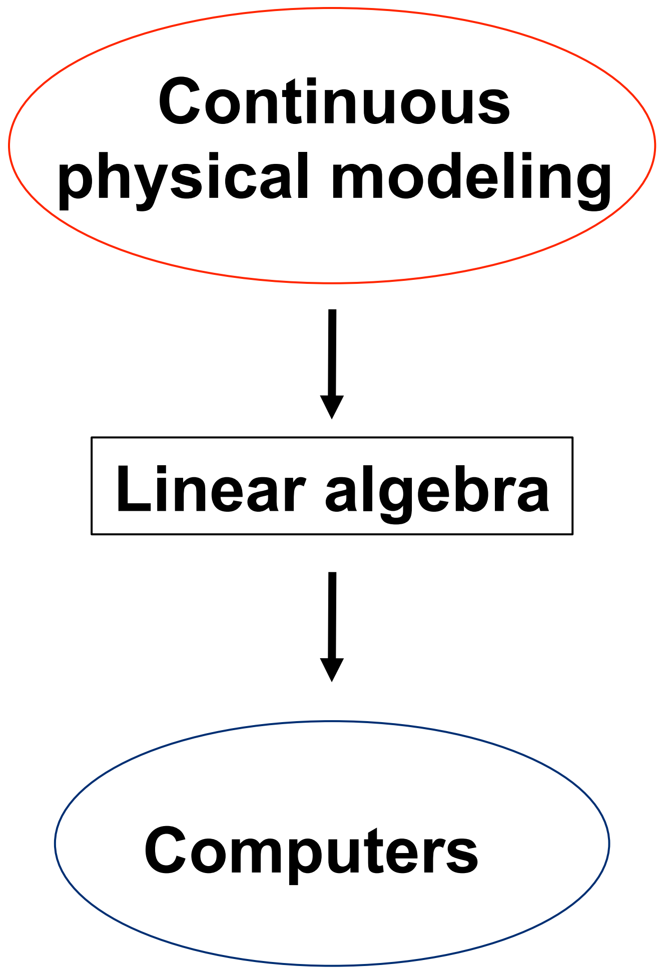
# *Conjugate gradients, sparse matrix-vector multiplication, graphs, and meshes*

Thanks to Aydin Buluc, Umit Catalyurek, Alan Edelman, and Kathy Yelick for some of these slides.

# *The middleware of scientific computing*



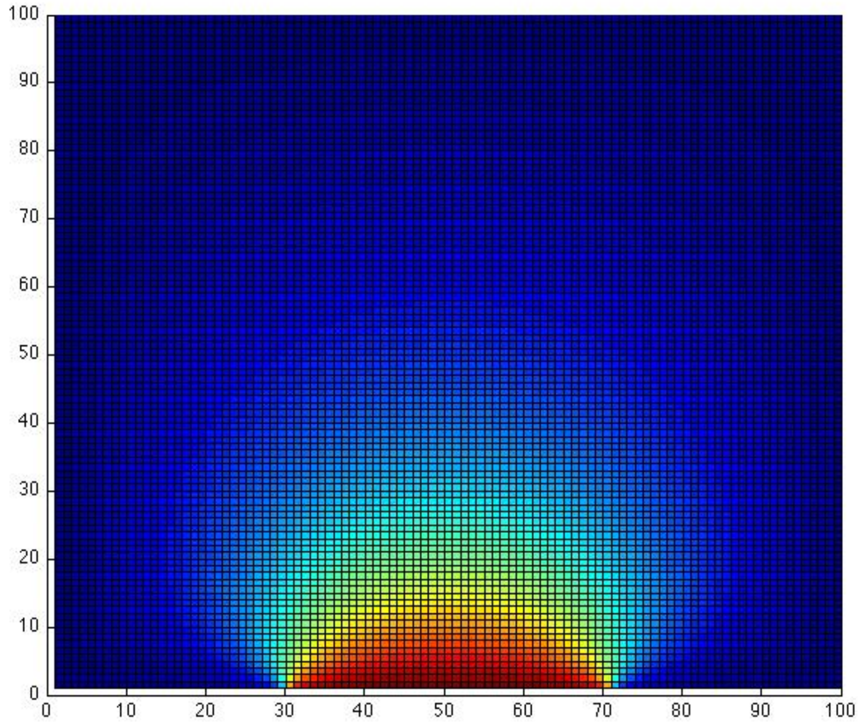

$$Ax = b$$

## *Example:  The Temperature Problem*

- A cabin in the snow
- Wall temperature is 0°, except for a radiator at 100°
- What is the temperature in the interior?

# *Example:  The Temperature Problem*

- A cabin in the snow (a square region ☺)
- Wall temperature is 0°, except for a radiator at 100°
- What is the temperature in the interior?



# The physics: Poisson's equation

$$\nabla^2 u(x,y) \equiv \frac{\partial^2 u}{\partial x^2}(x,y) + \frac{\partial^2 u}{\partial y^2}(x,y) = f(x,y)$$

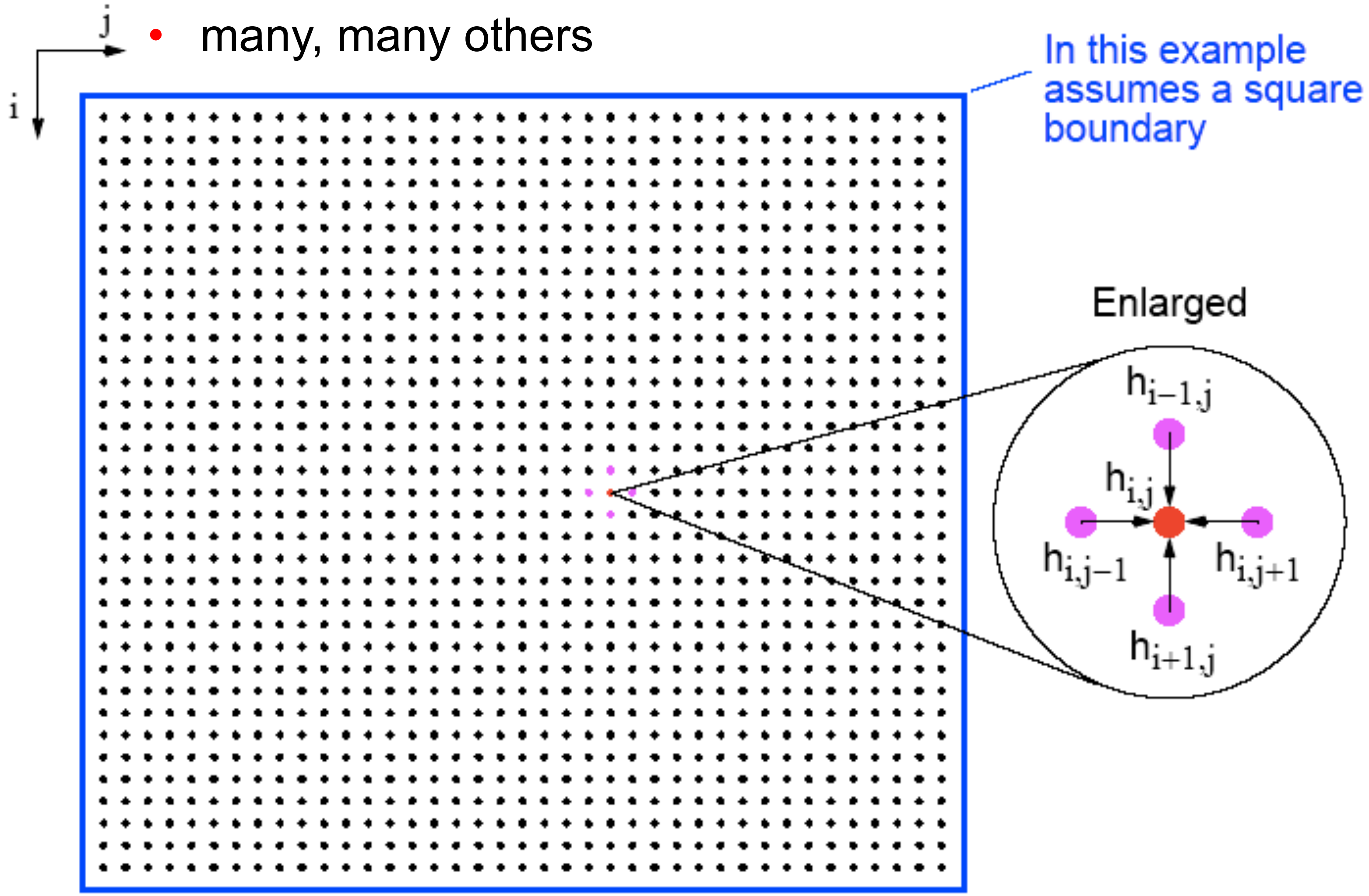
for $(x,y) \in R = \{ (x,y) \mid a < x < b,\ c < y < d \}$, and

$$u(x,y) = g(x,y)$$

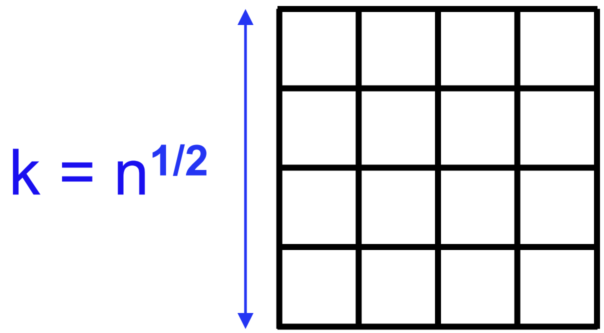
for $(x,y)$ on the boundary of $R$.

