CS 267: Applications of Parallel Computers

Graph Partitioning

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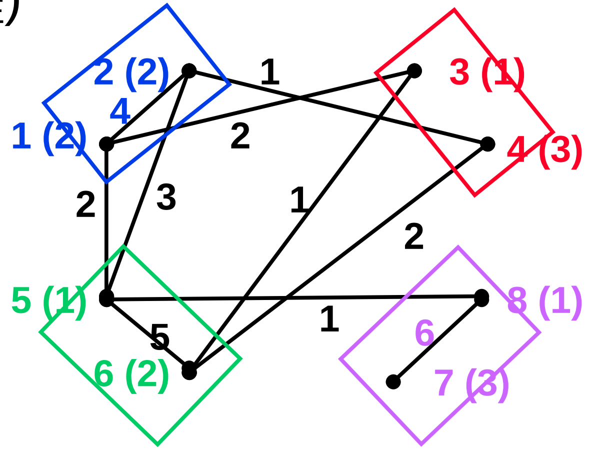
Outline of Graph Partitioning Lectures

- Review definition of Graph Partitioning problem
- Overview of heuristics
- Partitioning with Nodal Coordinates
    - Planar graphs
    - How well can graphs be partitioned in theory?
    - Graphs in higher dimensions
- Partitioning without Nodal Coordinates
- Multilevel Acceleration
    - BIG IDEA, appears often in scientific computing
- Comparison of Methods and Applications

Definition of Graph Partitioning

- Given a graph $G = (N, E, W_N, W_E)$
  - N = nodes (or vertices),
  - E = edges
  - W_N = node weights
  - W_E = edge weights



- Ex: N = {tasks}, W_N = {task costs}, edge (j,k) in E means task j sends $W_E(j,k)$ words to task k
- Choose a partition $N = N_1 \cup N_2 \cup \ldots \cup N_P$ such that
  - The sum of the node weights in each N_j is "about the same"
  - The sum of all edge weights of edges connecting all different pairs N_j and N_k is minimized
- Ex: balance the work load, while minimizing communication
- Special case of $N = N_1 \cup N_2$: Graph Bisection

Applications

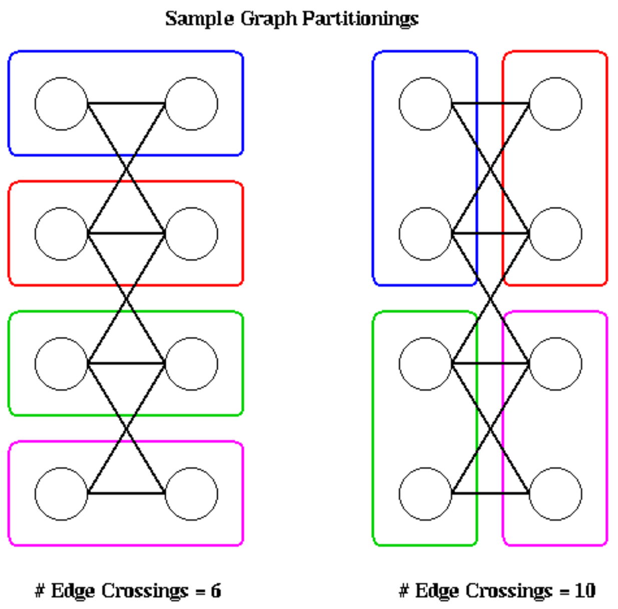
- Telephone network design
  - Original application, algorithm due to Kernighan
- Load Balancing while Minimizing Communication
- Sparse Matrix times Vector Multiplication
  - Solving PDEs
  - N = {1,…,n},   (j,k) in E if A(j,k) nonzero,
  - W_N(j) = #nonzeros in row j, W_E(j,k) = 1
- VLSI Layout
  - N = {units on chip}, E = {wires}, W_E(j,k) = wire length
- Sparse Gaussian Elimination
  - Used to reorder rows and columns to increase parallelism, and to decrease “fill-in”
- Data mining and clustering
- Physical Mapping of DNA

Cost of Graph Partitioning

- Many possible partitionings to search
- Just to divide in 2 parts there are:

  n choose n/2 ~

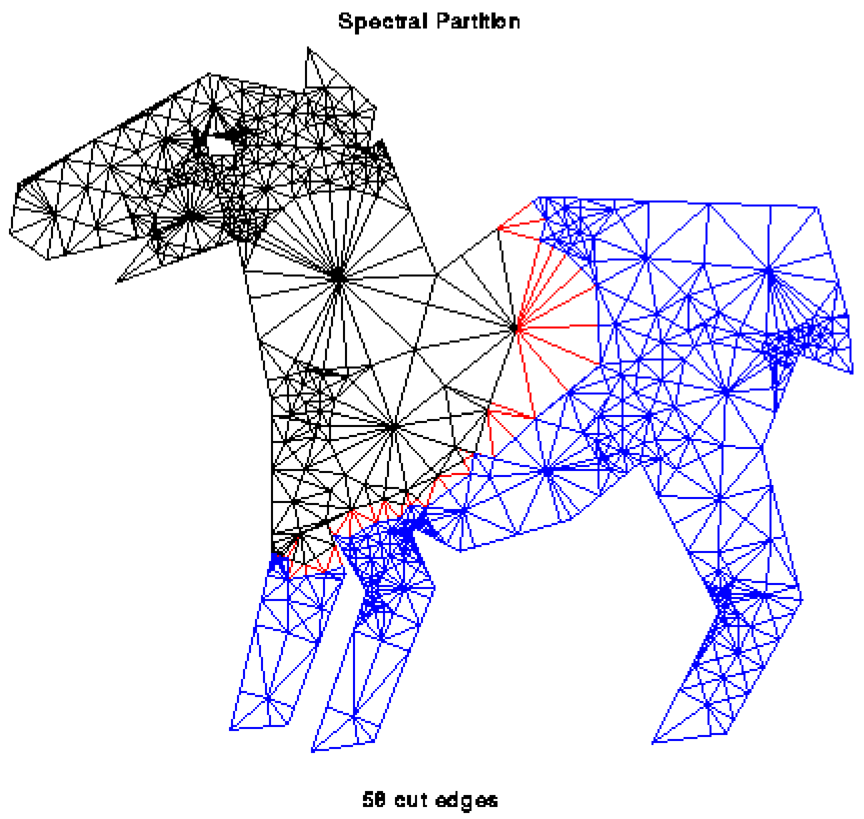
  sqrt(2n/pi)*2^n possibilities



- Choosing optimal partitioning is NP-complete
  - (NP-complete = we can prove it is a hard as other well-known hard problems in a class Nondeterministic Polynomial time)
  - Only known exact algorithms have cost = exponential(n)
- We need good heuristics

First Heuristic: Repeated Graph Bisection

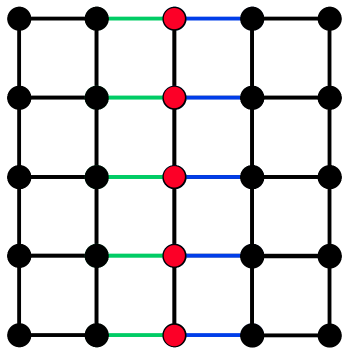
- To partition N into 2^k parts
  - bisect graph recursively k times
- Henceforth discuss mostly graph bisection



Edge Separators vs. Vertex Separators

- Edge Separator: E_s (subset of E) separates G if removing E_s from E leaves two ~equal-sized, disconnected components of N: N_1 and N_2
- Vertex Separator: N_s (subset of N) separates G if removing N_s and all incident edges leaves two ~equal-sized, disconnected components of N: N_1 and N_2

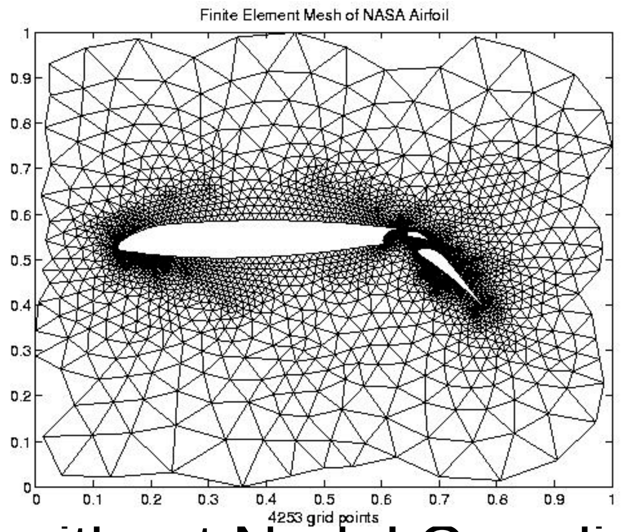
G = (N, E), Nodes N and Edges E
E_s = green edges or blue edges
N_s = red vertices



- Making an N_s from an E_s: pick one endpoint of each edge in E_s
  - $|N_s| <= |E_s|$?
- Making an E_s from an N_s: pick all edges incident on N_s
  - $|E_s| <= d * |N_s|$ where d is the maximum degree of the graph ?
- We will find Edge or Vertex Separators, as convenient

Overview of Bisection Heuristics

- Partitioning with Nodal Coordinates
  - Each node has x,y,z coordinates → partition space



- Partitioning without Nodal Coordinates
  - E.g., Sparse matrix of Web documents
    - A(j,k) = # times keyword j appears in URL k
- Multilevel acceleration (BIG IDEA)
  - Approximate problem by "coarse graph," do so recursively

Nodal Coordinates: How Well Can We Do?

