Multigrid

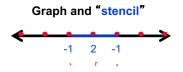
James Demmel

www.cs.berkeley.edu/~demmel/ma221_Spr20

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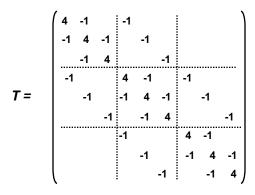
Poisson's equation in 1D: $\partial^2 u/\partial x^2 = f(x)$

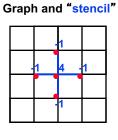
$$T = \begin{pmatrix} 2 & -1 \\ -1 & 2 & -1 \\ & -1 & 2 & -1 \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix}$$



2D Poisson's equation

° Similar to the 1D case, but the matrix *T* is now

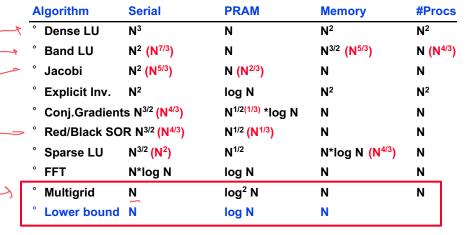




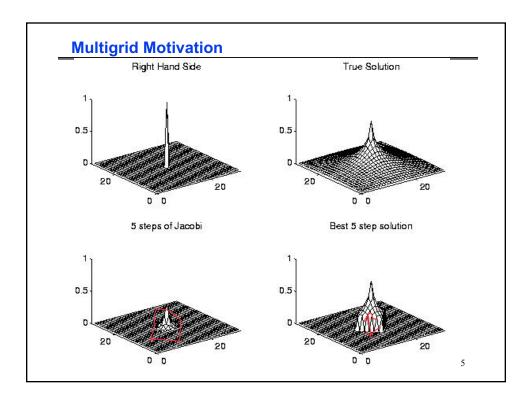
° 3D is analogous

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Algorithms for 2D (3D) Poisson Equation (N = n^2 (n^3) vars)



PRAM is an idealized parallel model with zero cost communication



Multigrid Motivation

- Recall that Jacobi, SOR, CG, or any other sparsematrix-vector-multiply-based algorithm can only move information one grid cell at a time
 - Take at least n steps to move information across n x n grid
- $^{\circ}$ Can show that decreasing error by fixed factor c<1 takes $\Omega(\log n)$ steps
 - Convergence to fixed error < 1 takes $\Omega(\log n)$ steps
- Therefore, converging in O(1) steps requires moving information across grid faster than to one neighboring grid cell per step
 - · One step can't just do sparse-matrix-vector-multiply

Big Idea used in multigrid and elsewhere

- ° If you are far away, problem looks simpler
 - For gravity: approximate earth, distant galaxies, ... by point masses
- ° Can solve such a coarse approximation to get an approximate solution, iterating if necessary
 - Solve coarse approximation problem by using an even coarser approximation of it, and so on recursively
- Ex: Multigrid for solving PDE in O(n) time
 - Use coarser mesh to get approximate solution of Poisson's Eq.
- Ex: Fast Multipole Method, Barnes-Hut for computing gravitational forces on n particles in O(n log n) time:
 - · Approximate particles in box by total mass, center of gravity
 - Good enough for distant particles; for close ones, divide box recursively
- Ex: Graph Partitioning (used to parallelize SpMV)
 - Replace graph to be partitioned by a coarser graph (CS267 for details)

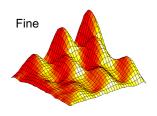
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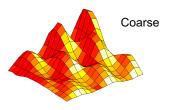
Fine and Coarse Approximations Fine Coarse Spr 2020 Math 221 8

Multigrid Overview

° Basic Algorithm:

- Replace problem on fine grid by an approximation on a coarser grid
- Solve the coarse grid problem approximately, and use the solution as a starting guess for the fine-grid problem, which is then iteratively updated
- Solve the coarse grid problem recursively, i.e. by using a still coarser grid approximation, etc.
- Success depends on coarse grid solution being a good approximation to the fine grid





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Multigrid uses Divide-and-Conquer in 2 Ways

° First way:

