CS 267 Sources of Parallelism and Locality in Simulation – Part 2

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Recap of Last Lecture

- 4 kinds of simulations
  - Discrete Event Systems
  - Particle Systems
  - Ordinary Differential Equations (ODEs)
  - Partial Differential Equations (PDEs) (today)
- Common problems:
  - Load balancing
    - May be due to lack of parallelism or poor work distribution
    - Statically, divide grid (or graph) into blocks
    - Dynamically, if load changes significantly during run
  - Locality
    - Partition into large chunks with low surface-to-volume ratio
      - To minimize communication
    - Distributed particles according to location, but use irregular spatial decomposition (e.g., quad tree) for load balance
  - Constant tension between these two
    - Particle-Mesh method: can't balance particles (moving), balance mesh (fixed) and keep particles near mesh points without communication

Partial Differential Equations
PDEs

Continuous Variables, Continuous Parameters

Examples of such systems include

- **Elliptic problems (steady state, global space dependence)**
  - **Electrostatic or Gravitational Potential: Potential(position)**
- **Hyperbolic problems (time dependent, local space dependence):**
  - **Sound waves: Pressure(position,time)**
- **Parabolic problems (time dependent, global space dependence)**
  - **Heat flow: Temperature(position, time)**
  - **Diffusion: Concentration(position, time)**

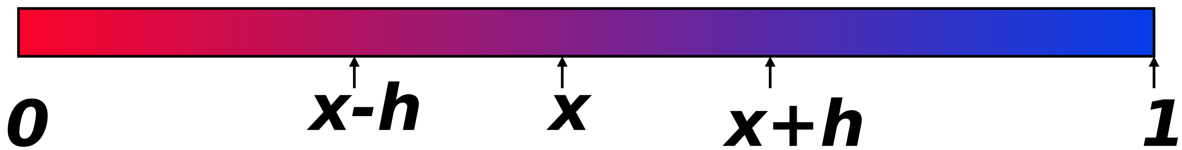
Global vs Local Dependence

- **Global means either a lot of communication, or tiny time steps**
- **Local arises from finite wave speeds: limits communication**

Many problems combine features of above

- **Fluid flow: Velocity,Pressure,Density(position,time)**
- **Elasticity: Stress,Strain(position,time)**

Example: Deriving the Heat Equation



Consider a simple problem

- A bar of uniform material, insulated except at ends
- Let *u(x,t)* be the temperature at position *x* at time *t*
- Heat travels from *x-h* to *x+h* at rate proportional to:

$$\frac{d\,u(x,t)}{dt} = C * \frac{(u(x-h,t)-u(x,t))/h - (u(x,t)-u(x+h,t))/h}{h}$$

- As $h \rightarrow 0$, we get the heat equation:

$$\frac{d\,u(x,t)}{dt} = C * \frac{d^2\,u(x,t)}{dx^2}$$

Details of the Explicit Method for Heat

$$\frac{d\, u(x,t)}{dt} = C * \frac{d^2}{dx^2} u(x,t)$$

- Discretize time and space using explicit approach (forward Euler) to approximate time derivative:

$$(u(x,t+\delta) - u(x,t))/\delta = C\ [\ (u(x-h,t)-u(x,t))/h - (u(x,t)- u(x+h,t))/h\ ] / h$$
$$= C\ [u(x-h,t) - 2*u(x,t) + u(x+h,t)]/h^2$$

Solve for $u(x,t+\delta)$:

$$u(x,t+\delta) = u(x,t)+ C*\delta /h^2 *(u(x-h,t) - 2*u(x,t) + u(x+h,t))$$

- Let $z = C*\delta /h^2$, simplify:

$$u(x,t+\delta) = z* u(x-h,t) + (1-2z)*u(x,t) + z*u(x+h,t)$$

- Change variable x to j*h, t to i*δ, and u(x,t) to u[j,i]

u[j,i+1]= z*u[j-1,i]+ (1-2*z)*u[j,i]+ z*u[j+1,i]

Explicit Solution of the Heat Equation

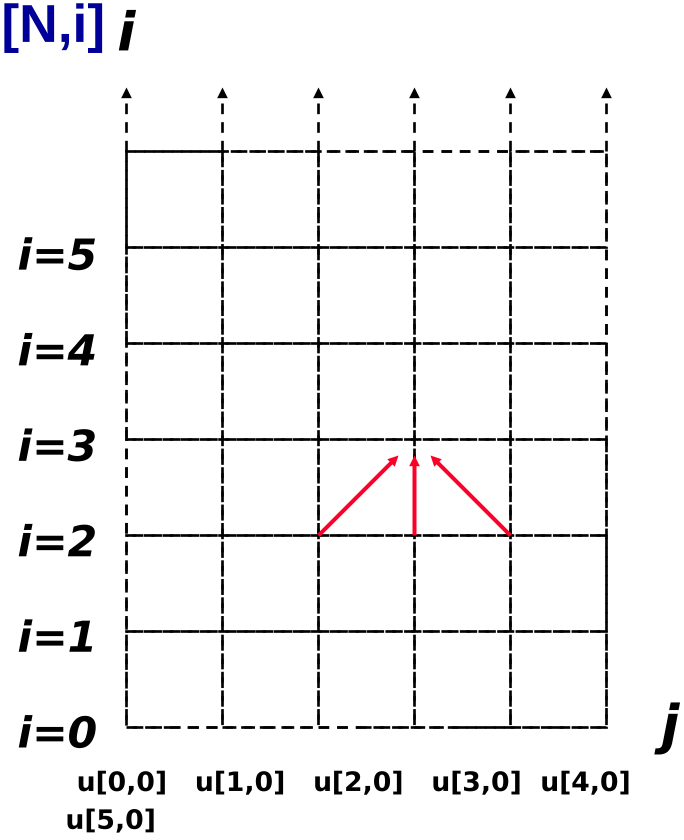
- Use "finite differences" with u[j,i] as the temperature at
  - **time t= i*δ (i = 0,1,2,…) and position x = j*h (j=0,1,…,N=1/h)**
  - **initial conditions on u[j,0]**
  - **boundary conditions on u[0,i] and u[N,i]**
- At each timestep i = 0,1,2,...

For j=0 to N

u[j,i+1]= z*u[j-1,i]+ (1-2*z)*u[j,i] + z*u[j+1,i]

where z =C*δ/h^2

- This corresponds to
  - Matrix-vector-multiply by T (next slide)
  - Combine nearest neighbors on grid

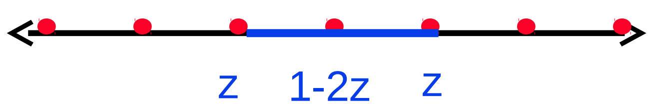


Matrix View of Explicit Method for Heat

- u[j,i+1]= z*u[j-1,i]+ (1-2*z)*u[j,i] + z*u[j+1,i],   same as:
- u[:, i+1] = T * u[:, i] where T is tridiagonal:

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

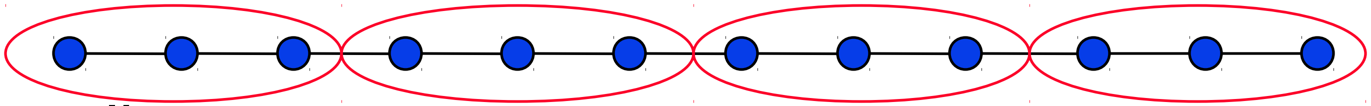
Graph and "3 point stencil"



- L called Laplacian (in 1D)
- For a 2D mesh (5 point stencil) the Laplacian is pentadiagonal
    - More on the matrix/grid views later

Parallelism in Explicit Method for PDEs

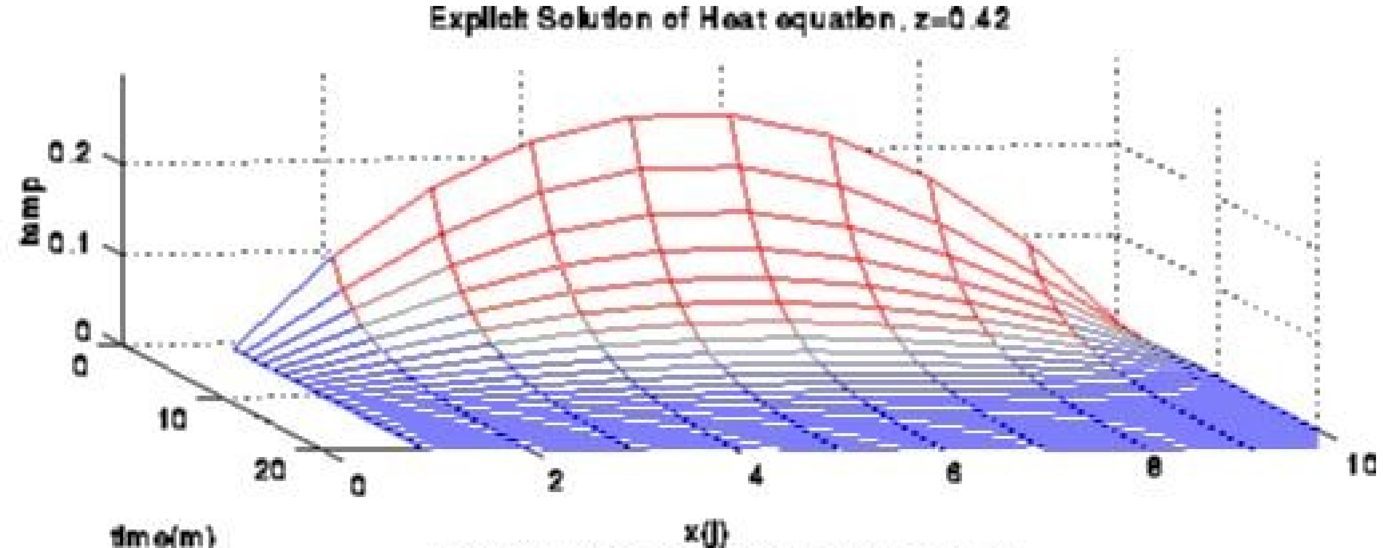
- Sparse matrix vector multiply, via Graph Partitioning
- Partitioning the space (x) into p chunks
  - good load balance (assuming large number of points relative to p)
  - minimize communication (least dependence on data outside chunk)