- Consider a special case:
  - A graph with nodal coordinates
  - The graph is planar
- A planar graph can be drawn in plane without edge crossings
- Ex: m x m grid of m^2 nodes: $\exists$ vertex separator N_S with $|N_S| = m = \mathrm{sqrt}(|N|)$ (see last slide for m=5)
- *Theorem* (Tarjan, Lipton, 1979): If G is planar, $\exists$ N_S such that
  - $N = N_1 \cup N_S \cup N_2$ is a partition,
  - $|N_1| <= 2/3\ |N|$ and $|N_2| <= 2/3\ |N|$
  - $|N_S| <= \mathrm{sqrt}(8 * |N|)$
- Theorem motivates intuition of following algorithms

Nodal Coordinates: Inertial Partitioning

- For a graph in 2D, choose line with half the nodes on one side and half on the other
  - In 3D, choose a plane, but consider 2D for simplicity
- Choose a line L, and then choose an $L^{\perp}$ perpendicular to it, with half the nodes on either side

1. **Choose a line L through the points**

   L given by a*(x-xbar)+b*(y-ybar)=0,

   with $a^2+b^2=1$; (a,b) is unit vector $\perp$ to L

2. **Project each point to the line**

   For each nj = (xj,yj), compute coordinate

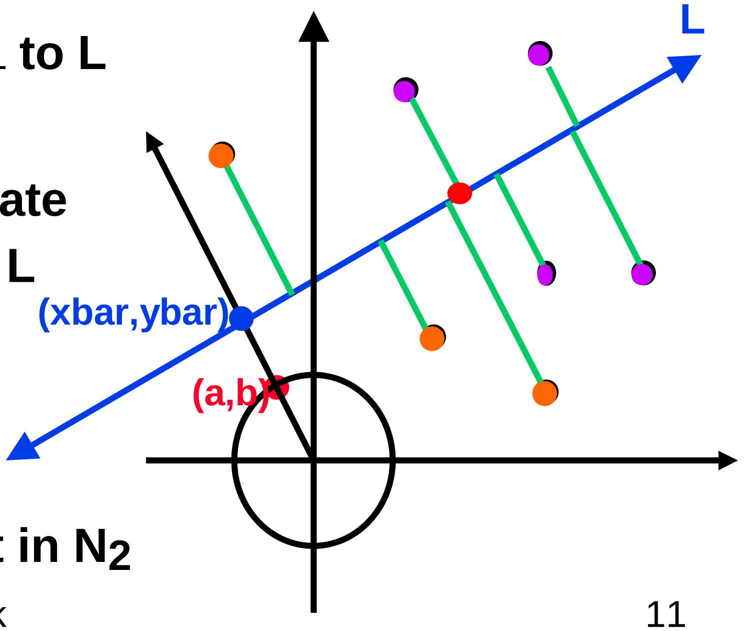
   S_j = -b*(x_j-xbar) + a*(y_j-ybar) along L

3. **Compute the median**

   Let Sbar = median(S_1,…,S_n)

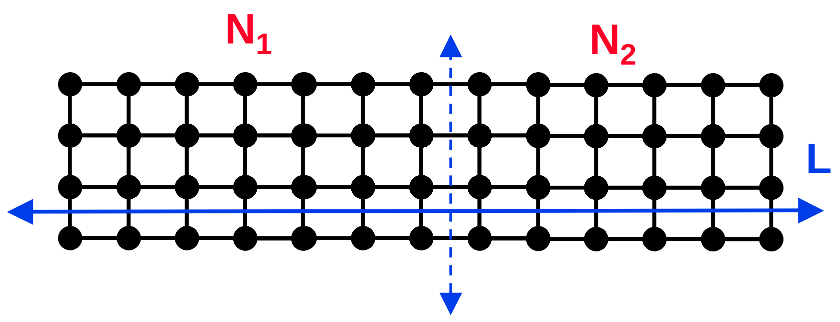
4. **Use median to partition the nodes**

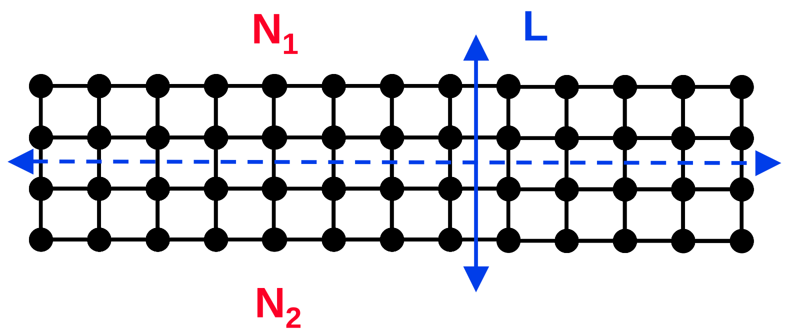
   Let nodes with S_j < Sbar be in N_1, rest in N_2



Inertial Partitioning: Choosing L

- Clearly prefer L on left below

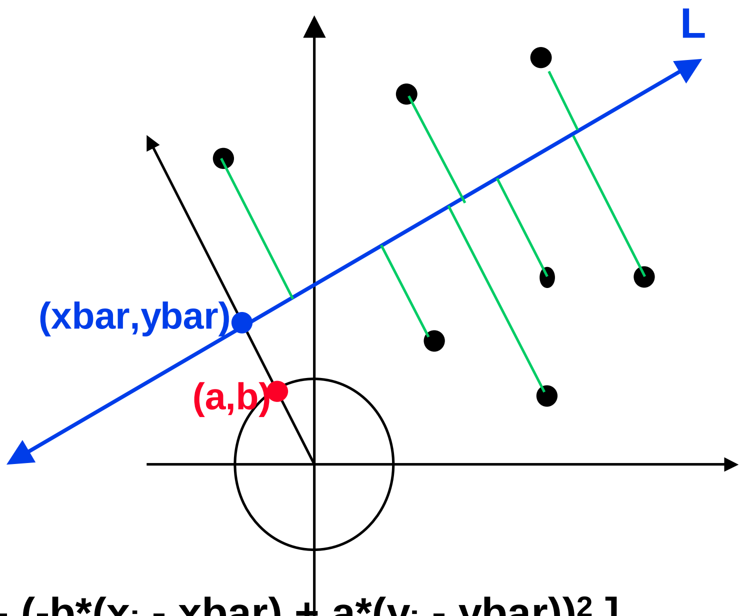




- Mathematically, choose L to be a total least squares fit of the nodes
    - Minimize sum of squares of distances to L (green lines on last slide)
    - Equivalent to choosing L as axis of rotation that minimizes the moment of inertia of nodes (unit weights) - source of name

Inertial Partitioning: choosing L (continued)

(a,b) is unit vector perpendicular to L



Σ_j (length of j-th green line)^2

$= \Sigma_j$ [$(x_j$ - xbar$)^2$ + $(y_j$ - ybar$)^2$ - (-b*$(x_j$ - xbar) + a*$(y_j$ - ybar$))^2$]

… Pythagorean Theorem

$= a^2 * \Sigma_j (x_j - \text{xbar})^2 + 2*a*b* \Sigma_j (x_j - \text{xbar})*(x_j - \text{ybar}) + b^2 \Sigma_j (y_j - \text{ybar})^2$

$= a^2 * X1 + 2*a*b* X2 + b^2 * X3$

$= [a\ b] * \begin{bmatrix} X1 & X2 \\ X2 & X3 \end{bmatrix} * \begin{bmatrix} a \\ b \end{bmatrix}$

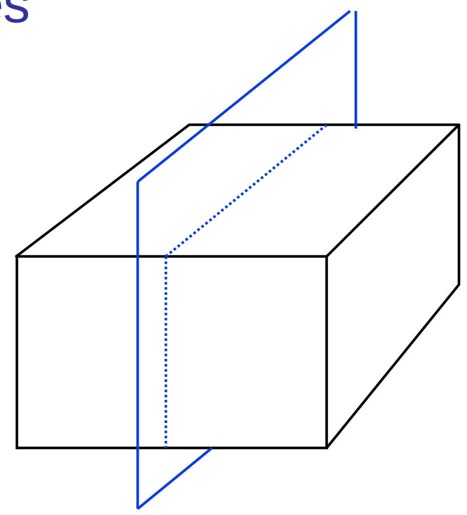
Minimized by choosing

(xbar , ybar) = $(\Sigma_j x_j , \Sigma_j y_j)$ / N = center of mass

(a,b) = eigenvector of smallest eigenvalue of $\begin{bmatrix} X1 & X2 \\ X2 & X3 \end{bmatrix}$

Nodal Coordinates: Random Spheres

- Generalize nearest neighbor idea of a planar graph to higher dimensions
- For intuition, consider a the graph defined by a regular 3D mesh
- An n by n by n mesh of $|N| = n^3$ nodes
  - Edges to 6 nearest neighbors
  - Partition by taking plane parallel to 2 axes
  - Cuts $n^2 = |N|^{2/3} = O(|E|^{2/3})$ edges
- For the general graphs
  - Need a notion of well-shaped
  - (Any graph fits in 3D without crossings!)

