractal



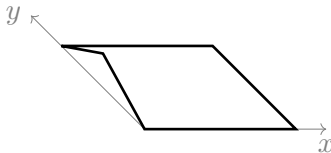
- the solution $u(x, y, z)$ of $-\nabla^2 u = 1$ with $g = 0$ gives the expected time for a Brownian motion to first hit $\partial\Omega$

minimal surface equation

2. *minimal surface equation (MSE)* with Dirichlet b.c.s:

$$-\nabla \cdot \left(\frac{\nabla u}{\sqrt{1 + |\nabla u|^2}} \right) = 0 \quad \text{with } u|_{\partial\Omega} = g.$$

- a nonlinear elliptic PDE in 2D
- here: square domain $\Omega = [0, 1] \times [0, 1]$
- the solution $u(x, y)$ gives the height of a zero-gravity soap bubble which spans a wire frame with height $z = g(x, y)$:



today's talk: mostly elliptic PDEs

both examples **1** & **2**

- are well-posed elliptic PDE BVPs
- seek solution u from an ∞ -dimensional vector space
- *main idea*: a PDE BVP is a system of ∞ eqns in ∞ unknowns

fine print:

- both examples derivable from variational principles, thus well-posed
- the “ ∞ -dimensional vector space” is a Sobolev space such as $H^1(\Omega)$

approximation: finite difference method

- most problems are not solvable exactly, so we
 - approximate by N equations in N unknowns
 - where $N \in \mathbb{Z}^+$ so $N \ll \infty$
- one method is *finite differences* (FDM), based on

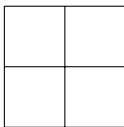
$$f'(x) = \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h} \approx \frac{f(x+h) - f(x)}{h}$$

- for the 2D Poisson equation:

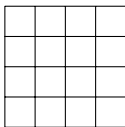
$$u_{xx} + u_{yy} \approx \frac{u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{ij}}{h^2}$$

structured grids notation

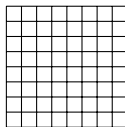
- a *structured grid* is a product of 1D grids
- consider sequence of such grids $\Omega^{(k)}$ on squares or cubes
- notation: *level k* grid has spacing h_k in each direction



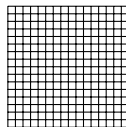
$\Omega^{(0)}$



$\Omega^{(1)}$



...

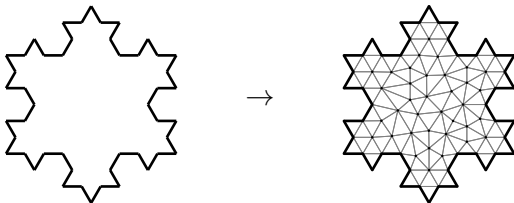


$\Omega^{(k)}$

- N_k is the number of equations and of unknowns
- “increasing resolution” means $h_k \rightarrow 0$ and $N_k \rightarrow \infty$
 - a.k.a. “refinement”
 - $N_k = O(h_k^{-d})$ grid points in d dimensions
 - typically: $N_{k+1} \approx 2^d N_k$

approximation: finite element method (FEM)

- FEM discretization is well-suited to unstructured meshes of arbitrary polygonal/polyhedral domains
 - e.g. triangulate the snowflake:



- FEM uses the *weak form* of the PDE
- example: for the Poisson equation it is

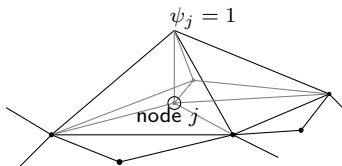
$$\int_{\Omega} \nabla u \cdot \nabla v = \int_{\Omega} f v \quad \forall v \in H_0^1(\Omega)$$

- derivation: multiply PDE by v and integrate by parts
- Fall 2018: graduate seminar in FEM

finite element method

in more detail, the FEM uses

- a triangular/quadrilateral/tetrahedral/etc. mesh of N nodes on Ω
- an N -dimensional subspace $\mathcal{X} \subset H^1(\Omega)$
- basis of *hat functions* $\psi_j(x, y)$
 - $\psi_j(x_i, y_i) = 0$ if $i \neq j$
 - $\psi_j(x_j, y_j) = 1$



then the FEM

- defines

$$u(x, y) = \sum_j u_j \psi_j(x, y)$$

for unknown coefficients $\mathbf{u} = \{u_j\} \in \mathbb{R}^N$ (N unknowns)

