

CS 267: Applications of Parallel Computers

Lecture 17 - Structured Grids

James Demmel

www.cs.berkeley.edu/~demmel/cs267_Spr15

Motifs

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

Topic of this lecture

	Embed	SPEC	DB	Games	ML	HPC	Health	Image	Speech	Music	Browser
Finite State Mach.											
Circuits											
Graph Algorithms											
Structured Grid											
Dense matrix											
Sparse Matrix											
Spectral (FFT)											
Dynamic Prog											
N-Body											
Backtrack/ B&B											
Graphical Models											
Unstructured Grid											

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Outline

- Review of Poisson Equation
- Jacobi's method
- Red-Black SOR method
- Conjugate Gradient (topic of Lecture 16)
- Multigrid
- (Later lecture: FFTs)

Solving PDEs

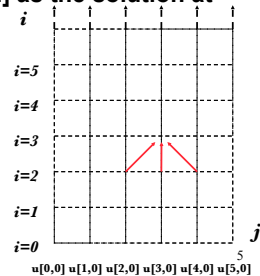
- Hyperbolic problems (waves):
 - Sound wave(position, time)
 - Use explicit time-stepping
 - Solution at each point depends on neighbors at previous time
- Elliptic (steady state) problems:
 - Electrostatic Potential (position)
 - Everything depends on everything else
 - This means locality is harder to find than in hyperbolic problems
- Parabolic (time-dependent) problems:
 - Temperature(position,time)
 - Involves an elliptic solve at each time-step
- Focus on elliptic problems
 - Canonical example is the Poisson equation

$$\partial^2 u / \partial x^2 + \partial^2 u / \partial y^2 + \partial^2 u / \partial z^2 = f(x,y,z)$$

Explicit Solution of PDEs

- Often used for hyperbolic PDEs
- Stability limits size of time-step
- Computation corresponds to
 - Matrix vector multiply
 - Combine nearest neighbors on grid
- Use finite differences with $u[j,i]$ as the solution at
 - time $t = i \cdot \delta$ ($i = 0, 1, 2, \dots$) and
 - position $x = j \cdot h$ ($j = 0, 1, \dots, N = 1/h$)
 - initial conditions on $u[j, 0]$
 - boundary conditions on $u[0, i]$ and $u[N, i]$

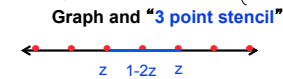
- At each timestep $i = 0, 1, 2, \dots$
 - For $j=1$ to $N-1$
 - $u[j, i+1] = z \cdot u[j-1, i] + (1-2z) \cdot u[j, i] + z \cdot u[j+1, i]$
- where $z = C \cdot \delta / h^2$



Matrix View of Explicit Method for Heat Equation

- $u[j, i+1] = z \cdot u[j-1, i] + (1-2z) \cdot u[j, i] + z \cdot u[j+1, i]$
- $u[:, i+1] = T \cdot u[:, i]$ where T is tridiagonal:

$$T = \begin{pmatrix} 1-2z & z & & & \\ z & 1-2z & z & & \\ & z & 1-2z & z & \\ & & z & 1-2z & z \\ & & & z & 1-2z \end{pmatrix} = I - z \cdot L, \quad L = \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix}$$



- L called Laplacian (in 1D)
- For a 2D mesh (5 point stencil) the Laplacian has 5 diagonals
- For a 3D mesh there are 7 diagonals

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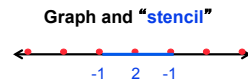
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Poisson's equation in 1D: $\partial^2 u / \partial x^2 = f(x)$

Solve $Tu = f$ for u where

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



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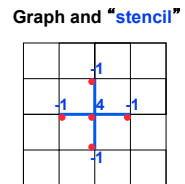
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2D Poisson's equation

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

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



- 3D is analogous

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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 $O(N^2)$