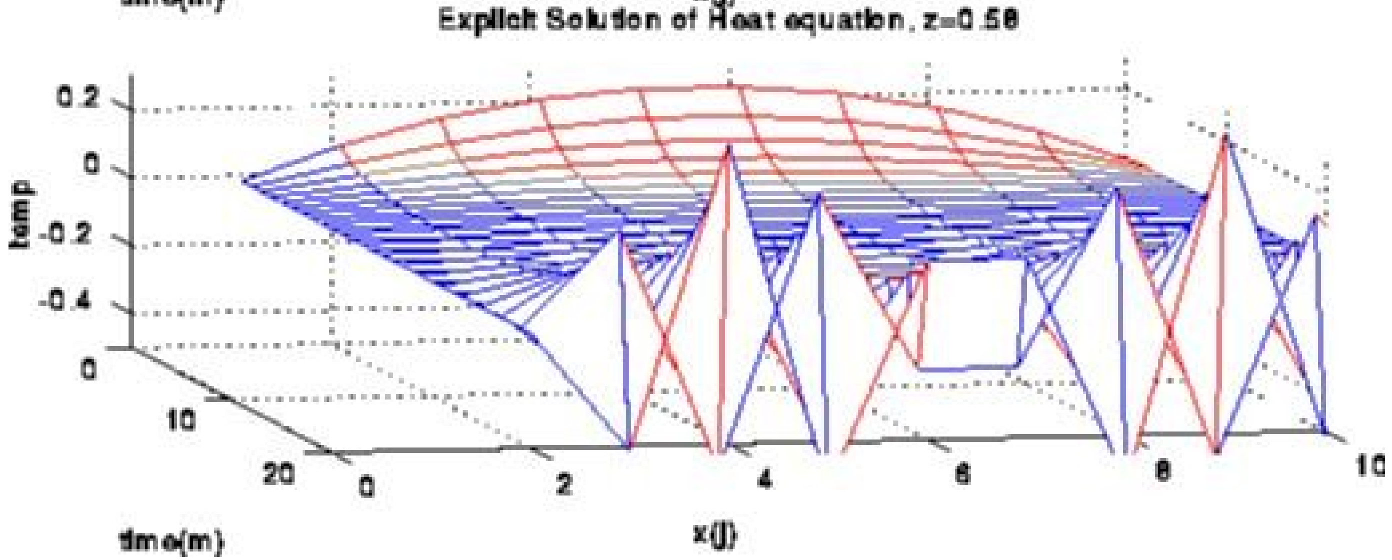


- Generalizes to
  - multiple dimensions.
  - arbitrary graphs (= arbitrary sparse matrices).

- Explicit approach often used for hyperbolic equations
  - Finite wave speed, so only depend on nearest chunks
- Problem with explicit approach for heat (parabolic):
  - numerical instability.
  - solution blows up eventually if $z = C\delta/h^2 > .5$
  - need to make the time step δ very small when h is small: $\delta < .5*h^2/C$

Instability in Solving the Heat Equation Explicitly





Implicit Solution of the Heat Equation

$$\frac{d\, u(x,t)}{dt} = C * \frac{d^2}{dx^2} u(x,t)$$

- Discretize time and space using implicit approach (Backward Euler) to approximate time derivative:

  $(u(x,t+\delta) - u(x,t))/dt = C^*(u(x-h,t+\delta) - 2^*u(x,t+\delta) + u(x+h,\ t+\delta))/h^2$

  $u(x,t) = u(x,t+\delta) - C^*\delta/h^2\ ^*(u(x-h,t+\delta) - 2^*u(x,t+\delta) + u(x+h,t+\delta))$

- Let $z = C^*\delta/h^2$ and change variable t to $i^*\delta$, x to j^*h and u(x,t) to u[j,i]

  $(I + z\ ^*L)^*\ u[:,\ i+1] = u[:,i]$

- Where I is identity and

  L is Laplacian as before

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

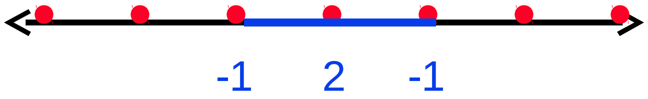
Implicit Solution of the Heat Equation

- The previous slide derived Backward Euler
  - **(I + z *L)* u[:, i+1] = u[:,i]**
- But the Trapezoidal Rule has better numerical properties:

  (I + (z/2)*L) * u[:,i+1]= (I - (z/2)*L) *u[:,i]
- Again **I** is the identity matrix and **L** is:

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

Graph and "stencil"

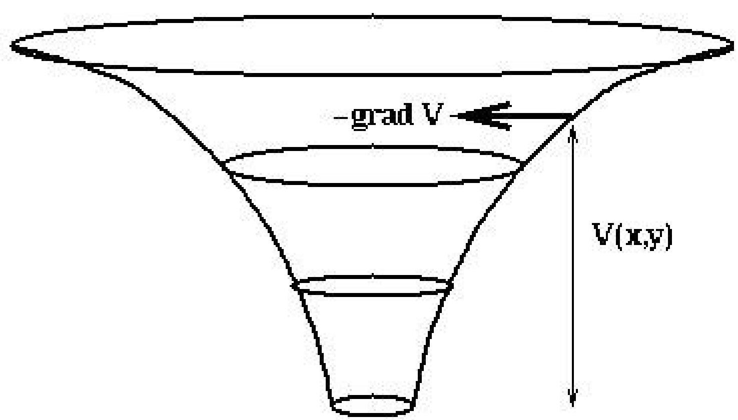


- Other problems (elliptic instead of parabolic) yield Poisson's equation (Lx = b in 1D)

Relation of Poisson to Gravity, Electrostatics

- Poisson equation arises in many problems
- E.g., force on particle at (x,y,z) due to particle at 0 is
  $-(x,y,z)/r^3$, where $r = \mathrm{sqrt}(x^2 + y^2 + z^2)$
- Force is also gradient of potential V = -1/r
  = -(d/dx V, d/dy V, d/dz V) = -grad V
- V satisfies Poisson's equation (try working this out!)

Relationship of Potential V and Force –grad V in 2D



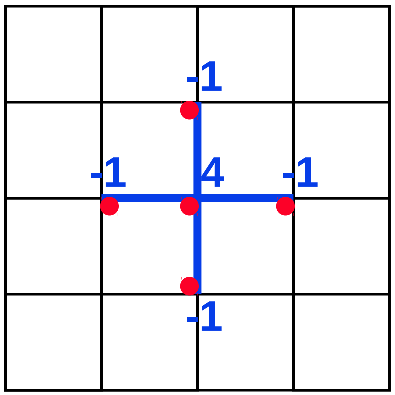
$$\frac{d^2V}{dx^2} + \frac{d^2V}{dy^2} + \frac{d^2V}{dz^2} = 0$$

2D Implicit Method

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

$$
L = \left(\begin{array}{ccc|ccc|ccc}
4 & -1 & & -1 & & & & & \\
-1 & 4 & -1 & & -1 & & & & \\
 & -1 & 4 & & & -1 & & & \\
\hline
-1 & & & 4 & -1 & & -1 & & \\
 & -1 & & -1 & 4 & -1 & & -1 & \\
 & & -1 & & -1 & 4 & & & -1 \\
\hline
 & & & -1 & & & 4 & -1 & \\
 & & & & -1 & & -1 & 4 & -1 \\
 & & & & & -1 & & -1 & 4
\end{array}\right)
$$

Graph and "5 point stencil"



3D case is analogous (7 point stencil)

- Multiplying by this matrix (as in the explicit case) is simply nearest neighbor computation on 2D grid.
- To solve this system, there are several techniques.

