# Multigrid 

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## Review of Previous Lectures and Outline

${ }^{\circ}$ Review Poisson equation
${ }^{\circ}$ Overview of Methods for Poisson Equation

- Jacobi's method
${ }^{\circ}$ Gauss-Seidel method
${ }^{\circ}$ Red-Black SOR method
${ }^{\circ}$ FFT
${ }^{\circ}$ Multigrid


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

$$
T=\left(\begin{array}{ccccc}
2 & -1 & & & \\
-1 & 2 & -1 & & \\
& -1 & 2 & -1 & \\
& & -1 & 2 & -1 \\
& & & -1 & 2
\end{array}\right) \xrightarrow{\text { Graph and "stencil" }}
$$

## 2D Poisson's equation

${ }^{\circ}$ Similar to the 1D case, but the matrix $T$ is now

${ }^{\circ} 3 \mathrm{D}$ is analogous

## Algorithms for 2D (3D) Poisson Equation ( $\mathrm{N}=\mathrm{n}^{2}\left(\mathrm{n}^{3}\right)$ vars)

| Algorithm | Serial | PRAM | Memory | \#Procs |
| :---: | :---: | :---: | :---: | :---: |
| - Dense LU | $\mathrm{N}^{3}$ | N | $\mathrm{N}^{2}$ | $\mathrm{N}^{2}$ |
| - Band LU | $\mathbf{N}^{2}\left(\mathbf{N}^{7 / 3}\right)$ | N | $\mathrm{N}^{3 / 2}\left(\mathrm{~N}^{5 / 3}\right)$ | $\mathrm{N}\left(\mathrm{N}^{4 / 3}\right)$ |
| - Jacobi | $\mathrm{N}^{2}\left(\mathrm{~N}^{5 / 3}\right)$ | $\mathbf{N}\left(\mathrm{N}^{2 / 3}\right)$ | N | N |
| - Explicit Inv. | $\mathrm{N}^{2}$ | $\log N$ | $\mathrm{N}^{2}$ | $\mathrm{N}^{2}$ |
| - Conj.Gradient | $\mathrm{N}^{\mathbf{3 / 2}}\left(\mathrm{N}^{4 / 3}\right)$ | $\mathbf{N}^{1 / 2(1 / 3)} \boldsymbol{l o g} \mathbf{N}$ | N | N |
| - Red/Black SOR | R $\mathbf{N}^{\mathbf{3} 2}\left(\mathbf{N}^{4 / 3}\right)$ | $\mathbf{N}^{1 / 2}\left(\mathbf{N}^{1 / 3}\right)$ | N | N |
| - Sparse LU | $\mathrm{N}^{3 / 2}\left(\mathrm{~N}^{2}\right)$ | $\mathbf{N}^{1 / 2}$ | $N^{*} \log \mathbf{N}\left(\mathbf{N}^{4 / 3}\right)$ | N |
| - FFT | $N^{*} \log N$ | $\log N$ | N | N |
| - Multigrid | N | $\log ^{2} \mathbf{N}$ | N | N |
| - Lower bound | N | $\log N$ | N |  |

PRAM is an idealized parallel model with zero cost communication

## Multigrid Motivation

${ }^{\circ}$ 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 $\mathbf{n}$ steps to move information across $\mathbf{n} \times \mathbf{n}$ grid
${ }^{\circ}$ Can show that decreasing error by fixed factor $\mathrm{c}<1$ takes $\Omega(\log n)$ steps
- Convergence to fixed error < 1 takes $\Omega(\log n)$ steps
${ }^{\circ}$ Therefore, converging in $\mathrm{O}(1)$ 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


## Multigrid Motivation

Right Hand Side
True Solution


5 steps of Jacobi



Best 5 step solution


## Big Idea used in multigrid and elsewhere

${ }^{\circ}$ If you are far away, problem looks simpler

- For gravity: approximate earth, distant galaxies, ... by point masses
${ }^{\circ}$ 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
${ }^{\circ}$ Ex: Multigrid for solving PDE in O(n) time
- Use coarser mesh to get approximate solution of Poisson's Eq.
${ }^{\circ}$ 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
${ }^{\circ}$ Ex: Graph Partitioning (used to parallelize SpMV)
- Replace graph to be partitioned by a coarser graph (CS267 for details)