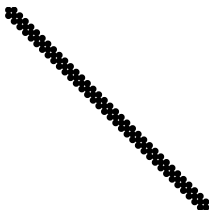
- requires the weak form to hold for all $v = \psi_i$ (N eqns)

sparse matrices

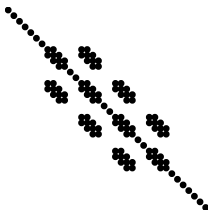
- both methods ($F \stackrel{D}{E} M$) produce *sparse matrices*
- for example, the Poisson equation becomes a linear system

$$A\mathbf{u} = \mathbf{b}$$

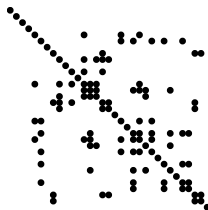
- $A \in \mathbb{R}^{N \times N}$ is sparse
- A is symmetric positive definite (SPD)
- *pro tip*: Matlab's `spy(A)` shows nonzero structure



Poisson 1D (either method)



MSE FDM 2D square



Poisson FEM 2D snowflake

nonlinear PDEs make sparse matrices too

- $F_{\mathbb{E}}^D M$ applied to a nonlinear elliptic PDE BVP gives a nonlinear (algebraic) system of N equations in N unknowns:

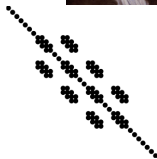
$$\mathbf{F}(\mathbf{u}) = 0$$

- $\mathbf{F} : \mathbb{R}^N \rightarrow \mathbb{R}^N$ is a nonlinear function
 - call $\mathbf{F}(\mathbf{w})$ the *residual* if \mathbf{w} is a guess at the solution
- usually apply Newton's method to solve:

$$J_{\mathbf{F}}(\mathbf{u}_{\ell}) \mathbf{s} = -\mathbf{F}(\mathbf{u}_{\ell})$$

$$\mathbf{u}_{\ell+1} = \mathbf{u}_{\ell} + \mathbf{s}$$

- $J_{\mathbf{F}}(\mathbf{w}) \in \mathbb{R}^{N \times N}$ is the Jacobian of \mathbf{F}
 - it is a sparse matrix (right)



MSE FDM 2D square

Outline

how to approximately solve a PDE

what is an “optimal solver”?

multigrid

barriers & extensions to optimality

define “optimal”

- consider N equations in N unknowns: $\mathbf{F}(\mathbf{u}) = 0$
 - residual $\mathbf{F} : \mathbb{R}^N \rightarrow \mathbb{R}^N$ is generally nonlinear
 - $\mathbf{F}(\mathbf{w}) = \mathbf{b} - A\mathbf{w}$ in the linear case

definition. an algorithm which solves $\mathbf{F}(\mathbf{u}) = 0$ in $O(N)$ work,
as $N \rightarrow \infty$, is *optimal*

- if you have ever tried solving big, nontrivially-coupled systems of equations, you'll conclude optimality is generally hopeless

slide full of caveats

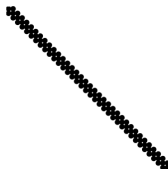
in the definition “an algorithm which solves $\mathbf{F}(\mathbf{u}) = 0$ in $O(N)$ work, as $N \rightarrow \infty$, is *optimal*”:

- “solves” means: generates \mathbf{u}_n so that $\frac{\|\mathbf{F}(\mathbf{u}_n)\|}{\|\mathbf{F}(\mathbf{u}_0)\|} \leq \text{tol}$
 - where \mathbf{u}_0 is an initial guess
 - in linear case $A\mathbf{u} = \mathbf{b}$, given any rounding error, only $O(\kappa(A)\epsilon_{\text{mach}})$ accuracy is possible anyway¹
- “ $O(N)$ ” hides constant; may depend on tol but not on N
- “work” = (count of floating point operations)
 - or runtime, but timing on modern computers is really messy
- “ $N \rightarrow \infty$ ” limit is notional only
 - real computers run out of memory
 - **optimal algorithms are often memory-limited** (that’s a *feature*)