# Many Physical Models Use Stencil Computations

- PDE models of heat, fluids, structures, …
- Weather, airplanes, bridges, bones, …
- Game of Life
- many, many others



# *Model Problem: Solving Poisson's equation for temperature*



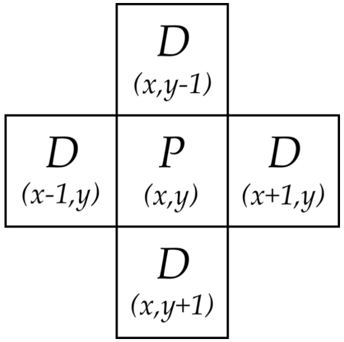

- Discrete approximation to Poisson's equation:

$$t(i) = \frac{1}{4}\left( t(i-k) + t(i-1) + t(i+1) + t(i+k) \right)$$

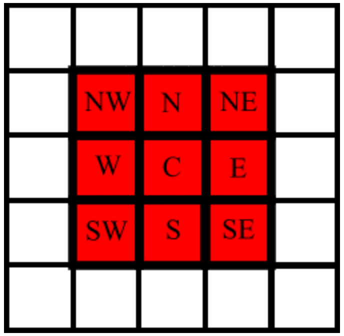
- Intuitively:

Temperature at a point is the average
of the temperatures at surrounding points

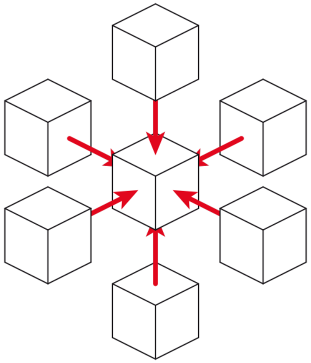
# Examples of stencils



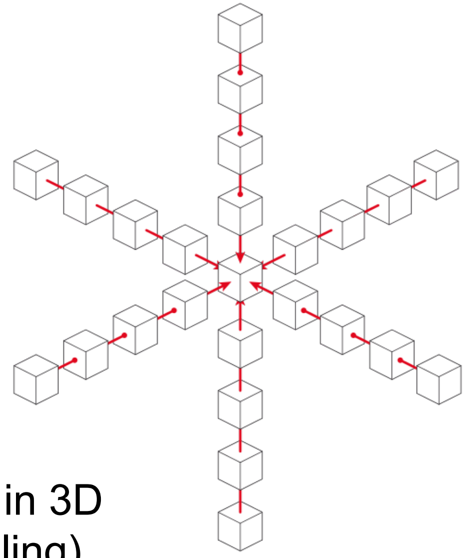

5-point stencil in 2D
(temperature problem)




9-point stencil in 2D
(game of Life)



7-point stencil in 3D
(3D temperature problem)

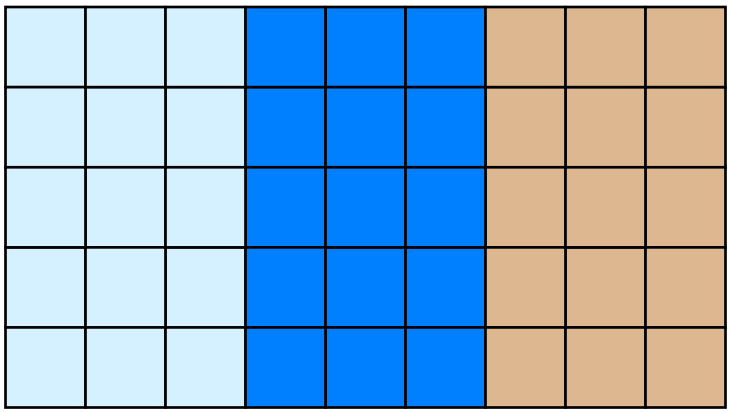


25-point stencil in 3D
(seismic modeling)

… and many more

# *Parallelizing Stencil Computations*

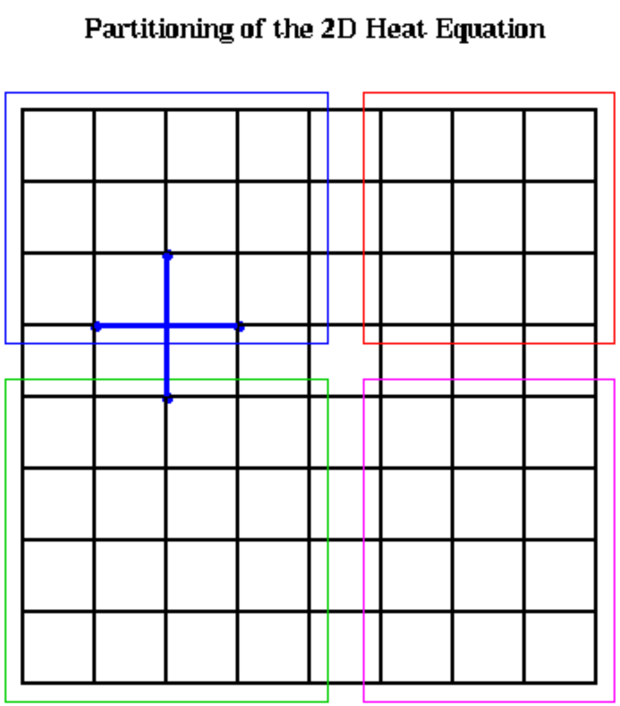
- Parallelism is simple
  - Grid is a regular data structure
  - Even decomposition across processors gives load balance
- Spatial locality limits communication cost
  - Communicate only boundary values from neighboring patches



- Communication volume
  - v = total # of boundary cells between patches

# *Two-dimensional block decomposition*

- n mesh cells, p processors
- Each processor has a patch of n/p cells
- Block row (or block col) layout: v = 2 * p * sqrt(n)
- 2-dimensional block layout: v = 4 * sqrt(p) * sqrt(n)



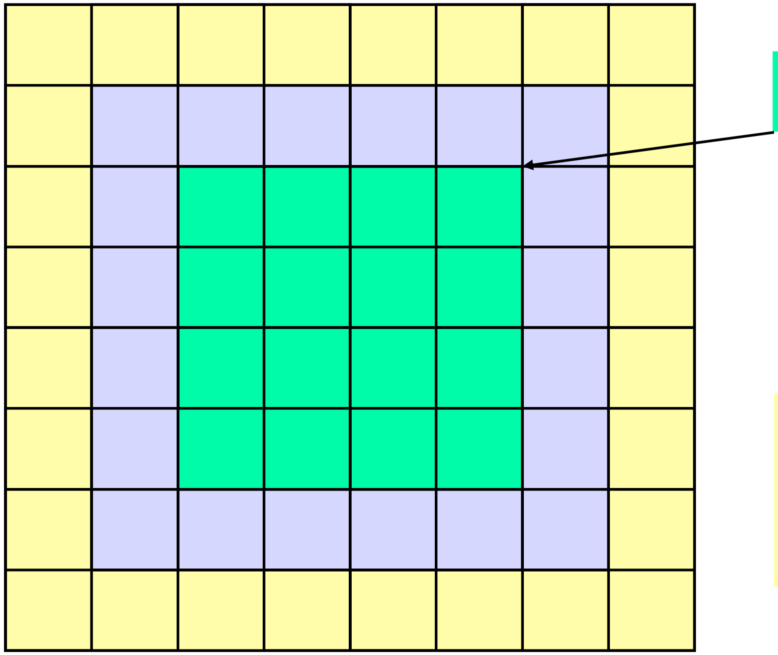
# Detailed complexity measures for data movement I: Latency/Bandwidth Model

<u>Moving data between processors by message-passing</u>

- Machine parameters:
  - $\alpha$ or $t_{startup}$ latency (message startup time in seconds)
  - $\beta$ or $t_{data}$ inverse bandwidth (in seconds per word)
  - between nodes of Triton, $\alpha \sim 2.2 \times 10^{-6}$ and $\beta \sim 6.4 \times 10^{-9}$
- Time to send & recv or bcast a message of $w$ words: $\alpha + w*\beta$
- $t_{comm}$ total commmunication time
- $t_{comp}$ total computation time
- Total parallel time: $t_p = t_{comp} + t_{comm}$

# Ghost Nodes in Stencil Computations

Comm cost = $\alpha$ * (#messages) + $\beta$ * (total size of messages)



**Green = my interior nodes**

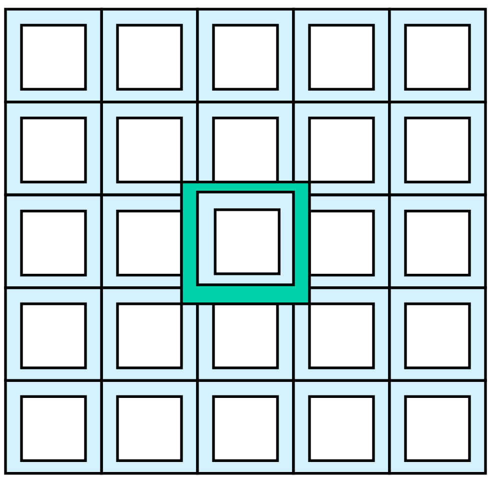
**Blue = my boundary nodes**

**Yellow**
**= neighbors' boundary nodes**
**= my "ghost nodes"**

- Keep a ghost copy of neighbors' boundary nodes
- Communicate every second iteration, not every iteration
- Reduces #messages, not total size of messages
- Costs extra memory and computation
- Can also use more than one layer of ghost nodes

# *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

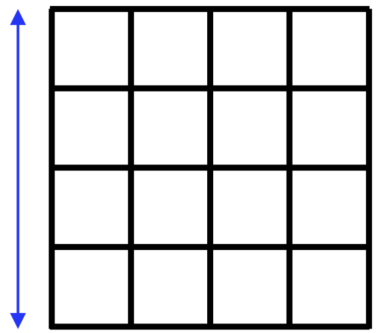


Implemented using "ghost" regions.