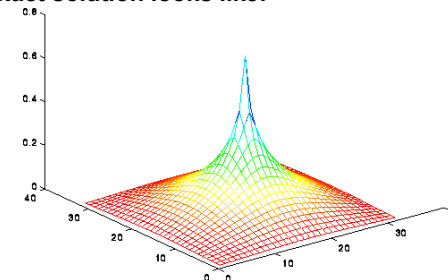
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Convergence of Nearest Neighbor Methods

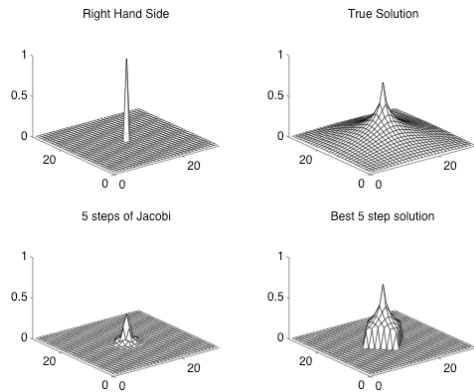
- Jacobi's method involves nearest neighbor computation on $n \times n$ grid ($N = n^2$)
 - So it takes $O(n) = O(\sqrt{N})$ iterations for information to propagate
- E.g., consider a rhs (b) that is 0, except the center is 1
- The exact solution looks like:



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Convergence of Nearest Neighbor Methods

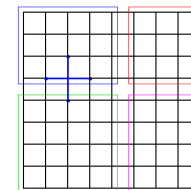


Takes $O(n)$ steps to propagate information across an $n \times n$ grid 13

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
 - if each processor owns n^2/p elements to update
 - amount of data communicated, $n/p^{1/2}$ per neighbor, relatively small if $n \gg p$



Want to take $s \gg 1$ iterations

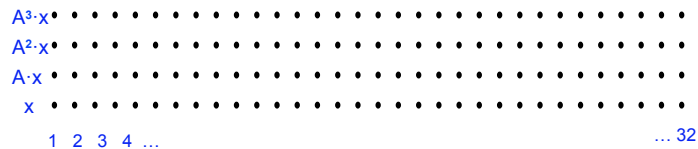
All the communication-avoiding techniques for Matrix-powers kernel (i.e. repeated SpMV's) from Lecture 16 may be used

Reduce communication cost of s iterations to 1 iteration 14

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Communication Avoiding Jacobi:

- Replace k iterations of $y = A \cdot x$ with $[Ax, A^2x, \dots, A^kx]$

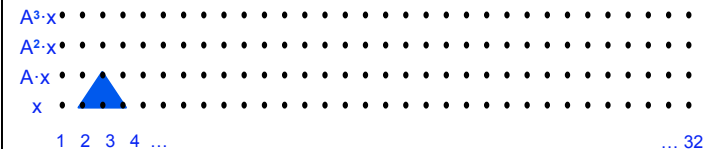


- Example: A tridiagonal, $n=32$, $k=3$
- Like Matrix-Powers Kernel, but simpler:
 - Don't need to store A explicitly (it's Jacobi)
 - Only need to save A^kx

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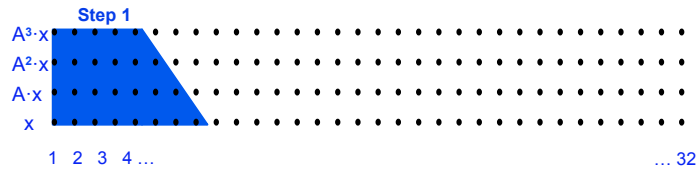


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Communication Avoiding Jacobi:

- Replace k iterations of $y = A \cdot x$ with $[Ax, A^2x, \dots, A^kx]$
- Sequential Algorithm