¹for students of MATH 614

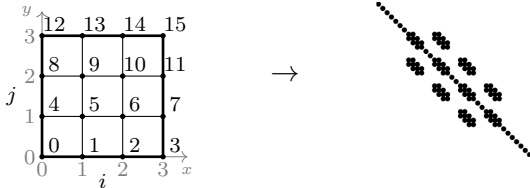
example: tridiagonal matrices

- an easy example of optimality
- Gauss elimination solves $A\mathbf{u} = \mathbf{b}$ in $8N - 6 = O(N)$ flops
 - need to avoid pivoting
- for SPD tridiagonal matrices, use Cholesky decomposition, again $O(N)$
- the 1D Poisson problem $-u'' = f$, and generally all ODE BVPs, have optimal solution methods



non-example: banded direct methods in 2D,3D

- for structured-grid FDM method on PDEs in 2D and 3D the bandwidth of A grows as $N \rightarrow \infty$
- for example, for MSE on $\Omega = [0, 1] \times [0, 1]$:



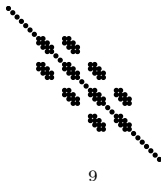
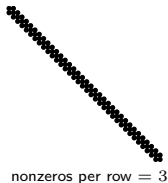
- if bandwidth p then Cholesky does $O(Np^2)$ work
- thus for direct methods for PDE problems on structured grids with m points in each direction:
 - $N = m^2$ and $p = m$ so $O(N^2)$ work in 2D
 - $N = m^3$ and $p = m^2$ so $O(N^{7/3})$ work in 3D
- variable reordering like “minimum degree” helps ... but not enough

sparse matrices from PDEs have $O(N)$ mat-vec

- if
 - $A \in \mathbb{R}^{N \times N}$ is sparse, with
 - number of nonzeros per row bounded independent of Nthen the *work of computing $A\mathbf{v}$* is $O(N)$
- computing $A\mathbf{v}$ is called a “mat-vec”
- condition is automatic for structured grids and any FEM
- for typical FEM on an unstructured mesh,

$$(\text{nonzeros in row } j \text{ of } A) = \text{degree}(\text{node } j) + 1$$

so cost of $A\mathbf{v}$ is $O((\max \text{ degree})N)$

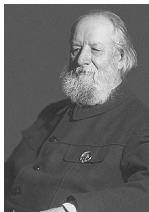


Krylov methods

- for most numerical analysts of the 1980s and 1990s, “sparse mat-vecs are $O(N)$ ” was the new hope
- because naval engineer A. Krylov (1931) observed that the solution to $A\mathbf{u} = \mathbf{b}$ may be well-approximated by \mathbf{v} in

$$\mathcal{K}_m(A, \mathbf{b}) = \text{span} \left\{ \mathbf{b}, A\mathbf{b}, A^2\mathbf{b}, \dots, A^m\mathbf{b} \right\}$$

- computing $\mathbf{v} \in \mathcal{K}_m(A, \mathbf{b})$ costs $O(mN)$
 - $\mathbf{v} \in \mathcal{K}_m(A, \mathbf{b}) \iff \mathbf{v} = p_m(A)\mathbf{b}$
- to solve $A\mathbf{u} = \mathbf{b}$ we want $\mathbf{u} = A^{-1}\mathbf{b} \approx p_m(A)\mathbf{b}$



conjugate gradients

- example: *conjugate gradients* (CG) is a Krylov method
 - A must be SPD
 - CG generates the “best” iterates \mathbf{u}_m from a Krylov space
 - the error $\mathbf{e}_m = \mathbf{u}_m - \mathbf{u}$ is minimal in norm $\|\cdot\|_A$
 - work per CG iteration is $O(N)$
 - thus work is $O(mN)$ for m iterations
- if $\kappa = \kappa_2(A)$ is the condition number of A then

$$\frac{\|\mathbf{e}_m\|_A}{\|\mathbf{e}_0\|_A} \leq 2 \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^m$$