Adds memory overhead

# *Model Problem: Solving Poisson's equation for temperature*

$k = n^{1/2}$



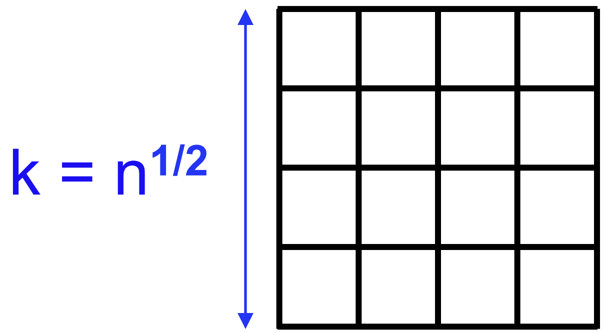
- Discrete approximation to Poisson's equation:

$$t(i) = \frac{1}{4} \left( t(i-k) + t(i-1) + t(i+1) + t(i+k) \right)$$

- Intuitively:

Temperature at a point is the average
of the temperatures at surrounding points

# *Model Problem: Solving Poisson's equation for temperature*



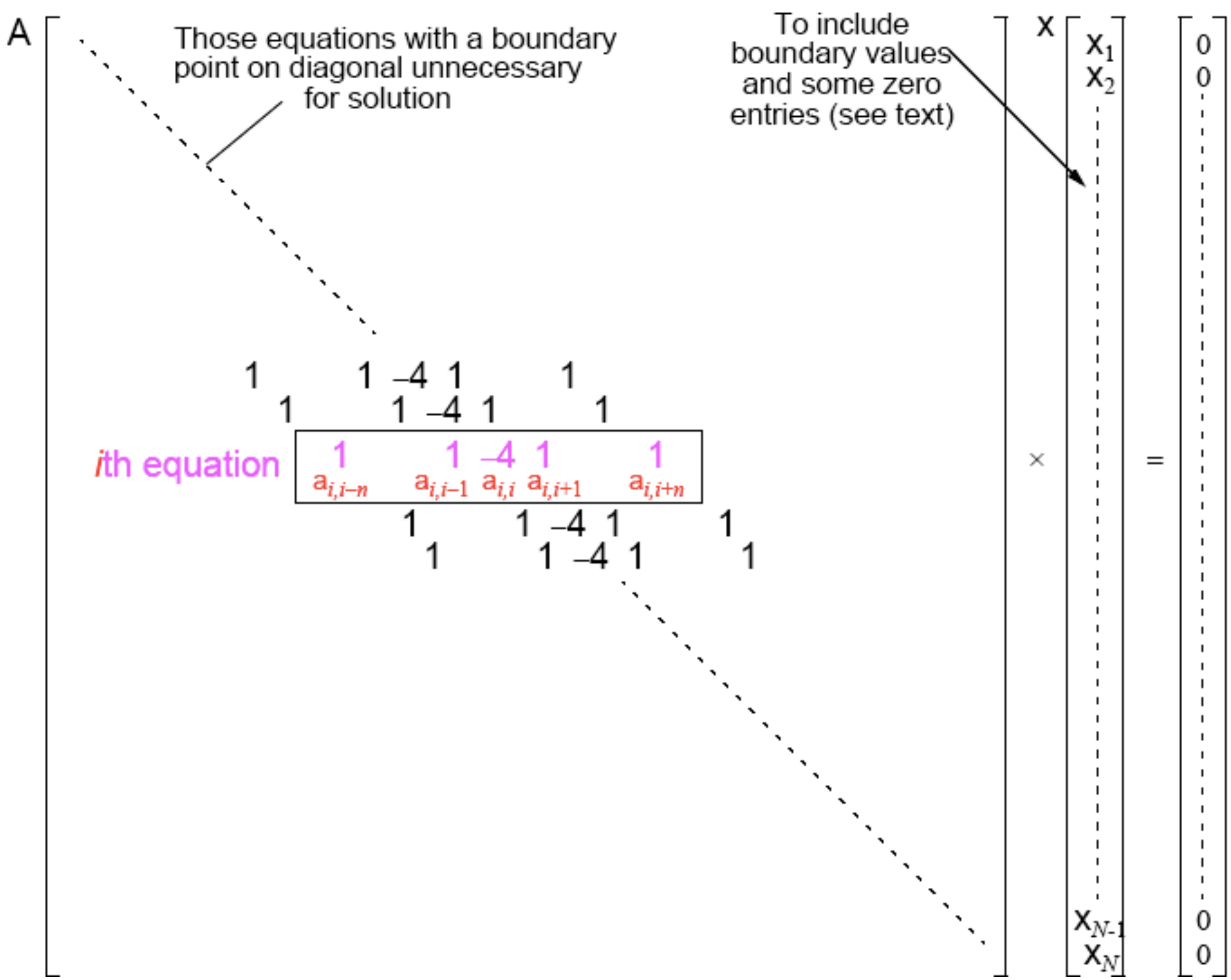

- For each i from 1 to n, except on the boundaries:

$$-t(i-k) - t(i-1) + 4*t(i) - t(i+1) - t(i+k) = 0$$

- n equations in n unknowns: A*t = b
- Each row of A has at most 5 nonzeros
- In three dimensions, $k = n^{1/3}$ and each row has at most 7 nzs

# A Stencil Computation Solves a System of Linear Equations

- Solve $Ax = b$ for $x$
- Matrix $A$, right-hand side vector $b$, unknown vector $x$
- $A$ is *sparse*: most of the entries are 0



# Conjugate gradient iteration to solve A*x=b

$x_0 = 0, \quad r_0 = b, \quad d_0 = r_0$ (these are all <u>vectors</u>)

**<u>for</u>** $k = 1, 2, 3, \ldots$

$\alpha_k = (r^T_{k-1} r_{k-1}) / (d^T_{k-1} A d_{k-1})$ step length

$x_k = x_{k-1} + \alpha_k d_{k-1}$ approximate solution

$r_k = r_{k-1} - \alpha_k A d_{k-1}$ residual = $b - Ax_k$

$\beta_k = (r^T_k r_k) / (r^T_{k-1} r_{k-1})$ improvement

$d_k = r_k + \beta_k d_{k-1}$ search direction

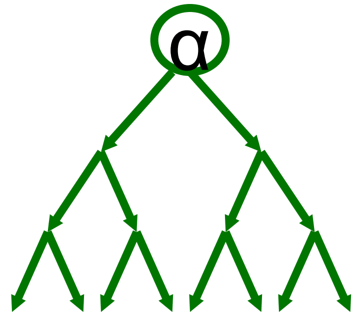
- One matrix-vector multiplication per iteration
- Two vector dot products per iteration
- Four n-vectors of working storage

# *Vector and matrix primitives for CG*

- DAXPY: $v = \alpha^*v + \beta^*w$ (vectors v, w; scalars α, β)
  - Broadcast the scalars α and β, then independent * and +
  - comm volume = 2p, span = log n
- DDOT: $\alpha = v^T{}^*w = \Sigma_j v[j]^*w[j]$ (vectors v, w; scalar α)
  - Independent *, then + reduction
  - comm volume = p, span = log n
- Matvec: $v = A^*w$ (matrix A, vectors v, w)
  - The hard part
  - But all you need is a subroutine to compute v from w
  - Sometimes you don't need to store A (e.g. temperature problem)
  - Usually you do need to store A, but it's *sparse* ...

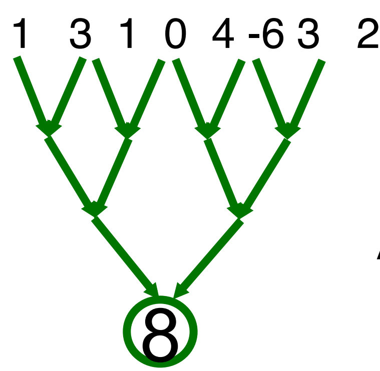
# *Broadcast and reduction*

- Broadcast of 1 value to p processors in log p time




Broadcast

- Reduction of p values to 1 in log p time
- Takes advantage of associativity in +, *, min, max, etc.




Add-reduction

# *Where's the data (temperature problem)?*

- The matrix A: Nowhere!!