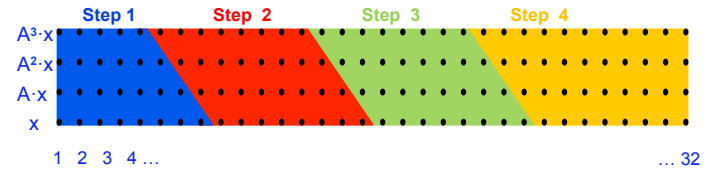


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Communication Avoiding Jacobi:

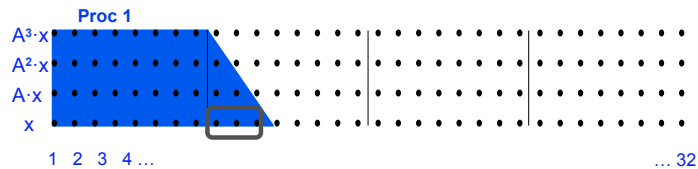
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- Example: A tridiagonal, $n=32$, $k=3$
- Like Matrix-Powers Kernel, but simpler:
 - Don't need to store A explicitly (it's Jacobi)
 - Only need to save A^kx – move $O(n)$ words instead of $\Theta(kn)$

Communication Avoiding Jacobi:

- Replace k iterations of $y = A \cdot x$ with $[Ax, A^2x, \dots, A^kx]$
- Parallel Algorithm

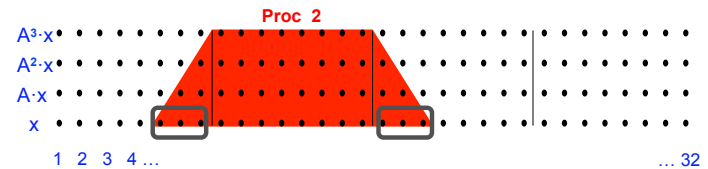


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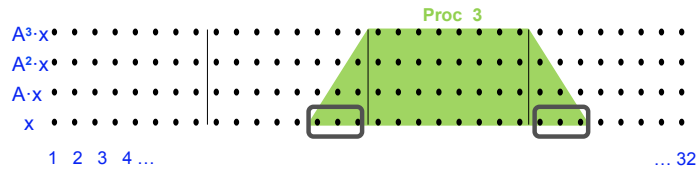


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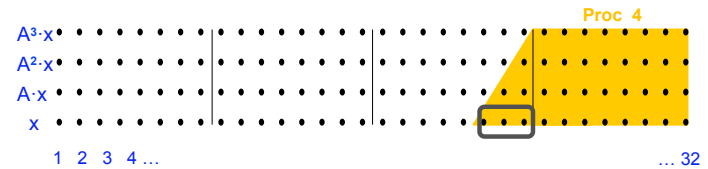


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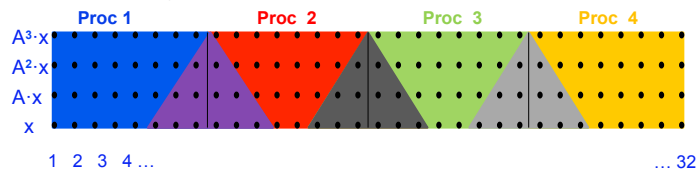


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Communication Avoiding Jacobi:

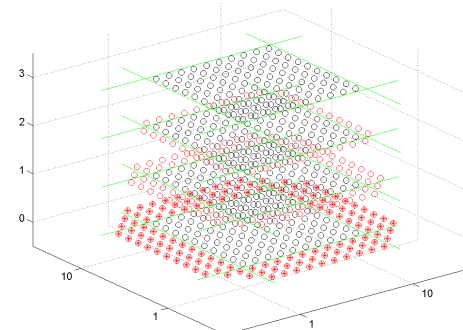
- Replace k iterations of $y = A \cdot x$ with $[Ax, A^2x, \dots, A^kx]$
- Parallel Algorithm



- Example: A tridiagonal, $n=32$, $k=3$
- Entries in overlapping regions (triangles) computed redundantly
- Send $O(1)$ messages instead of $O(k)$