## Fine and Coarse Approximations



Fine


Coarse

## Multigrid Overview

## ${ }^{\circ}$ 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.
${ }^{\circ}$ Success depends on coarse grid solution being a good approximation to the fine grid


## Multigrid uses Divide-and-Conquer in 2 Ways

${ }^{\circ}$ First way:

- Solve problem on a given grid by calling Multigrid on a coarse approximation to get a good guess to refine
${ }^{\circ}$ 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 Multgrid responsible for suppressing coefficients of sine curves of the lower half of the frequencies in the error (pictures later)


## Multigrid Sketch in 1D

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


## Multigrid Sketch (1D and 2D)

${ }^{\circ}$ Consider a $2^{m}+1$ grid in 1D ( $2^{m}+1$ by $2^{m}+1$ grid in 2D) for simplicity

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

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

$\mathbf{P}^{(2)}: 5$ by 5 grid of points 3 by 3 grid of unknowns
Points labeled 1 are part of next coarser grid

$\mathbf{P}^{(1)}: 3$ by 3 grid of points 1 by 1 grid of unknowns


## Multigrid Operators (write on board)

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


## Multigrid V-Cycle Algorithm (write on board)

Function MGV ( b(i), $\mathbf{x}(\mathrm{i})$ )
... Solve $T(i)^{*} x(i)=b(i)$ given $b(i)$ and an initial guess for $x(i)$
... return an improved $\mathrm{x}(\mathrm{i})$
if ( $\mathrm{i}=1$ )
compute exact solution $\mathbf{x}(1)$ of $\mathbf{P}^{(1)} \quad$ only 1 unknown
return $\mathrm{x}(1)$
else

$$
\begin{aligned}
& x(i)=S(i)(b(i), x(i)) \\
& r(i)=T(i)^{\star} x(i)-b(i) \\
& d(i)=\ln (i-1)(M G V(R(i)(r(i)), 0)) \\
& x(i)=x(i)-d(i) \\
& x(i)=S(i)(b(i), x(i)) \\
& \text { return } x(i)
\end{aligned}
$$

improve solution by
damping high frequency error compute residual
solve $\mathrm{T}(\mathrm{i})^{\star} \mathrm{d}(\mathrm{i})=\mathrm{r}(\mathrm{i})$ recursively
correct fine grid solution
improve solution again

## Why is this called a V-Cycle?

${ }^{\circ}$ Just a picture of the call graph
${ }^{\circ}$ In time a V-cycle looks like the following


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

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

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

## 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 $\mathrm{i}=2$ to m

$$
x(i)=\operatorname{MGV}(b(i), \ln (i-1)(x(i-1)))
$$

${ }^{\circ}$ In other words:

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


## Full Multigrid Cost Analysis

Full Multigrid Cyele

${ }^{\circ}$ One V-cycle for each call to FMG

- people also use "W cycles" and other compositions
${ }^{\circ}$ \#Flops: $\quad \Sigma_{\mathrm{i}=1}^{\mathrm{m}} \mathrm{O}\left(4^{\mathrm{i}}\right)=\mathbf{O}\left(4^{\mathrm{m}}\right)=\mathbf{O}$ (\# unknowns)


## Complexity of Solving Poisson's Equation

${ }^{\circ}$ Theorem: error after one FMG call $\leq \mathrm{c} \cdot$ error before, where $\mathrm{c}<\mathbf{1 / 2}$, independent of \# unknowns
${ }^{\circ}$ 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
${ }^{\circ}$ Total complexity just proportional to cost of one FMG call

The Solution Operator S(i) - Details (on board)
${ }^{\circ}$ The solution operator, $\mathbf{S}(\mathbf{i})$, is a weighted Jacobi
${ }^{\circ}$ Consider the 1D problem

${ }^{\circ}$ At level $i$, pure Jacobi replaces:

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

${ }^{\circ}$ Weighted Jacobi uses:

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

${ }^{\circ}$ 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)