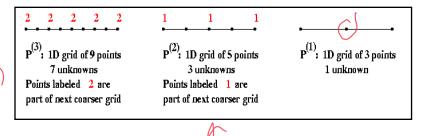
 Solve problem on a given grid by calling Multigrid on a coarse approximation to get a good guess to refine

Second way:

- · Think of error as a sum of sine curves of different frequencies
- · Same idea as FFT solution, but not explicit in algorithm
- Each call to Multigrid responsible for suppressing coefficients of sine curves of the lower half of the frequencies in the error (pictures later)

Multigrid Sketch in 1D

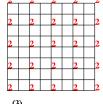
- ° Consider a 2^m+1 grid in 1D for simplicity
- Let P⁽ⁱ⁾ be the problem of solving the discrete Poisson equation on a 2ⁱ+1 grid in 1D. Write linear system as T(i) * x(i) = b(i)
- $^{\circ}\ P^{(m)}\,,\,P^{(m\text{-}1)}\,,\,\dots\,,\,P^{(1)}$ is sequence of problems from finest to coarsest



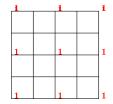
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Multigrid Sketch (1D and 2D)

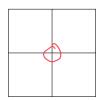
- ° Consider a 2m+1 grid in 1D (2m+1 by 2m+1 grid in 2D) for simplicity
- Let P⁽ⁱ⁾ be the problem of solving the discrete Poisson equation on a 2ⁱ+1 grid in 1D (2ⁱ+1 by 2ⁱ+1 grid in 2D)
 - Write linear system as T(i) * x(i) = b(i)
- $^{\circ}\ P^{(m)}\ , P^{(m-1)}\ , \ \dots\ , P^{(1)}$ is sequence of problems from finest to coarsest



P⁽³⁾: 9 by 9 grid of points 7 by 7 grid of unknowns Points labeled 2 are part of next coarser grid



P⁽²⁾: 5 by 5 grid of points 3 by 3 grid of unknowns Points labeled 1 are part of next coarser grid



P⁽¹⁾: 3 by 3 grid of points 1 by 1 grid of unknowns

Multigrid Operators (write on board)

- For problem P⁽ⁱ⁾:
 - · b(i) is the RHS and
 - · x(i) is the current estimated solution

both live on grids of size 2i-1

- All the following operators just average values on neighboring grid points (so information moves fast on coarse grids)
- The restriction operator R(i) maps P⁽ⁱ⁾ to P⁽ⁱ⁻¹⁾
 - Restricts problem on fine grid P⁽ⁱ⁾ to coarse grid P⁽ⁱ⁻¹⁾
 - · Uses sampling or averaging
 - b(i-1)= R(i) (b(i))
- The interpolation operator In(i-1) maps approx. solution x(i-1) to x(i)
 - Interpolates solution on coarse grid P⁽ⁱ⁻¹⁾ to fine grid P⁽ⁱ⁾
 - x(i) = In(i-1)(x(i-1))
- The solution operator S(i) takes $P^{(i)}$ and improves solution x(i)
 - · Uses "weighted" Jacobi or SOR on single level of grid
 - x improved (i) = S(i) (b(i), x(i))
- Overall algorithm, then details of operators

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```
Multigrid V-Cycle Algorithm (write on board, Matlab code on webpage)
```