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Remotely Dependent Entries for $[x, Ax, A^2x, A^3x]$, 2D Laplacian



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References for Optimizing Stencils (1/2)

- **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/
- **Autotuning stencils and multigrid (Mary Hall @ Utah)**
super-scidac.org/
- **Polyhedral tiling (Michelle Strout @ Colorado)**
www.cs.colostate.edu/~mstrout/Papers/pubs-poly.php

References for Optimizing Stencils (2/2)

- 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***
 - $u(i,j,m+1) = (u(i-1,j,m) + u(i+1,j,m) \dots$

some of the values for $m+1$ are already available

 - $u(i,j,m+1) = (u(i-1,j,latest) + u(i+1,j,latest) \dots$

where latest is either m or $m+1$

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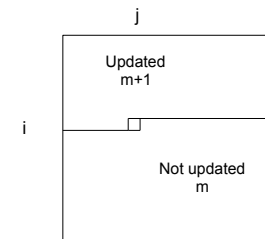
Gauss-Seidel

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

```

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

```



- **Cannot be parallelized, because of dependencies** 28

Gauss-Seidel

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

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for i = 1 to n
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                + b(i,j)) / 4

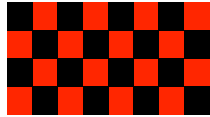
```

- 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
              + u(i,j,m)) / 4
forall red points u(i,j)
  u(i,j,m+1) = (u(i-1,j,m+1) + ... black neighbors
              + u(i,j,m)) / 4

```



- 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

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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:

$$u(i,j,m+1) = u(i,j,m) + \text{correction}(i,j,m)$$
- If "correction" is a good direction to move, then one should move even further in that direction by some factor $w > 1$

$$u(i,j,m+1) = u(i,j,m) + w * \text{correction}(i,j,m)$$
- Called **successive overrelaxation (SOR)**
- Parallelizes like Jacobi
- Can prove $w = 2/(1 + \sin(\pi/(n+1)))$ 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

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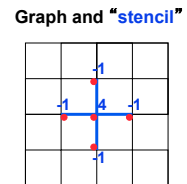
Conjugate Gradient Algorithm for Solving $Ax=b$

- Initial guess x
- $r = b - A*x, j=1$
- Repeat
 - $\rho = r^T r$... dot product
 - If $j=1, p = r$, else $\beta = \rho / \text{old_rho}, p = r + \beta * p$, 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
 - $\text{old_rho} = \rho; j=j+1$
- Until ρ small enough
 - Converges in $O(n) = O(N^{1/2})$ steps, like SOR, but more general
 - Can be reorganized to use matrix powers kernel $[Ax, A^2x, \dots, A^kx]$
 - "Communication Avoiding Krylov Subspace Methods,"
 - M. Hoemmen, UCB PhD Thesis, bebop.cs.berkeley.edu, 2010

2D Poisson's equation

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

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



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Multigrid Motivation

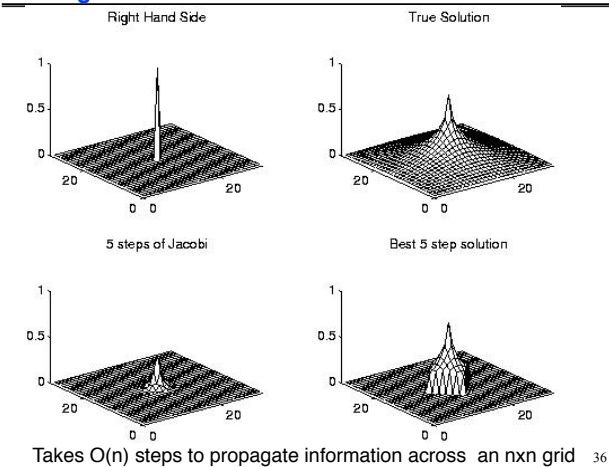
- Recall that Jacobi, SOR, CG, or any other sparse-matrix-vector-multiply-based algorithm can only move information one grid cell at a time
 - Take at least n steps to move information across $n \times n$ grid
- Therefore, converging in $O(1)$ steps requires moving information across grid faster than to one neighboring grid cell per step
 - One step can't just do sparse-matrix-vector-multiply

