CS 267: Applications of Parallel Computers

Lecture 16 - Structured Grids

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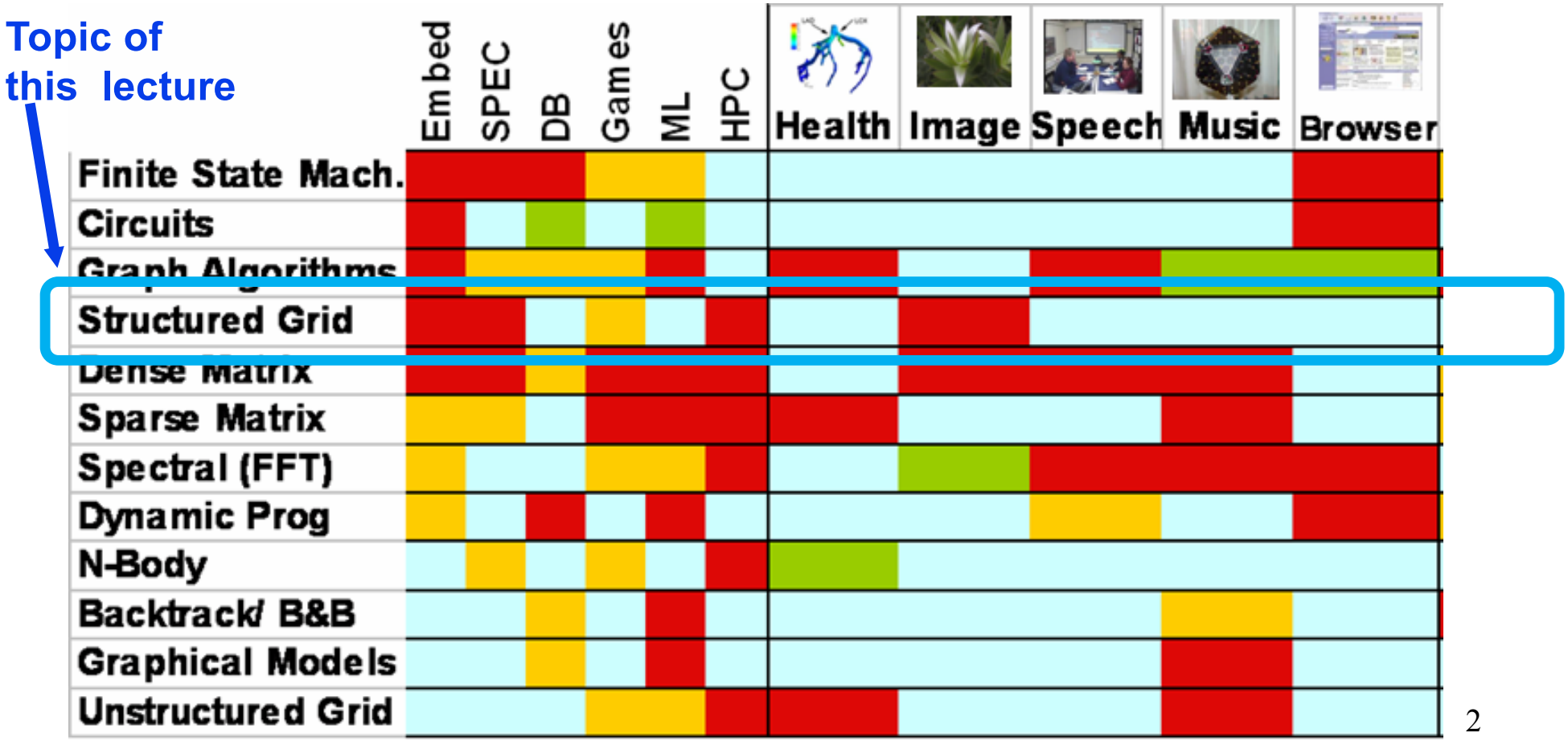
Motifs

The Motifs (formerly "Dwarfs") from
"The Berkeley View" (Asanovic et al.)
Motifs form key computational patterns



Outline

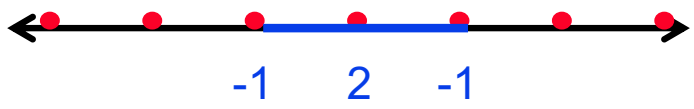
- Review of Poisson Equation
- Jacobi's method
- Red-Black SOR method
- Conjugate Gradient (topic of Lecture 15)
- Multigrid
- (Later lecture: FFTs)

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

Solve Tu = f for u where

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

Graph and "stencil"

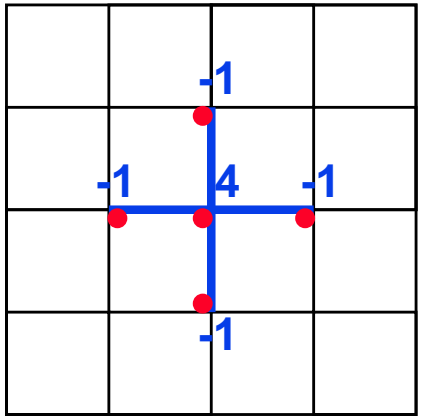


2D Poisson's equation

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

$$T = \begin{pmatrix} 4 & -1 & & -1 & & & & & \\ -1 & 4 & -1 & & -1 & & & & \\ & -1 & 4 & & & -1 & & & \\ -1 & & & 4 & -1 & & -1 & & \\ & -1 & & -1 & 4 & -1 & & -1 & \\ & & -1 & & -1 & 4 & & & -1 \\ & & & -1 & & & 4 & -1 & \\ & & & & -1 & & -1 & 4 & -1 \\ & & & & & -1 & & -1 & 4 \end{pmatrix}$$

Graph and "stencil"



- 3D is analogous

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

Algorithm	Serial	PRAM	Memory	#Procs
° Dense LU	N^3	N	N^2	N^2
° Band LU	N^2 ($N^{7/3}$)	N	$N^{3/2}$ ($N^{5/3}$)	N ($N^{4/3}$)
° Jacobi	N^2 ($N^{5/3}$)	N ($N^{2/3}$)	N	N
° Explicit Inv.	N^2	log N	N^2	N^2
° Conj.Gradients	$N^{3/2}$ ($N^{4/3}$)	$N^{1/2(1/3)}$ *log N	N	N
° Red/Black SOR	$N^{3/2}$ ($N^{4/3}$)	$N^{1/2}$ ($N^{1/3}$)	N	N
° Sparse LU	$N^{3/2}$ (N^2)	$N^{1/2}$	N*log N ($N^{4/3}$)	N
° FFT	N*log N	log N	N	N
° Multigrid	N	$\log^2$ N	N	N
° Lower bound	N	log N	N	

PRAM is an idealized parallel model with zero cost communication

Reference: James Demmel, Applied Numerical Linear Algebra, SIAM, 1997.

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Jacobi's Method

- To derive Jacobi's method, write Poisson as:

  u(i,j) = (u(i-1,j) + u(i+1,j) + u(i,j-1) + u(i,j+1) + b(i,j))/4

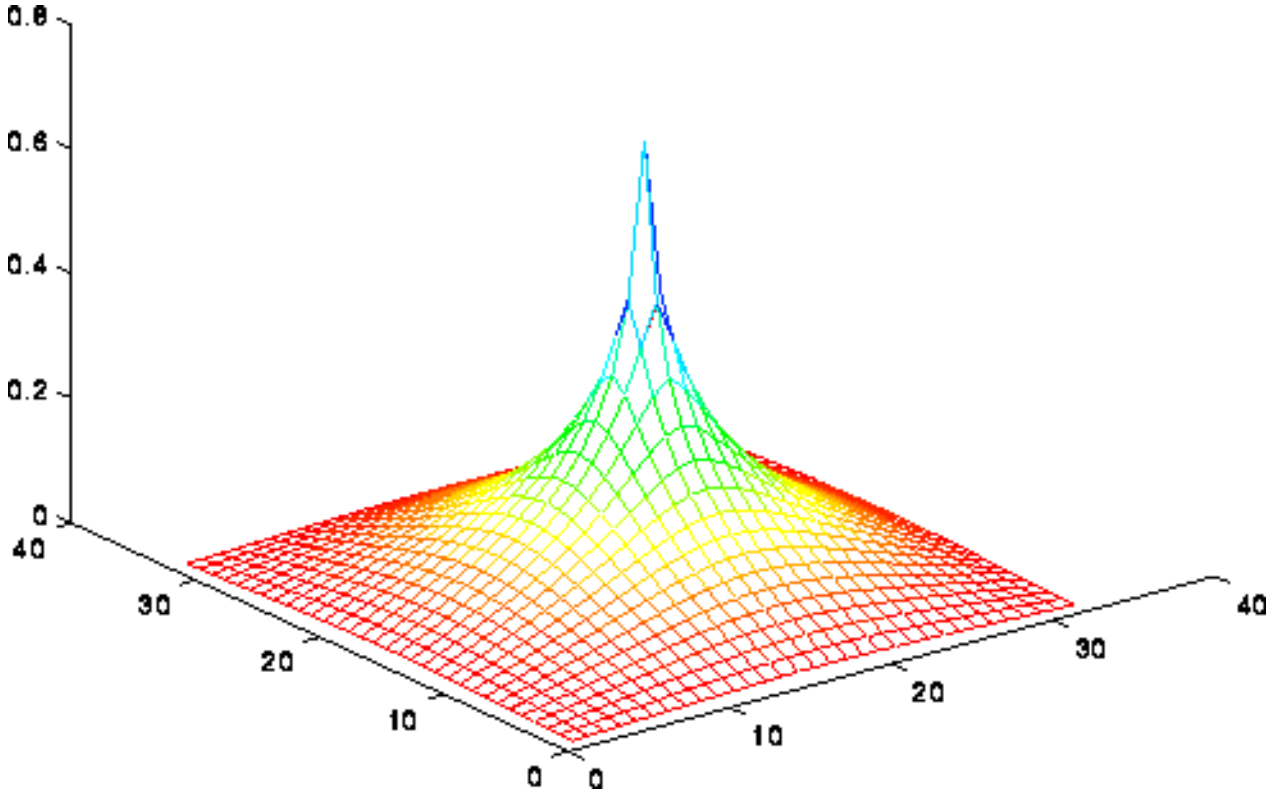
- Let u(i,j,m) be approximation for u(i,j) after m steps

  u(i,j,m+1) = (u(i-1,j,m) + u(i+1,j,m) + u(i,j-1,m) +
  u(i,j+1,m) + b(i,j)) / 4

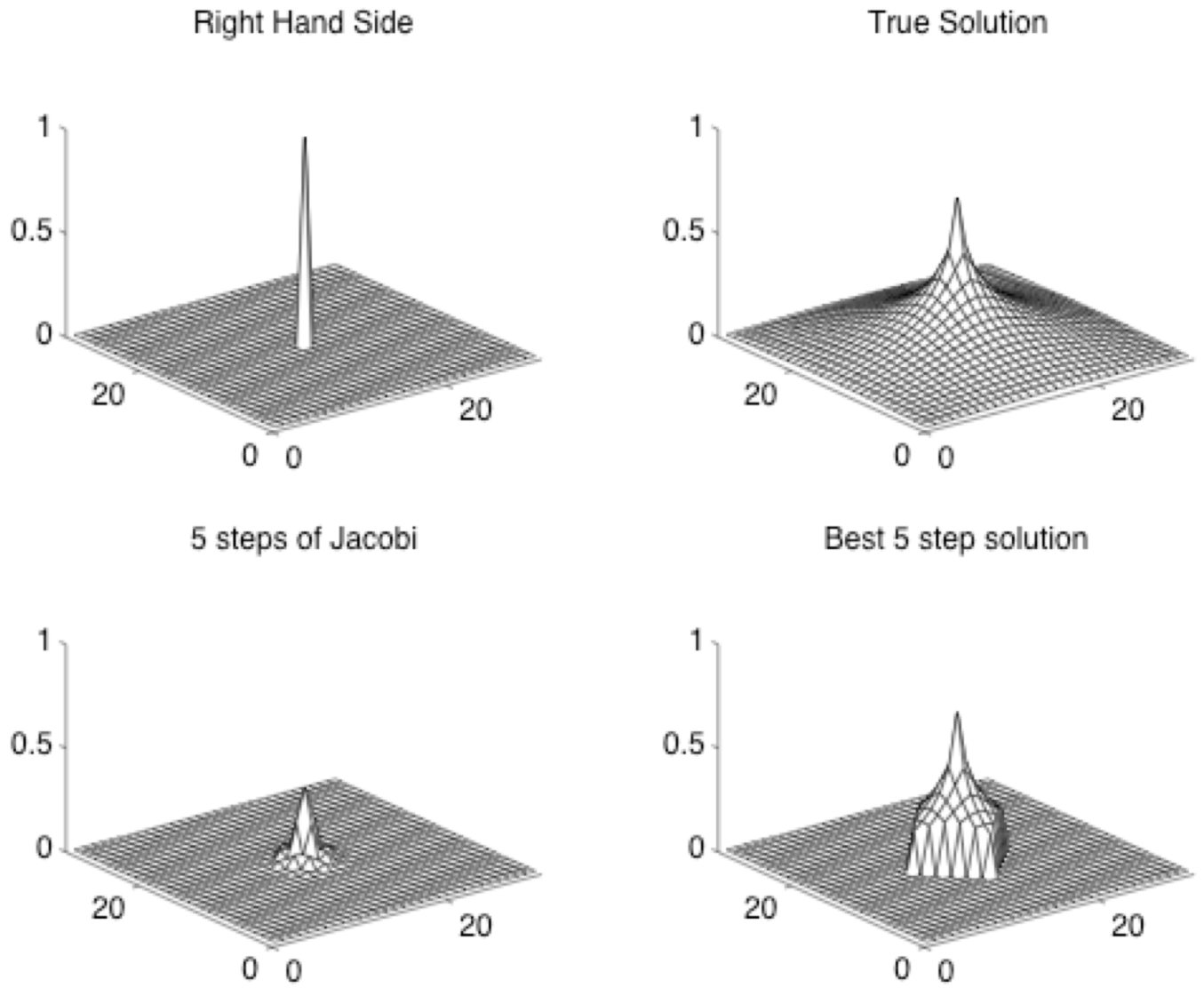
- I.e., u(i,j,m+1) is a weighted average of neighbors
- Motivation: u(i,j,m+1) chosen to exactly satisfy equation at (i,j)
- Steps to converge proportional to problem size, $N=n^2$
- Therefore, serial complexity is $O(N^2)$

Convergence of Nearest Neighbor Methods

- Jacobi's method involves nearest neighbor computation on nxn grid ($N = n^2$)
  - So it takes O(n) = O(sqrt(N)) iterations for information to propagate
- E.g., consider a rhs (b) that is 0, except the center is 1
- The exact solution looks like:



Convergence of Nearest Neighbor Methods



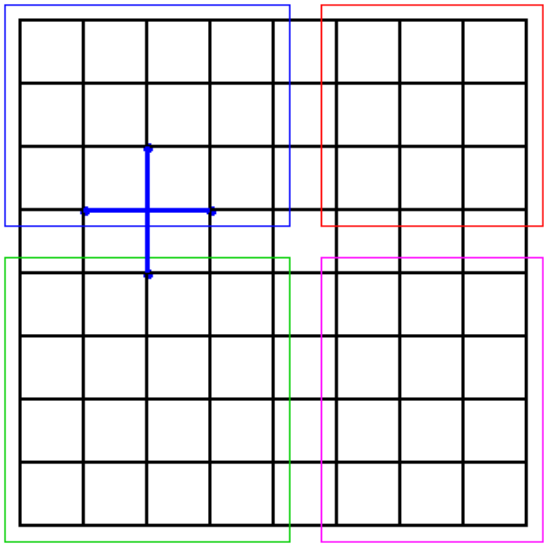
Takes O(n) steps to propagate information across an nxn grid

Parallelizing Jacobi's Method

- **Reduces to sparse-matrix-vector multiply by (nearly) T**

  U(m+1) = (T/4 - I) * U(m) + B/4

- **Each value of U(m+1) may be updated independently**
  - **keep 2 copies for iterations m and m+1**
- **Requires that boundary values be communicated**
  - **each processor owns n^2/p elements to update**
  - **amount of data communicated, $n/p^{1/2}$ per neighbor, relatively small if n>>p**



Want to take s>>1 iterations

All the communication-avoiding techniques for Matrix-powers kernel (i.e. repeated SpMVs) from Lecture 15 may be used

Reduce communication cost of s iterations to 1 iteration

References for Optimizing Stencils (1/2)