- it follows that $m = O(\sqrt{\kappa})$ iterations are needed

CG iterations increase with N

- unfortunately, if A is from FDM applied to the Poisson equation then

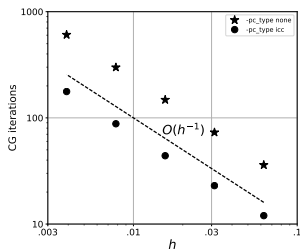
$$\kappa_2(A) = O(h^{-2})$$

- the number of CG iterations m increases with $N = O(h^{-d})$

- $m = O(N^{1/2})$ in 2D
 $\implies O(N^{3/2})$ solver
- $m = O(N^{1/3})$ in 3D
 $\implies O(N^{4/3})$ solver

- other Krylov methods are similar
- general reminder:

a Krylov method can only be optimal if the number of iterations m is bounded independently of N



preconditioning

- by ~ 1995 it was clear that Krylov methods by themselves were not the answer for solving big PDE problems
- but you don't have to accept the given system $A\mathbf{u} = \mathbf{b}$
- *definition.* given invertible M ,
 - $(M^{-1}A)\mathbf{u} = M^{-1}\mathbf{b}$ is the *left-preconditioned* system
 - $(AM^{-1})M\mathbf{u} = \mathbf{b}$ is the *right-preconditioned* system
- new condition numbers $\kappa_2(M^{-1}A)$ or $\kappa_2(AM^{-1})$ can be much smaller
- “ M^{-1} ” must be a cheap method for this to help
 - e.g. Meijerink & van der Vorst (1977): incomplete LU and Cholesky factorizations

where we stand: an optimality lemma

- *lemma.* as $N \rightarrow \infty$, if $A \in \mathbb{R}^{N \times N}$ is SPD and if a symmetric preconditioning method produces bounded condition numbers,

$$\kappa_2(M^{-1}A) \leq B,$$

where $B > 0$ is independent of N , then preconditioned CG is an optimal solver

- *optimality goal:* find preconditioners which make $\kappa_2(M^{-1}A)$ bounded independent of N
- *multigrid* is such a preconditioner

Outline

how to approximately solve a PDE

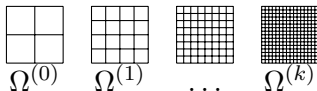
what is an “optimal solver”?

multigrid

barriers & extensions to optimality

multigrid: what it does

- given sequence of grids $\{\Omega^{(j)}\}_0^k$



- given initial guess \mathbf{w} on the finest grid $\Omega^{(k)}$, a multigrid cycle (e.g. a “V cycle”) approximately solves $A\mathbf{u} = \mathbf{b}$

function VCYCLE($A, \mathbf{b}, \mathbf{w}, l$)

if $l == 0$ **then**

 solve $A\mathbf{v} = \mathbf{b}$, e.g. by a direct solver

else

 improve \mathbf{w} on the level l grid

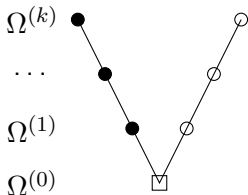
$\mathbf{r}^C = (\text{restrict } \mathbf{r} = \mathbf{b} - A\mathbf{w} \text{ to } \Omega^{(l-1)})$

$\mathbf{z}^C = \text{VCYCLE}(A^C, \mathbf{r}^C, 0, l-1)$

$\mathbf{v} \leftarrow \mathbf{v} + (\text{interpolate } \mathbf{z}^C \text{ to } \Omega^{(l)})$