```
Function MGV (b(i), x(i))
```

- ... Solve T(i)*x(i) = b(i) given b(i) and an initial guess for x(i)
- ... return an improved x(i)

if (i = 1)

compute exact solution x(1) of $P^{(1)}$ only 1 unknown

return x(1)

else

improve solution by x(i) = S(i) (b(i), x(i))

damping high frequency error

compute residual r(i) = T(i)*x(i) - b(i)

d(i) = In(i-1) (MGV(R(i) (r(i)), 0))solve T(i)*d(i) = r(i) recursively

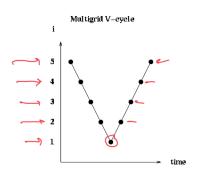
x(i) = x(i) - d(i)correct fine grid solution x(i) = S(i) (b(i), x(i))improve solution again

return x(i)

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Why is this called a V-Cycle?

- ° Just a picture of the call graph
- ° In time a V-cycle looks like the following



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Cost (#flops) of a V-Cycle for 2D Poisson

- ° Constant work per mesh point (average with neighbors)
- ° Work at each level in a V-cycle is O(the number of unknowns)
- ° Cost of Level i is O((2ⁱ-1)²) = O(4 i)
- ° If finest grid level is m, total time is:

$$\Sigma_{i=1}^{m} O(4^{i}) = O(4^{m}) = O(\# unknowns)$$

Full Multigrid (FMG)

- ° Intuition:
 - · improve solution by doing multiple V-cycles
 - · avoid expensive fine-grid (high frequency) cycles
 - · analysis of why this works is beyond the scope of this class

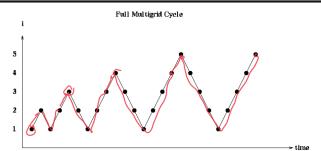
```
Function FMG (b(m), x(m))
... return improved x(m) given initial guess
compute the exact solution x(1) of P(1) ←
for i=2 to m
```

x(i) = MGV (b(i), In (i-1) (x(i-1)))

- ° In other words:
 - · Solve the problem with 1 unknown
 - Given a solution to the coarser problem, $P^{(i-1)}$, map it to starting guess for $P^{(i)}$
 - · Solve the finer problem using the Multigrid V-cycle

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Full Multigrid Cost Analysis