- Halide – Jonathan Ragan-Kelley et al
  - domain specific language for optimizing image processing pipelines, including stencil operations
- Bebop.cs.berkeley.edu
  - "Autotuning Stencil Codes for Cache-Based Multicore Platforms", K. Datta, UCB PhD thesis, 2009,
  - "Avoiding Communication in Computing Krylov Subspaces," J. Demmel, M. Hoemmen, M. Mohiyuddin, K. Yelick, 2007
  - "Optimization and Performance Modeling of Stencil Computations on Modern Microprocessors", K. Datta, S. Kamil, S. Williams, L. Oliker, J.Shalf, K. Yelick, SIAM Review, 2008
- SEJITS – sejits.org (Armando Fox et al @ UCB)

  "Bringing parallel performance to python with domain-specific selective embedded just-in-time specialization"
- Pochoir – stencil compiler (Charles Leiserson @ MIT)

  people.csail.mit.edu/yuantang/

References for Optimizing Stencils (2/2)

- Autotuning stencils and multigrid (Mary Hall @ Utah)
  super-scidac.org/
- Polyhedral tiling (Michelle Strout @ Colorado)
  www.cs.colostate.edu/~mstrout/Papers/pubs-poly.php
- Ian Foster et al, on grids (SC2001)
- "Efficient out-of-core algorithms for linear relaxation using blocking covers," C. Leiserson, S. Rao, S. Toledo, FOCS, 1993
- "Data flow and storage allocation for the PDQ-5 program on the Philco-2000," C. Pfeifer, CACM, 1963

Improvements to Jacobi

- Similar to Jacobi: u(i,j,m+1) will be computed as a linear combination of neighbors
  - Numeric coefficients and update order are different
- 2 improvements
  - Use "most recent values" of u that are available, since these are probably more accurate
  - Update value of u(m+1) "more aggressively" at each step
- First, note that while evaluating *sequentially*
  - u(i,j,m+1) = (u(i-1,j,m) + u(i+1,j,m) …

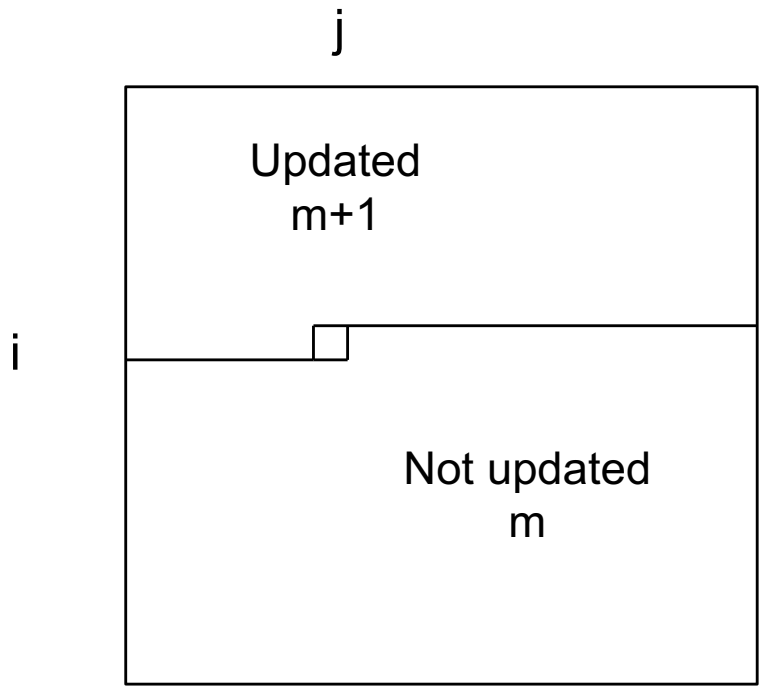
  some of the values for m+1 are already available
  - u(i,j,m+1) = (u(i-1,j,latest) + u(i+1,j,latest) …

  where latest is either m or m+1

Gauss-Seidel

- Updating left-to-right row-wise order, we get the Gauss-Seidel algorithm

```
for i = 1 to n
  for j = 1 to n
    u(i,j,m+1) = (u(i-1,j,m+1) + u(i+1,j,m) + u(i,j-1,m+1) + u(i,j+1,m)
                 + b(i,j)) / 4
```



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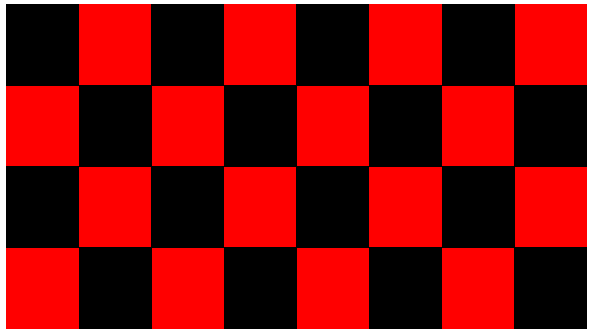
```

- Cannot be parallelized, because of dependencies, so instead we use a "red-black" order