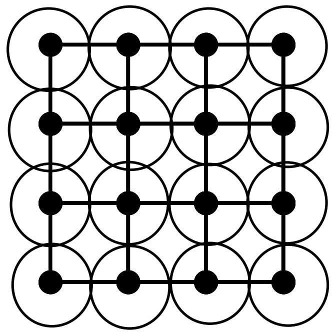


Random Spheres: Well Shaped Graphs

- Approach due to Miller, Teng, Thurston, Vavasis
- Def: A k-ply neighborhood system in d dimensions is a set $\{D_1,\ldots,D_n\}$ of closed disks in R^d such that no point in R^d is strictly interior to more than k disks
- Def: An (α,k) overlap graph is a graph defined in terms of $\alpha >= 1$ and a k-ply neighborhood system $\{D_1,\ldots,D_n\}$: There is a node for each D_j, and an edge from j to i if expanding the radius of the smaller of D_j and D_i by $>\alpha$ causes the two disks to overlap

Ex: n-by-n mesh is a (1,1) overlap graph

Ex: Any planar graph is (α,k) overlap for some α,k



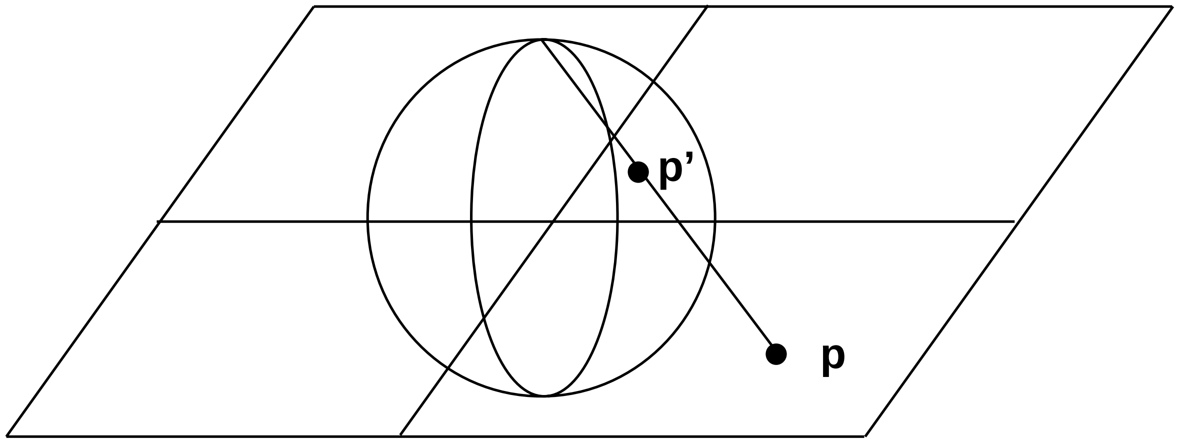
2D Mesh is (1,1) overlap graph

Generalizing Lipton/Tarjan to Higher Dimensions

- *Theorem* (Miller, Teng, Thurston, Vavasis, 1993): Let G=(N,E) be an (α,k) overlap graph in d dimensions with n=|N|. Then there is a vertex separator N_s such that
  - $N = N_1 \cup N_s \cup N_2$ and
  - N_1 and N_2 each has at most n*(d+1)/(d+2) nodes
  - N_s has at most $O(\underline{\alpha} * k^{1/d} * n^{(d-1)/d})$ nodes
- When d=2, same as Lipton/Tarjan
- Algorithm:
  - Choose a sphere S in R^d
  - Edges that S "cuts" form edge separator E_s
  - Build N_s from E_s
  - Choose "randomly", so that it satisfies Theorem with high probability

Stereographic Projection

- Stereographic projection from plane to sphere
  - In d=2, draw line from p to North Pole, projection p’ of p is where the line and sphere intersect



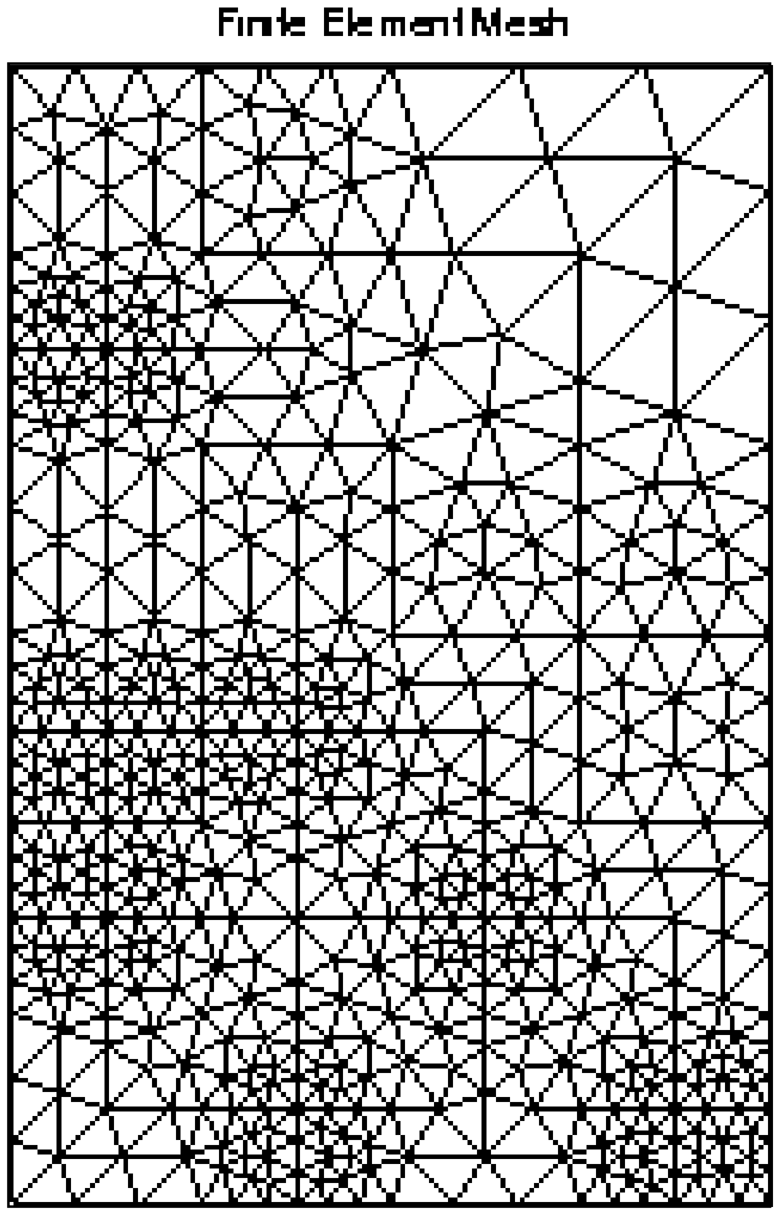
$p = (x,y)$ $p' = (2x,2y,x^2 + y^2 - 1) / (x^2 + y^2 + 1)$

  - Similar in higher dimensions

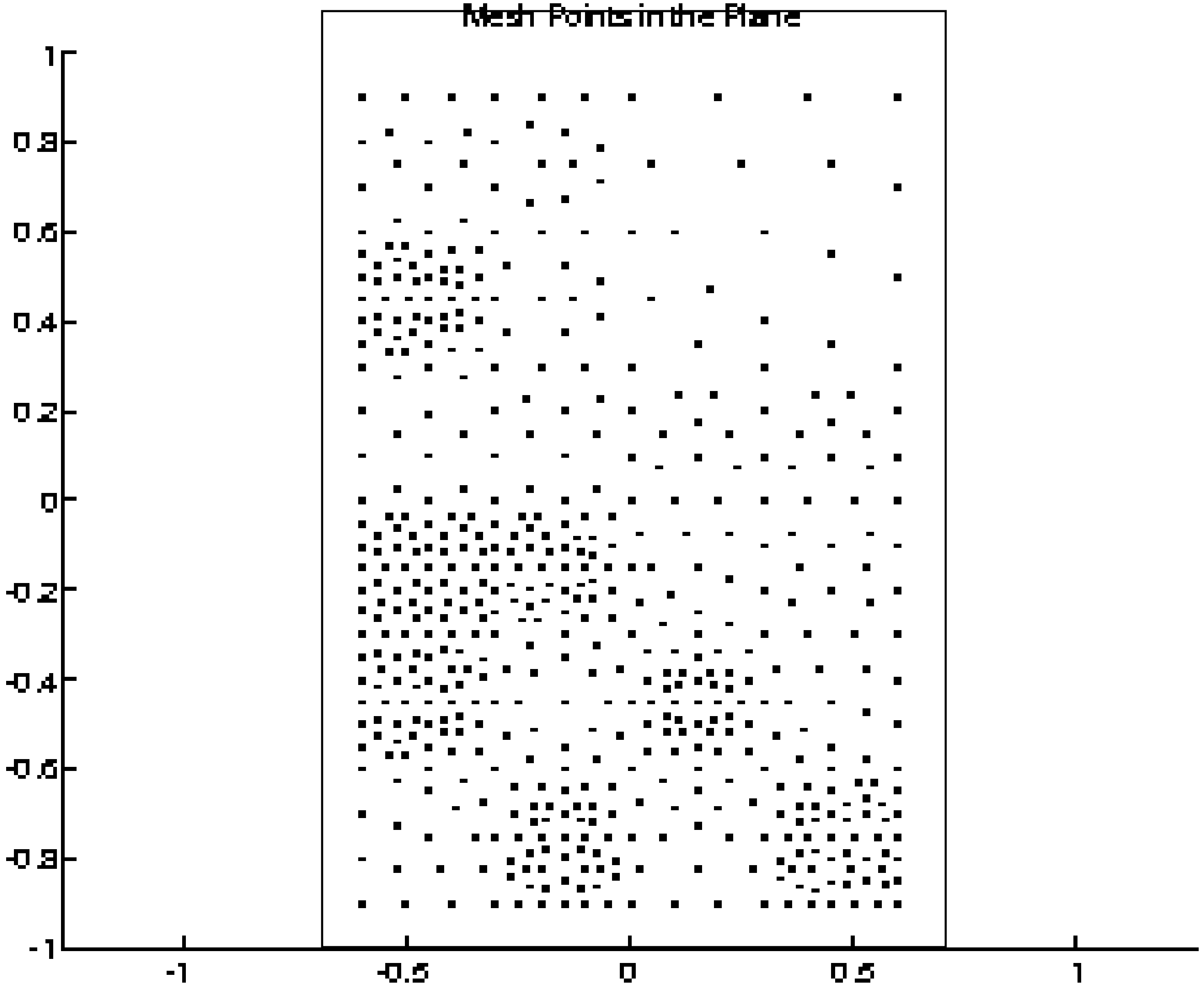
Choosing a Random Sphere

- Do stereographic projection from R^d to sphere in R^{d+1}
- Find centerpoint of projected points
  - Any plane through centerpoint divides points ~evenly
  - There is a linear programming algorithm, cheaper heuristics
- *Conformally map* points on sphere
  - *Rotate* points around origin so centerpoint at (0,…0,r) for some r
  - *Dilate* points (unproject, multiply by sqrt((1-r)/(1+r)), project)
    - this maps centerpoint to origin (0,…,0)
- Pick a random plane through origin
  - Intersection of plane and sphere is circle
- Unproject circle
  - yields desired circle C in R^d
- Create N_s: j belongs to N_s if α*D_j intersects C