- ° One V-cycle for each call to FMG
 - people also use "W cycles" and other compositions
- ° #Flops: $\sum_{i=1}^{m} O(4^{i}) = O(4^{m}) = O(\# unknowns)$

Complexity of Solving Poisson's Equation

- Theorem: error after one FMG call ≤ c · error before, where c < 1/2, independent of # unknowns</p>
- ° Corollary: We can make the error < any fixed tolerance in a fixed number of steps, independent of size of finest grid
- * This is the most important convergence property of MG, distinguishing it from all other methods, which converge more slowly for large grids
- Total complexity just proportional to cost of one FMG call

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The Solution Operator S(i) – Details (on board)

- ° The solution operator, S(i), is a weighted Jacobi
- ° Consider the 1D problem



At level i, pure Jacobi replaces:

$$x(j) := 1/2 (x(j-1) + x(j+1) + b(j))$$

in notation from lecture: $R_J = I - T/2$

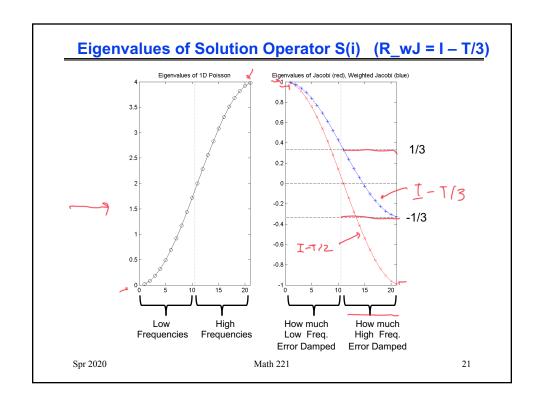
Weighted Jacobi uses:

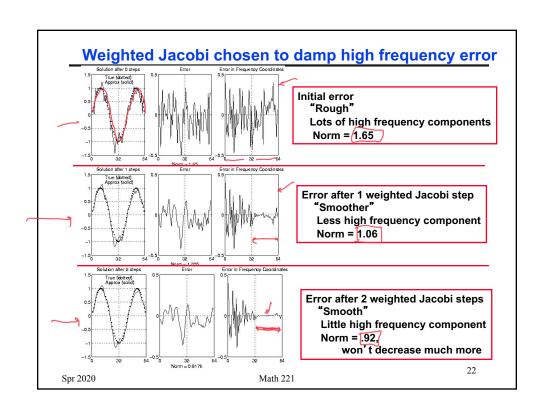
$$x(j) := 1/3 (x(j-1) + x(j) + x(j+1) + b(j))$$

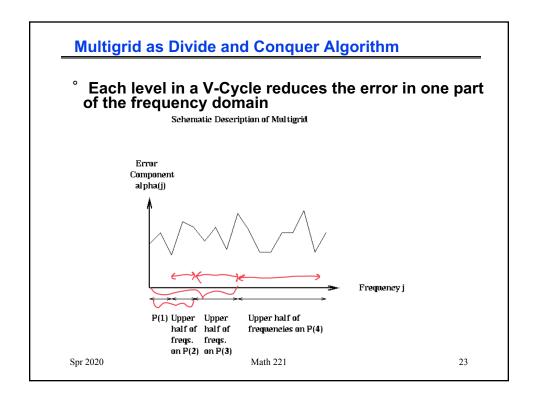
R wJ = I - T/3

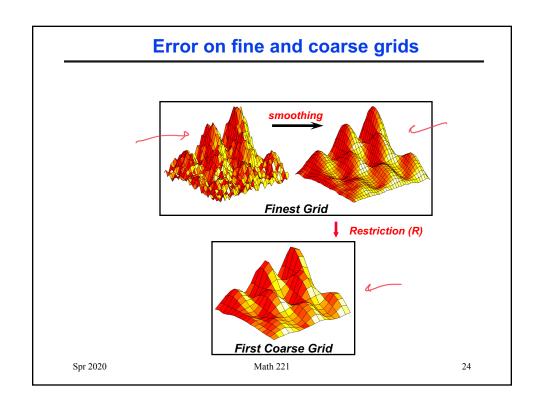
- ° In 2D, similar average of nearest neighbors
 - Chosen so that "high frequency" eigenvector components of error get decreased by as much as possible (1/3)

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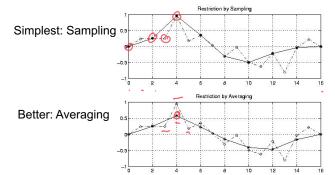






The Restriction Operator R(i) - Details The restriction operator, R(i), takes

- - a problem P(i) with Right-Hand-Side (RHS) b_{fine} and
 - maps it to a coarser problem P(i-1) with RHS b_{coarse} = R(i)(b_{fine})
- In 1D, average values of neighbors
 - Simplest: Sampling: bcoarse(k) = bfine(k)
 - Better: Averaging: bcoarse(k) = 1/4 * bfine(k-1) + 1/2 * bfine(k) + 1/4 * bfine(k+1)