```
forall black points u(i,j)
  u(i,j,m+1) = (u(i-1,j,m) + …  red neighbors
forall red points u(i,j)
  u(i,j,m+1) = (u(i-1,j,m+1) + … black neighbors
```



- For general graph, use "graph coloring"
  - Can use repeated Maximal Independent Sets to color
  - Graph(T) is bipartite => 2 colorable (red and black)
  - Nodes for each color can be updated simultaneously
  - Same optimizations, using submatrices

Successive Overrelaxation (SOR)

- Red-black Gauss-Seidel converges twice as fast as Jacobi, but there are twice as many parallel steps, so the same in practice
- To motivate next improvement, write basic step in algorithm as:

  u(i,j,m+1) = u(i,j,m) + correction(i,j,m)

- If "correction" is a good direction to move, then one should move even further in that direction by some factor w>1

  u(i,j,m+1) = u(i,j,m) + w * correction(i,j,m)

- Called successive overrelaxation (SOR)
- Parallelizes like Jacobi
- Can prove w = 2/(1+sin(π/(n+1))) for best convergence for Poisson
  - Number of steps to converge = parallel complexity = O(n), instead of O(n^2) for Jacobi
  - Serial complexity O(n^3) = O($N^{3/2}$), instead of O(n^4) = O(N^2) for Jacobi

Conjugate Gradient Algorithm for Solving Ax=b

- Initial guess x
- r = b – A*x, j=1
- Repeat
  - rho = r^T*r … dot product
  - If j=1, p = r, else beta = rho/old_rho, p = r + beta*p, endif … saxpy
  - q = A*p … sparse matrix vector multiply, or stencil
  - alpha = rho / p^T * q … dot product
  - x = x + alpha * p … saxpy
  - r = r – alpha * q … saxpy
  - old_rho = rho; j=j+1
- Until rho small enough

- Converges in O(n) = O($N^{1/2}$) steps, like SOR, but more general
- Can be reorganized to use matrix powers kernel [Ax,A^2x,…,A^kx]
  - "Communication Avoiding Krylov Subspace Methods," M. Hoemmen, UCB PhD Thesis, bebop.cs.berkeley.edu, 2010

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° **Lower bound**	**N**	**log N**	**N**	

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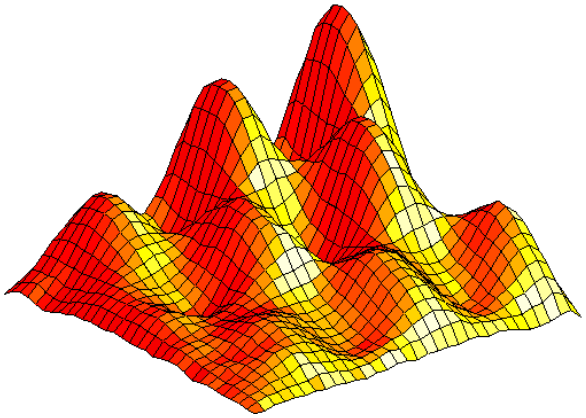
Multigrid Motivation

- Recall that Jacobi, SOR, CG, or any other sparse-matrix-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
- 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

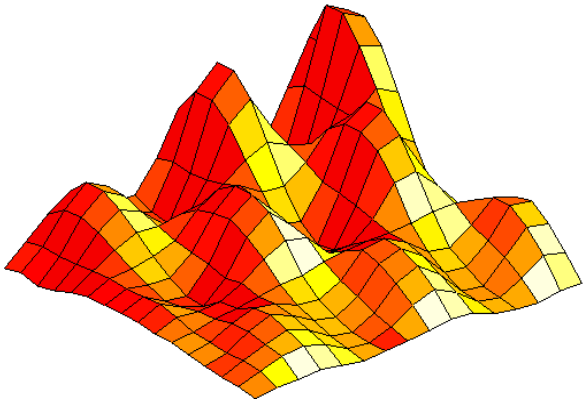
Big Idea used in multigrid and elsewhere

- 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: Graph Partitioning (used to parallelize SpMV)
  - Replace graph to be partitioned by a coarser graph
- 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

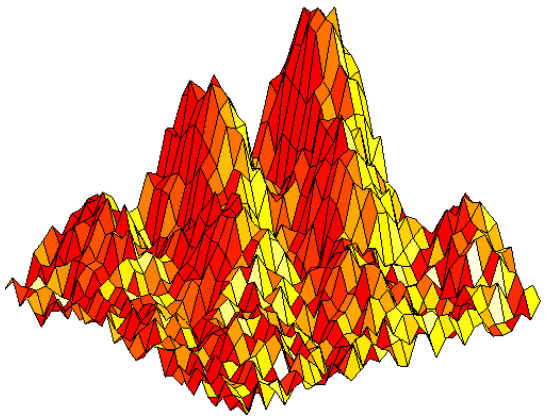
Fine and Coarse Approximations



Fine

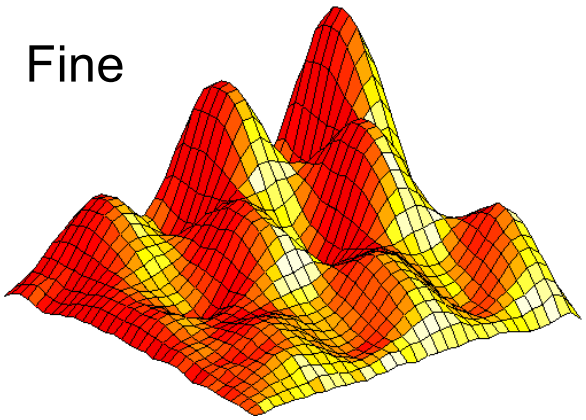


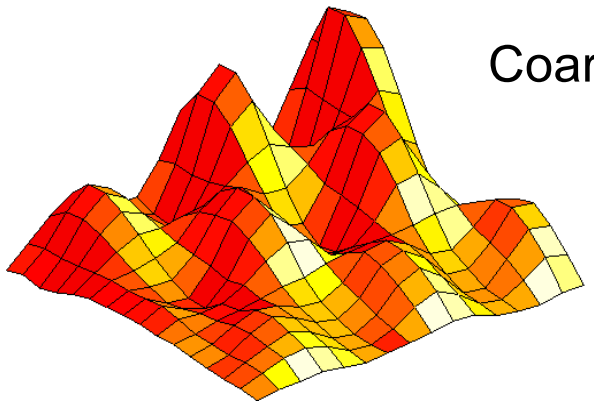
Coarse



Multigrid Overview

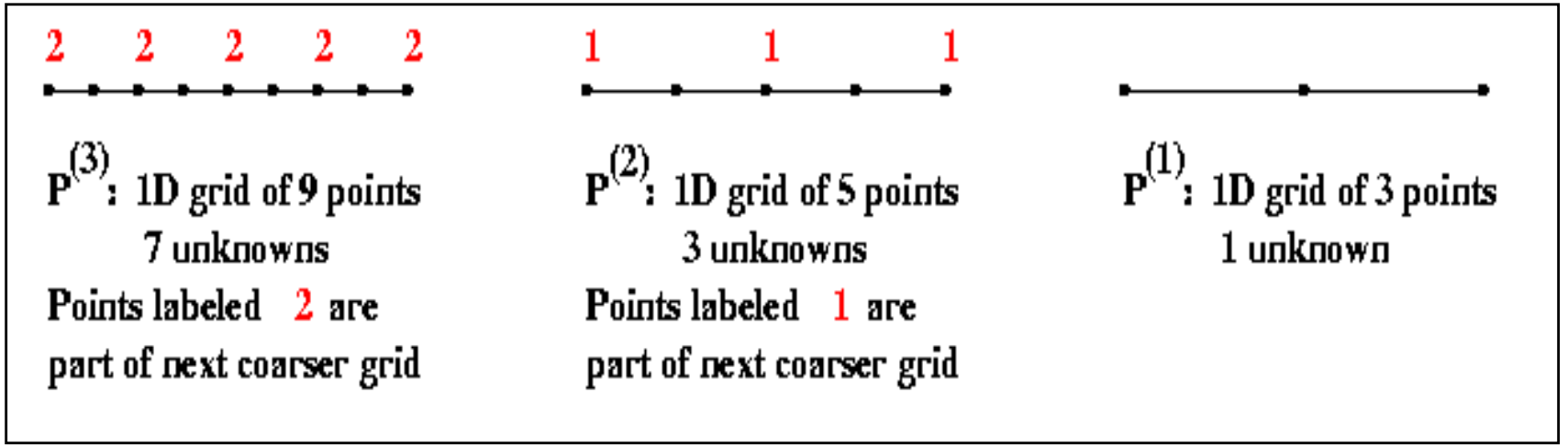
- **Basic Algorithm:**
  - **Replace problem on fine grid by an approximation on a coarser grid**
  - **Solve the coarse grid problem approximately, and use the solution as a starting guess for the fine-grid problem, which is then iteratively updated**
  - **Solve the coarse grid problem recursively,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





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 2^i+1 grid in 1D (2^i-1 unknowns plus 2 boundaries)
  - Write linear system as T(i) * x(i) = b(i)
- $P^{(m)}$, $P^{(m-1)}$, … , $P^{(1)}$ is sequence of problems from finest to coarsest



Multigrid Sketch in 2D

- Consider a 2^m+1 by 2^m+1 grid in 2D
- Let $P^{(i)}$ be the problem of solving the discrete Poisson equation on a 2^i+1 by 2^i+1 grid in 2D
  - Write linear system as T(i) * x(i) = b(i)
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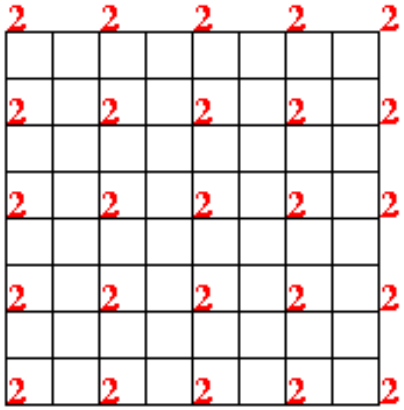
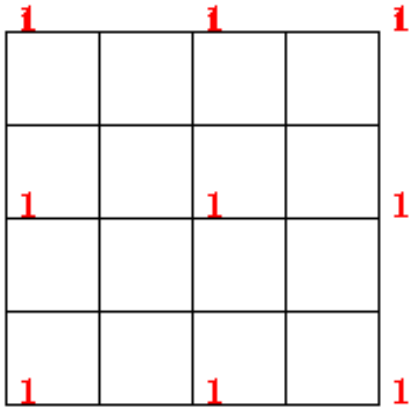
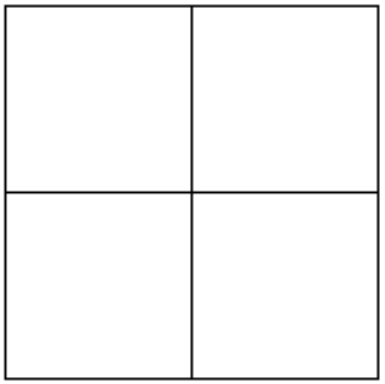


$P^{(3)}$: 9 by 9 grid of points
7 by 7 grid of unknowns
Points labeled 2 are
part of next coarser grid



$P^{(2)}$: 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

- For problem $P^{(i)}$ at varying coarsening levels (i, grid size grows with i):
  - b(i) is the Right Hand Side (RHS) and
  - x(i) is the current estimated solution

  } both live on grids of size 2^i-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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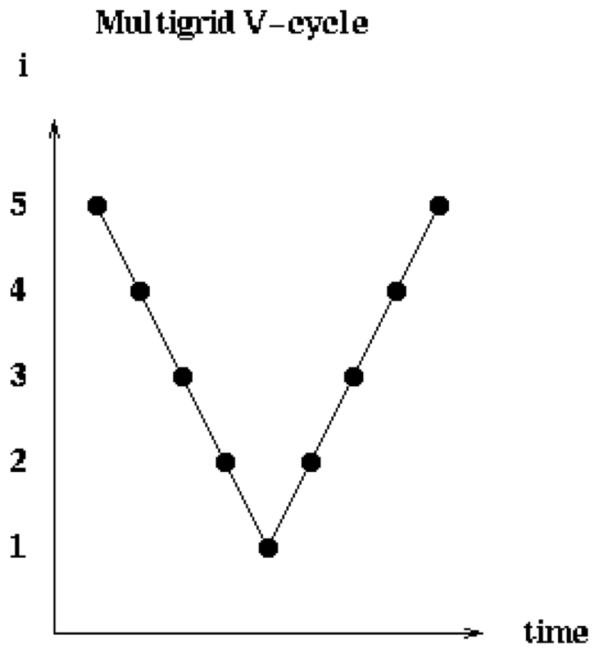
- All the following operators just average values on neighboring grid points (so information moves fast on coarse grids)
- The restriction operator R(i) maps $P^{(i)}$ to $P^{(i-1)}$
  - Restricts problem on fine grid $P^{(i)}$ to coarse grid $P^{(i-1)}$
  - Uses sampling or averaging
  - b(i-1)= R(i) (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

Multigrid V-Cycle Algorithm