Random Sphere Algorithm (Gilbert)



Random Sphere Algorithm (Gilbert)



Random Sphere Algorithm (Gilbert)

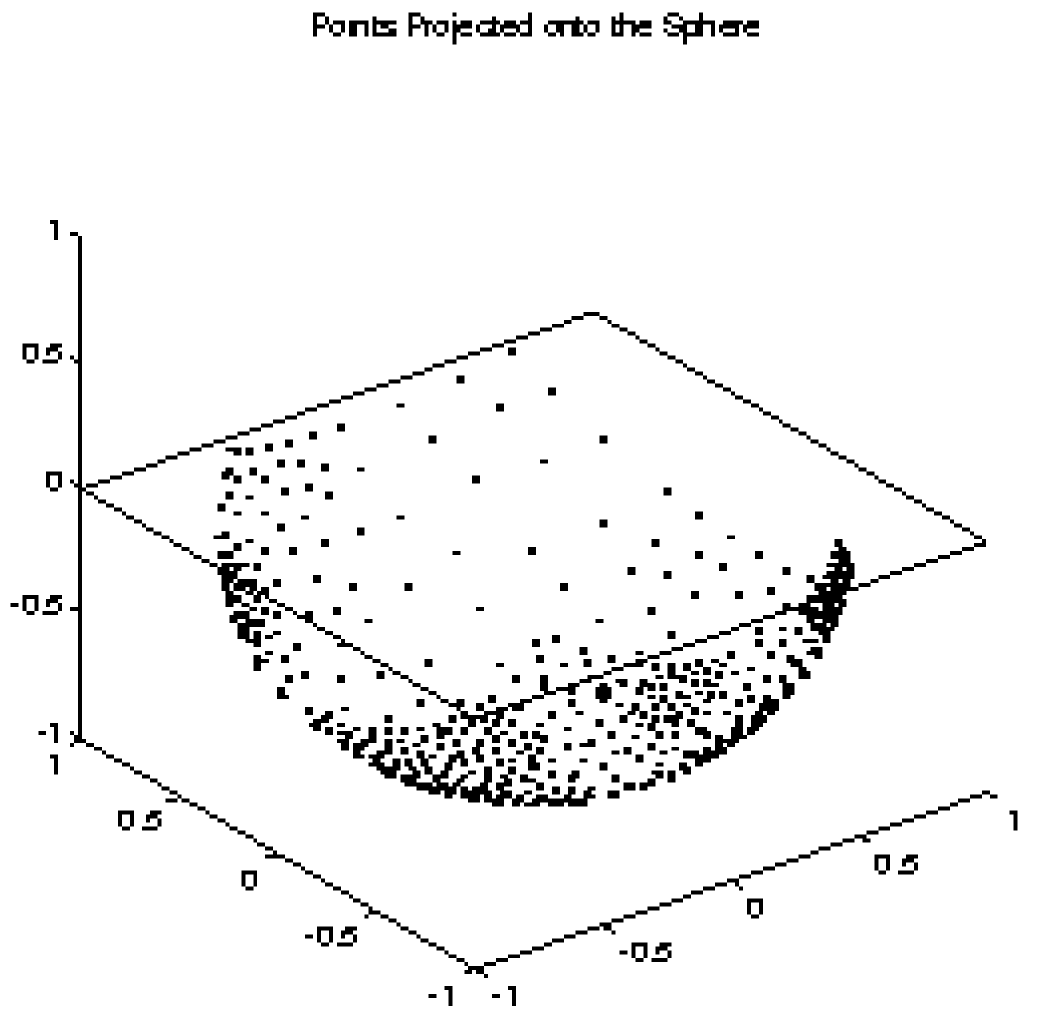
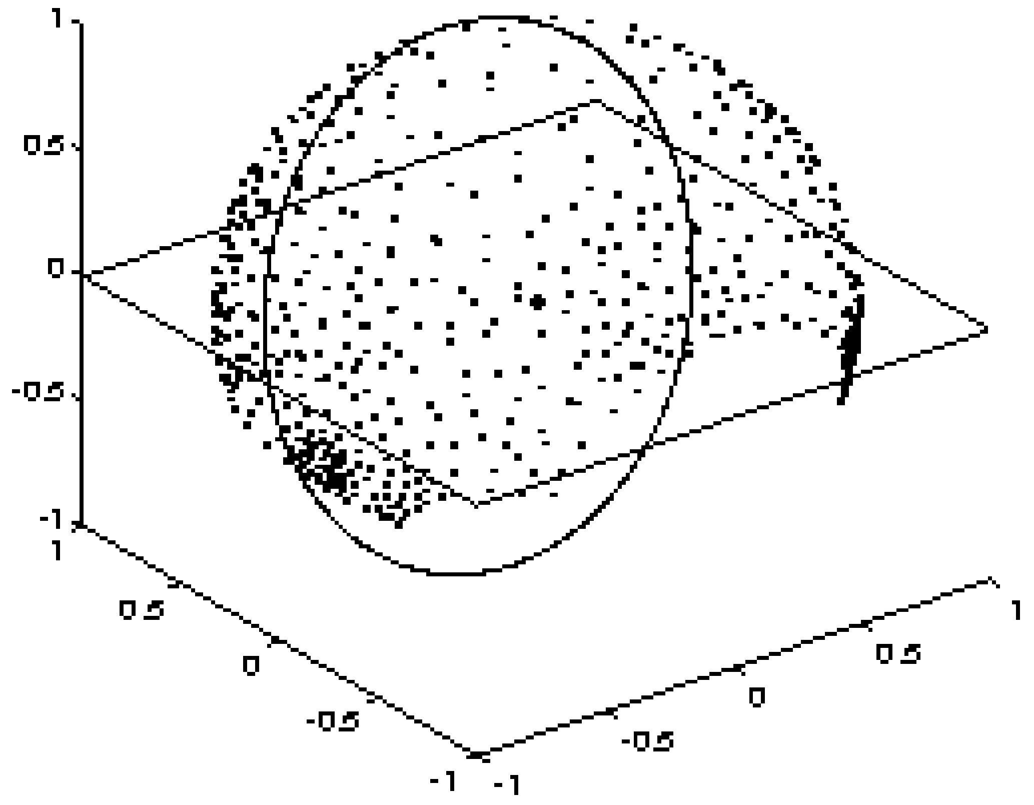


Figure 3: Projected mesh points. The large dot is the centerpoint.

Random Sphere Algorithm (Gilbert)



Random Sphere Algorithm (Gilbert)