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Multigrid Motivation



Big Idea used in multigrid and elsewhere

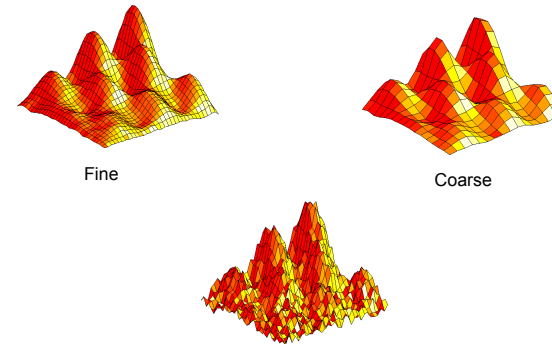
- If you are far away, problem looks simpler
 - For gravity: approximate earth, distant galaxies, ... by point masses
- Can solve such a coarse approximation to get an approximate solution, iterating if necessary
 - Solve coarse approximation problem by using an even coarser approximation of it, and so on recursively
- Ex: Graph Partitioning (used to parallelize SpMV)
 - Replace graph to be partitioned by a coarser graph
- 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

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Fine and Coarse Approximations



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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



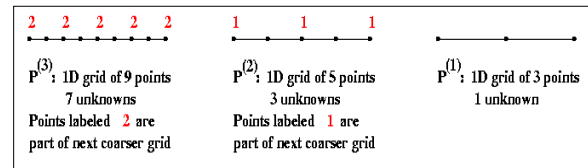
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Multigrid Sketch in 1D

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



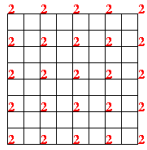
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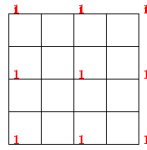
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Multigrid Sketch in 2D

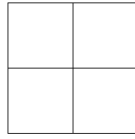
- Consider a 2^{m+1} by 2^{m+1} grid in 2D
- Let $P^{(i)}$ be the problem of solving the discrete Poisson equation on a 2^{i+1} by 2^{i+1} grid in 2D
 - Write linear system as $T^{(i)} * x^{(i)} = b^{(i)}$
- $P^{(m)}, P^{(m-1)}, \dots, P^{(1)}$ is sequence of problems from finest to coarsest



$P^{(3)}$: 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

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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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Multigrid Operators

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Multigrid Operators

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Multigrid Operators

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 } 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 $ln^{(i-1)}$ maps approx. solution $x^{(i-1)}$ to $x^{(i)}$
 - Interpolates solution on coarse grid $P^{(i-1)}$ to fine grid $P^{(i)}$
 - $x^{(i)} = ln^{(i-1)}(x^{(i-1)})$
- The **solution operator $S^{(i)}$** takes $P^{(i)}$ and improves solution $x^{(i)}$
 - Uses "weighted" Jacobi or SOR on single level of grid
 - $x^{(i)}_{improved} = S^{(i)}(b^{(i)}, x^{(i)})$
- Overall algorithm, then details of operators

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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
     $x^{(i)} = S^{(i)}(b^{(i)}, x^{(i)})$                 solve recursively
                                                improve solution by damping
                                                high frequency error
     $r^{(i)} = T^{(i)}x^{(i)} - b^{(i)}$                 compute residual
     $d^{(i)} = ln^{(i-1)}(MGV(R^{(i)}(r^{(i)}), 0))$     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  $x^{(i)}$ 
    