Algorithms for 2D (3D) Poisson Equation (N 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	$N^{3/2}$ $(N^{4/3})$	$N^{1/2}$ $(N^{4/3})$	N	N
• Sparse LU	$N^{3/2}$ (N^2)	$N^{1/2}$ $(N^{2/3})$	$N*\log N$ $(N^{4/3})$	$N(N^{4/3})$
• FFT	$N*\log N$	$\log N$	N	N
• Multigrid	N	$\log^2 N$	N	N
• Lower bound	N	$\log N$	N	

All entries in "Big-Oh" sense (constants omitted)

PRAM is an idealized parallel model with zero cost communication

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

Overview of Algorithms

- Sorted in two orders (roughly):
  - from slowest to fastest on sequential machines.
  - from most general (works on any matrix) to most specialized (works on matrices "like" T).
- Dense LU: Gaussian elimination; works on any N-by-N matrix.
- Band LU: Exploits the fact that T is nonzero only on sqrt(N) diagonals nearest main diagonal.
- Jacobi: Essentially does matrix-vector multiply by T in inner loop of iterative algorithm.
- Explicit Inverse: Assume we want to solve many systems with T, so we can precompute and store inv(T) "for free", and just multiply by it (but still expensive).
- Conjugate Gradient: Uses matrix-vector multiplication, like Jacobi, but exploits mathematical properties of T that Jacobi does not.
- Red-Black SOR (successive over-relaxation): Variation of Jacobi that exploits yet different mathematical properties of T. Used in multigrid schemes.
- Sparse LU: Gaussian elimination exploiting particular zero structure of T.
- FFT (Fast Fourier Transform): Works only on matrices *very* like T.
- Multigrid: Also works on matrices like T, that come from elliptic PDEs.
- Lower Bound: Serial (time to print answer); parallel (time to combine N inputs).
- Details in class notes and www.cs.berkeley.edu/~demmel/ma221.

Mflop/s Versus Run Time in Practice

- Problem: Iterative solver for a convection-diffusion problem; run on a 1024-CPU NCUBE-2.
- Reference: Shadid and Tuminaro, SIAM Parallel Processing Conference, March 1991.

Solver	Flops	CPU Time(s)	Mflop/s
Jacobi	3.82×10^{12}	2124	1800
Gauss-Seidel	1.21×10^{12}	885	1365
Multigrid	2.13×10^{9}	7	318

- Which solver would you select?

Summary of Approaches to Solving PDEs

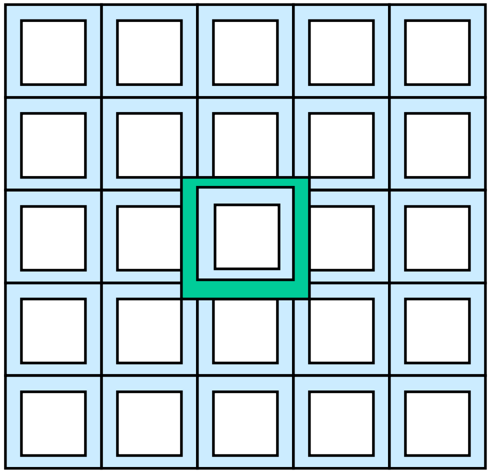
- As with ODEs, either explicit or implicit approaches are possible
  - Explicit, sparse matrix-vector multiplication
  - Implicit, sparse matrix solve at each step
    - Direct solvers are hard (more on this later)
    - Iterative solves turn into sparse matrix-vector multiplication
      - Graph partitioning
- Grid and sparse matrix correspondence:
  - Sparse matrix-vector multiplication is nearest neighbor “averaging” on the underlying mesh
- Not all nearest neighbor computations have the same efficiency
  - Depends on the mesh structure (nonzero structure) and the number of Flops per point.

Comments on practical meshes

- Regular 1D, 2D, 3D meshes
  - Important as building blocks for more complicated meshes
- Practical meshes are often irregular
  - Composite meshes, consisting of multiple “bent” regular meshes joined at edges
  - Unstructured meshes, with arbitrary mesh points and connectivities
  - Adaptive meshes, which change resolution during solution process to put computational effort where needed

Parallelism in Regular meshes

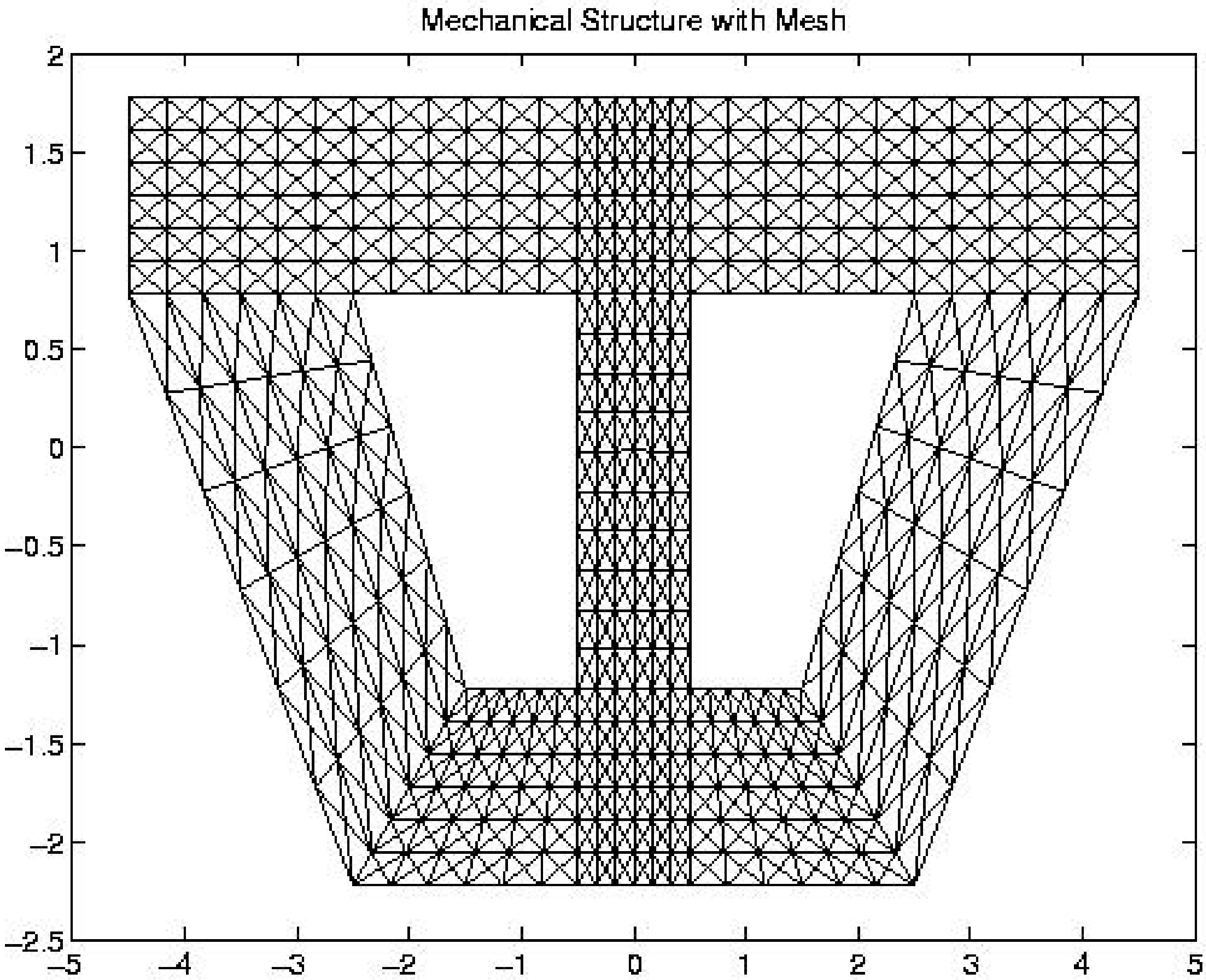
- Computing a Stencil on a regular mesh
  - need to communicate mesh points near boundary to neighboring processors.
    - Often done with ghost regions
  - Surface-to-volume ratio keeps communication down, but
    - Still may be problematic in practice



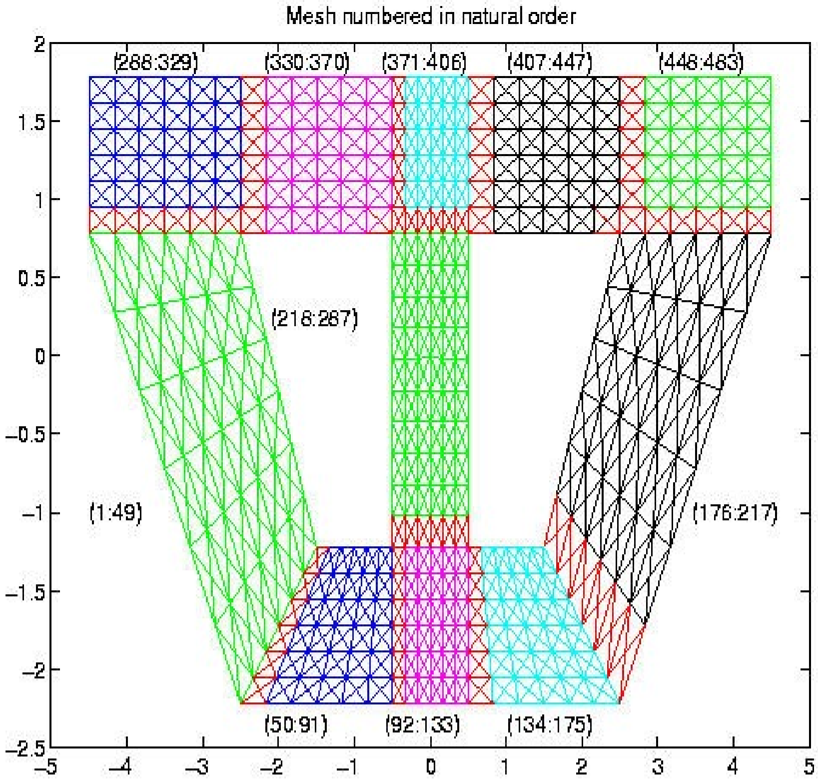
Implemented using "ghost" regions.