```
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                                           solve recursively
      x(i) = S(i) (b(i), x(i))                   improve solution by damping
                                                      high frequency error
      r(i)  = T(i)*x(i) - b(i)                   compute residual
      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)
```

This is called a V-Cycle

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



Complexity of a V-Cycle

- On a serial machine
  - Work at each point in a V-cycle is O(the number of unknowns)
  - Cost of Level i is $(2^i-1)^2 = O(4^i)$ for a 2D grid
  - If finest grid level is m, total time is:

$$\sum_{i=1}^{m} O(4^i) = O(4^m) \quad \text{for a 2D grid}$$

$$= O(\#\text{ unknowns}) \text{ in general}$$

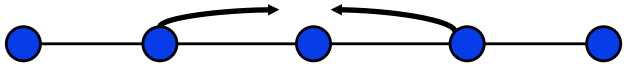
- On an ideal parallel machine (PRAM)
  - with one processor per grid point and free communication, each step in the V-cycle takes constant time
  - Total V-cycle time is O(m) = O(log #unknowns)

Complexity of Solving Poisson's Equation

- **Theorem: error after one call to multigrid**
  - **error_after ≤ .5 * error_before**
  - **independent of # unknowns**
  - **➔At least 1 bit each time**
- **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**

The Solution Operator S(i) - Details