```

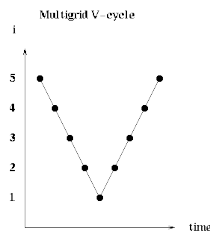
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This is called a V-Cycle

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



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Complexity of a V-Cycle

- On a serial machine
 - Work at each point in a V-cycle is $O(\text{the number of unknowns})$
 - 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:

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

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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 ... from coarse to fine mesh

x(i) = MG (b(i), ln (i-1) (x(i-1)))

◦ In other words:

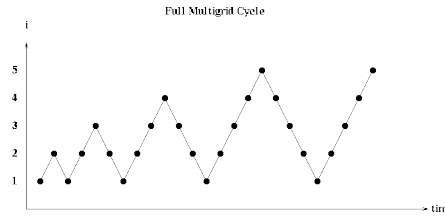
- Solve the problem with 1 unknown
- Given a solution to the coarser problem, $P^{(i-1)}$, map it to starting guess for $P^{(i)}$
- Solve the finer problem using the Multigrid V-cycle

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Full Multigrid Cost Analysis



◦ One V for each call to FMG

- people also use Ws and other compositions

◦ Serial time: $\sum_{i=1}^m O(4^i) = O(4^m) = O(\# \text{ unknowns})$

◦ PRAM time: $\sum_{i=1}^m O(i) = O(m^2) = O(\log^2 \# \text{ unknowns})$

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Complexity of Solving Poisson's Equation

• Theorem: error after one call to multigrid

- error_after $\leq .5 * \text{error_before}$
- 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

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Complexity of Solving Poisson's Equation

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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:

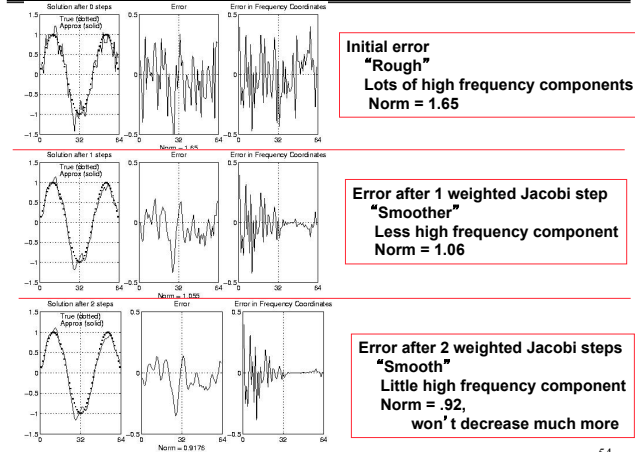
$$x(j) := 1/3 (x(j-1) + x(j) + x(j+1) + b(j))$$
- In 2D, similar average of nearest neighbors

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Weighted Jacobi chosen to damp high frequency error



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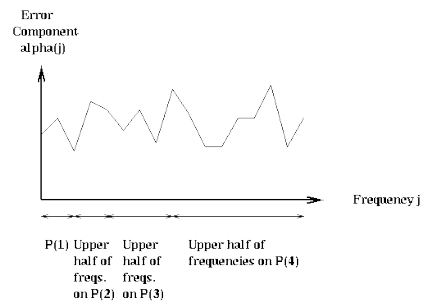
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Multigrid as Divide and Conquer Algorithm

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

Schematic Description of Multigrid



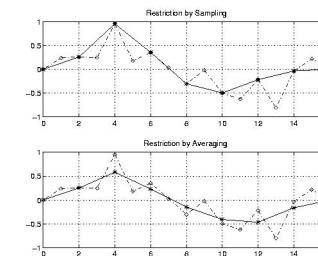