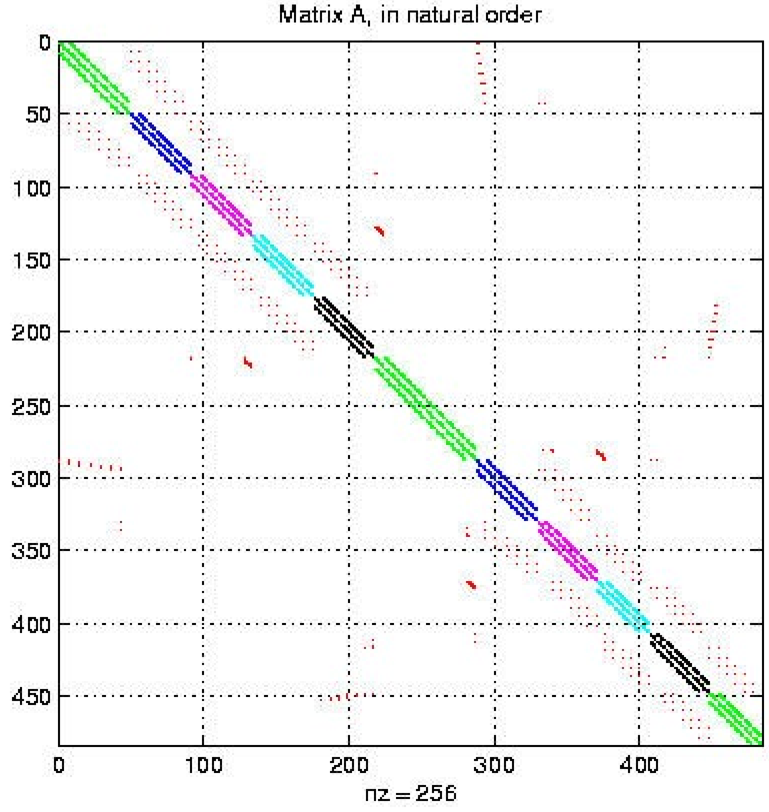
Adds memory overhead

Composite mesh from a mechanical structure



Converting the mesh to a matrix

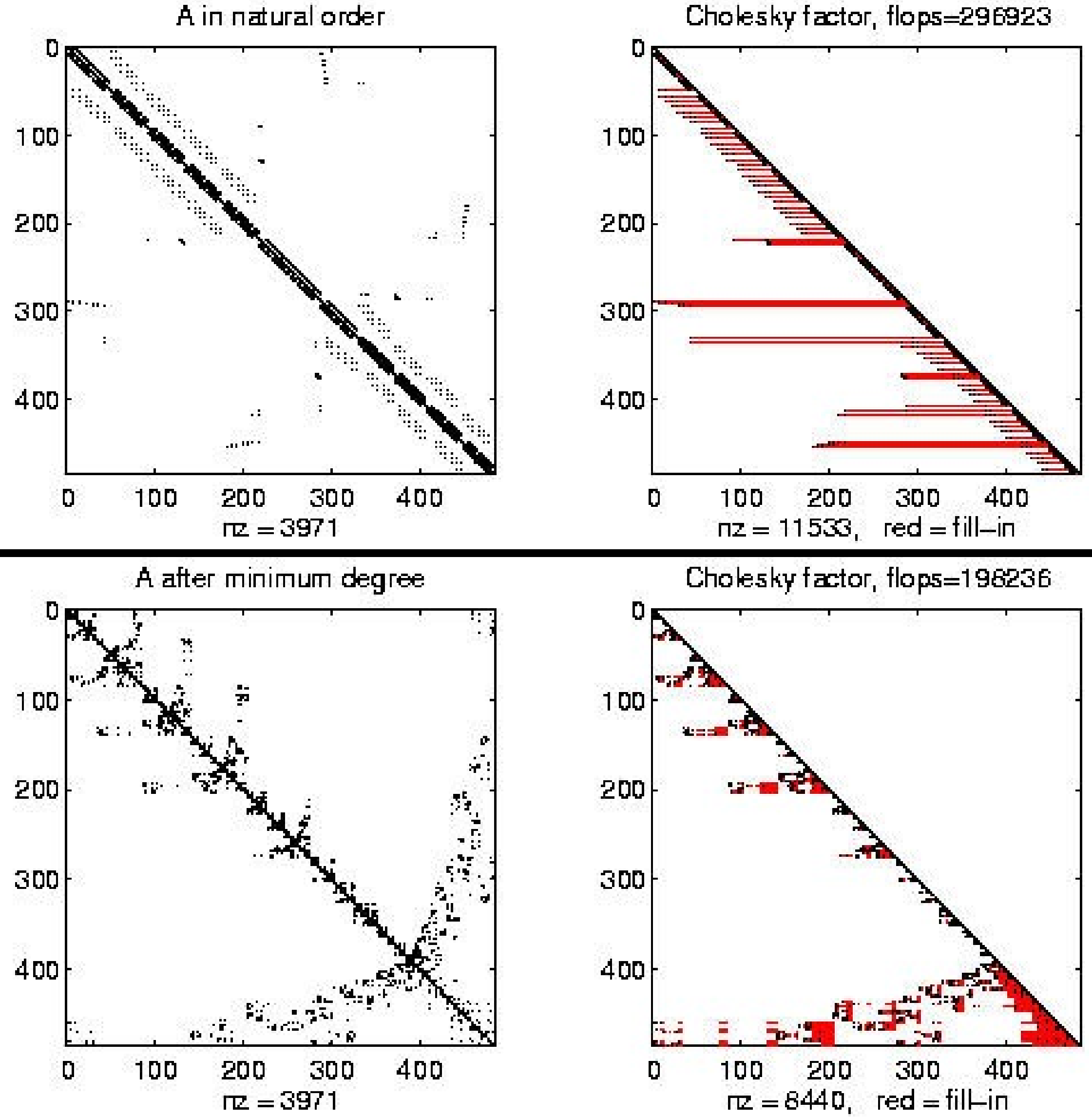




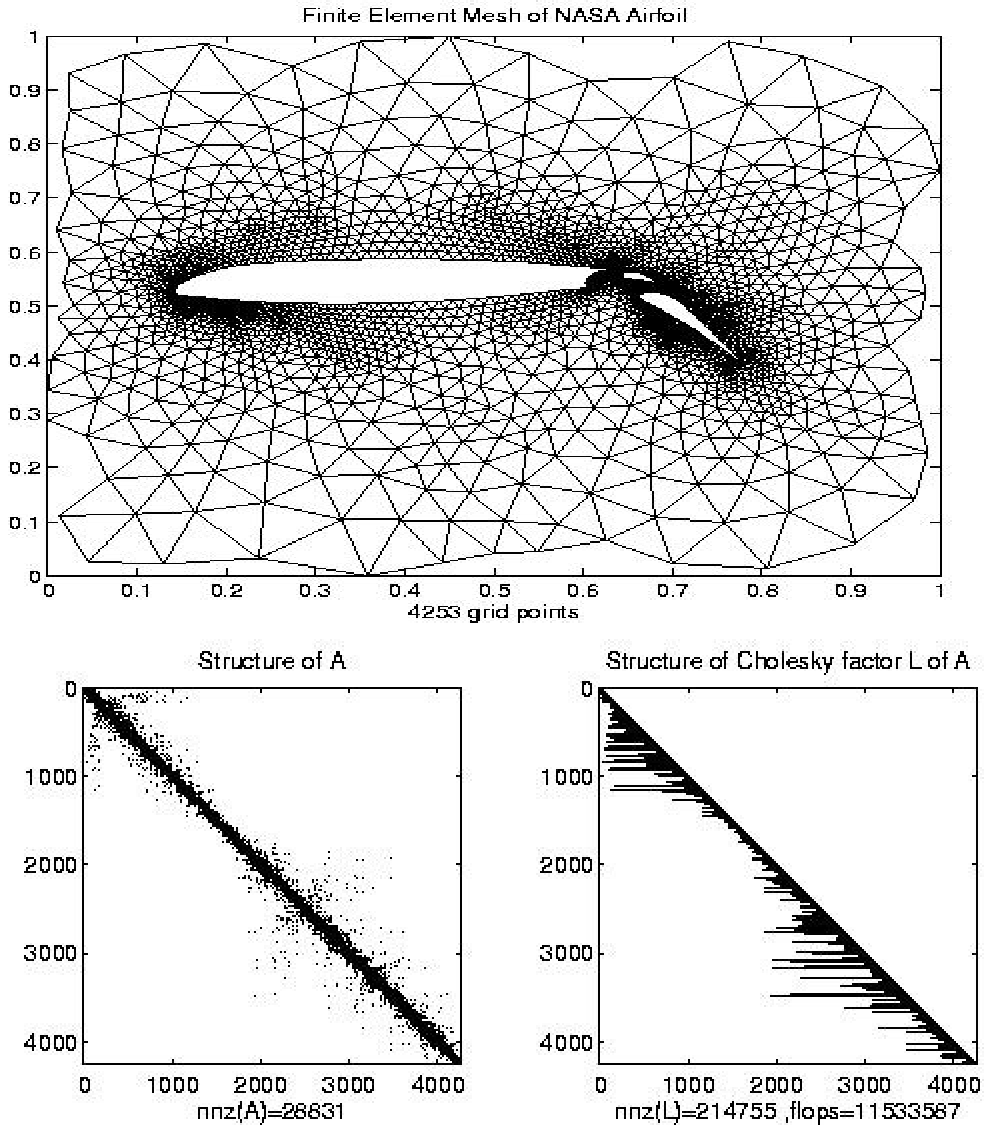
Example of Matrix Reordering Application