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



- At level i, pure Jacobi replaces:

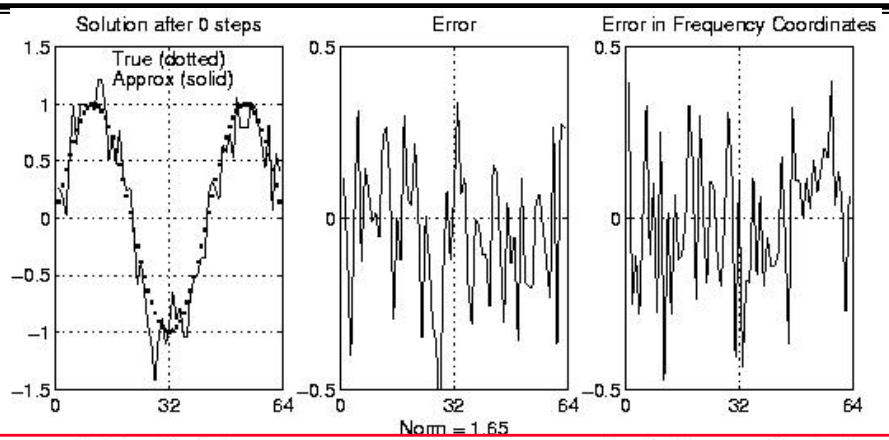
  x(j) := 1/2 (x(j-1) + x(j+1) + b(j))

- Weighted Jacobi uses:

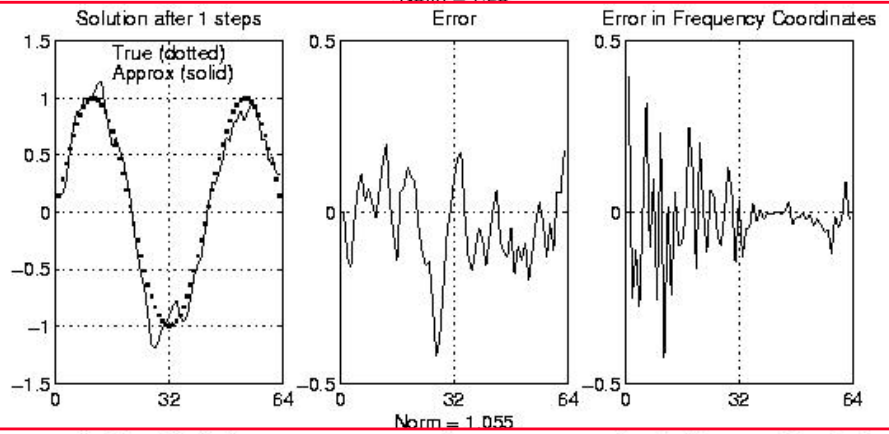
  x(j) := 1/3 (x(j-1) + x(j) + x(j+1) + b(j))

- In 2D, similar average of nearest neighbors

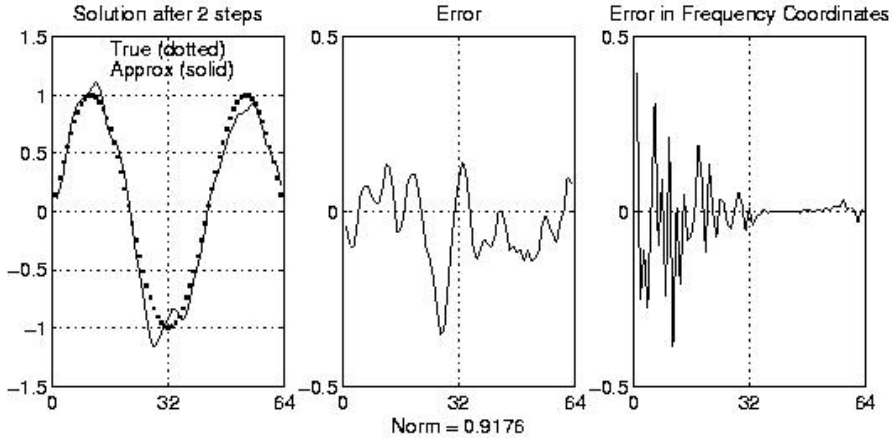
Weighted Jacobi chosen to damp high frequency error



Initial error
- **"Rough"**
- **Lots of high frequency components**
- **Norm = 1.65**



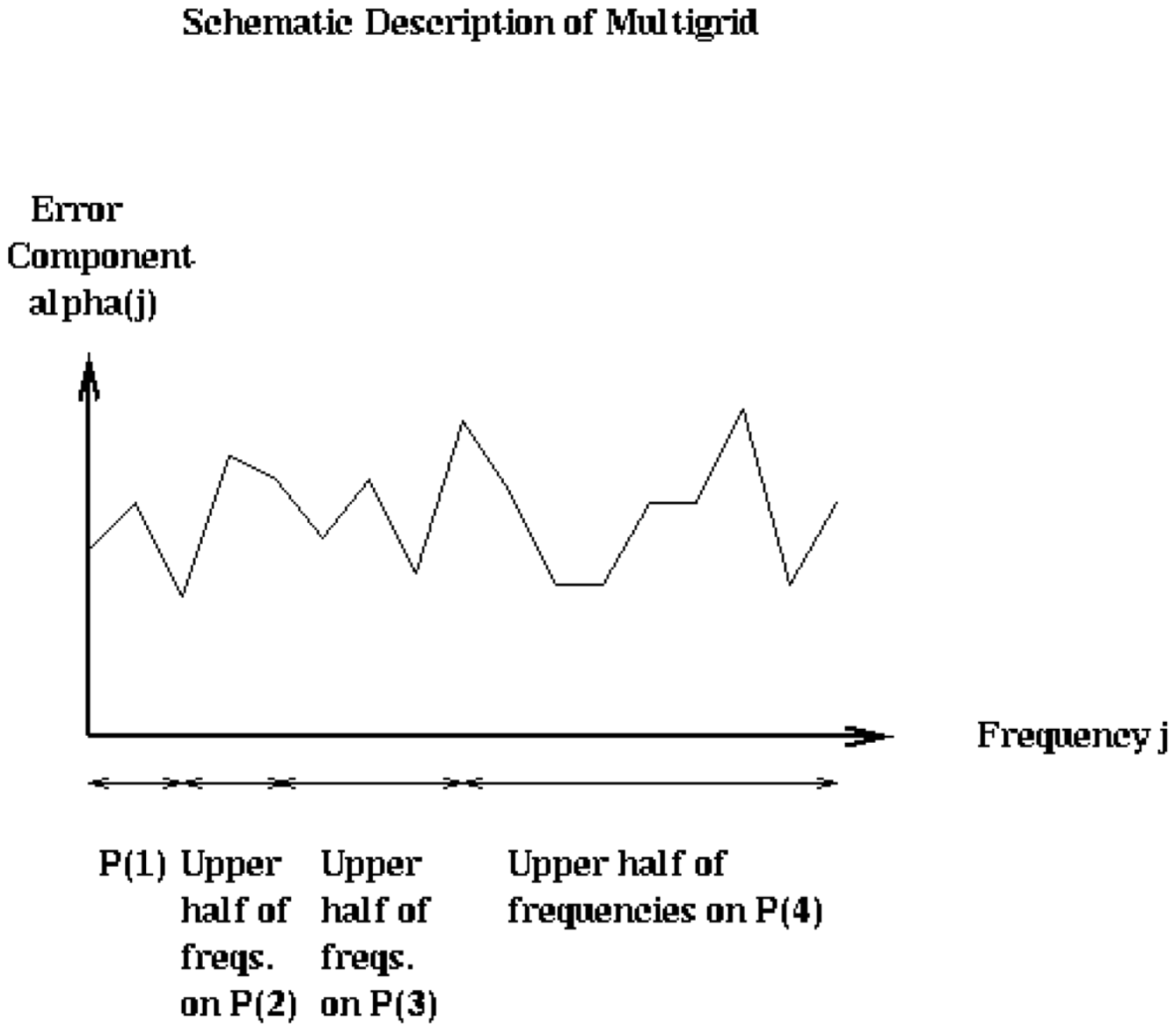
Error after 1 weighted Jacobi step
- **"Smoother"**
- **Less high frequency component**
- **Norm = 1.06**



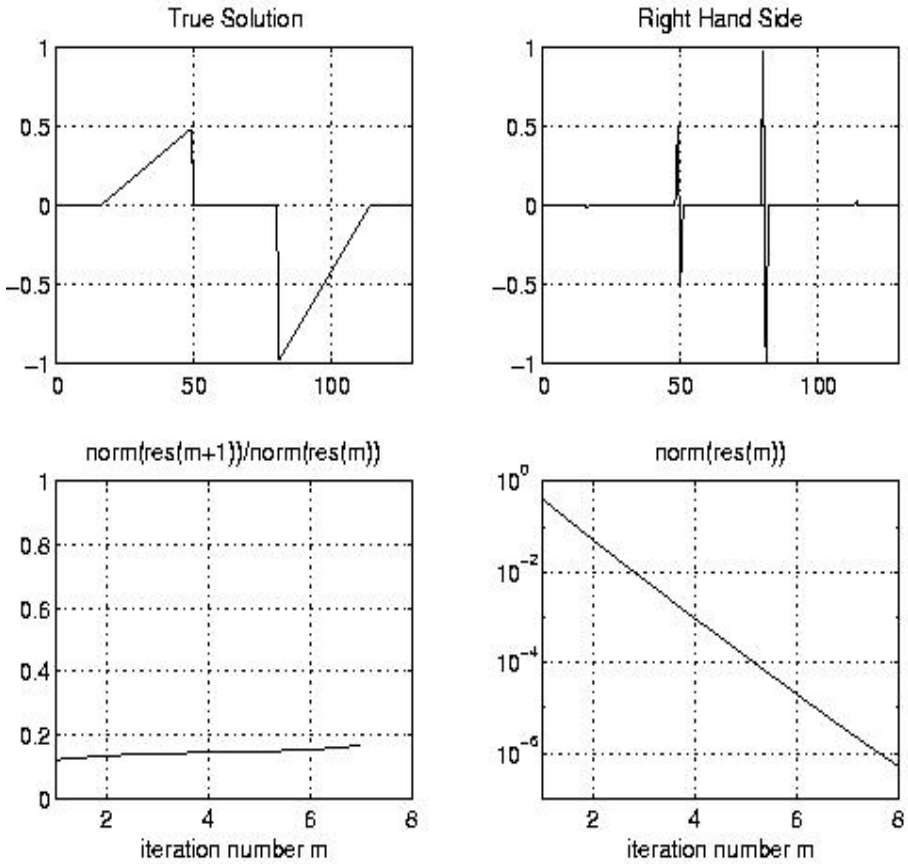
Error after 2 weighted Jacobi steps
- **"Smooth"**
- **Little high frequency component**
- **Norm = .92,**
- **won't decrease much more**

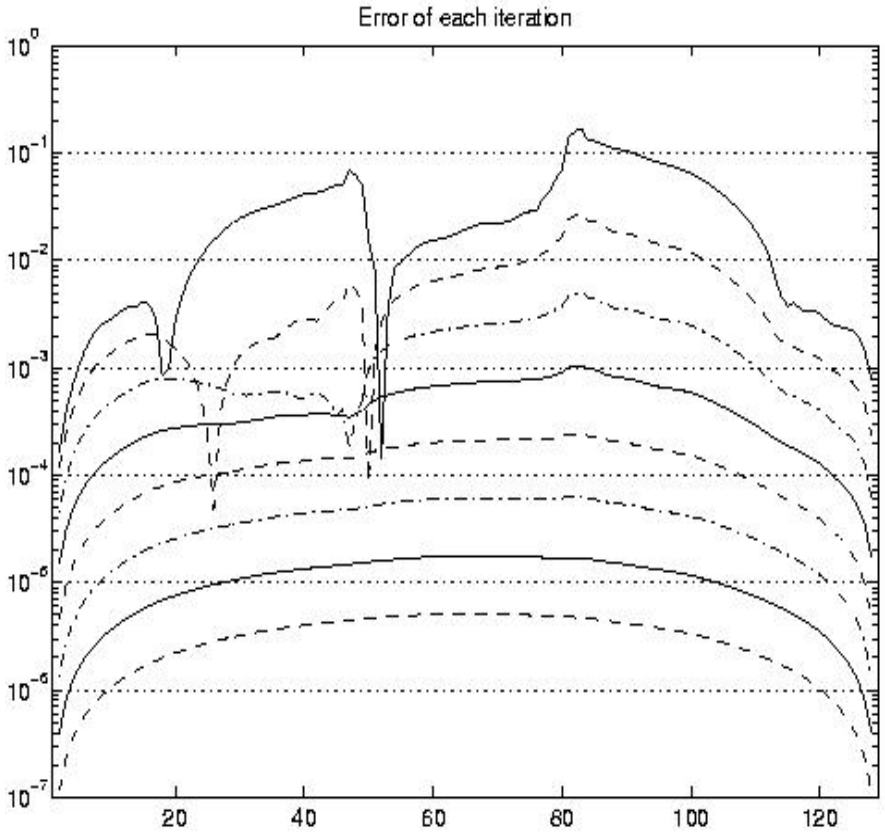
Multigrid as Divide and Conquer Algorithm

° Each level in a V-Cycle reduces the error in one part of the frequency domain

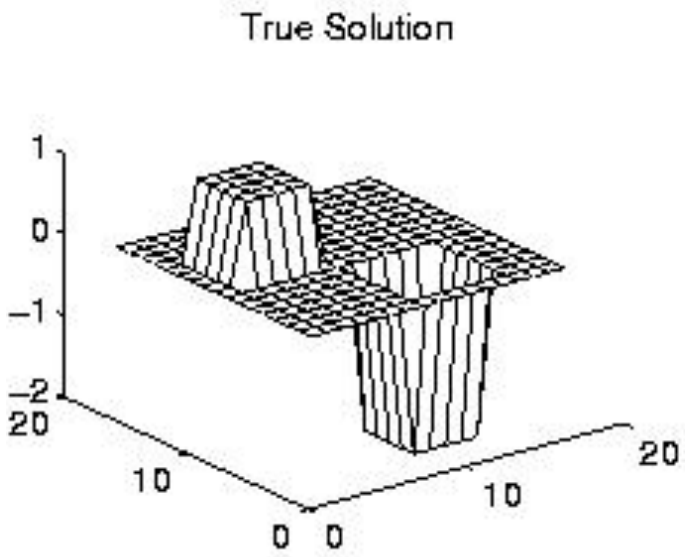


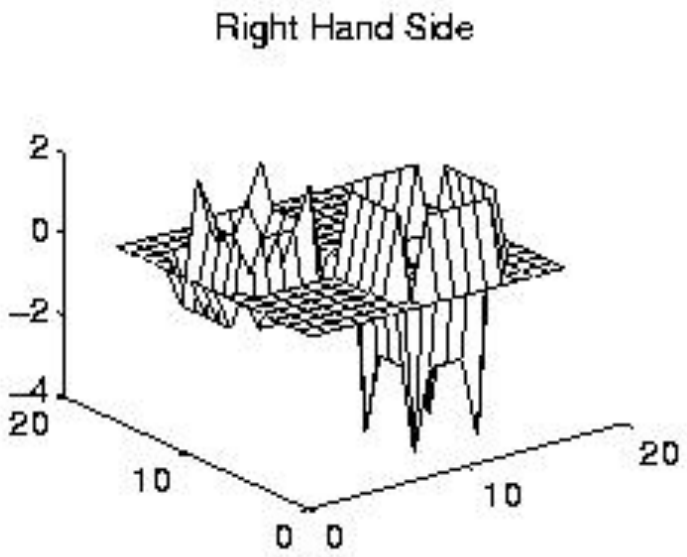
Convergence Picture of Multigrid in 1D

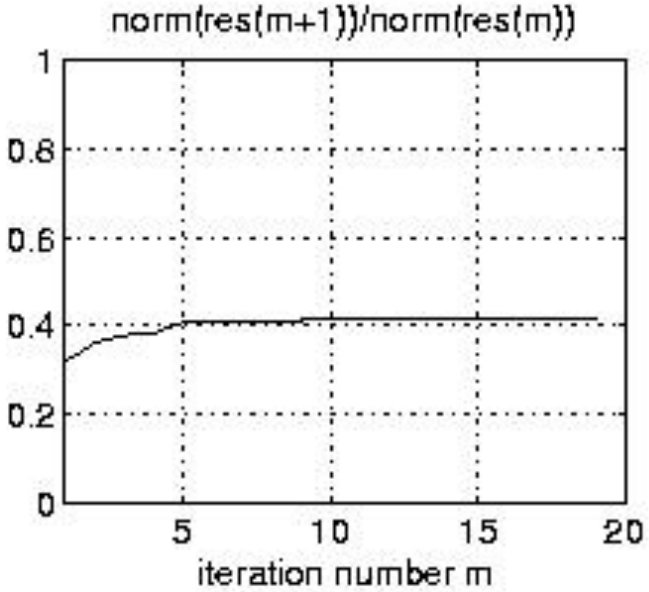


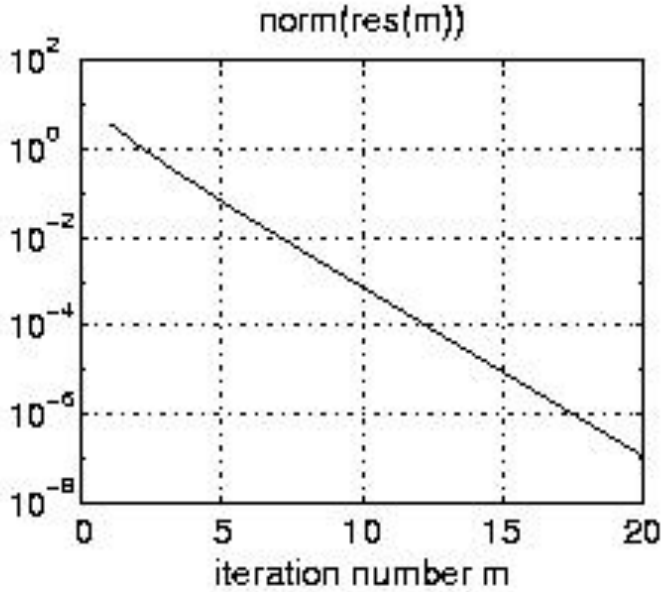


Convergence Picture of Multigrid in 2D



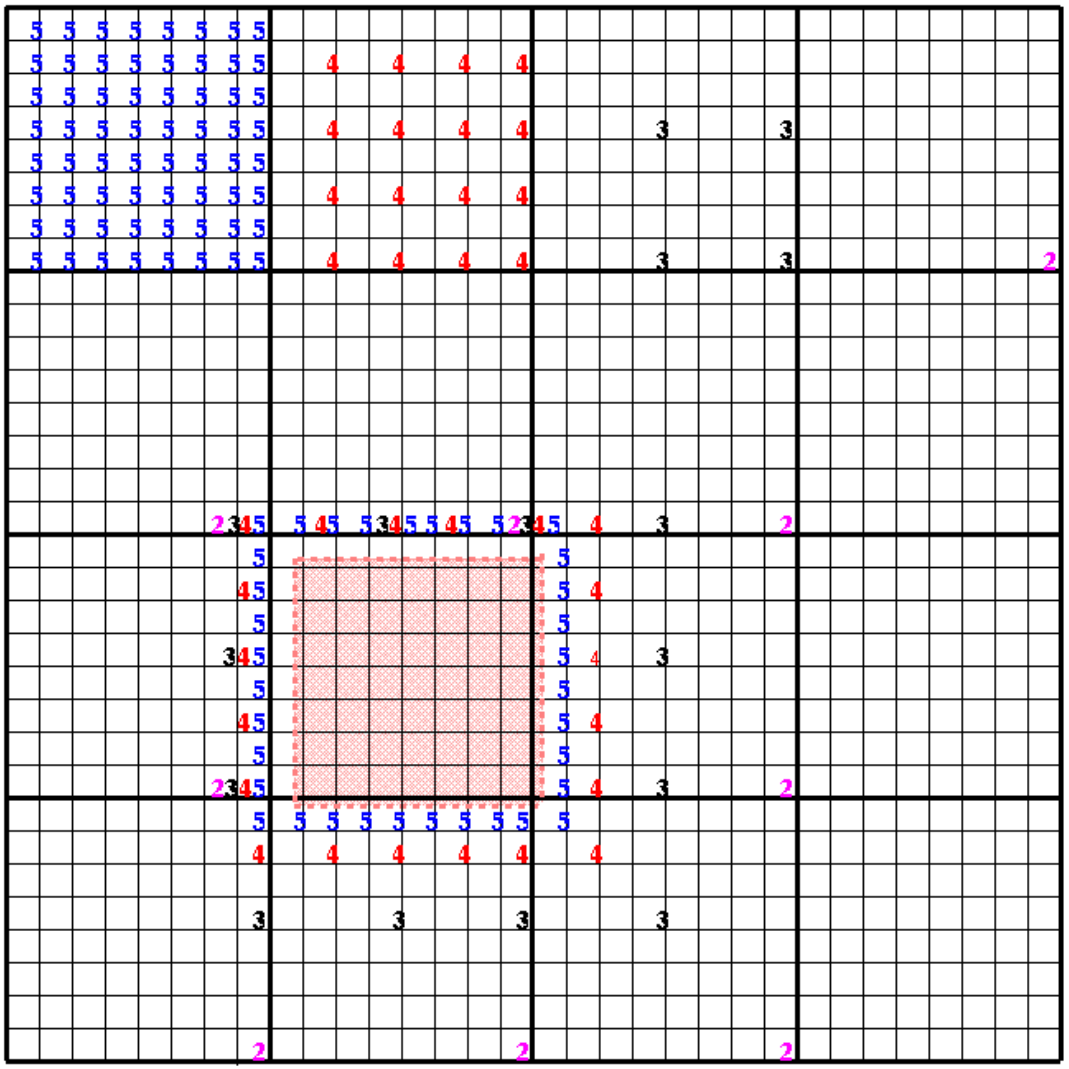






Parallel 2D Multigrid