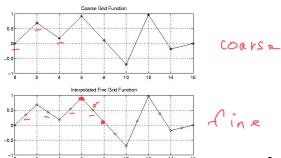


° In 2D, average with all 8 neighbors (N,S,E,W,NE,NW,SE,SW) Spr 2020

Interpolation Operator In(i-1): details

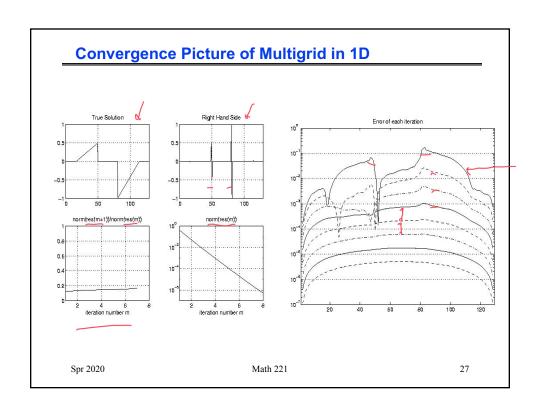
The interpolation operator In(i-1), takes a function x_{coarse} on a coarse grid $P^{(i-1)}$, and produces a function x_{fine} on a fine grid $P^{(i)}$:

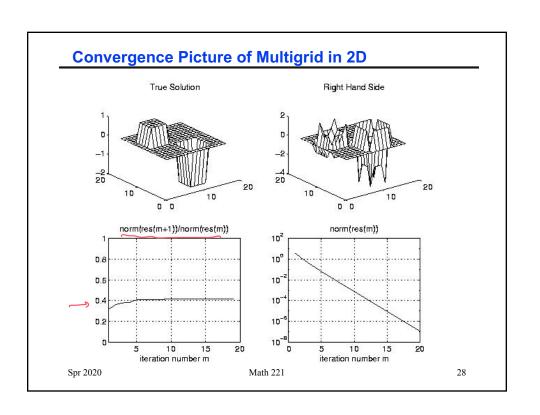
- ° x_{fine} = In(i-1)(x_{coarse})
- ° In 1D, linearly interpolate nearest coarse neighbors
 - xfine(k) = xcoarse(k) if the fine grid point k is also a coarse one, else
 - xfine(k) = 1/2 * xcoarse(left of k) + 1/2 * xcoarse(right of k)



In 2D, interpolation requires averaging with 4 nearest neighbors (NW,SW,NE,SE)

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```
Multigrid V-Cycle Algorithm Analysis (1/2)
Function MGV (b(i), x(i))
  ... Solve T(i)*x(i) = b(i) given b(i) and an initial guess for x(i)
  ... return an improved x(i)
 if (i = 1)
     compute exact solution x(1) of P^{(1)}
                                                 only 1 unknown
     return x(1)
  else
     x(i) = S(i) (b(i), x(i))
                                                  x(i) = S \cdot x(i) + b(i)/3 
     r(i) = T(i)*x(i) - b(i)
                                                  r(i) = T(i)*x(i) - b(i) \longleftarrow
     d(i) = In(i-1) (MGV(R(i) (r(i)), 0))
                                                 d(i) = In \cdot (T(i-1)^{-1} \cdot (R \cdot r(i)))
              (Note: we assume recursive solve is exact, for ease of analysis)
     x(i) = x(i) - d(i)
                                                 x(i) = x(i) - d(i)
     x(i) = S(i) (b(i), x(i))
                                                 x(i) = S \cdot x(i) + b(i)/3
     return x(i)
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```

Multigrid V-Cycle Algorithm Analysis (2/2)