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The Restriction Operator R(i) - Details

- The restriction operator, R(i), takes
 - a problem P⁽ⁱ⁾ with RHS b(i) and
 - maps it to a coarser problem P⁽ⁱ⁻¹⁾ with RHS b(i-1)
- In 1D, average values of neighbors
 - $x_{coarse}(i) = 1/4 * x_{fine}(i-1) + 1/2 * x_{fine}(i) + 1/4 * x_{fine}(i+1)$



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

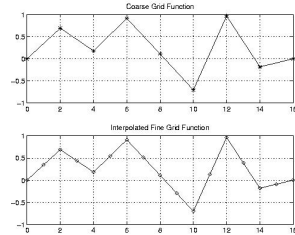
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Interpolation Operator $I_n(i-1)$: details

- The interpolation operator $I_n(i-1)$, takes a function on a coarse grid $P^{(i-1)}$, and produces a function on a fine grid $P^{(i)}$
- In 1D, linearly interpolate nearest coarse neighbors
 - $x_{\text{fine}}(i) = x_{\text{coarse}}(i)$ if the fine grid point i is also a coarse one, else
 - $x_{\text{fine}}(i) = 1/2 * x_{\text{coarse}}(\text{left of } i) + 1/2 * x_{\text{coarse}}(\text{right of } i)$



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

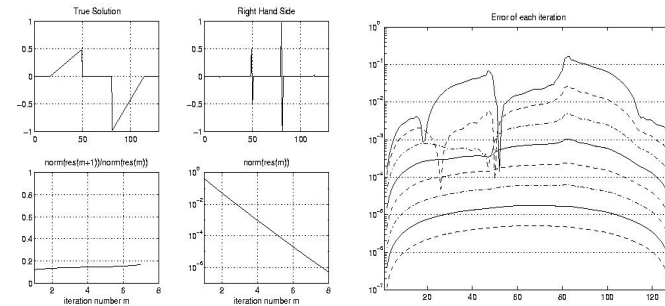


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Convergence Picture of Multigrid in 1D

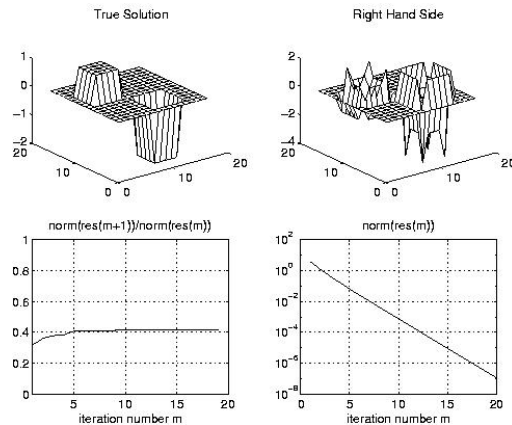


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Convergence Picture of Multigrid in 2D



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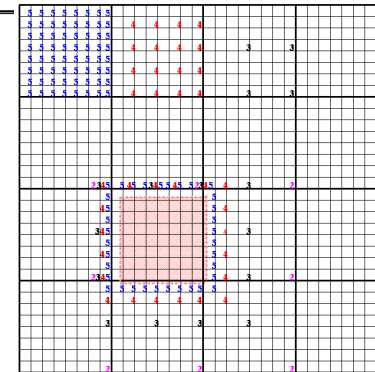
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Parallel 2D Multigrid

- 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 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 $j \geq k$, 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

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Comparison of Methods (in $O(\cdot)$ 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 $\alpha \gg \beta$

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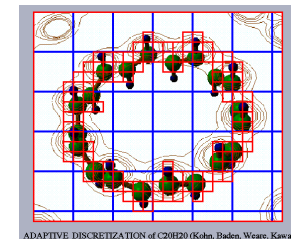
Practicalities

- 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, so flops = $O(1000)$
 - In 2D, the surface to communicate is $4 \times 1000^{1/2} \approx 128$, or 13%
 - In 3D, the surface is $1000 \cdot 8^3 \approx 500$, or 50%
- See Tuminaro and Womble, SIAM J. Sci. Comp., v14, n5, 1993 for analysis of MG on 1024 nCUBE2