## Eigenvalues of Solution Operator S(i)




## Weighted Jacobi chosen to damp high frequency error



## Multigrid as Divide and Conquer Algorithm

## ${ }^{\circ}$ Each level in a V-Cycle reduces the error in one part of the frequency domain

Schematic Description of Multigrid



## Error on fine and coarse grids



## The Restriction Operator R(i) - Details

${ }^{\circ}$ The restriction operator, R(i), takes

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

${ }^{\circ}$ In 2D, average with all 8 neighbors (N,S,E,W,NE,NW,SE,SW)


## Interpolation Operator $\ln (\mathrm{i}-1)$ : details

${ }^{\circ}$ The interpolation operator $\ln (\mathrm{i}-1)$, takes a function $\mathrm{x}_{\text {coarse }}$ on a coarse grid $\mathbf{P}^{(i-1)}$, and produces a function $\mathrm{x}_{\text {fine }}$ on a fine grid $\mathbf{P}^{(i)}$ :

。 $\mathrm{x}_{\text {fine }}=\ln (\mathrm{i}-1)\left(\mathrm{x}_{\text {coarse }}\right)$

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


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



## Convergence Picture of Multigrid in 1D



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## Convergence Picture of Multigrid in 2D

True Solution


Right Hand Side



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## Multigrid V-Cycle Algorithm Analysis (1/2)

Function MGV ( b(i), $\mathbf{x ( i )}$ )
... 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 $\mathbf{x}(1)$ of $\mathbf{P}^{(1)}$ only 1 unknown
return $\mathrm{x}(1)$
else
(Note: we assume recursive solve is exact, for ease of analysis)

$$
\begin{aligned}
& x(i)=x(i)-d(i) \\
& x(i)=S(i)(b(i), x(i))
\end{aligned}
$$

$$
\begin{aligned}
& x(i)=x(i)-d(i) \\
& x(i)=s \cdot x(i)+b(i) / 3
\end{aligned}
$$

return $x(i)$

$$
\begin{aligned}
& \mathbf{x}(\mathrm{i})=\mathbf{S}(\mathrm{i})(\mathrm{b}(\mathrm{i}), \mathbf{x}(\mathrm{i})) \\
& x(i)=S \cdot x(i)+b(i) / 3 \\
& r(i)=T(i)^{*} x(i)-b(i) \\
& r(i)=T(i)^{\star} x(i)-b(i) \\
& \mathrm{d}(\mathrm{i})=\ln (\mathrm{i}-1)\left(\operatorname{MGV}(\mathbf{R}(\mathrm{i})(\mathrm{r}(\mathrm{i}), 0)) \quad \mathrm{d}(\mathrm{i})=\mathbf{P} \cdot\left(\mathrm{T}(\mathrm{i}-1)^{-1} \cdot(\mathrm{R} \cdot \mathrm{r}(\mathrm{i}))\right)\right.
\end{aligned}
$$

## Multigrid V-Cycle Algorithm Analysis (2/2)

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

$$
\begin{aligned}
& x(i)=S \cdot x(i)+b(i) / 3 \\
& r(i)=T(i)^{\star} x(i)-b(i) \\
& d(i)=P \cdot\left(T(i-1)^{-1} \cdot(R \cdot r(i))\right) \\
& x(i)=x(i)-d(i) \\
& x(i)=S \cdot x(i)+b(i) / 3
\end{aligned}
$$

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

Substitute each equation into later ones to get

$$
e(i)=S \cdot\left(I-P \cdot\left(T(i-1)^{-1} \cdot(R \cdot T(i))\right)\right) \cdot S \cdot e(i) \equiv M \cdot e(i)
$$

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)

${ }^{\circ}$ What does it mean to do Multigrid anyway?
${ }^{\circ}$ 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?
${ }^{\circ}$ Need to define $\mathbf{R}()$ and $\operatorname{In}()$
- How do we convert from coarse to fine mesh and back?
- How do we define coarse matrix (no longer formula, like Poisson)
${ }^{\circ}$ Need to define S()
- How do we damp "high frequency" error?
${ }^{\circ}$ Dealing with coarse meshes efficiently
- Should we switch to another solver on coarsest meshes?