```
Goal: combine these equations to get formula for error e(i) = x(i) - x:
```

```
subtract x = S \cdot x + b(i)/3 to get e(i) = S \cdot e(i) subtract x = S \cdot x + b(i)/3 to get e(i) = S \cdot e(i) subtract 0 = T(i) \cdot x - b(i) to get e(i) = T(i) \cdot e(i) d(i) = In \cdot (T(i-1)^{-1} \cdot (R \cdot r(i))) assume coarse problem solved exactly subtract x = x to get e(i) = e(i) - d(i) subtract x = x \cdot x + b(i)/3 to get e(i) = S \cdot e(i)
```

Substitute each equation into later ones to get

$$e(i) = S \cdot (I - \underline{In} \cdot (T(i-1)^{-1} \cdot (\underline{R} \cdot T(i)))) \cdot S \cdot e(i) = M \cdot e(i)$$

Theorem: For 1D Poisson problem, the eigenvalues of M are either 0 or 1/9, independent of dimension.

This means multigrid converges in a bounded number of steps, independent of dimension.

Generalizing Multigrid beyond Poisson, to unstructured meshes (1/2)

- What does it mean to do Multigrid anyway?
- Need to be able to coarsen grid (hard problem)
 - · Can't just pick "every other grid point" anymore
 - · How to make coarse graph approximate fine one
 - · What if there are no grid points?
- Need to define R() and In()
 - · How do we convert from coarse to fine mesh and back?
 - How do we define coarse matrix (no longer formula, like Poisson)
- Need to define S()
 - · How do we damp "high frequency" error?
- Dealing with coarse meshes efficiently
 - · Should we switch to another solver on coarsest meshes?

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Generalizing Multigrid beyond Poisson, to unstructured meshes (2/2)

- Given original problem, how do we generate a sequence of coarse approximations?
- For finite element problems, could regenerate matrix starting on coarser mesh
 - Need access to original physical problem and finite element modeling system, i.e. a lot more than just the original matrix, so it may be impossible
 - · What does "coarse" mean, once very coarse?
- Geometric Multigrid
 - Assume we know (x,y,z) coordinates of underlying mesh, and matrix
 - Generate coarse mesh points, analogous to taking every other point in regular mesh
 - Retriangulate to get new mesh
 - Use finite element shape functions on coarse mesh to project fine matrix to coarse one

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- Algebraic Multigrid
 - Don't even have (x,y,z) coordinates, just matrix

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Geometric Multigrid

Need matrix, (x,y,z) coordinates of mesh points

- · Not minimum information (just matrix), but a little more
- · Based on work of Guillard, Chan, Smith

° Finite element intuition

- · Goal is to compute function, represented by values at points
- · Think of approximation by piecewise linear function connecting points
 - Easy in 1D, need triangulated mesh in 2D, 3D uses tetrahedra

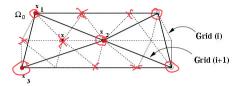
° Geometric coarsening

- · Pick a subset of coarse points "evenly spaced" among fine points
 - Use Maximal Independent Sets
 - Try to keep important points, like corners, edges of object
- · Retriangulate coarse points
 - Try to approximate answer by piecewise linear function on new triangles
- Let columns of P ("prolongator") be values at fine grid points given values at coarse ones
 - Generalizes Interpolation operator "In" from before
- $A_{coarse} = P^T A_{fine} P$ Galerkin method
- For Poisson: P = In, $P^T = 2*R$, $T_{coarse} = 2*P^T*T_{fine}*P$

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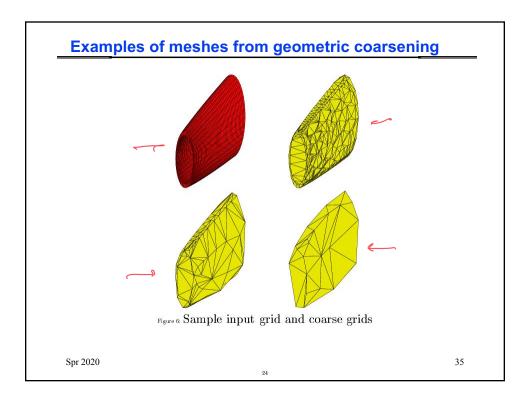
Example of Geometric Coarsening



Simple Greedy Algorithm:

repeat
pick unmarked vertex
mark it and its neighbors
until no unmarked vertices

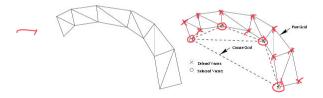
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What can go wrong