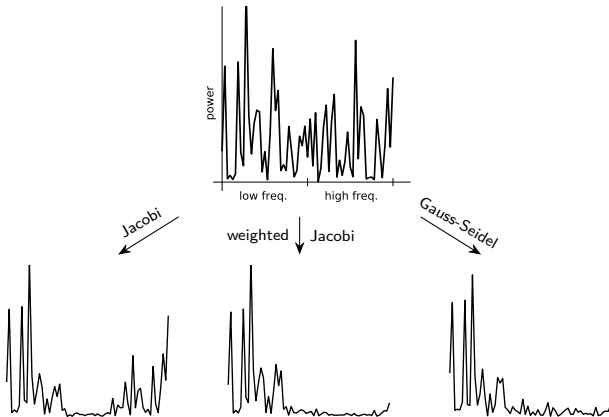
 improve \mathbf{v} some more on the level l grid

return \mathbf{v}



multigrid uses cheap smoothers

- *question*: what does “improve w on the level l grid” mean?
answer: **smoothing**
- many classical linear iterations are smoothing
 - e.g. weighted Jacobi and Gauss-Seidel using A
 - fast $O(N)$ operations
 - single iteration reduces high-frequency components of the error



multigrid: why it is $O(N)$

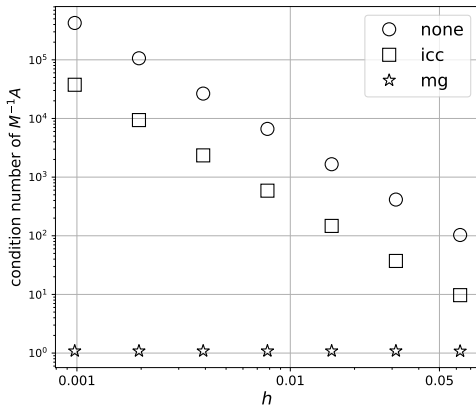
- multigrid is a systematic way of combining two actions
 - *smoothing*: filter out high frequencies of the error on your grid
 - *coarsening*: transfer to an easier grid
 - frequencies that were “medium-low” are now “high”
- restricting and interpolating on $\Omega^{(l)}$ is $O(N_l)$
- a single step of the smoother on $\Omega^{(l)}$ is $O(N_l)$
- thus total work on $\Omega^{(l)}$ is CN_l for fixed C
- then the total work of a V-cycle is a finite geometric series:

$$\begin{aligned} & (\Omega^{(k)} \text{ work}) + (\Omega^{(k-1)} \text{ work}) + \cdots + (\Omega^{(1)} \text{ work}) + (\Omega^{(0)} \text{ work}) \\ &= CN_k + CN_{k-1} + \cdots + CN_1 + C_0 \\ &= CN_k + C \frac{N_k}{2^d} + \cdots + C \left(\frac{1}{2^d} \right)^{k-1} N_k + C_0 \\ &\leq 2CN_k + C_0 \end{aligned}$$

- re the coarsest grid ... who cares! ... C_0 is independent of N

multigrid on Poisson

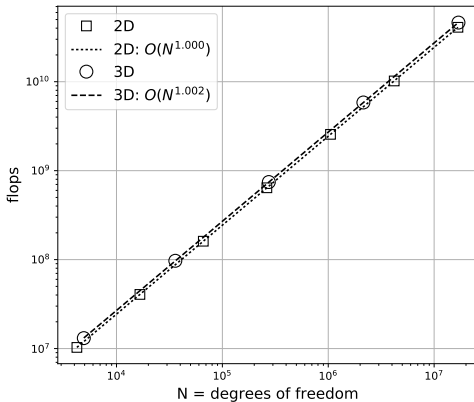
- V-cycle-preconditioned CG iterations on $\Omega = [0, 1]^2$ Poisson



values of $\kappa_2(M^{-1}A)$ for 2D problem

multigrid on Poisson: evidence of optimality

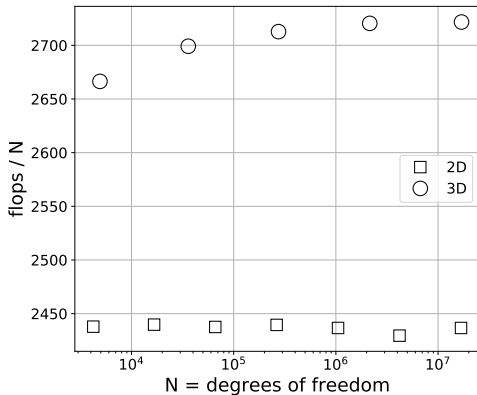
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direct demonstration of $O(N)$ work