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

## ${ }^{\circ}$ Given original problem, how do we generate a sequence of coarse approximations?

${ }^{\circ}$ 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?
${ }^{\circ}$ 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
${ }^{\circ}$ Algebraic Multigrid
- Don't even have ( $x, y, z$ ) coordinates, just matrix


## 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
${ }^{\circ}$ 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
- $\mathbf{A}_{\text {coarse }}=\mathbf{P}^{\boldsymbol{\top}} \mathbf{A}_{\text {fine }} \mathbf{P}$ - Galerkin method

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## Example of Geometric Coarsening



## Examples of meshes from geometric coarsening



Figre : Sample input grid and coarse grids

## 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:


## How to coarsen carefully

Example - classify vertices - modify graph


Figure 1: Modify graph


Figure 2: New mesh - fixed mesh

## Algebraic Multigrid

- No information beyond matrix needed
${ }^{\circ}$ Galerkin still used to get $\mathbf{A}_{\text {coarse }}=\mathbf{P}^{\boldsymbol{\top}} \mathbf{A}_{\text {fine }} \mathbf{P}$
- Prolongator $\mathbf{P}$ defined purely algebraically
- Cluster fine grid points into nearby groups
- Can use Maximal Independent Sets or Graph Partitioning
- Use magnitude of entries of $A_{\text {fine }}$ 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(Afine)
- Easy to implement (just SpMVs with Afine )
- Chebyshev chooses $p(y)$ such that
- |1-p(y) y|=min over interval $\left[\lambda^{*}, \lambda_{\max }\right]$ estimated to contain eigenvalues of $A_{\text {fine }}$


## 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

## Methods: $\mu$ FE modeling

## Mechanical Testing $\mathrm{E}, \varepsilon_{\text {yield }}, \sigma_{\mathrm{ult}}$, etc.



Micro-Computed Tomography $\mu \mathrm{CT}$ @ $22 \mu \mathrm{~m}$ resolution

Source: Mark Adams, PPPL
3D image

$\mu$ FE mesh
2.5 mm cube $44 \mu \mathrm{~m}$ elements


## 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

$80 \mu \mathrm{~m}$ w/ shell


## 131K dof / proc - Flops/sec/proc

## . 47 Teraflops - 4088 processors



## Conclusions

## ${ }^{\circ}$ 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
${ }^{\circ}$ 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"


## Extra slides

## Parallel 2D Multigrid

## ${ }^{\circ}$ Multigrid on 2D requires nearest neíghbor (up to 8) computation at each level of the grid

## ${ }^{\circ}$ Start with $\mathrm{n}=2^{\mathrm{m}}+1$ by $2^{m}+1$ grid (here $\mathrm{m}=5$ )

- Use an s by s processor grid (here $\mathrm{s}=4$ )

|  | 55 | 5 | 55 | 5 | 55 | 55 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
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|  | 55 | 5 | 5 | 5 | 55 | 55 |  | 4 | 4 | , | , | 4 | 4 | 4 |  |  |  |  |  |  |  |  |  |  |  |  |
|  | 55 | 5 | 55 | 5 | 55 | 55 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
|  | 55 | 5 | 5 | 5 | 55 | 55 |  | , | , | , |  | , | 4 | 4 |  |  | 3 |  |  | 3 |  |  |  |  |  |  |
|  | 55 | 5 | 55 | 5 | 55 | 55 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
|  | 55 | 5 | 5 | 5 | 55 | 55 |  | 6 | 4 | $\checkmark$ |  | , | 4 | 4 |  |  |  |  |  |  |  |  |  |  |  |  |
|  | 55 | 5 | 5 | 5 | 55 | 55 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
|  | 5 5. | 5 | 5. | 5 | 5 | 55 |  | , |  |  |  | , | 4 | , |  |  |  |  |  |  |  |  |  |  |  |  |
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|  |  |  |  |  |  | 315 |  |  |  |  |  |  | 5 | 15 |  |  | 3 |  |  | , |  |  |  |  |  |  |
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|  |  |  |  |  |  | 45 |  |  |  |  |  |  |  |  | 5 |  |  |  |  |  |  |  |  |  |  |  |
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|  |  |  |  |  |  | 345 |  |  |  |  |  |  |  |  | 5 |  | 3 |  |  |  |  |  |  |  |  |  |
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|  |  |  |  |  |  | 45 |  |  |  |  |  |  |  |  | 5 |  |  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  | 5 |  |  |  |  |  |  |  |  | 5 |  |  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  | 24.5 |  |  |  |  |  |  |  |  | 5 |  | 3 |  |  | 2 |  |  |  |  |  |  |
|  |  |  |  |  |  | 5 |  | 5 | 5 | 5 | 5 | 5 | - 5 | 5 | 5 |  |  |  |  |  |  |  |  |  |  |  |
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|  |  |  |  |  |  | 2 |  |  |  |  |  |  |  | 2 |  |  |  |  |  | 2 |  |  |  |  |  |  |