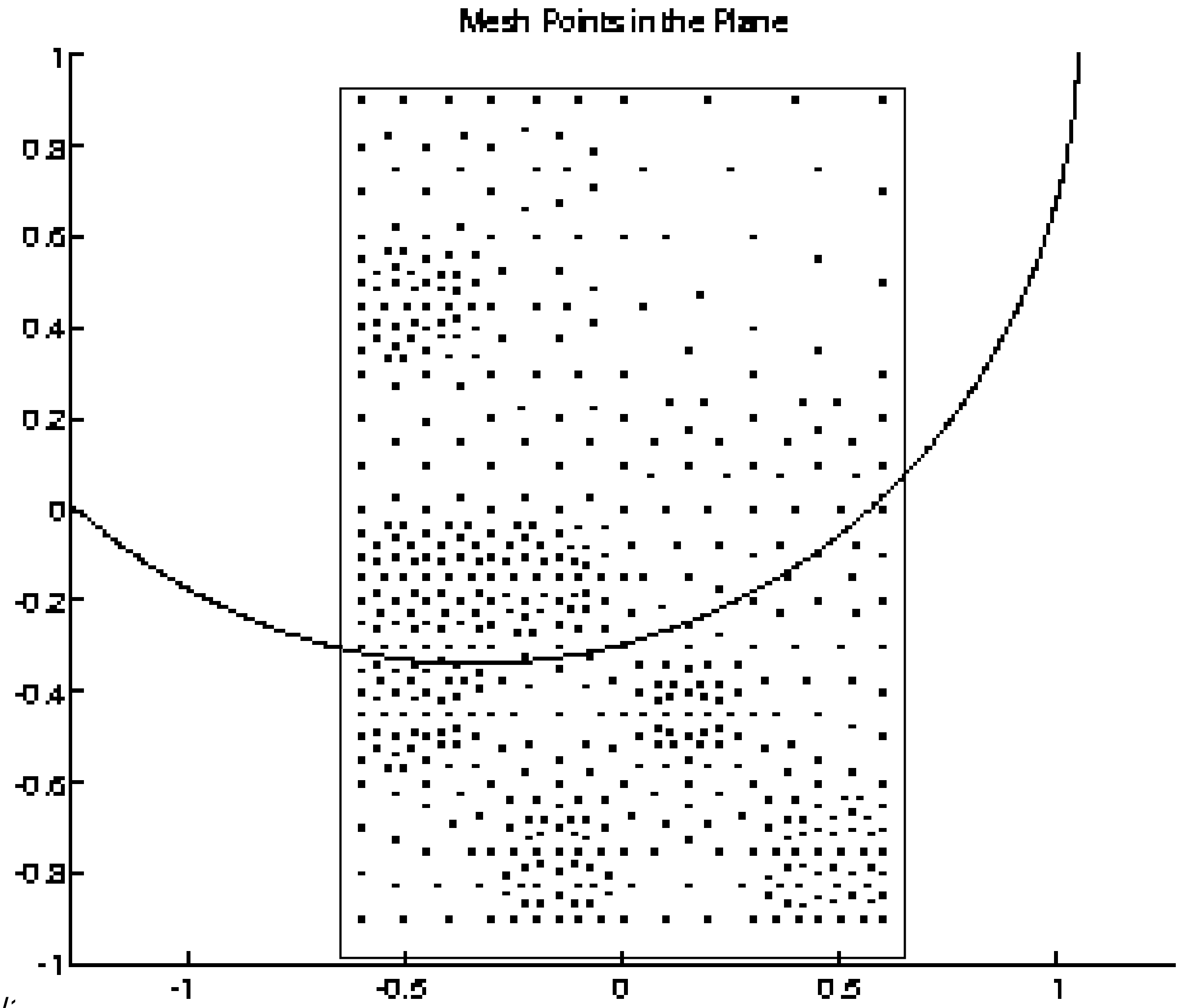


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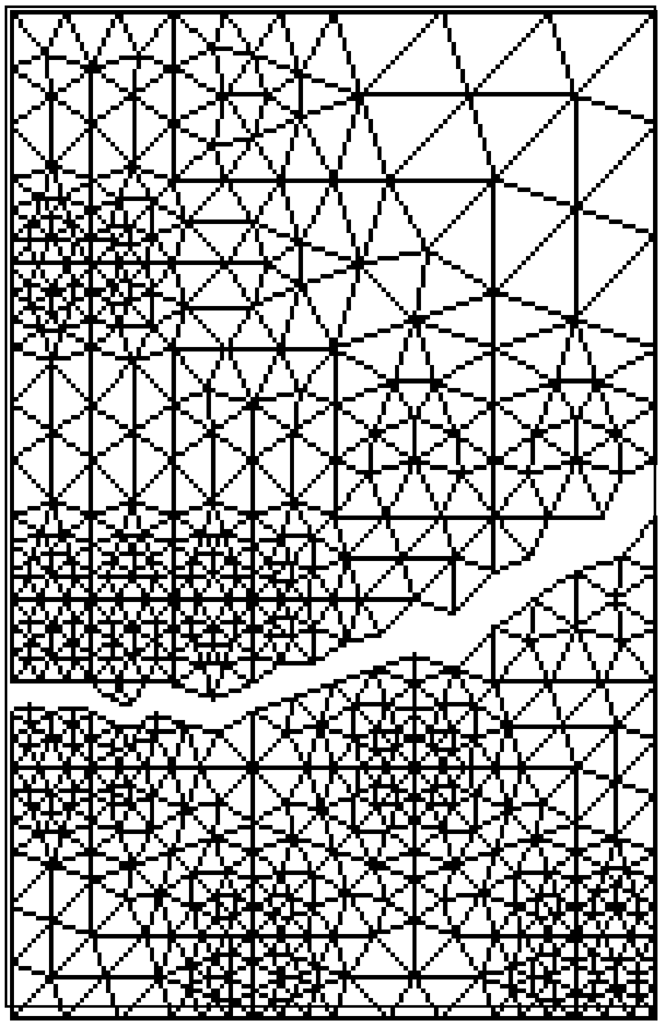
Figure 5: The separating circle projected back to the plane.

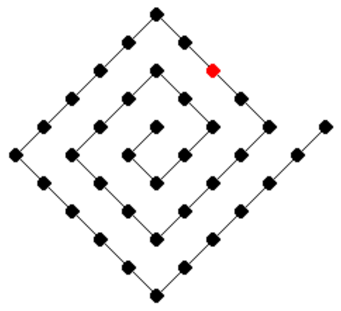
Partition of the Original Mesh



42 cut edges

Nodal Coordinates: Summary

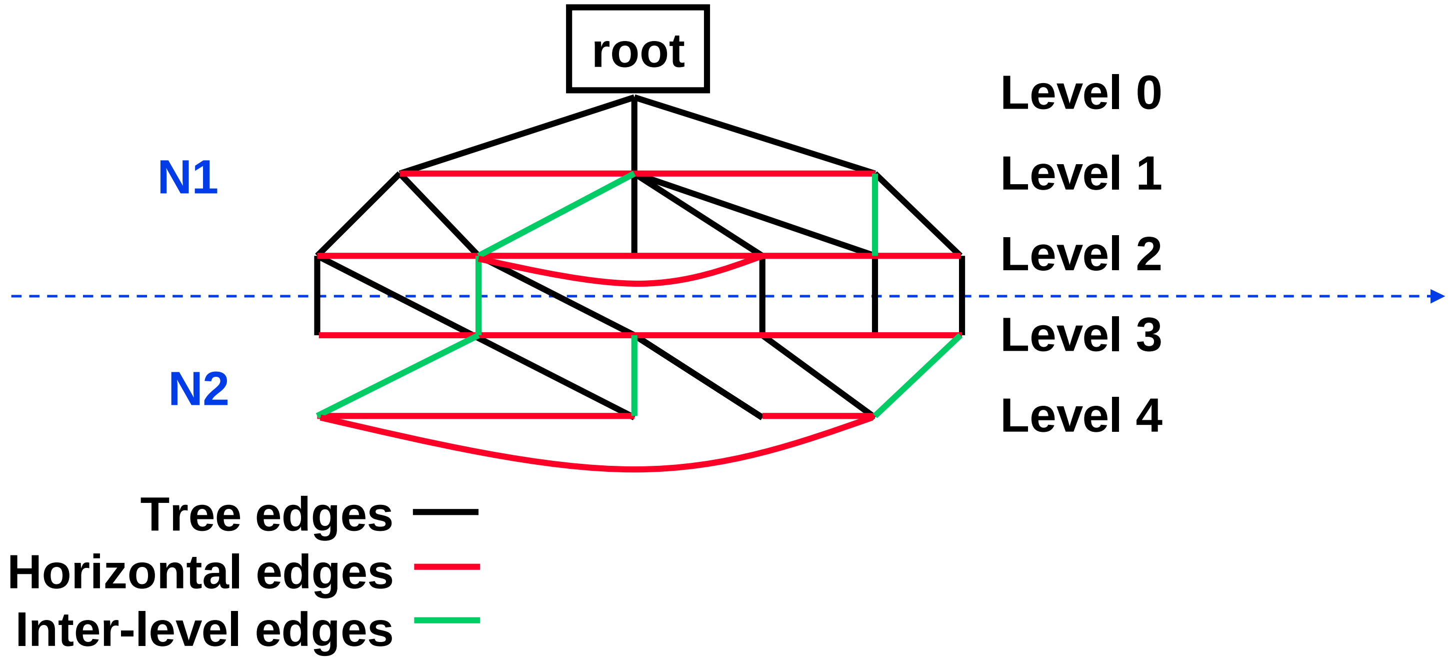
- Other variations on these algorithms
- Algorithms are efficient
- Rely on graphs having nodes connected (mostly) to “nearest neighbors” in space
  - algorithm does not depend on where actual edges are!
- Common when graph arises from physical model
- Ignore edges, but can be used as good starting guess for subsequent partitioners that do examine edges
- Can do poorly if graph connection is not spatial:



- Details at
  - www.cs.berkeley.edu/~demmel/cs267/lecture18/lecture18.html
  - www.parc.xerox.com/spl/members/gilbert (tech reports and SW)
  - www-sal.cs.uiuc.edu/~steng

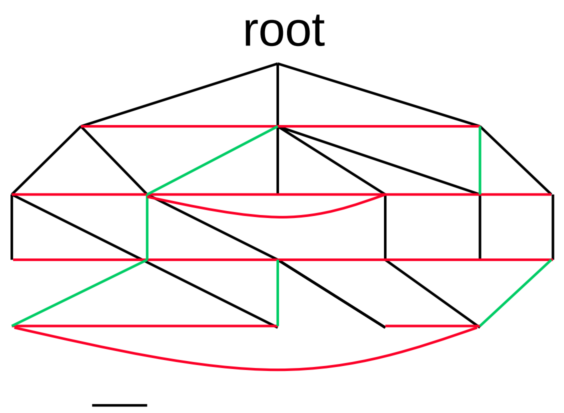
Coordinate-Free: Breadth First Search (BFS)

- Given G(N,E) and a root node r in N, BFS produces
  - A subgraph T of G (same nodes, subset of edges)
  - T is a tree rooted at r
  - Each node assigned a level = distance from r