- Care needed so coarse grid preserves geometric features of fine grid
 - Label fine grid points as corner, edge, face, interior
 - Delete edges between same-labeled points in different features
 - Ex: delete edges between points on different faces
 - Keeps feature represented on coarse meshes

Pathological example:



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Example - classify vertices - modify graph Surface vertices Corner vertices Figure 1: Modify graph Figure 2: New mesh - fixed mesh Spr 2020

Algebraic Multigrid

- ° No information beyond matrix needed
- ° Galerkin still used to get Acoarse =(P^T/Afine(P)
- Prolongator P defined purely algebraically
 - · Cluster fine grid points into nearby groups
 - Can use Maximal Independent Sets or Graph Partitioning
 - Use magnitude of entries of Afine to cluster
 - · Associate one coarse grid node to each group
 - To interpolate coarse grid values to associated fine grid point, can use properties of PDE, eg elasticity:
 - Rigid body modes of coarse grid point
 - Let coarse grid point have 6 dof (3 translation, 3 rotation)
 - Can be gotten from QR factorization of submatrix of Afine
 - · Can also apply smoother to resulting columns of P
 - "Smoothed Aggregation"
- Based on work of Vanek, Mandel, Brezina, Farhat, Roux, Bulgakov, Kuhn ...

Parallel Smoothers for Unstructured Multigrid

- Weighted Jacobi
 - Easy to implement, hard to choose weight
- Gauss-Seidel
 - Works well, harder to parallelize because of triangular solve
- Polynomial Smoothers
 - Chebyshev polynomial p(A_{fine})
 - Easy to implement (just SpMVs with Afine)
 - Chebyshev chooses p(y) such that
 - [1 p(y) y] = min over interval $[\lambda^*, \lambda_{max}]$ estimated to contain eigenvalues of Afine

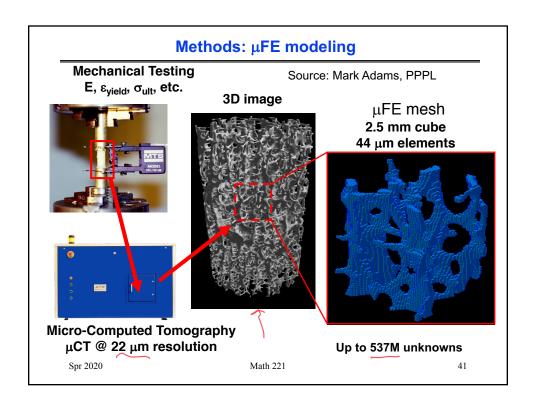
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Source of Unstructured Finite Element Mesh: Vertebra

Study failure modes of trabecular Bone under stress

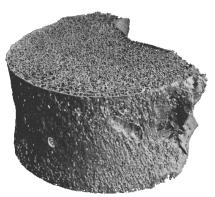


Source: M. Adams, H. Bayraktar, T. Keaveny, P. Papadopoulos, A. Gupta Spr 2020 Math 221



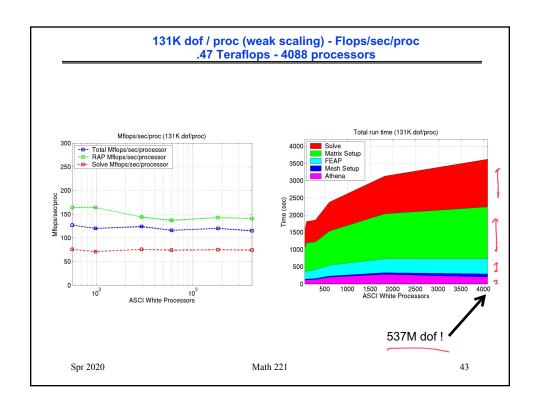
Vertebral Body With Shell

- Large deformation elasticity
- 6 load steps (3% strain)
- Scaled speedup
 - ~131K dof/processor
- 7 to 537 million dof
- 4 to 292 nodes
- IBM SP Power3
 - 14 of 16 procs/node used
 - Up to 4088 processors
- Double/Single Colony switch
- Gordon Bell Prize, 2004
- Clinical application to predicting chance of fracture due to osteoporosis



 $80 \mu m w/ shell$

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Conclusions

Multigrid can be very fast

- Provably "optimal" (does O(N) flops to compute N unknowns) for many problems in which one can show that using a coarse grid gives a good approximation
- · Can be parallelized effectively

Multigrid can be complicated to implement

- · Lots of software available (see web page for pointers)
 - PETSc (includes many iterative solvers, interfaces to other packages, Python interface, runs in parallel)
 - ACTS (repository for PETSc and other packages)
 - Offers periodic short courses on using these packages
 - MGNET
- Sample Matlab implementation for 1D and 2D Poisson
 - See class web page under "Matlab Programs for Homework Assignments"



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Parallel 2D Multigrid

- Multigrid on 2D requires nearest neighbor (up to 8) computation at each level of the grid
- Start with n=2^m+1 by 2^m+1 grid (here m=5)
- Use an s by s processor grid (here s=4)

Communication pattern for Multigrid on 33 by 33 mesh with 4 by 4 processor grid In top processor row, grid points labeled m are updated in problem P(m) of multigrid Pink processor owns grid points inside pink box In lower half of graph, grid points labeled m need to be communicated to pink processor in problem P(m) of multigrid