- The vectors x, b, r, d:
  - Each vector is one value per stencil point
  - Divide stencil points among processors, n/p points each

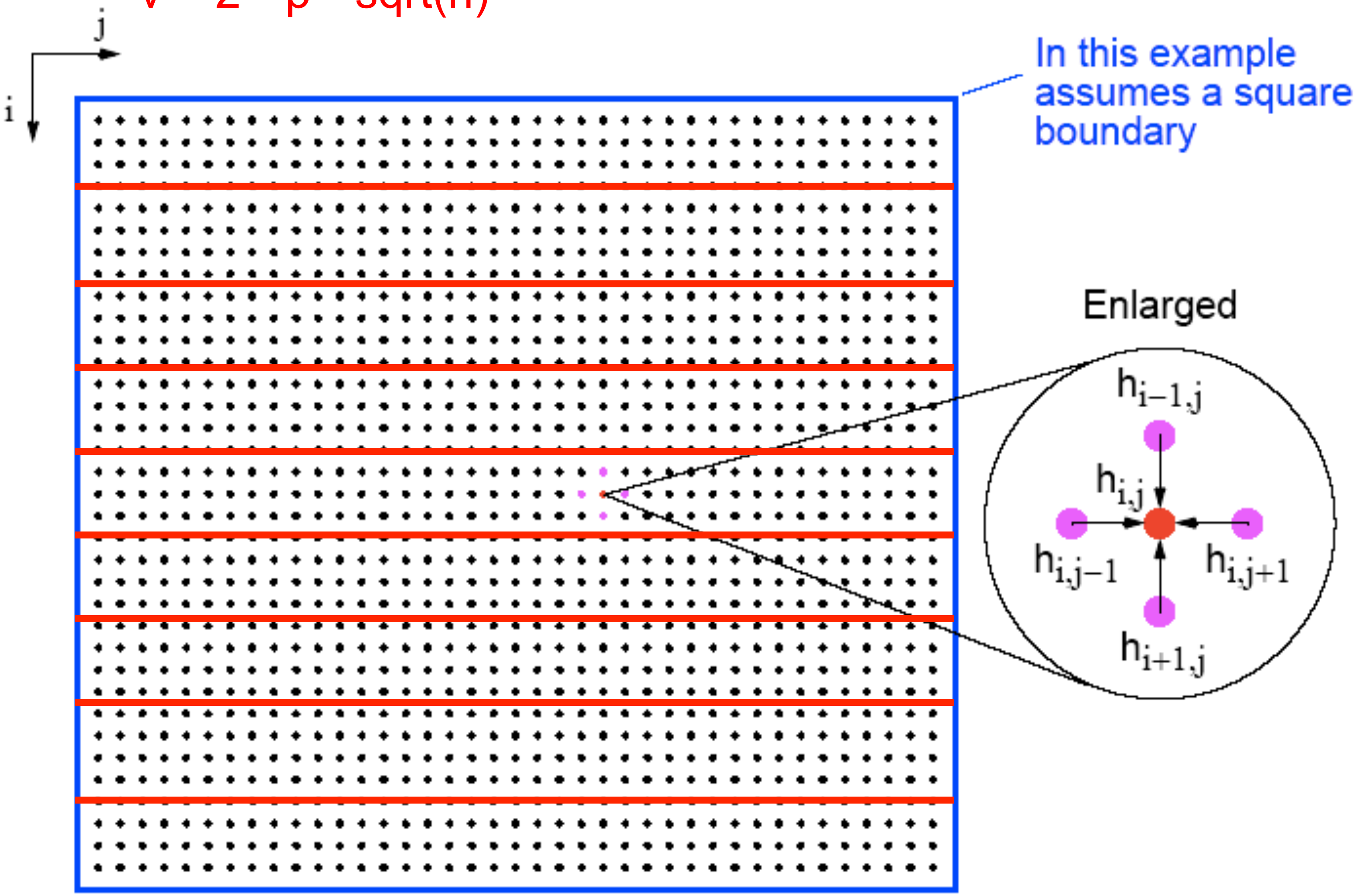
- How do you divide up the sqrt(n) by sqrt(n) region of points?

- Block row (or block col) layout: v = 2 * p * sqrt(n)

- 2-dimensional block layout: v = 4 * sqrt(p) * sqrt(n)

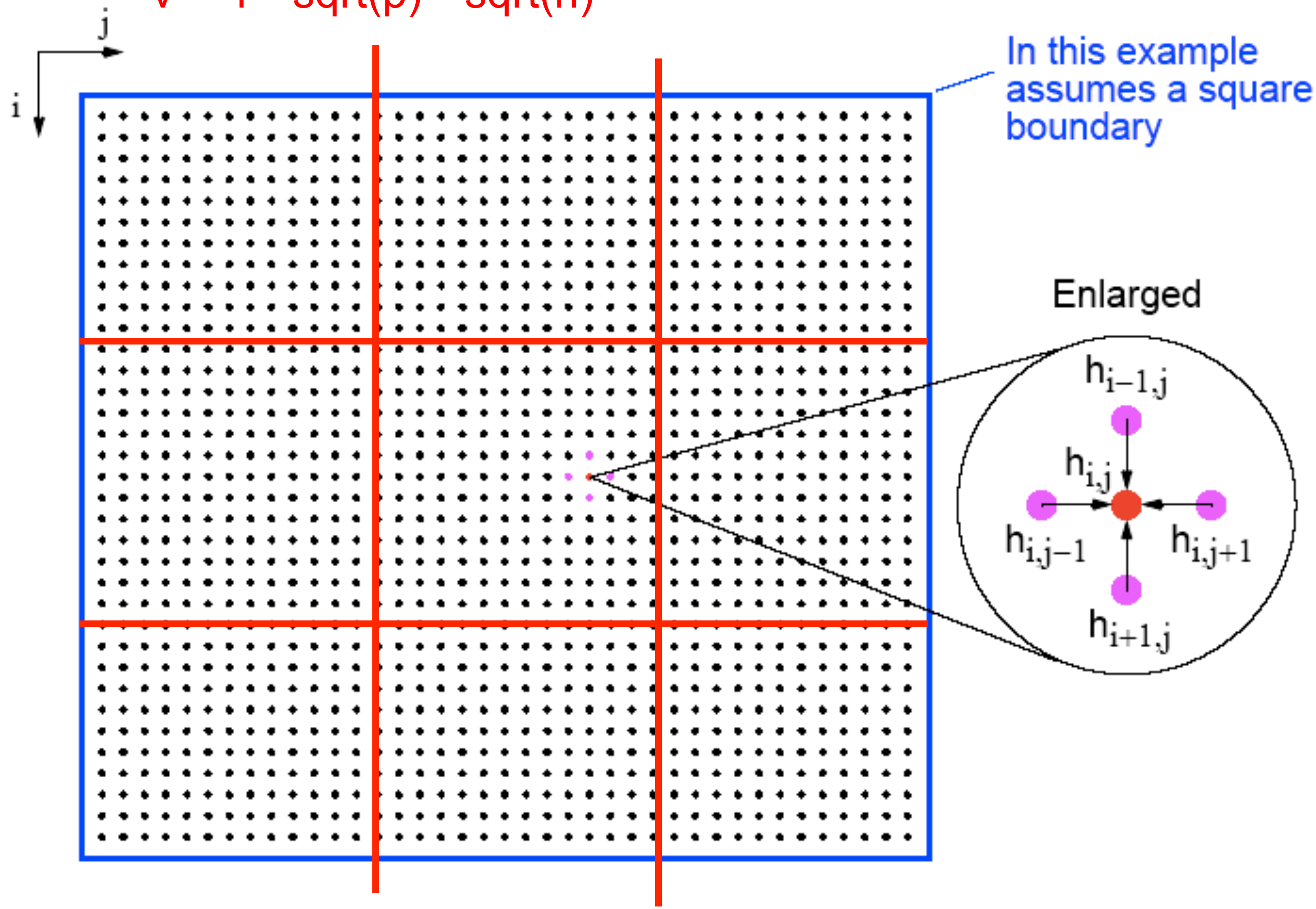
# How do you partition the sqrt(n) by sqrt(n) stencil points?

- First version: number the grid by rows
- Leads to a block row decomposition of the region
- v = 2 * p * sqrt(n)



# How do you partition the sqrt(n) by sqrt(n) stencil points?

- Second version: 2D block decomposition
- Numbering is a little more complicated
- v = 4 * sqrt(p) * sqrt(n)



# *Where's the data (temperature problem)?*

- The matrix A: Nowhere!!
- The vectors x, b, r, d:
  - Each vector is one value per stencil point
  - Divide stencil points among processors, n/p points each
- How do you divide up the sqrt(n) by sqrt(n) region of points?
- Block row (or block col) layout: v = 2 * p * sqrt(n)
- 2-dimensional block layout: v = 4 * sqrt(p) * sqrt(n)

# *The Landscape of Ax = b Algorithms*

| | Gaussian elimination | Iterative |
|---|---|---|
| Any matrix | **Pivoting LU** | **GMRES, BiCGSTAB, …** |
| Symmetric positive definite matrix | **Cholesky** | **Conjugate gradient** |

**More General** ↕ **More Robust**

**More Robust** ↔ **Less Storage**

# *Conjugate gradient in general*

- CG can be used to solve *any* system $Ax = b$, if …

# *Conjugate gradient in general*

- CG can be used to solve *any* system $Ax = b$, if …
- The matrix $A$ is *symmetric* ($a_{ij} = a_{ji}$) …
- … and *positive definite* (all eigenvalues > 0).

# Conjugate gradient in general

- CG can be used to solve *any* system $Ax = b$, if …
- The matrix $A$ is *symmetric* ($a_{ij} = a_{ji}$) …
- … and *positive definite* (all eigenvalues > 0).