Breadth First Search

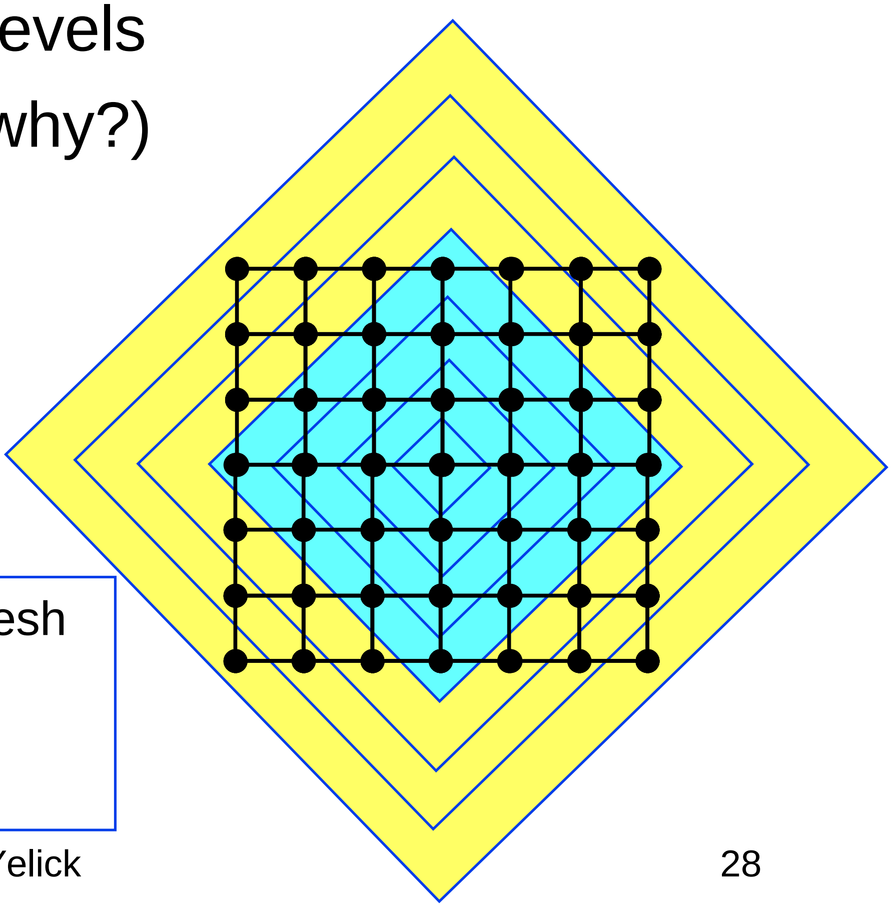
- Queue (First In First Out, or FIFO)
  - Enqueue(x,Q) adds x to back of Q
  - x = Dequeue(Q) removes x from front of Q
- Compute Tree $T(N_T,E_T)$



```
N_T = {(r,0)}, E_T = empty set          … Initially T = root r, which is at level 0
Enqueue((r,0),Q)                        … Put root on initially empty Queue Q
Mark r                                  … Mark root as having been processed
While Q not empty                       … While nodes remain to be processed
    (n,level) = Dequeue(Q)              … Get a node to process
    For all unmarked children c of n
        N_T = N_T U (c,level+1)         …  Add child c to N_T
        E_T = E_T U (n,c)               …  Add edge (n,c) to E_T
        Enqueue((c,level+1),Q))         … Add child c to Q for processing
        Mark c                          … Mark c as processed
    Endfor
Endwhile
```

Partitioning via Breadth First Search

- BFS identifies 3 kinds of edges
  - Tree Edges - part of T
  - Horizontal Edges - connect nodes at same level
  - Interlevel Edges - connect nodes at adjacent levels
- No edges connect nodes in levels differing by more than 1 (why?)
- BFS partioning heuristic
  - N = N_1 U N_2, where
    - N_1 = {nodes at level <= L},
    - N_2 = {nodes at level > L}
  - Choose L so $|N_1|$ close to $|N_2|$



BFS partition of a 2D Mesh using center as root:
N1 = levels 0, 1, 2, 3
N2 = levels 4, 5, 6

Coordinate-Free: Kernighan/Lin

- Take a initial partition and iteratively improve it
    - Kernighan/Lin (1970), cost = $O(|N|^3)$ but easy to understand
    - Fiduccia/Mattheyses (1982), cost = $O(|E|)$, much better, but more complicated
- Given $G = (N,E,W_E)$ and a partitioning $N = A \cup B$, where $|A| = |B|$
    - $T = \text{cost}(A,B) = \Sigma$ {W(e) where e connects nodes in A and B}
    - Find subsets X of A and Y of B with $|X| = |Y|$
    - Swapping X and Y should decrease cost:
        - newA = A - X U Y   and   newB = B - Y U X
        - newT = cost(newA , newB) < cost(A,B)
- Need to compute newT efficiently for many possible X and Y, choose smallest

Kernighan/Lin: Preliminary Definitions

- T = cost(A, B),   newT = cost(newA, newB)
- Need an efficient formula for newT; will use
  - E(a) = external cost of a in A = S {W(a,b) for b in B}
  - I(a) = internal cost of a in A = S {W(a,a') for other a' in A}
  - D(a) = cost of a in A   = E(a) - I(a)
  - E(b), I(b) and D(b) defined analogously for b in B
- Consider swapping X = {a} and Y = {b}
  - newA = A - {a} U {b},   newB = B - {b} U {a}
- newT = T - (D(a) + D(b) - 2*w(a,b)) = T - gain(a,b)
  - gain(a,b) measures improvement gotten by swapping a and b
- Update formulas
  - newD(a') = D(a') + 2*w(a',a) - 2*w(a',b)   for a' in A, a' != a
  - newD(b') = D(b') + 2*w(b',b) - 2*w(b',a)   for b' in B, b' != b

Kernighan/Lin Algorithm

```
Compute  T = cost(A,B) for initial A, B                     … cost = $O(|N|^2)$
Repeat
    … One pass greedily computes |N|/2 possible X,Y to swap, picks best
    Compute costs D(n) for all n in N                          … cost = $O(|N|^2)$
    Unmark all nodes in N                                      … cost = $O(|N|)$
    While there are unmarked nodes                             … |N|/2 iterations
        Find an unmarked pair (a,b) maximizing gain(a,b)       … cost = $O(|N|^2)$
        Mark a and b (but do not swap them)                    … cost = $O(1)$
        Update D(n) for all unmarked n,
            as though a and b had been swapped                 … cost = $O(|N|)$
    Endwhile
        … At this point we have computed a sequence of pairs
        …  (a1,b1), … , (ak,bk)   and gains gain(1),…., gain(k)
        … where k = |N|/2, numbered in the order in which we marked them
    Pick m maximizing Gain = $\Sigma_{k=1 \text{ to } m}$ gain(k)          … cost = $O(|N|)$
        … Gain is reduction in cost from swapping (a1,b1) through (am,bm)
    If Gain > 0 then   … it is worth swapping
        Update newA = A - { a1,…,am } U { b1,…,bm }            … cost = $O(|N|)$
        Update newB = B - { b1,…,bm } U { a1,…,am }            … cost = $O(|N|)$
        Update T = T - Gain                                    … cost = $O(1)$
    endif
Until Gain <= 0
```

Comments on Kernighan/Lin Algorithm

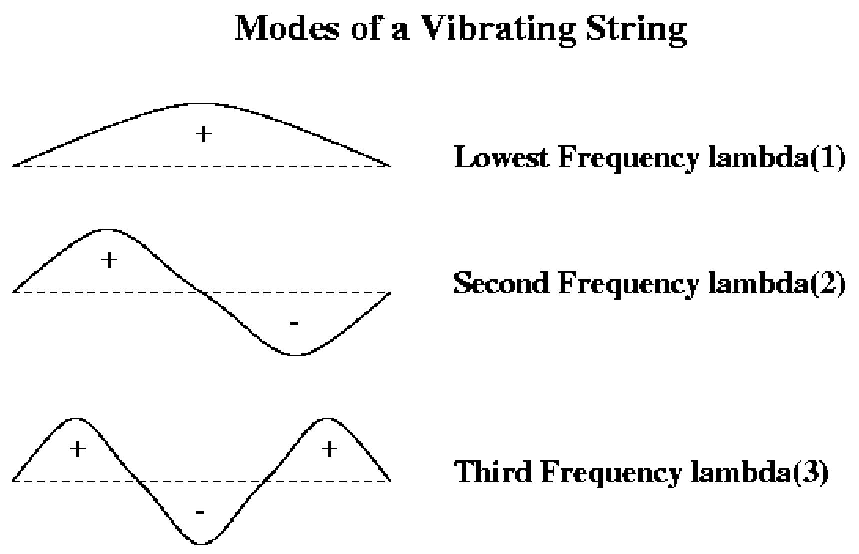
- Most expensive line show in red
- Some gain(k) may be negative, but if later gains are large, then final Gain may be positive
    - can escape "local minima" where switching no pair helps
- How many times do we Repeat?
    - K/L tested on very small graphs (|N|<=360) and got convergence after 2-4 sweeps
    - For random graphs (of theoretical interest) the probability of convergence in one step appears to drop like $2^{-|N|/30}$

Coordinate-Free: Spectral Bisection

- Based on theory of Fiedler (1970s), popularized by Pothen, Simon, Liou (1990)
- Motivation, by analogy to a vibrating string
- Basic definitions
- Vibrating string, revisited
- Implementation via the Lanczos Algorithm
  - To optimize sparse-matrix-vector multiply, we graph partition
  - To graph partition, we find an eigenvector of a matrix associated with the graph
  - To find an eigenvector, we do sparse-matrix vector multiply
  - No free lunch ...