When performing
Gaussian Elimination
Zeros can be filled ☹

Matrix can be reordered
to reduce this fill
But it's not the same
ordering as for
parallelism



Irregular mesh: NASA Airfoil in 2D (direct solution)



Irregular mesh: Tapered Tube (multigrid)

Example of Prometheus meshes

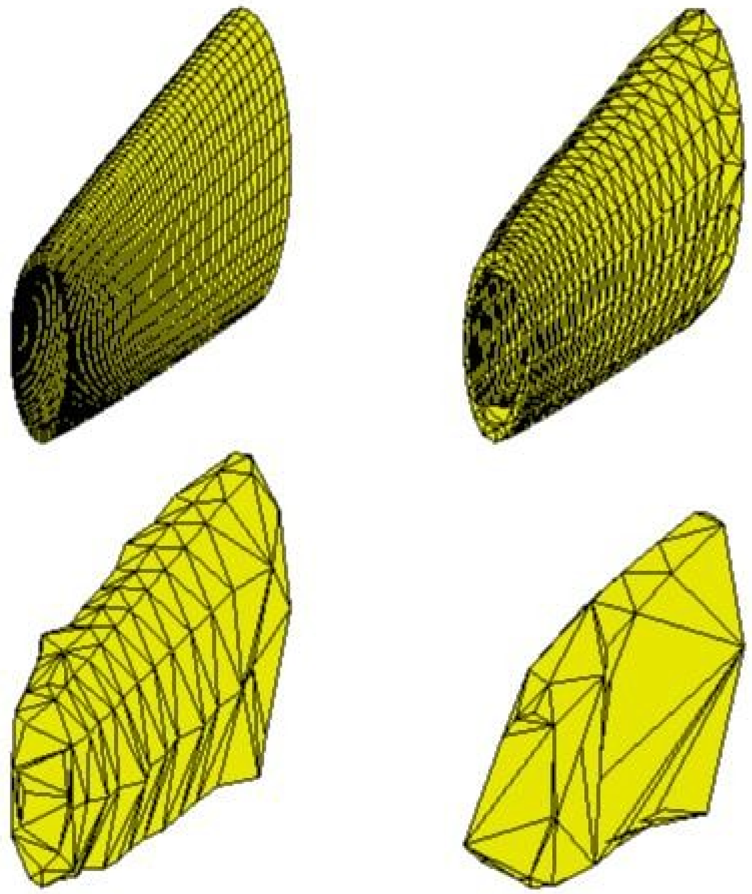
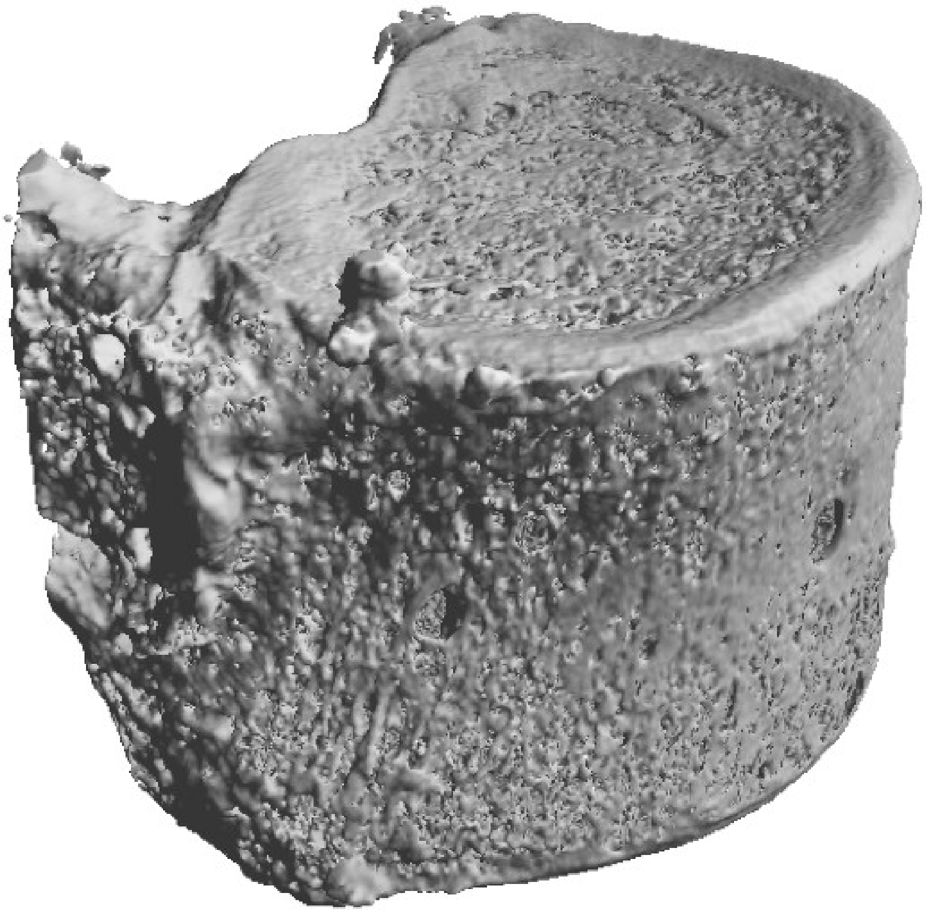


Figure 6: Sample input grid and coarse grids

Source of Unstructured Finite Element Mesh: Vertebra

Study failure modes of trabecular Bone under stress

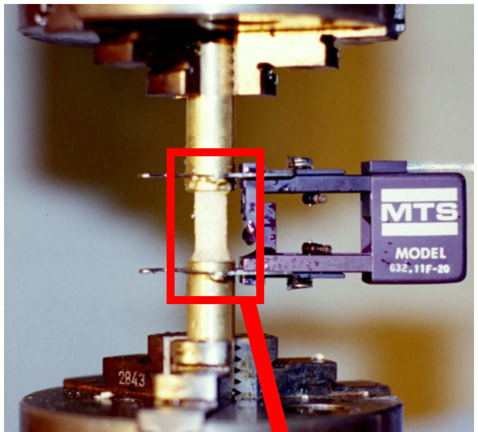


Source: M. Adams, H. Bayraktar, T. Keaveny, P. Papadopoulos, A. Gupta

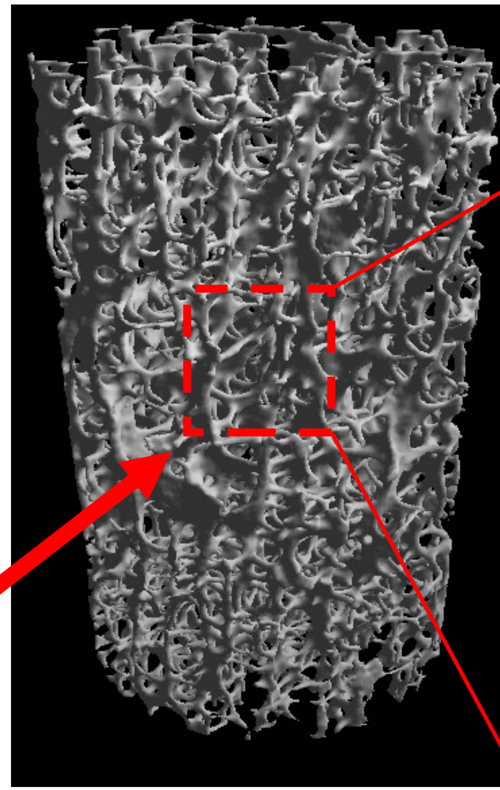
Methods: µFE modeling (Gordon Bell Prize, 2004)

Mechanical Testing
E, ε_{yield}, σ_{ult}, etc.