- Symmetric positive definite matrices occur a lot in scientific computing & data analysis!

# *Conjugate gradient in general*

- CG can be used to solve *any* system $Ax = b$, if …
- The matrix $A$ is *symmetric* ($a_{ij} = a_{ji}$) …
- … and *positive definite* (all eigenvalues > 0).

- Symmetric positive definite matrices occur a lot in scientific computing & data analysis!

- But usually the matrix isn't just a stencil.
- Now we do need to store the matrix $A$. Where's the data?

# *Conjugate gradient in general*

- CG can be used to solve *any* system $Ax = b$, if …
- The matrix $A$ is *symmetric* ($a_{ij} = a_{ji}$) …
- … and *positive definite* (all eigenvalues > 0).

- Symmetric positive definite matrices occur a lot in scientific computing & data analysis!

- But usually the matrix isn't just a stencil.
- Now we do need to store the matrix $A$. Where's the data?

- The key is to use graph data structures and algorithms.

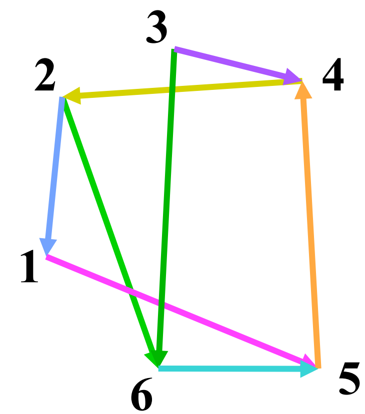
# *Vector and matrix primitives for CG*

- DAXPY: $v = \alpha * v + \beta * w$ (vectors v, w; scalars α, β)
  - Broadcast the scalars α and β, then independent * and +
  - comm volume = 2p, span = log n
- DDOT: $\alpha = v^T * w = \Sigma_j v[j] * w[j]$ (vectors v, w; scalar α)
  - Independent *, then + reduction
  - comm volume = p, span = log n
- Matvec: $v = A * w$ (matrix A, vectors v, w)
  - The hard part
  - But all you need is a subroutine to compute v from w
  - Sometimes you don't need to store A (e.g. temperature problem)
  - Usually you do need to store A, but it's *sparse* ...

# Graphs and Sparse Matrices

- Sparse matrix is a representation of a (sparse) graph

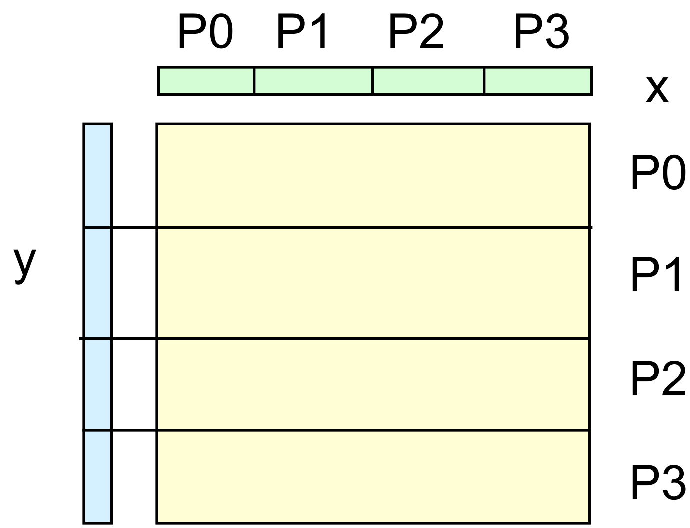
| | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| 1 | 1 | | | | 1 | |
| 2 | 1 | 1 | | | | 1 |
| 3 | | | 1 | 1 | | 1 |
| 4 | | 1 | | 1 | | |
| 5 | | | | 1 | 1 | |
| 6 | | | | | 1 | 1 |




- Matrix entries are edge weights
- Number of nonzeros per row is the vertex degree
- Edges represent data dependencies in matrix-vector multiplication

# Parallel Dense Matrix-Vector Product (Review)

- y = A*x, where A is a dense matrix




- Layout:
  - 1D by rows
- Algorithm:

  Foreach processor j

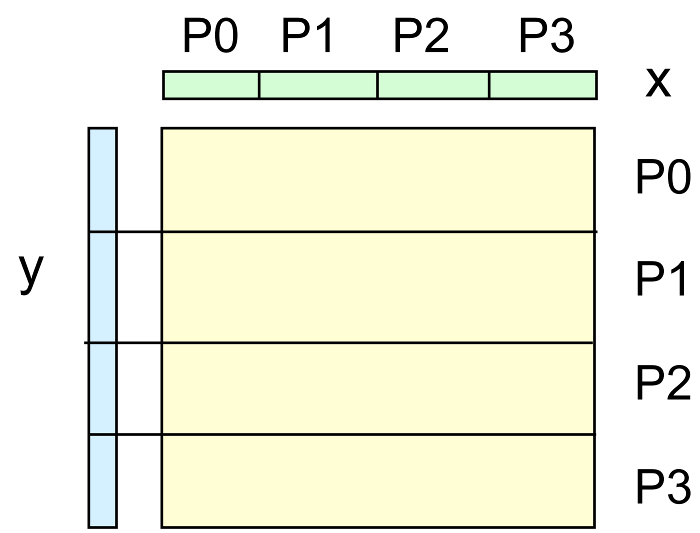
  Broadcast X(j)

  Compute A(p)*x(j)
- A(i) is the n by n/p block row that processor Pi owns
- Algorithm uses the formula

  $Y(i) = A(i)*X = \Sigma_j A(i)*X(j)$

# *Parallel sparse matrix-vector product*

- Lay out matrix and vectors by rows
- y(i) = sum(A(i,j)*x(j))
- Only compute terms with A(i,j) ≠ 0




- Algorithm

  Each processor i:

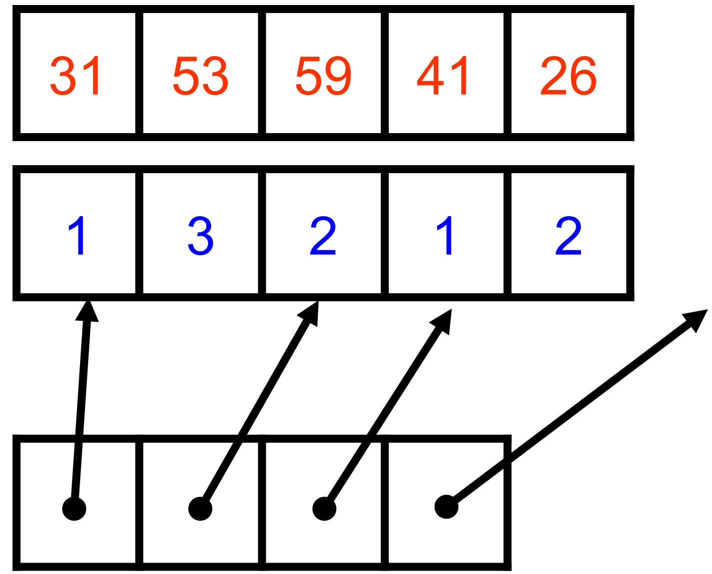
  Broadcast x(i)

  Compute y(i) = A(i,:)*x

- Optimizations
  - Only send each proc the parts of x it needs, to reduce comm
  - Reorder matrix for better locality by graph partitioning
  - Worry about balancing number of nonzeros / processor,
    if rows have very different nonzero counts

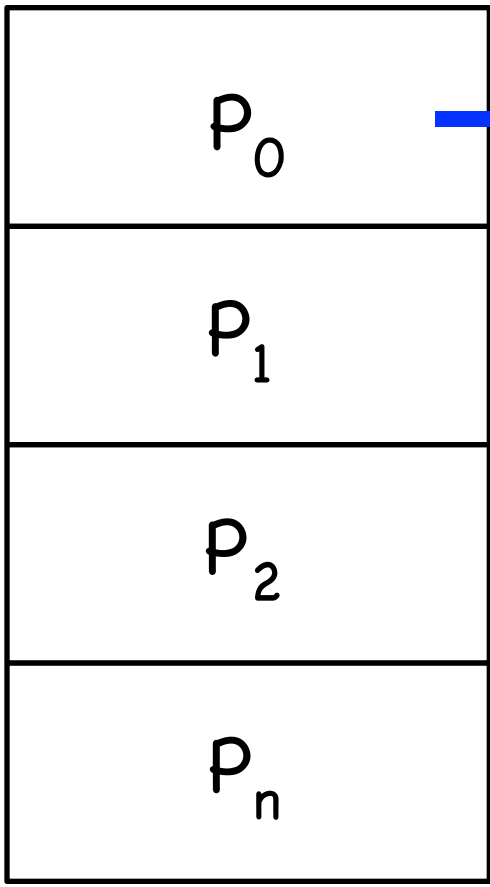
# *Data structure for sparse matrix A (stored by rows)*