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Performance Model of parallel 2D Multigrid (V-cycle)

- ° Assume 2m+1 by 2m+1 grid of points, n= 2m-1, N=n2
- ° Assume p = 4^k processors, arranged in 2^k by 2^k grid
 - Processors start with 2^{m-k} by 2^{m-k} subgrid of unknowns
- Consider V-cycle starting at level m
 - · At levels m through k of V-cycle, each processor does some work
 - At levels k-1 through 1, some processors are idle, because a 2^{k-1} by 2^{k-1} grid of unknowns cannot occupy each processor
- ° Cost of one level in V-cycle
 - If level j >= k, then cost =

O(4^{j-k}) Flops, proportional to the number of grid points/processor

+ O(1) α Send a constant # messages to neighbors

+ O(2^{j-k}) β Number of words sent

If level j < k, then cost =

O(1) Flops, proportional to the number of grid points/processor

+ O(1) α Send a constant # messages to neighbors

+ O(1) β Number of words sent

Sum over all levels in all V-cycles in FMG to get complexity

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Comparison of Methods (in O(.) sense)

	# Flops	# Messages	# Words sent
MG	N/p +	(log N) ²	(N/p) ^{1/2} +
	log p * log N		log p * log N
FFT	N log N / p	p ^{1/2}	N/p
SOR	N ^{3/2} /p	N ^{1/2}	N/p

- SOR is slower than others on all counts
- Flops for MG and FFT depends on accuracy of MG
- MG communicates less total data (bandwidth)
- ° Total messages (latency) depends ...
 - This coarse analysis can't say whether MG or FFT is better when $\alpha >\!\!> \beta$

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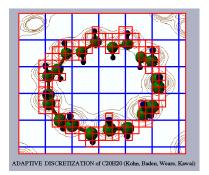
Practicalities

- ° In practice, we don't go all the way to P(1)
- ° In sequential code, the coarsest grids are negligibly cheap, but on a parallel machine they are not.
 - · Consider 1000 points per processor
 - In 2D, the surface to communicate is 4xsqrt(1000) ~= 128, or 13%
 - In 3D, the surface is 1000-83 ~= 500, or 50%
- See Tuminaro and Womble, SIAM J. Sci. Comp., v14, n5, 1993 for analysis of MG on 1024 nCUBE2
 - · on 64x64 grid of unknowns, only 4 per processor
 - efficiency of 1 V-cycle was .02, and on FMG .008
 - · on 1024x1024 grid
 - efficiencies were .7 (MG Vcycle) and .42 (FMG)
 - although worse parallel efficiency, FMG is 2.6 times faster that V-cycles alone
 - nCUBE had fast communication, slow processors

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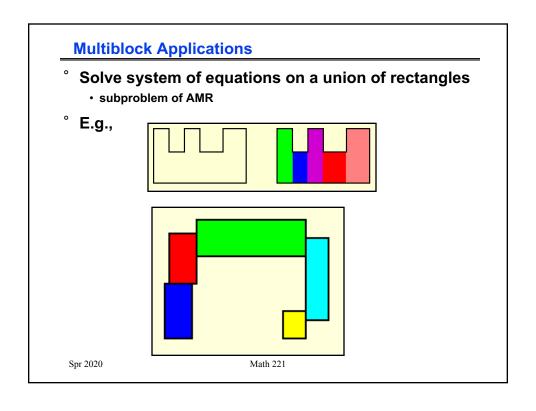
Multigrid on an Adaptive Mesh

- For problems with very large dynamic range, another level of refinement is needed
- Build adaptive mesh and solve multigrid (typically) at each level



° Can't afford to use finest mesh everywhere

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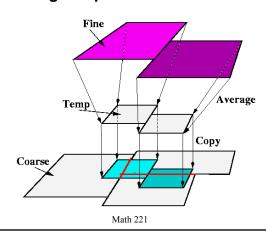


Adaptive Mesh Refinement

° Data structures in AMR

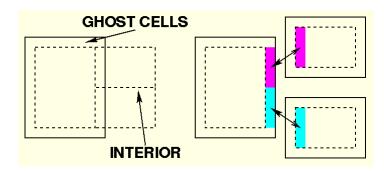
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- Usual parallelism is to assign grids on each level to processors
- ° Load balancing is a problem



Support for AMR

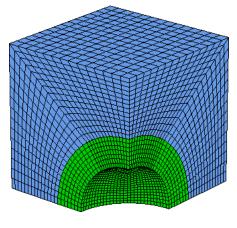
- ° Domains in Titanium designed for this problem
- ° Kelp, Boxlib, and AMR++ are libraries for this
- ° Primitives to help with boundary value updates, etc.



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Multigrid on an Unstructured Mesh

- Another approach to variable activity is to use an unstructured mesh that is more refined in areas of interest
- Adaptive rectangular or unstructured?
 - Numerics easier on rectangular
 - Supposedly easier to implement (arrays without indirection) but boundary cases tend to dominate code



Up to 39M unknowns on 960 processors, With 50% efficiency (Source: M. Adams)

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