Source: Mark Adams, PPPL

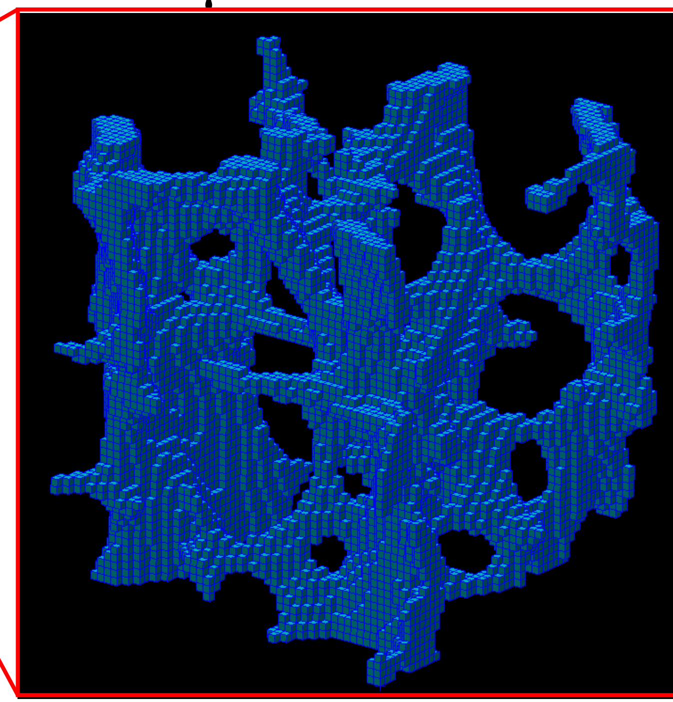


3D image



µFE mesh

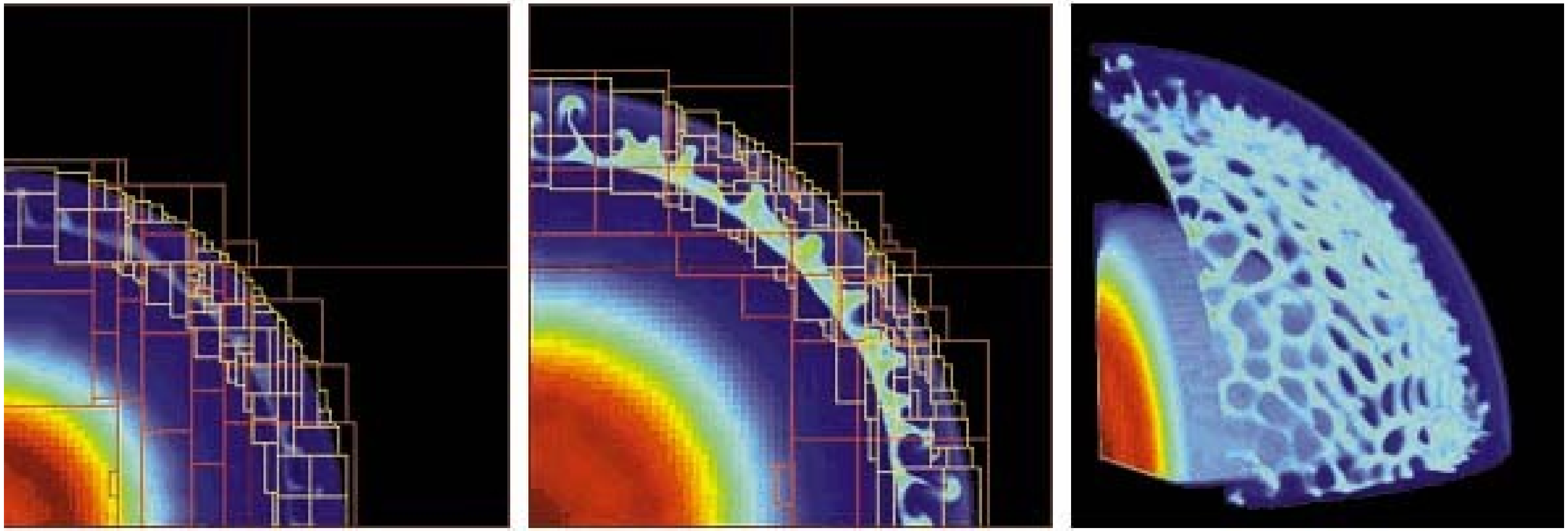
2.5 mm cube
44 µm elements



Micro-Computed Tomography
µCT @ 22 µm resolution

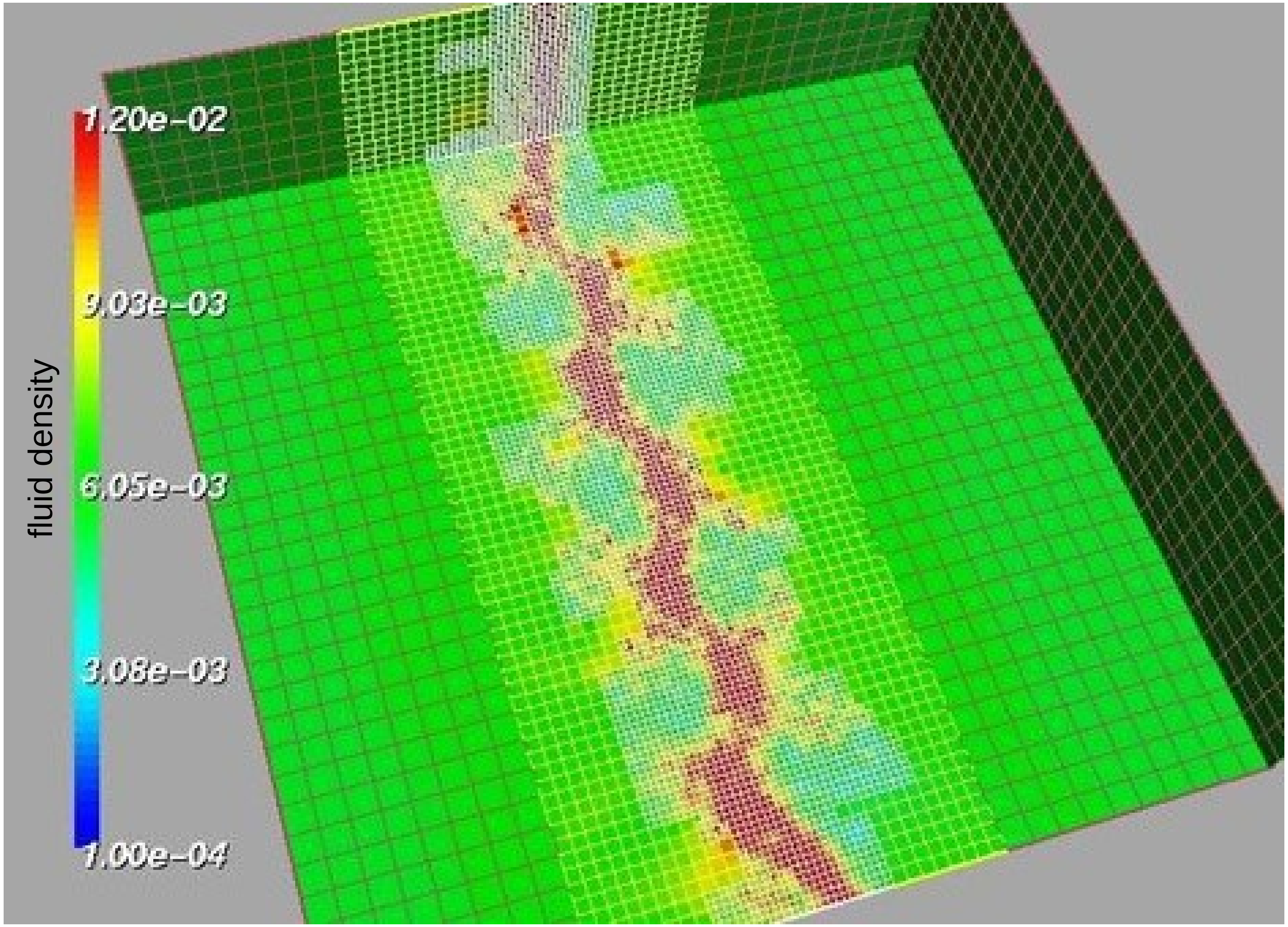
Up to 537M unknowns

Adaptive Mesh Refinement (AMR)



- Adaptive mesh around an explosion
  - Refinement done by estimating errors; refine mesh if too large
- Parallelism
  - Mostly between “patches,” assigned to processors for load balance
  - May exploit parallelism within a patch
- Projects:
  - Titanium (http://www.cs.berkeley.edu/projects/titanium)
  - Chombo (P. Colella, LBL), KeLP (S. Baden, UCSD), J. Bell, LBL

Adaptive Mesh



Shock waves in gas dynamics using AMR (Adaptive Mesh Refinement)
See: http://www.llnl.gov/CASC/SAMRAI/

Challenges of Irregular Meshes

- How to generate them in the first place
  - Start from geometric description of object
  - Triangle, a 2D mesh partitioner by Jonathan Shewchuk
  - 3D harder!
- How to partition them
  - ParMetis, a parallel graph partitioner
- How to design iterative solvers
  - PETSc, a Portable Extensible Toolkit for Scientific Computing
  - Prometheus, a multigrid solver for finite element problems on irregular meshes
- How to design direct solvers
  - SuperLU, parallel sparse Gaussian elimination