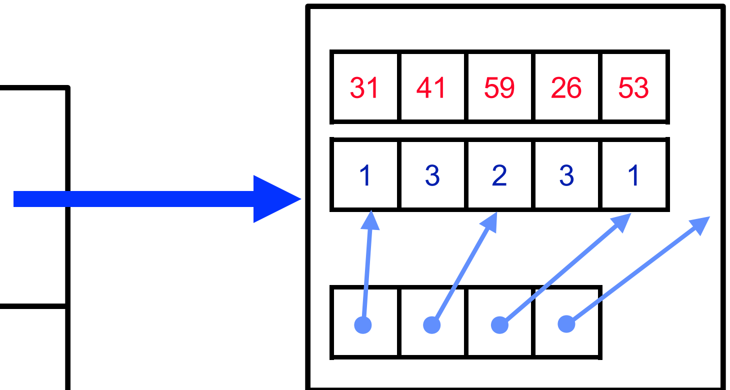
| | | |
|---|---|---|
| 31 | 0 | 53 |
| 0 | 59 | 0 |
| 41 | 26 | 0 |




- Full matrix:
  - 2-dimensional array of real or complex numbers
  - (nrows*ncols) memory
- Sparse matrix:
  - compressed row storage
  - about (2*nzs + nrows) memory

# Distributed-memory sparse matrix data structure

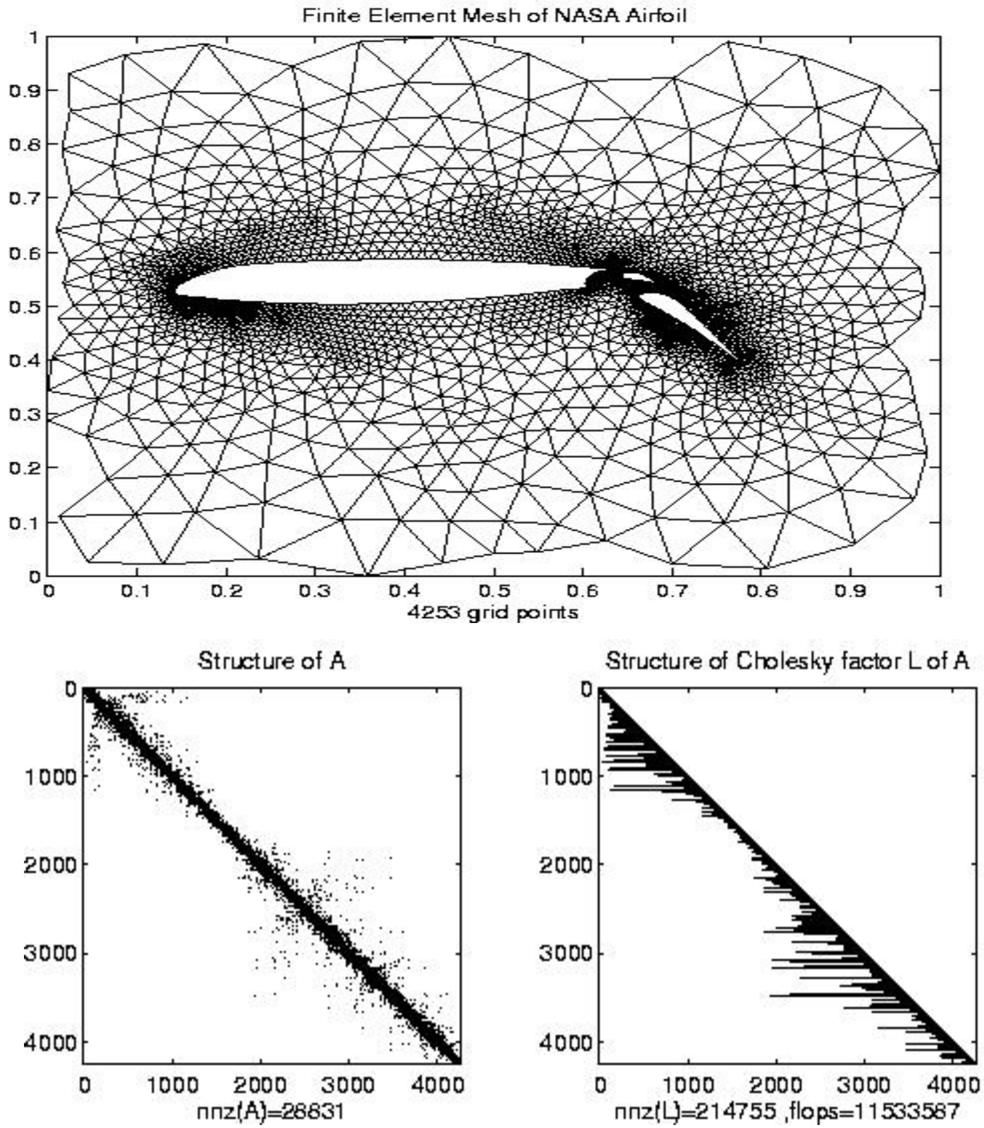


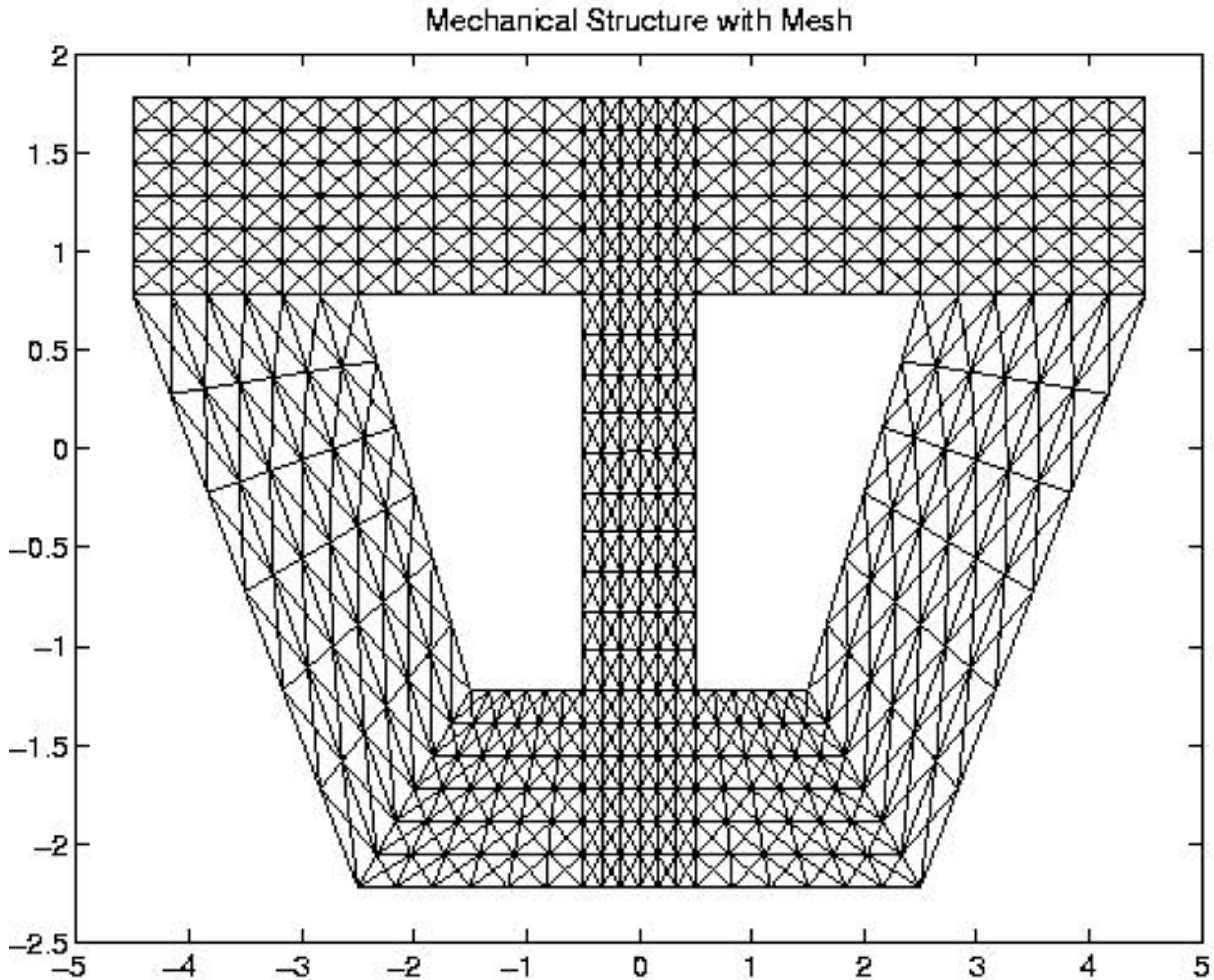

Each processor stores:

- # of local nonzeros
- range of local rows
- nonzeros in CSR form

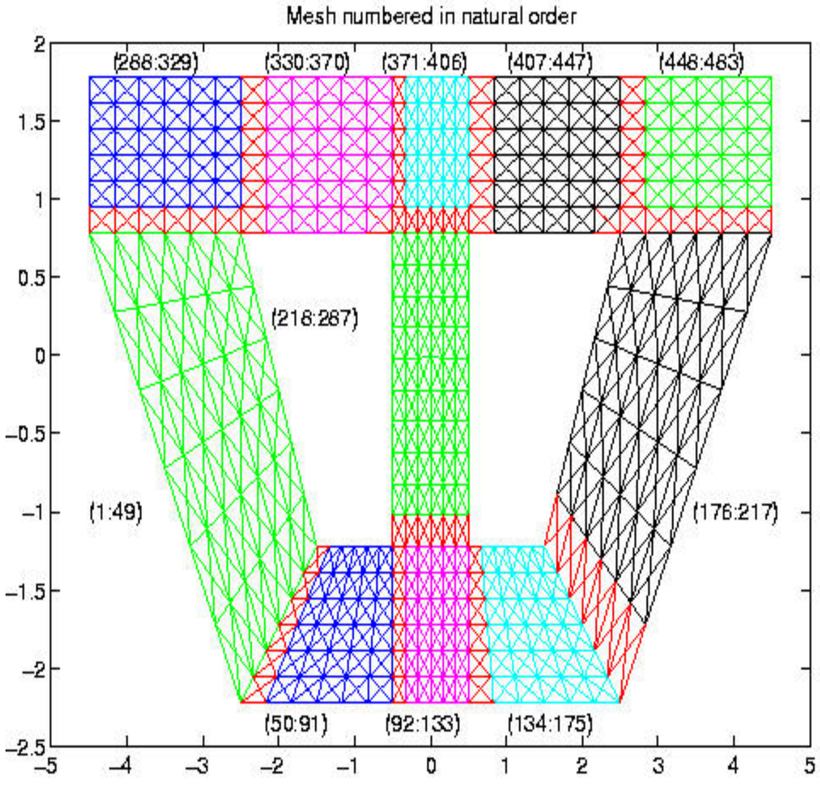
# *Irregular mesh: NASA Airfoil in 2D*

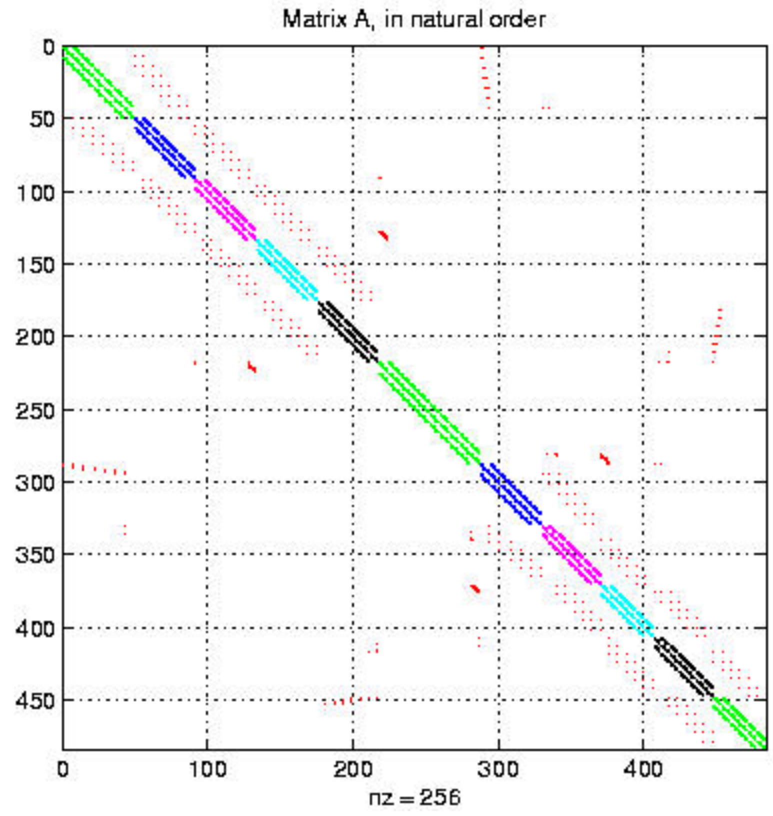


# *Composite Mesh from a Mechanical Structure*

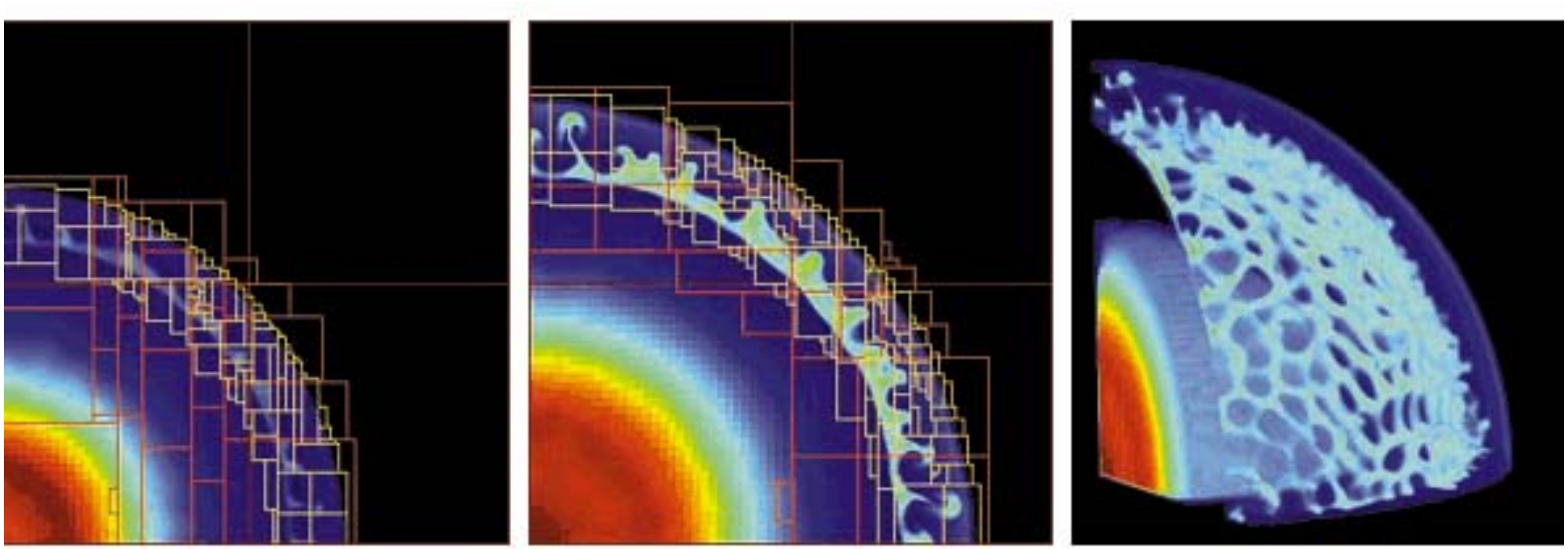


# Converting the Mesh to a Matrix



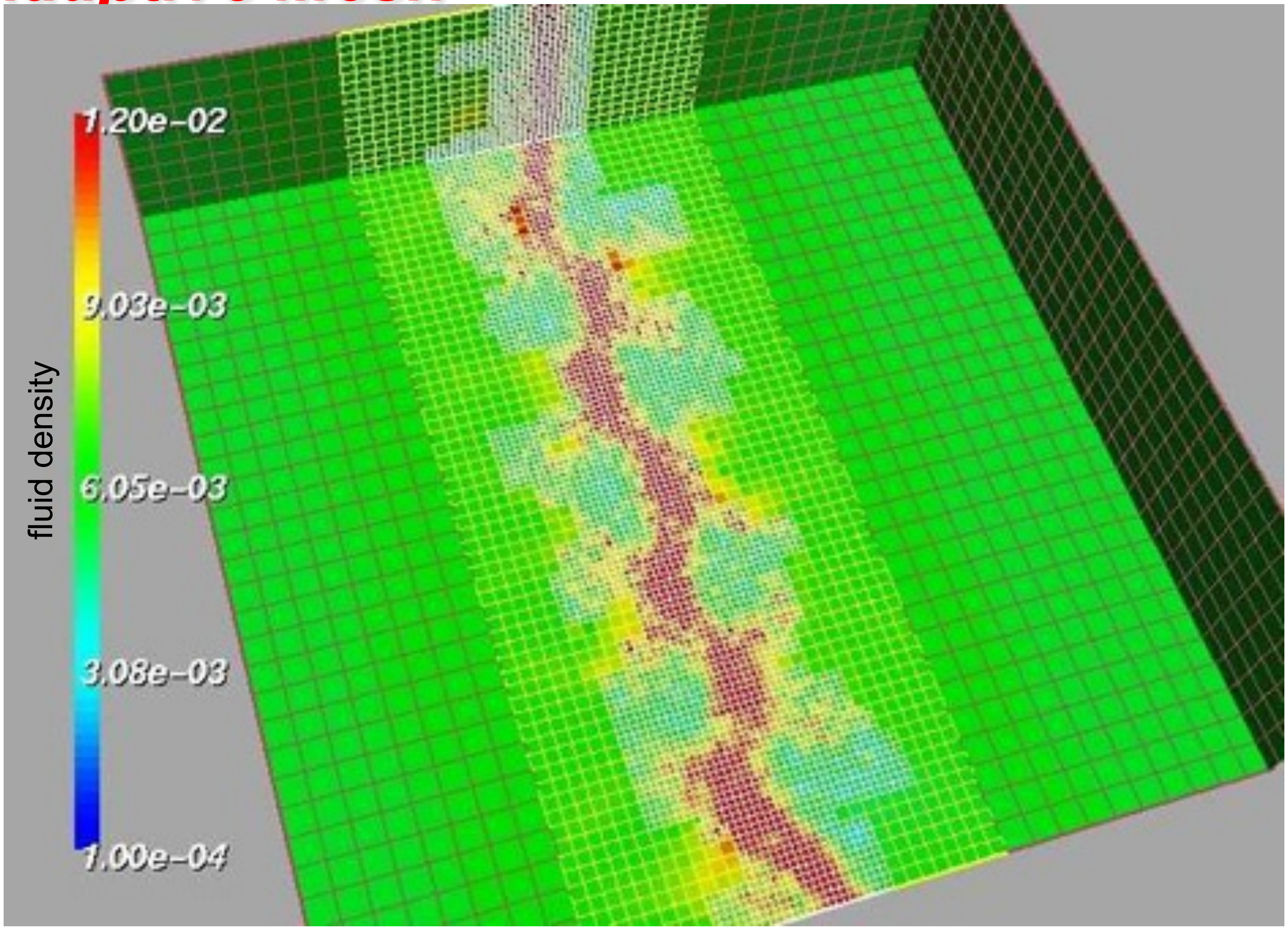



# *Adaptive Mesh Refinement (AMR)*



- Adaptive mesh around an explosion
- Refinement done by calculating errors