Communication pattern for Mul tigrid 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 $\mathrm{P}(\mathrm{m})$ of multigrid

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

${ }^{\circ}$ Assume $2^{\mathrm{m}}+\mathbf{1}$ by $\mathbf{2}^{\mathrm{m}}+\mathbf{1}$ grid of points, $\mathrm{n}=\mathbf{2}^{\mathrm{m}} \mathbf{- 1}, \mathrm{N}=\mathrm{n}^{\mathbf{2}}$
${ }^{\circ}$ 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
${ }^{\circ}$ 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
${ }^{\circ}$ Cost of one level in V-cycle
- If level $\mathbf{j}>=k$, then cost $=$

|  | $O\left(4^{j-k}\right)$ |
| ---: | :--- |
| $+O(1) \alpha$ | $\ldots$. Flops, proportional to the number of grid points/processor |
| $+O\left(2^{j-k}\right) \beta$ | $\ldots$. Number of words sent |

- If level $\mathbf{j}<\mathbf{k}$, then cost =

$$
O(1)
$$

$$
+\mathrm{O}(1) \alpha \quad \text {.... Send a constant \# messages to neighbors }
$$

$$
+O(1) \beta \quad \text {.... Number of words sent }
$$

- 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 | $N / p+$ <br> $\log p^{*} \log N$ | $(\log N)^{2}$ | $(N / p)^{1 / 2}+$ <br> $\log p^{*} \log N$ |
| FFT | $N \log N / p$ | $p^{1 / 2}$ | $N / p$ |
| SOR | $N^{3 / 2} / p$ | $N^{1 / 2}$ | $N / p$ |

${ }^{\circ}$ SOR is slower than others on all counts
${ }^{\circ}$ Flops for MG and FFT depends on accuracy of MG
${ }^{\circ}$ MG communicates less total data (bandwidth)

- Total messages (latency) depends ...
- This coarse analysis can't say whether MG or FFT is better when $\alpha \gg \beta$


## Practicalities

${ }^{\circ}$ In practice, we don't go all the way to $\mathbf{P}^{(1)}$
${ }^{\circ}$ 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 $4 x \operatorname{sqrt}(1000) \sim=128$, or $13 \%$
- In 3D, the surface is $1000-8^{3} \sim=500$, 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 $1024 \times 1024$ 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

Multigrid on an Adaptive Mesh
${ }^{\circ}$ For problems with very large dynamic range, another level of refinement is needed
${ }^{\circ}$ Build adaptive mesh and solve multigrid (typically) at each level


ADAPTIVE DISCRETIZATION of C20H20 (Kohn, Baden, Weare, Kawai)
${ }^{\circ}$ Can't afford to use finest mesh everywhere

## Multiblock Applications

- Solve system of equations on a union of rectangles
- subproblem of AMR
${ }^{\circ}$ E.g.,



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## Adaptive Mesh Refinement

${ }^{\circ}$ Data structures in AMR
${ }^{\circ}$ Usual parallelism is to assign grids on each level to processors
${ }^{\circ}$ Load balancing is a problem


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## Support for AMR

${ }^{\circ}$ Domains in Titanium designed for this problem
${ }^{\circ}$ Kelp, Boxlib, and AMR++ are libraries for this
${ }^{\circ}$ Primitives to help with boundary value updates, etc.

GHOST CELLS


## Multigrid on an Unstructured Mesh

${ }^{\circ}$ Another approach to variable activity is to use an unstructured mesh that is more refined in areas of interest

## ${ }^{\circ}$ 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)