 - on 64×64 grid of unknowns, only 4 per processor
 - efficiency of 1 V-cycle was .02, and on FMG .008
 - on 1024×1024 grid
 - efficiencies were .7 (MG Vcycle) 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

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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

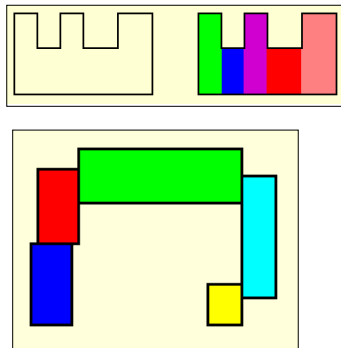
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Multiblock Applications

- Solve system of equations on a union of rectangles
 - subproblem of AMR
- E.g.,



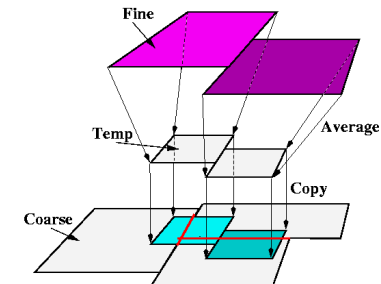
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Adaptive Mesh Refinement

- Data structures in AMR
- Usual parallelism is to assign grids on each level to processors
- Load balancing is a problem



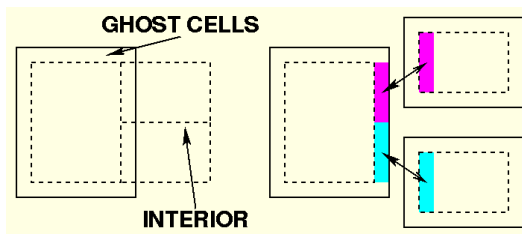
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Support for AMR

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



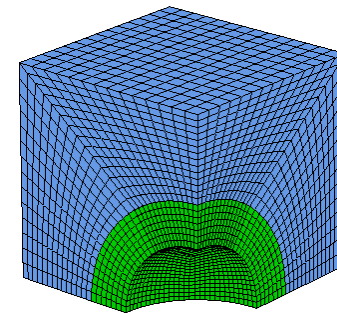
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Multigrid on an Unstructured Mesh

- 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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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?

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Irregular mesh: Tapered Tube (multigrid)

Example of Prometheus meshes

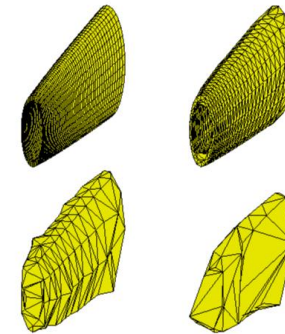


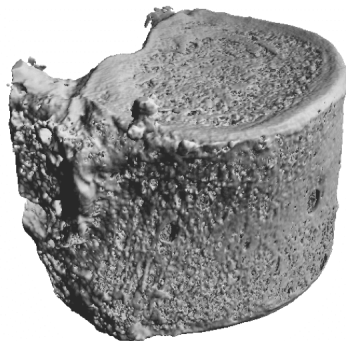
Figure 6 Sample input grid and coarse grids

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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

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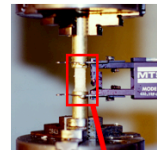
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Multigrid for nonlinear elastic analysis of bone

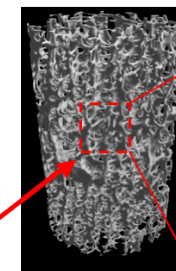
Gordon Bell Prize, 2004

Source: M. Adams et al

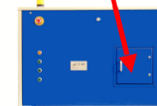
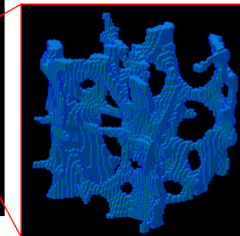
Mechanical testing
for material properties



3D image



μ FE mesh
2.5 mm³
44 μ m elements



Micro Computed
Tomography @
22 μ m resolution

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

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