- These are challenges to do sequentially, more so in parallel

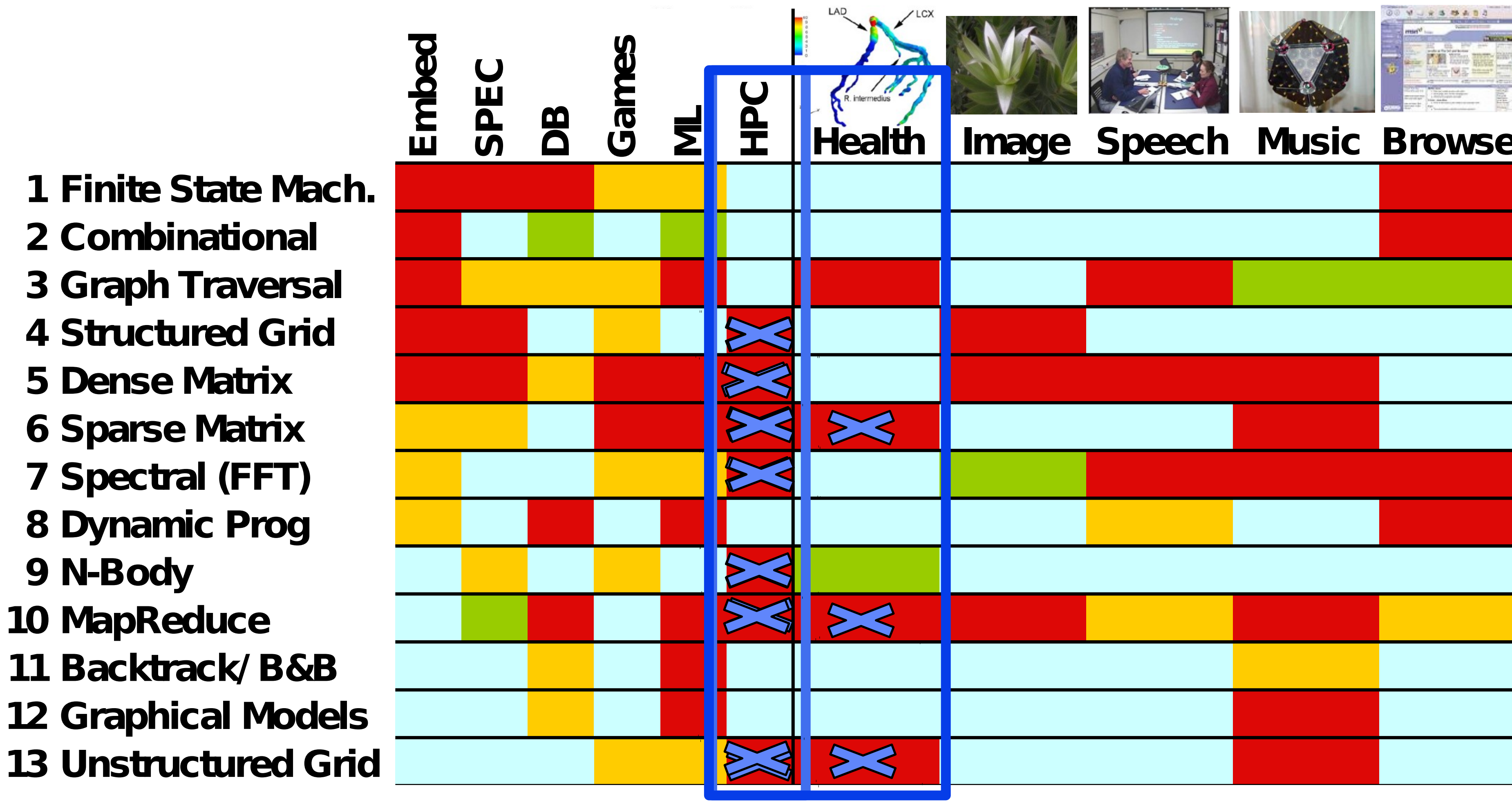
Summary – sources of parallelism and locality

- Current attempts to categorize main “kernels” dominating simulation codes
- “Seven Dwarfs” (P. Colella)
  - Structured grids
    - including locally structured grids, as in AMR
  - Unstructured grids
  - Spectral methods (Fast Fourier Transform)
  - Dense Linear Algebra
  - Sparse Linear Algebra
    - Both explicit (SpMV) and implicit (solving)
  - Particle Methods
  - Monte Carlo/Embarrassing Parallelism/Map Reduce (easy!)

What do commercial and CSE applications have in common?

Motif/Dwarf: Common Computational Methods

(Red Hot → Blue Cool)



Extra Slides

CS267 Final Projects

- Project proposal
  - Teams of 3 students, typically across departments
  - Interesting parallel application or system
  - Conference-quality paper
  - High performance is key:
    - Understanding performance, tuning, scaling, etc.
    - More important than the difficulty of problem
- Leverage
  - Projects in other classes (but discuss with me first)
  - Research projects

Project Ideas (from 2009)

- Applications
  - Implement existing sequential or shared memory program on distributed memory
  - Investigate SMP trade-offs (using only MPI versus MPI and thread based parallelism)
- Tools and Systems
  - Effects of reordering on sparse matrix factoring and solves
- Numerical algorithms
  - Improved solver for immersed boundary method
  - Use of multiple vectors (blocked algorithms) in iterative solvers

Project Ideas (from 2009)

- Novel computational platforms
  - Exploiting hierarchy of SMP-clusters in benchmarks
  - Computing aggregate operations on ad hoc networks (Culler)
  - Push/explore limits of computing on “the grid”
  - Performance under failures
- Detailed benchmarking and performance analysis, including identification of optimization opportunities
  - Titanium
  - UPC
  - IBM SP (Blue Horizon)

Phillip Colella's "Seven dwarfs"

High-end simulation in the physical sciences = 7 numerical methods:

1. Structured Grids (including locally structured grids, e.g. AMR)
2. Unstructured Grids
3. Fast Fourier Transform
4. Dense Linear Algebra
5. Sparse Linear Algebra
6. Particles
7. Monte Carlo

- Add 4 for embedded
  8. Search/Sort
  9. Finite State Machine
  10. Filter
  11. Combinational logic
- Then covers all 41 EEMBC benchmarks
- Revise 1 for SPEC
  - 7. Monte Carlo => Easily parallel (to add ray tracing)
- Then covers 26 SPEC benchmarks

Well-defined targets from algorithmic, software, and architecture standpoint

Slide from "Defining Software Requirements for Scientific Computing", Phillip Colella, 2004

Implicit Methods and Eigenproblems

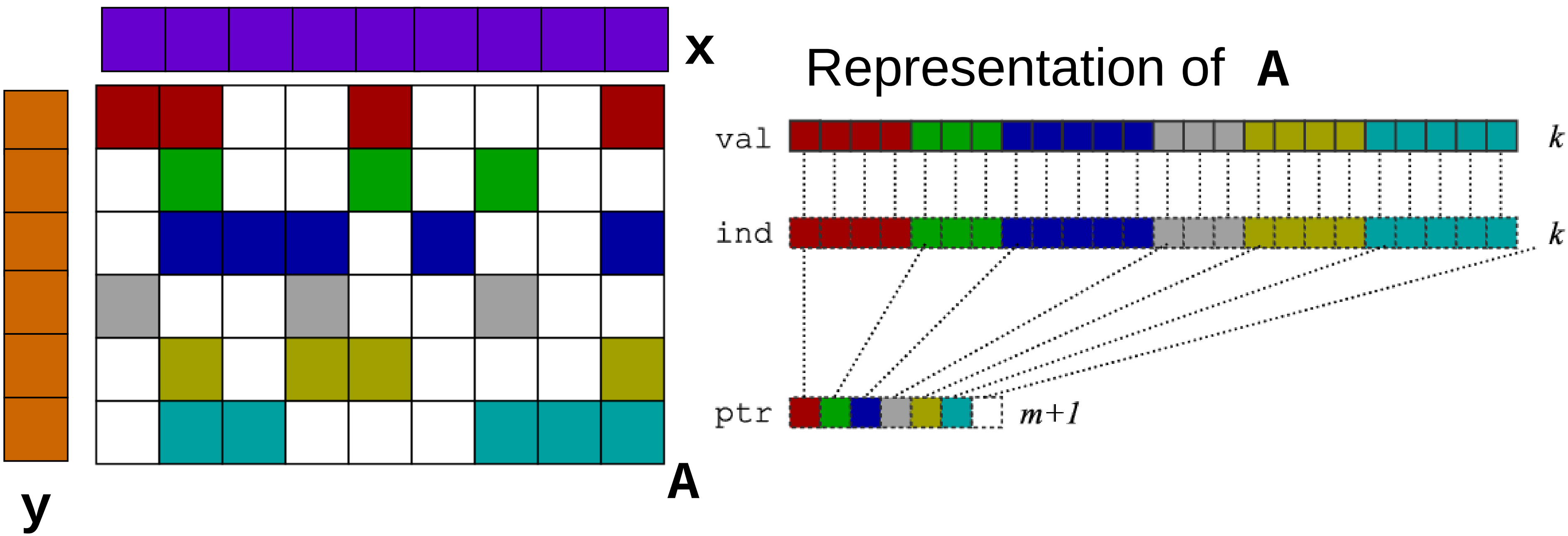
- Implicit methods for ODEs solve linear systems
- Direct methods (Gaussian elimination)
  - Called LU Decomposition, because we factor A = L*U.
  - Future lectures will consider both dense and sparse cases.
  - More complicated than sparse-matrix vector multiplication.
- Iterative solvers
  - Will discuss several of these in future.
    - Jacobi, Successive over-relaxation (SOR) , Conjugate Gradient (CG), Multigrid,...
  - Most have sparse-matrix-vector multiplication in kernel.
- Eigenproblems
  - Future lectures will discuss dense and sparse cases.
  - Also depend on sparse-matrix-vector multiplication, direct methods.