multigrid on Poisson: evidence of optimality

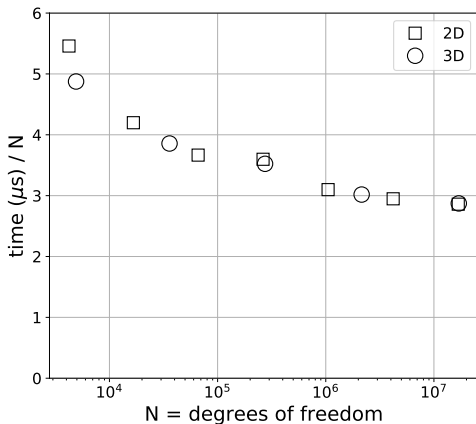
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i.e. constant amount of work per degree of freedom

multigrid on Poisson: evidence of optimality

- V-cycle-preconditioned CG iterations on $\Omega = [0, 1]^d$ Poisson



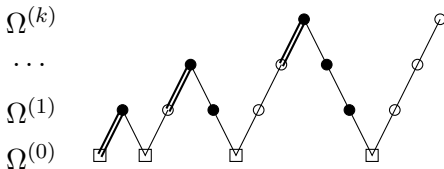
(almost) constant amount of time per degree of freedom

multigrid on MSE

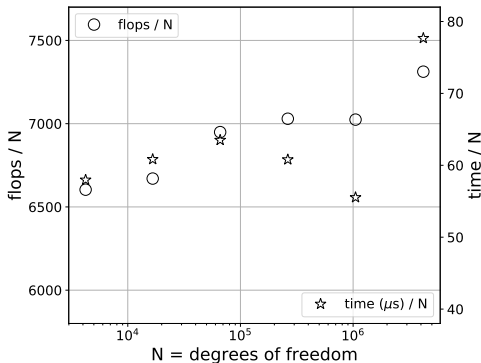
- recall the nonlinear MSE problem on $\Omega = [0, 1]^2$:

$$-\nabla \cdot \left(\frac{\nabla u}{\sqrt{1 + |\nabla u|^2}} \right) = 0 \quad \text{with } u|_{\partial\Omega} = g.$$

- solved by Newton iteration
- how to *find a convergent initial iterate* on a fine grid?
- multigrid solution is by nonlinear “F-cycle”
 - a.k.a. nested iteration with V-cycles
 - start* on coarse grid $\Omega^{(0)}$
 - interpolating upward supplies good initial iterate



multigrid on MSE: evidence of optimality



- on finest 2049×2049 grid with $N = 4 \times 10^6$:

$$\text{total flops} = N \left(\frac{\text{flops}}{N} \right) = (4 \times 10^6)(7 \times 10^3) \approx 3 \times 10^{10}$$

- runtime about 5 minutes total

algebraic multigrid

- what about multigrid on unstructured grids?
 - remember the snowflake?
 - for “geometric” multigrid (used so far) one needs subgrids and grid-based restriction and interpolation operations
- new idea ~1985 is *algebraic multigrid*
 - can be applied to *any* linear system $A\mathbf{u} = \mathbf{b}$
 - extracts analogs of “subgrid” and “smoother” and “interpolation” from A itself
 - ... but tends to need elliptic PDEish properties to actually work
 - active research area for e.g. spectral graph theory
 - by a new generation of applied mathematicians

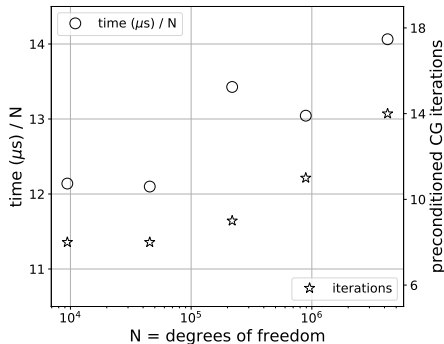
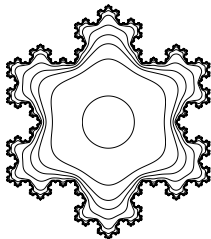
algebraic multigrid

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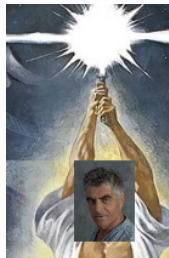
algebraic multigrid: evidence of (near-)optimality