# Adaptive Mesh




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

# Irregular mesh: Tapered Tube (Multigrid)

Example of Prometheus meshes

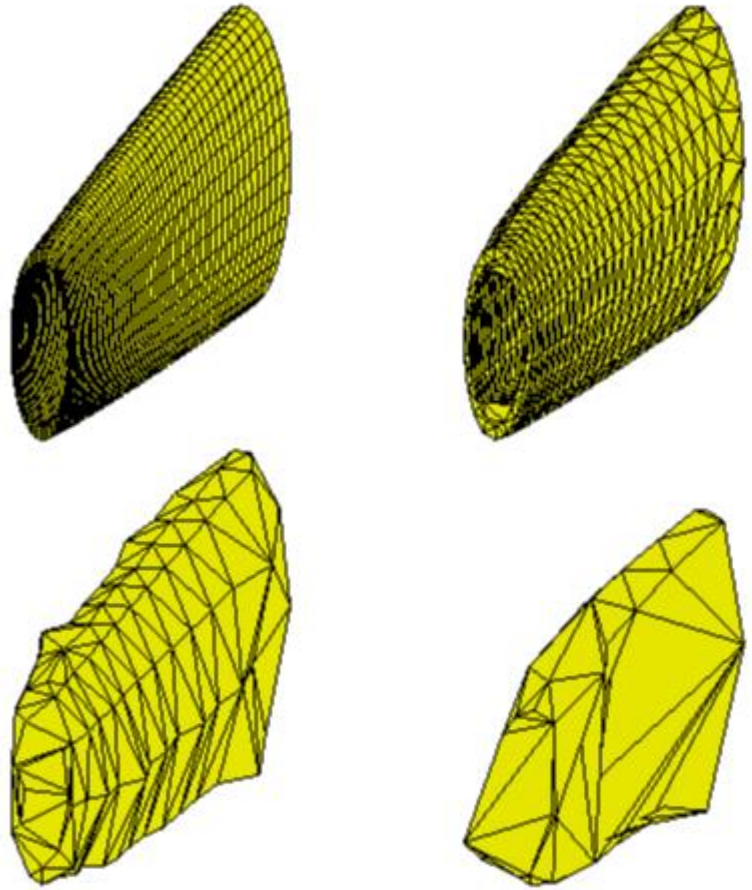
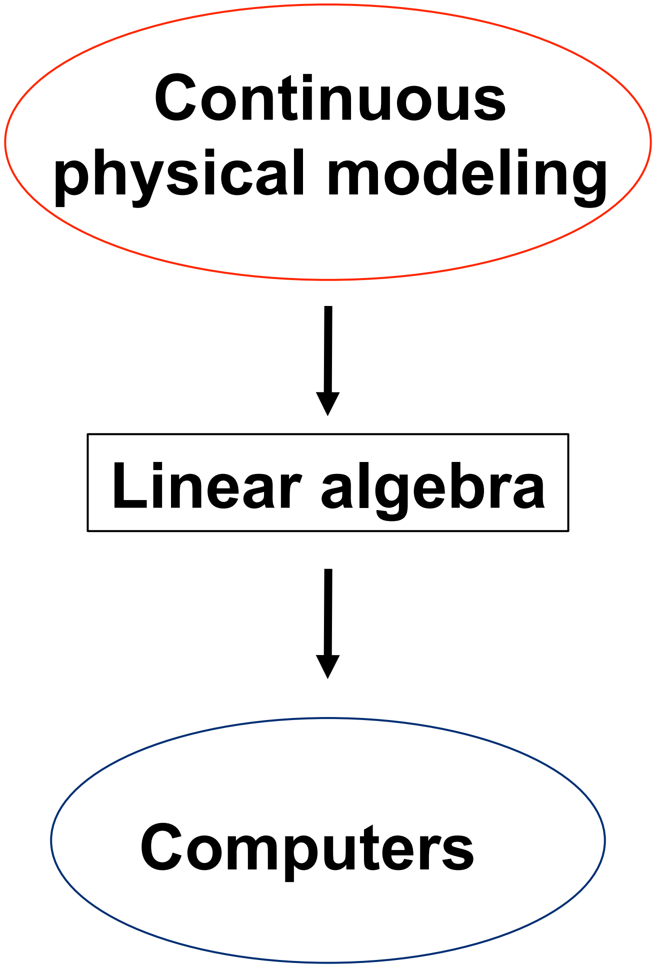
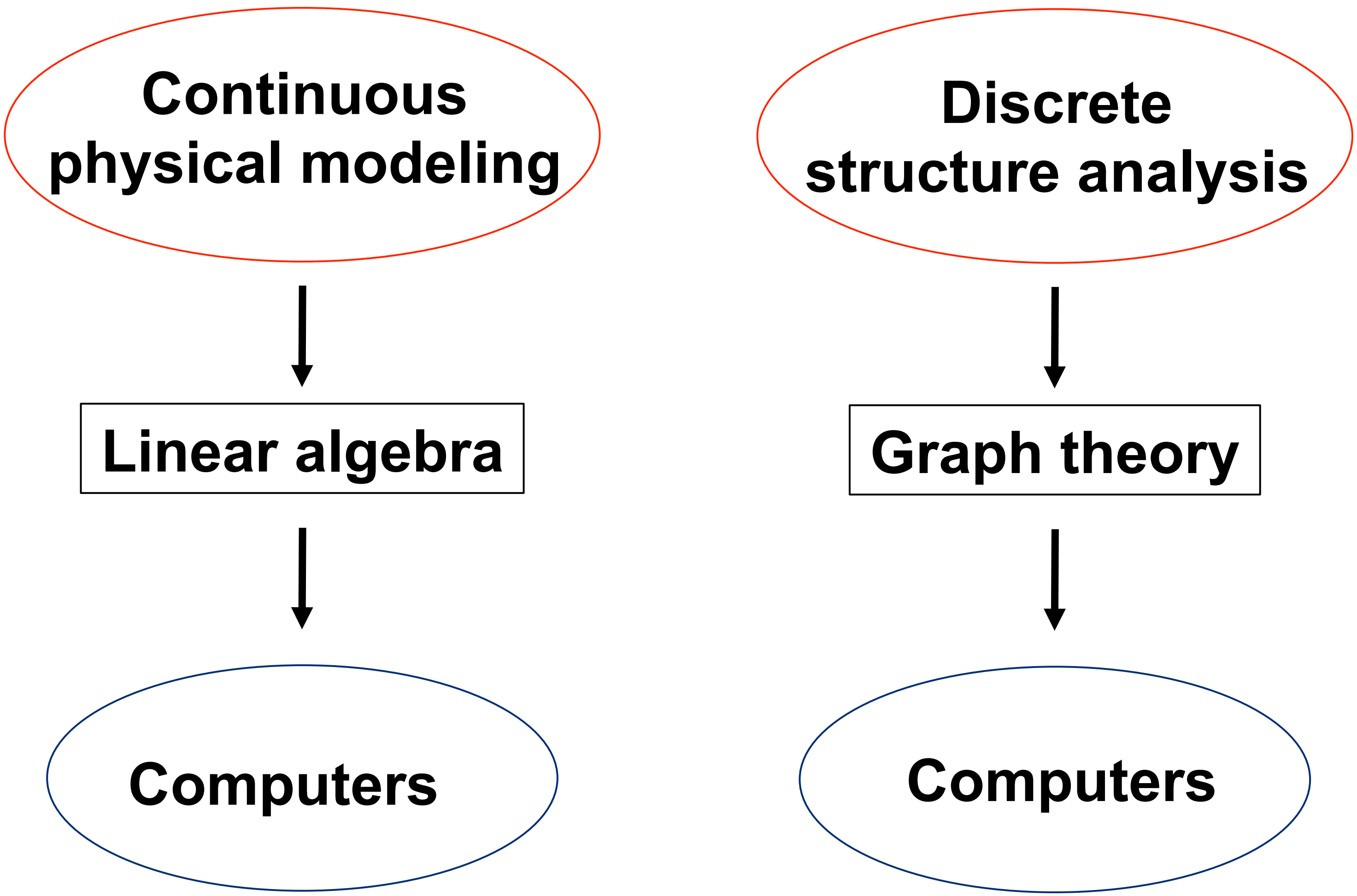


Figure 6: Sample input grid and coarse grids

# *Scientific computation and data analysis*



# *Scientific computation and data analysis*



# *Scientific computation and data analysis*