Motivation for Spectral Bisection

- Vibrating string
- Think of G = 1D mesh as masses (nodes) connected by springs (edges), i.e. a string that can vibrate
- Vibrating string has modes of vibration, or harmonics
- Label nodes by whether mode - or + to partition into N- and N+
- Same idea for other graphs (eg planar graph ~ trampoline)


Modes of a Vibrating String
+
Lowest Frequency lambda(1)
+
-
Second Frequency lambda(2)
+
+
-
Third Frequency lambda(3)

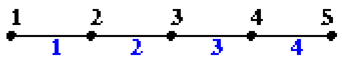
Basic Definitions

- *Definition*: The incidence matrix In(G) of a graph G(N,E) is an |N| by |E| matrix, with one row for each node and one column for each edge. If edge e=(i,j) then column e of In(G) is zero except for the i-th and j-th entries, which are +1 and -1, respectively.
- Slightly ambiguous definition because multiplying column e of In(G) by -1 still satisfies the definition, but this won't matter...
- *Definition*: The Laplacian matrix L(G) of a graph G(N,E) is an |N| by |N| symmetric matrix, with one row and column for each node. It is defined by
  - L(G) (i,i) = degree of node I (number of incident edges)
  - L(G) (i,j) = -1 if i != j and there is an edge (i,j)
  - L(G) (i,j) = 0 otherwise

Example of In(G) and L(G) for Simple Meshes

Incidence and Laplacian Matrices

Graph G

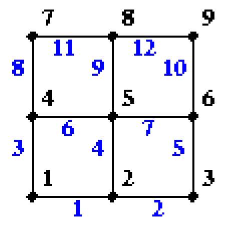


Incidence Matrix In(G)

$$\begin{array}{c|cccc|}
 & 1 & 2 & 3 & 4 \\
\hline
1 & -1 & & & \\
2 & 1 & -1 & & \\
3 & & 1 & -1 & \\
4 & & & 1 & -1 \\
5 & & & & 1
\end{array}$$

Laplacian Matrix L(G)

$$\begin{array}{c|ccccc|}
 & 1 & 2 & 3 & 4 & 5 \\
\hline
1 & 1 & -1 & & & \\
2 & -1 & 2 & -1 & & \\
3 & & -1 & 2 & -1 & \\
4 & & & -1 & 2 & -1 \\
5 & & & & -1 & 1
\end{array}$$



$$\begin{array}{c|cccccccccccc|}
 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 \\
\hline
1 & -1 & & 1 & & & & & & & & & \\
2 & 1 & -1 & & 1 & & & & & & & & \\
3 & & 1 & & & 1 & & & & & & & \\
4 & & & -1 & & & -1 & & 1 & & & & \\
5 & & & & -1 & & 1 & -1 & & 1 & & & \\
6 & & & & & -1 & & 1 & & & 1 & & \\
7 & & & & & & & & -1 & & & -1 & \\
8 & & & & & & & & & -1 & & 1 & -1 \\
9 & & & & & & & & & & -1 & & 1
\end{array}$$

$$\begin{array}{c|ccccccccc|}
 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \\
\hline
1 & 2 & -1 & & -1 & & & & & \\
2 & -1 & 3 & -1 & & -1 & & & & \\
3 & & -1 & 2 & & & -1 & & & \\
4 & -1 & & & 3 & -1 & & -1 & & \\
5 & & -1 & & -1 & 4 & -1 & & -1 & \\
6 & & & -1 & & -1 & 3 & & & -1 \\
7 & & & & -1 & & & 2 & -1 & \\
8 & & & & & -1 & & -1 & 3 & -1 \\
9 & & & & & & -1 & & -1 & 2
\end{array}$$

Nodes numbered in black

Edges numbered in blue

Properties of Laplacian Matrix

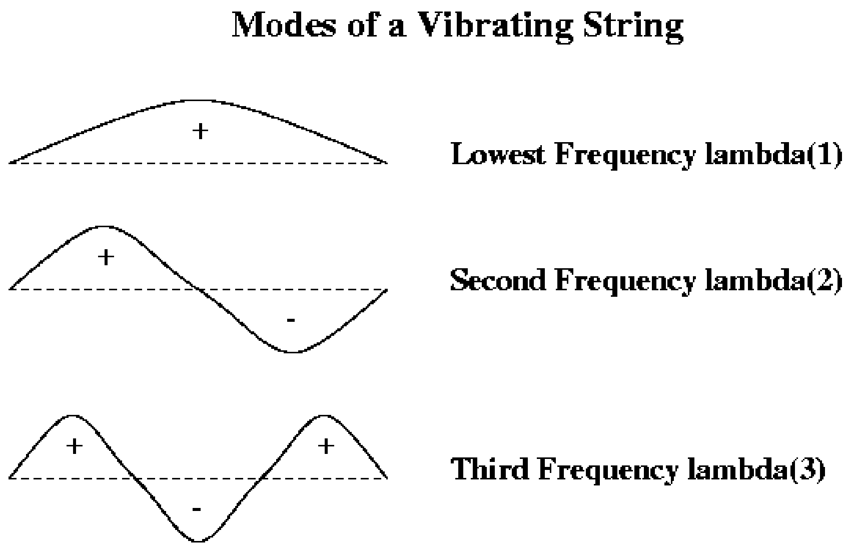
- *Theorem 1:* Given G, L(G) has the following properties (proof on web page)
  - L(G) is symmetric.
    - This means the eigenvalues of L(G) are real and its eigenvectors are real and orthogonal.
  - Rows of L sum to zero:
    - Let e = $[1,\dots,1]^T$, i.e. the column vector of all ones. Then L(G)*e=0.
  - The eigenvalues of L(G) are nonnegative:
    - $0 = \lambda_1 <= \lambda_2 <= \dots <= \lambda_n$
  - The number of connected components of G is equal to the number of λ_i equal to 0.
  - *Definition*: $\lambda_2(L(G))$ is the algebraic connectivity of G
    - The magnitude of λ_2 measures connectivity
    - In particular, λ_2 != 0 if and only if G is connected.

Spectral Bisection Algorithm

- Spectral Bisection Algorithm:
  - Compute eigenvector v_2 corresponding to $\lambda_2(L(G))$
  - For each node n of G
    - if $v_2(n) < 0$ put node n in partition N-
    - else put node n in partition N+
- Why does this make sense? First reasons...
  - *Theorem 2 (Fiedler, 1975):* Let G be connected, and N- and N+ defined as above. Then N- is connected. If no $v_2(n) = 0$, then N+ is also connected. (proof on web page)
  - Recall $\lambda_2(L(G))$ is the algebraic connectivity of G
  - *Theorem 3 (Fiedler):* Let $G_1(N,E_1)$ be a subgraph of G(N,E), so that G_1 is "less connected" than G. Then $\lambda_2(L(G)) <= \lambda_2(L(G))$, i.e. the algebraic connectivity of G_1 is less than or equal to the algebraic connectivity of G. (proof on web page)

Motivation for Spectral Bisection (recap)

- Vibrating string has modes of vibration, or harmonics
- Modes computable as follows
  - Model string as masses connected by springs (a 1D mesh)
  - Write down F=ma for coupled system, get matrix A
  - Eigenvalues and eigenvectors of A are frequencies and shapes of modes
- Label nodes by whether mode - or + to get N- and N+
- Same idea for other graphs (eg planar graph ~ trampoline)


Modes of a Vibrating String
+
Lowest Frequency lambda(1)
+
-
Second Frequency lambda(2)
+
+
-
Third Frequency lambda(3)

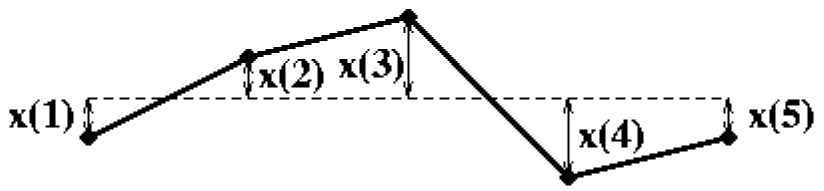
Details for Vibrating String Analogy

- Force on mass j = k*[x(j-1) - x(j)] + k*[x(j+1) - x(j)]
  = -k*[-x(j-1) + 2*x(j) - x(j+1)]
- F=ma yields m*x''(j) = -k*[-x(j-1) + 2*x(j) - x(j+1)] (*)
- Writing (*) for j=1,2,…,n yields

$$m * \frac{d^2}{dx^2}\begin{pmatrix} x(1) \\ x(2) \\ \ldots \\ x(j) \\ \ldots \\ x(n) \end{pmatrix} = -k*\begin{pmatrix} 2*x(1) - x(2) \\ -x(1) + 2*x(2) - x(3) \\ \ldots \\ -x(j-1) + 2*x(j) - x(j+1) \\ \ldots \\ 2*x(n-1) - x(n) \end{pmatrix} = -k*\begin{pmatrix} 2 & -1 & & & & \\ -1 & 2 & -1 & & & \\ & & \ldots & & & \\ & & -1 & 2 & -1 & \\ & & & & \ldots & \\ & & & & -1 & 2 \end{pmatrix} * \begin{pmatrix} x(1) \\ x(2) \\ \ldots \\ x(j) \\ \ldots \\ x(n) \end{pmatrix} = -k*L*\begin{pmatrix} x(1) \\ x(2) \\ \ldots \\ x(j) \\ \ldots \\ x(n) \end{pmatrix}$$

(-m/k) x'' = L*x

Vibrating Mass Spring System



Details for Vibrating String (continued)