- recall unstructured mesh on a snowflake polygon; level 2 at right
- generate level 5,6,7,8,9 approximations of the Koch fractal
- mesh them
- and test algebraic-multigrid-preconditioned CG method, on the Poisson equation $-\nabla^2 u = 1$, for optimality



wider applicability of multigrid

- multigrid was invented for Poisson and linear elliptic equations by Federenko (1962, 1964)
- but there was a period of darkness
- by 1980 or so optimism about multigrid was limited to one mathematician: Achi Brandt
 - a creator of algebraic multigrid,
 - and of a fully-nonlinear multigrid, the *full approximation scheme* (not covered here),
 - who started calling optimality “textbook multigrid efficiency,” which isn’t really helping
- since then, multigrid has succeeded on more and more applications
 - example: Brown et al. (2013), *Achieving textbook multigrid efficiency for hydrostatic ice flow*



Achi Brandt is my hero



Jed Brown, UAF MS
2006

Outline

how to approximately solve a PDE

what is an “optimal solver”?

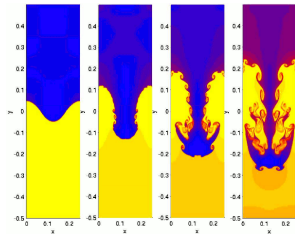
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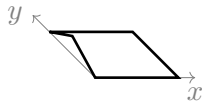
low regularity of solution

- multigrid is not always easy to make optimal
- consider nonlinear PDE BVP

- or a PDE system like Stokes flow
- or an implicit time step of Navier-Stokes

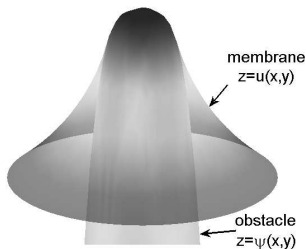


- try Newton-multigrid method
 - as we did with MSE
- *problem*: often # of Newton steps *and* Krylov steps grows as $h \rightarrow 0$ because of large gradients in the solution
- can demonstrate this with MSE for nonsmooth boundary conditions
 - not shown
 - Brandt suggests: combine multigrid & AMR



constrained problems

- other problems are not quite PDEs because they have inequality constraints
- causes two difficulties for Newton-multigrid methods:
 1. a free boundary implies low regularity (last slide)
 2. # of Newton steps is proportional to D/h where D is distance-to-move free boundary (from initial iterate)
- but there's another Brandt invention: *projected full approximation scheme*, a fully-nonlinear and constraint-adapted multigrid
- Max H. is working on it



numerical convergence, and spectral methods

- for a PDE BVP, as $h \rightarrow 0$ and $N \rightarrow \infty$ we **first want convergence to the continuum solution**
 - I have been assuming that our methods are convergent!
- spectral methods get very close to the continuum solution for very small N ... compared to F_{EM}^D
 - *if* the geometry is simple (rectangle)
 - *and* the solution is smooth
- often A is dense
- but with such a spectral method, even $O(N^3)$ solution of the discrete equations is often acceptable because N is small
- recalling these things shows that optimality is *not* the only good goal

optimality, by numerical DE subfield

- for all DE problems, one needs to define N , the number of discrete degrees of freedom, before we can talk optimality
- ODE IVP
 - for $y' = f(t, y)$ and $y(t) \in \mathbb{R}^q$
 - on $[0, T]$ with Δt spacing in time
 - define:

$$N := \frac{T}{\Delta t} q$$

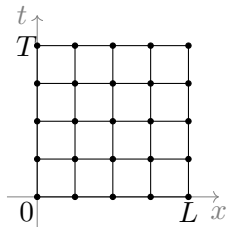
- with this N , all ODE IVP methods are already optimal

optimality, by numerical DE subfield

- for all DE problems, one needs to define N , the number of discrete degrees of freedom, before we can talk optimality
- ODE IVP already optimal ✓
- ODE BVP
 - $F_E^D M$ generate tridiagonal systems
 - already optimal

optimality, by numerical DE subfield

- for all DE problems, one needs to define N , the number of discrete degrees of freedom, before we can talk optimality
- ODE IVP already optimal ✓
- ODE BVP already optimal ✓
- hyperbolic PDE IBVP
 - for example, wave equation with reaction: $u_t + a(u) \cdot \nabla u = f(u)$
 - FVMs normally use explicit, CFL-limited time steps Δt
 - if we define $N = \frac{T}{\Delta t} \frac{L}{\Delta x}$, these methods are already optimal