ODEs and Sparse Matrices

- All these problems reduce to sparse matrix problems
  - Explicit: sparse matrix-vector multiplication (SpMV).
  - Implicit: solve a sparse linear system
    - direct solvers (Gaussian elimination).
    - iterative solvers (use sparse matrix-vector multiplication).
  - Eigenvalue/vector algorithms may also be explicit or implicit.
- Conclusion: SpMV is key to many ODE problems
  - Relatively simple algorithm to study in detail
  - Two key problems: locality and load balance

SpMV in Compressed Sparse Row (CSR) Format

CSR format is one of many possibilities

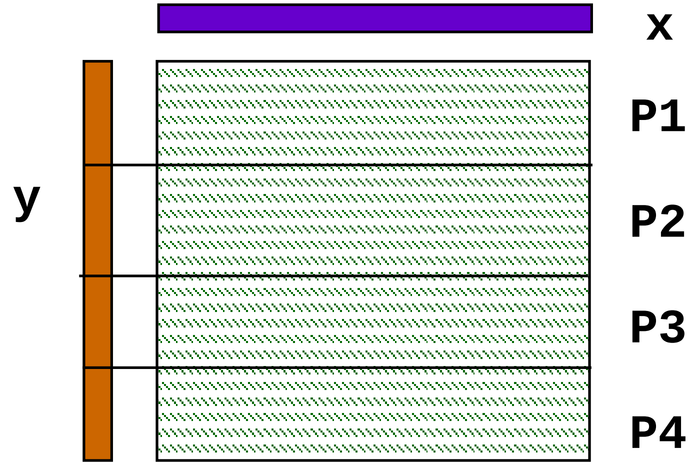


Matrix-vector multiply kernel: $y(i) \leftarrow y(i) + A(i,j) \cdot x(j)$

```
for each row i
  for k=ptr[i] to ptr[i+1] do
      y[i] = y[i] + val[k]*x[ind[k]]
```

Parallel Sparse Matrix-vector multiplication

- y = A*x, where A is a sparse n x n matrix

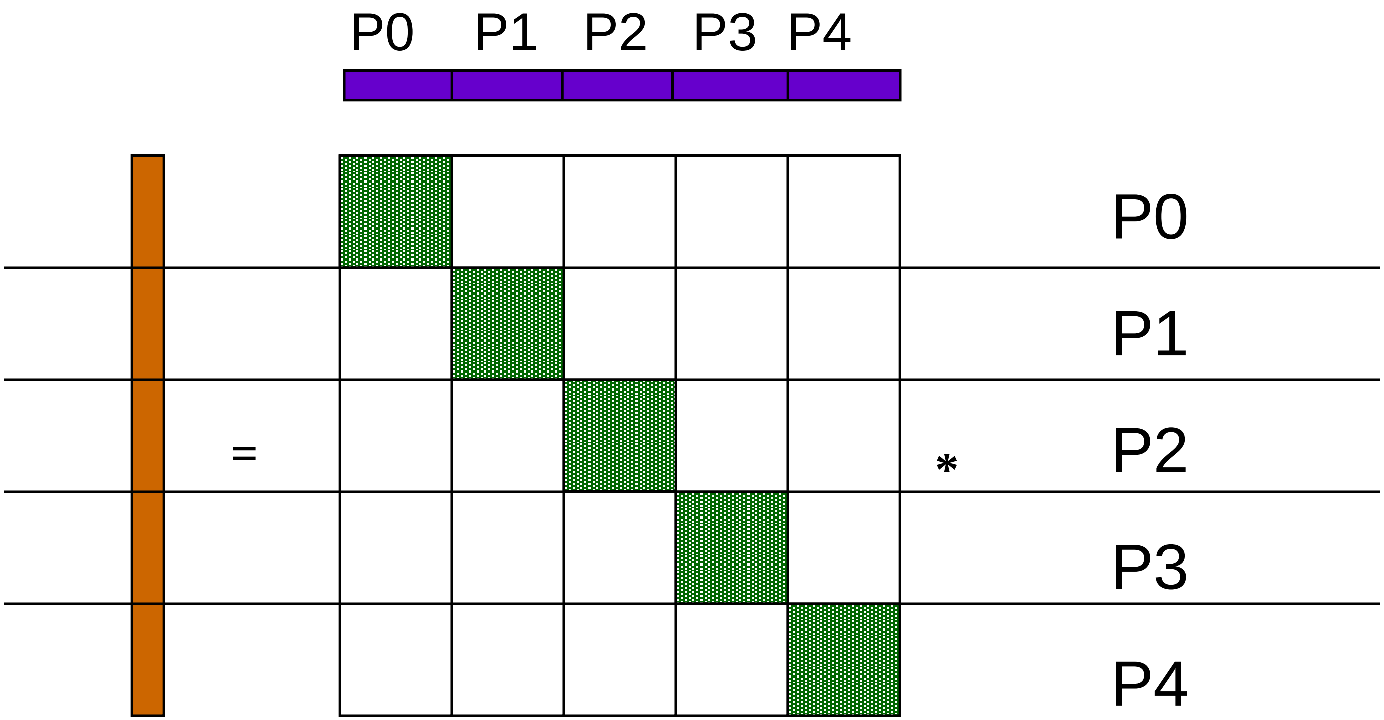


- Questions
  - which processors store
    - y[i], x[i], and A[i,j]
  - which processors compute
    - y[i] = sum (from 1 to n) A[i,j] * x[j]
      = (row i of A) * x   … a sparse dot product
- Partitioning
  - Partition index set {1,…,n} = N1 ∪ N2 ∪ … ∪ Np.
  - For all i in Nk, Processor k stores y[i], x[i], and row i of A
  - For all i in Nk, Processor k computes y[i] = (row i of A) * x
    - "owner computes" rule: Processor k compute the y[i]s it owns.

May require communication

Matrix Reordering via Graph Partitioning

- "Ideal" matrix structure for parallelism: block diagonal
  - p (number of processors) blocks, can all be computed locally.
  - If no non-zeros outside these blocks, no communication needed
- Can we reorder the rows/columns to get close to this?
  - Most nonzeros in diagonal blocks, few outside



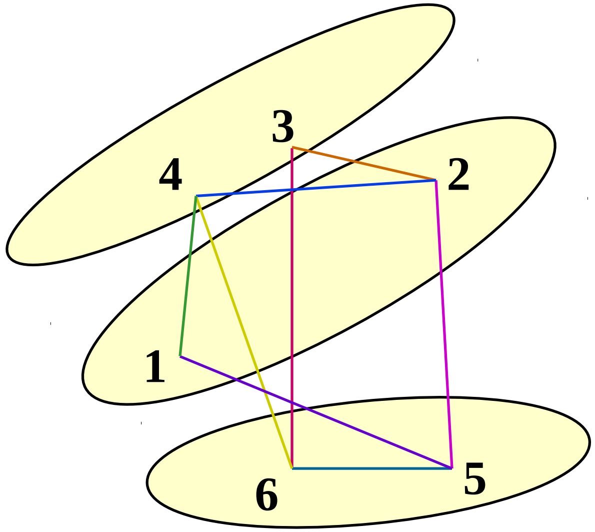
Goals of Reordering

- Performance goals
  - balance load (how is load measured?).
    - Approx equal number of nonzeros (not necessarily rows)
  - balance storage (how much does each processor store?).
    - Approx equal number of nonzeros
  - minimize communication (how much is communicated?).
    - Minimize nonzeros outside diagonal blocks
    - Related optimization criterion is to move nonzeros near diagonal
  - improve register and cache re-use
    - Group nonzeros in small vertical blocks so source (x) elements loaded into cache or registers may be reused (temporal locality)
    - Group nonzeros in small horizontal blocks so nearby source (x) elements in the cache may be used (spatial locality)
- Other algorithms reorder for other reasons
  - Reduce # nonzeros in matrix after Gaussian elimination
  - Improve numerical stability

Graph Partitioning and Sparse Matrices

- Relationship between matrix and graph

	1	2	3	4	5	6
1	1			1	1	
2		1	1	1	1	
3		1	1			1
4	1	1		1		1
5	1	1			1	1
6			1	1	1	1

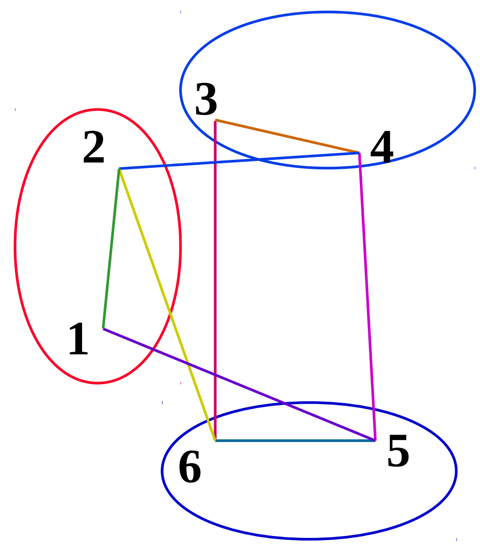


- Edges in the graph are nonzero in the matrix: here the matrix is symmetric (edges are unordered) and weights are equal (1)
- If divided over 3 procs, there are 14 nonzeros outside the diagonal blocks, which represent the 7 (bidirectional) edges

Graph Partitioning and Sparse Matrices

- Relationship between matrix and graph

	1	2	3	4	5	6
1	1	1			1	
2	1	1		1		1
3			1	1		1
4		1	1	1	1	
5	1			1	1	1
6		1	1		1	1



- A “good” partition of the graph has
  - equal (weighted) number of nodes in each part (load and storage balance).
  - minimum number of edges crossing between (minimize communication).
- Reorder the rows/columns by putting all nodes in one partition together.