- 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

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

- Assume 2^m+1 by 2^m+1 grid of points, $n= 2^m-1$, $N=n^2$
- 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

    $+ O(1)\ \alpha$ .... Send a constant # messages to neighbors

    $+ O(2^{j-k})\ \beta$ .... Number of words sent
  - If level j < k, then cost =

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

    $+ O(1)\ \alpha$ .... Send a constant # messages to neighbors

    $+ O(1)\ \beta$ .... Number of words sent
- Sum over all levels in all V-cycles to get complexity

Comparison of Methods (in O(.) sense)

	# Flops	# Messages	# Words sent
MG	N/p + log p * log N	$(\log N)^2$	$(N/p)^{1/2}$ + 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 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 $\alpha >> \beta$

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, so flops = O(1000)
  - In 2D, the surface to communicate is 4 x $1000^{1/2}$ ~= 128, or 13%
  - In 3D, the surface is 1000-8^3 ~= 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 V-cycle) and .42 (FMG)
    - although worse parallel efficiency, FMG is 2.6 times faster than V-cycles alone
  - nCUBE had fast communication, slow processors
- Today: Same problem in Chombo @ LBL
  - Communication of coarsest meshes

Multigrid on an Unstructured Mesh

- Need to partition graph for parallelism
- 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
  - Use "maximal independent sets" again
  - How to make coarse graph approximate fine one
- Need to define R() and In()
  - How do we convert from coarse to fine mesh and back?
- Need to define S()
  - How do we define coarse matrix (no longer formula, like Poisson)
- Dealing with coarse meshes efficiently
  - Should we switch to using fewer processors on coarse meshes?
  - Should we switch to another solver on coarse meshes?

Irregular mesh: Tapered Tube (multigrid)

Example of Prometheus meshes

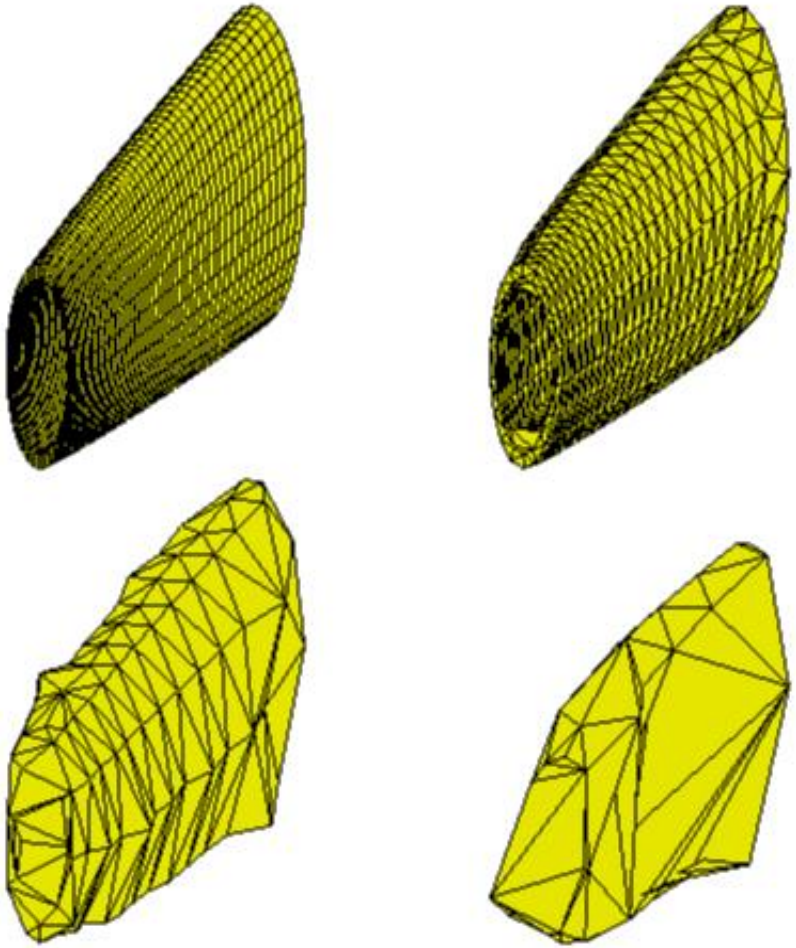


Figure 6: Sample input grid and coarse grids

Source of Unstructured Finite Element Mesh: Vertebra

Study failure modes of trabecular bone under stress

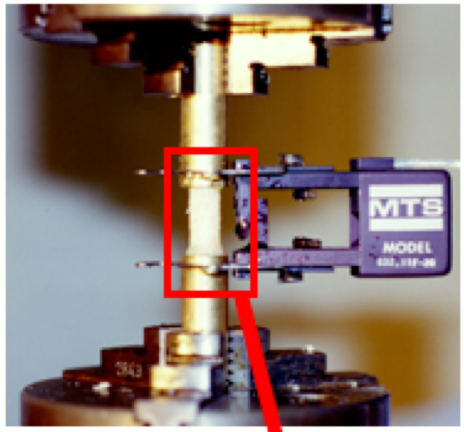
Source: M. Adams, H. Bayraktar, T. Keaveny, P. Papadopoulos, A. Gupta

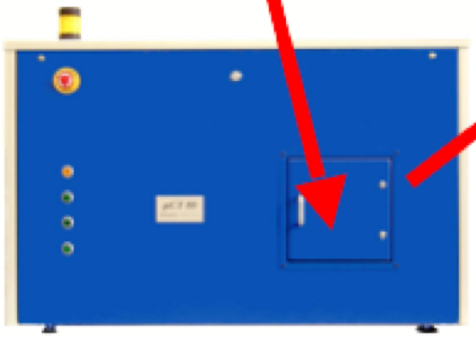
Multigrid for nonlinear elastic analysis of bone

Gordon Bell Prize, 2004

Source: M. Adams et al

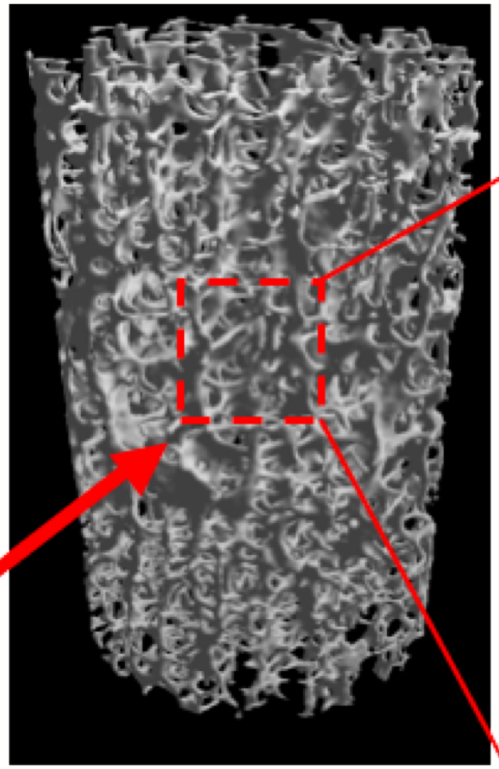
Mechanical testing for material properties



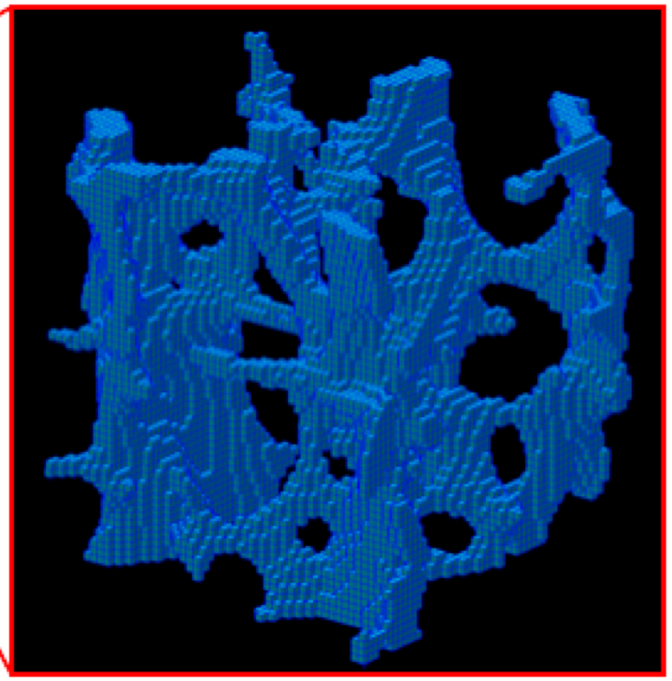


Micro Computed Tomography @ 22 μm resolution

3D image



μFE mesh
2.5 mm^3
44 μm elements



Up to
537M unknowns
4088 Processors (ASCI White)
70% parallel efficiency