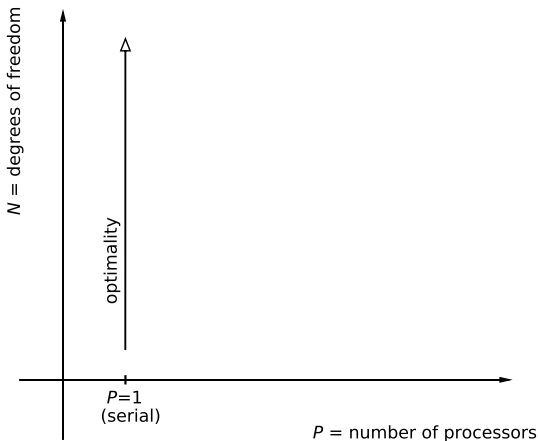


optimality, by numerical DE subfield

- for all DE problems, one needs to define N , the number of discrete degrees of freedom, before we can talk optimality
- ODE IVP already optimal ✓
- ODE BVP already optimal ✓
- hyperbolic PDE IBVP already optimal ✓
- PDE BVP optimal requires effort
- other PDE IBVP optimal requires effort
 - for example, advection-diffusion-reaction equation with reaction: $u_t + a(u) \cdot \nabla u = \nabla \cdot (D \nabla u) + f(u)$

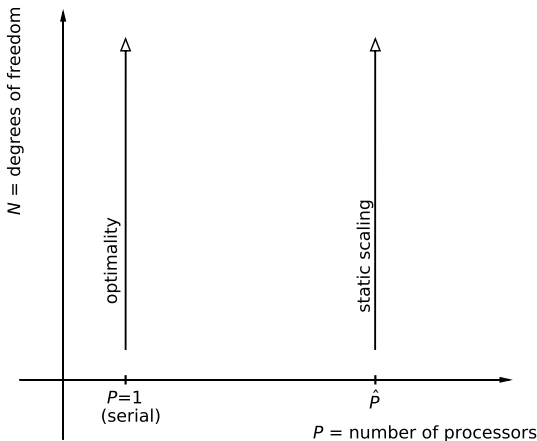
conflicting goal: parallel scaling

- sometimes you have a big machine with \hat{P} processors
 - everything so far has been serial ($P = 1$)
 - on graph below, runtime is third axis



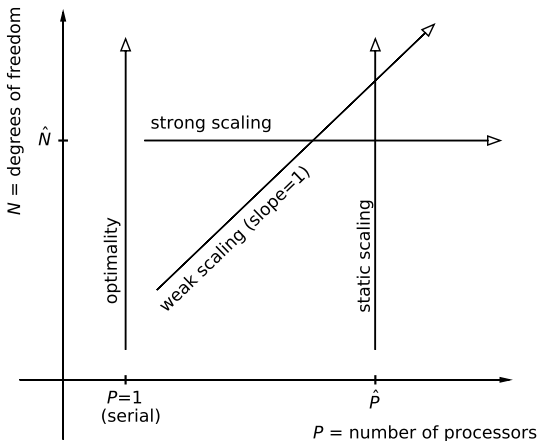
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conclusion

- in approximately solving your well-behaved PDE-type problem on a modern computer,

you should be solving the N equations in $O(N)$ work

as you head toward $N = \infty$ unknowns

- this is a good *goal* for PDE BVPs
- to achieve it you must exploit
 - the locality (sparsity) of the problem, and
 - correlation (smoothness) of the solution
- multigrid is the only real hope!?
- talk to me about PETSc ... I am writing a book about that

conclusion

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²for dense systems $A\mathbf{u} = \mathbf{b}$ the goal is $O(N^2)$... an open problem