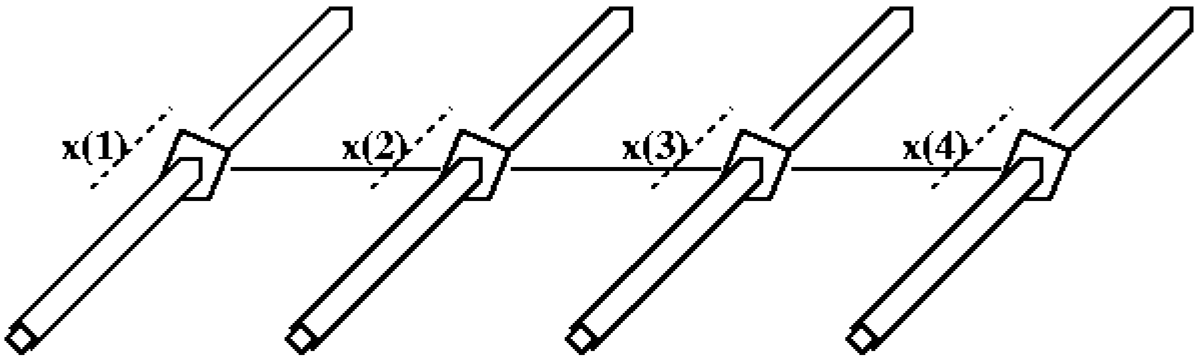
- $-(m/k)\, x'' = L*x$, where $x = [x_1, x_2, \ldots, x_n]^T$
- Seek solution of form $x(t) = \sin(\alpha*t) * x0$
  - $L*x0 = (m/k)*\alpha^2 * x0 = \lambda * x0$
  - For each integer i, get $\lambda = 2*(1-\cos(i*\pi/(n+1)))$, $x0 = \begin{pmatrix} \sin(1*i*\pi/(n+1)) \\ \sin(2*i*\pi/(n+1)) \\ \ldots \\ \sin(n*i*\pi/(n+1)) \end{pmatrix}$
  - Thus x0 is a sine curve with frequency proportional to i
  - Thus $\alpha^2 = 2*k/m *(1-\cos(i*\pi/(n+1))$ or $\alpha \sim \mathrm{sqrt}(k/m)*\pi*i/(n+1)$

- $L = \begin{pmatrix} 2 & -1 & & \\ -1 & 2 & -1 & \\ & \ldots & & \\ & & -1 & 2 \end{pmatrix}$ not quite L(1D mesh), but we can fix that ...

Motivation for Spectral Bisection

- Vibrating string has modes of vibration, or harmonics
- Modes computable as follows
  - Model string as masses connected by springs (a 1D mesh)
  - Write down F=ma for coupled system, get matrix A
  - Eigenvalues and eigenvectors of A are frequencies and shapes of modes
- Label nodes by whether mode - or + to get N- and N+
- Same idea for other graphs (eg planar graph ~ trampoline)

"Vibrating String" for Spectral Bisection

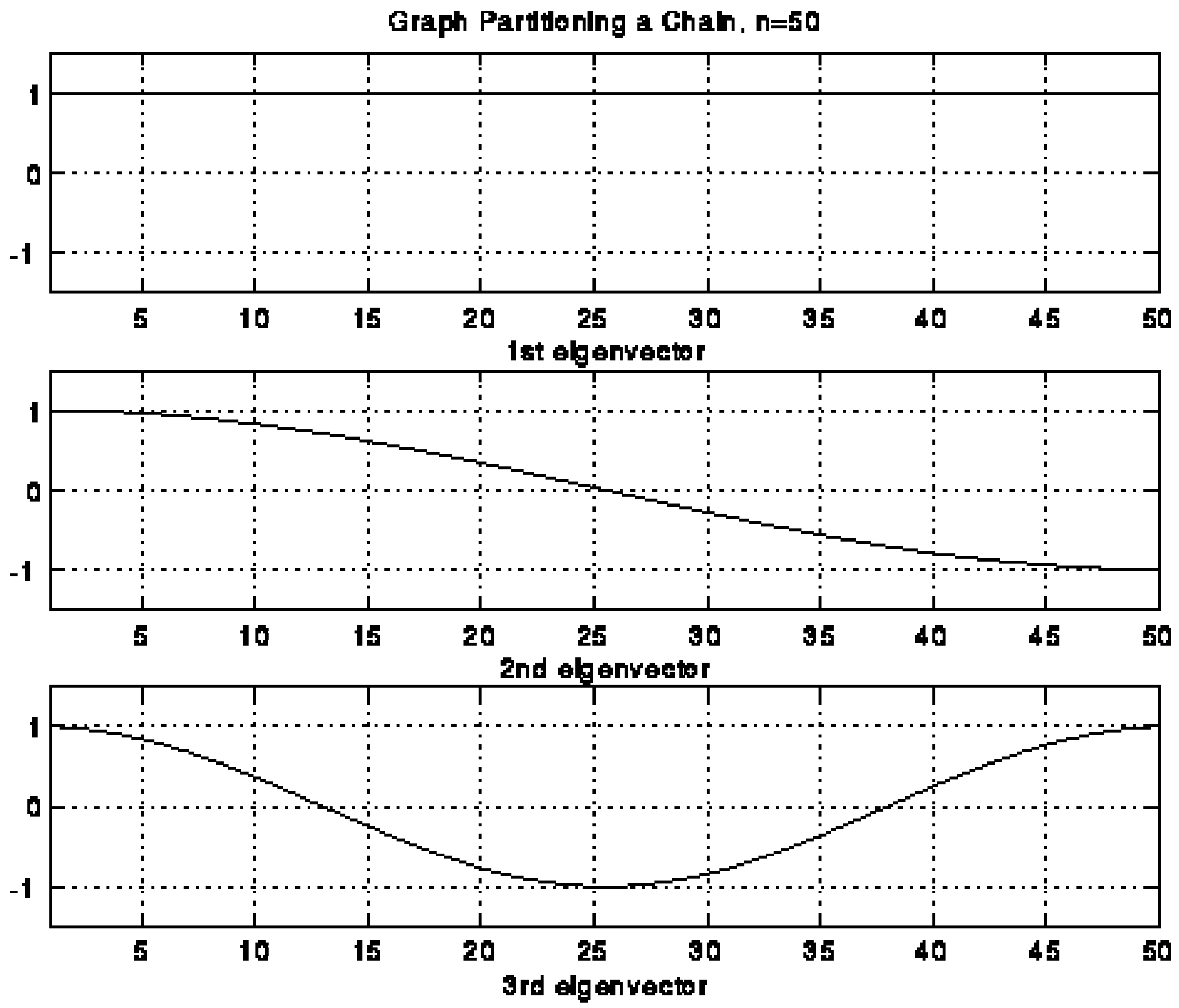


Eigenvectors of L(1D mesh)

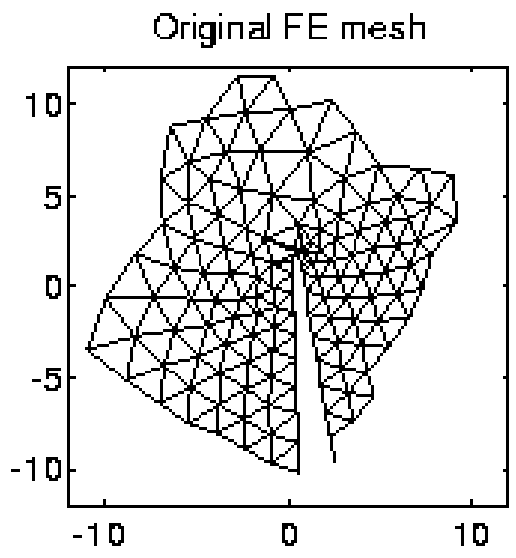
Eigenvector 1 (all ones)

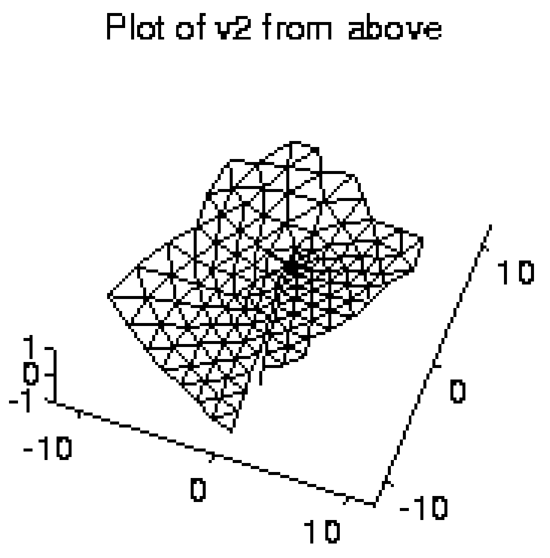
Eigenvector 2

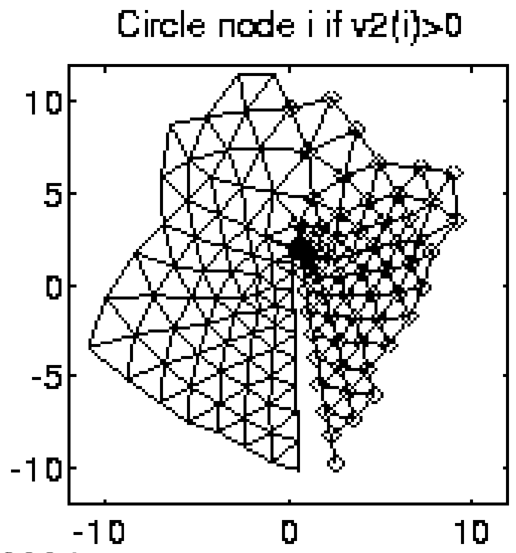
Eigenvector 3

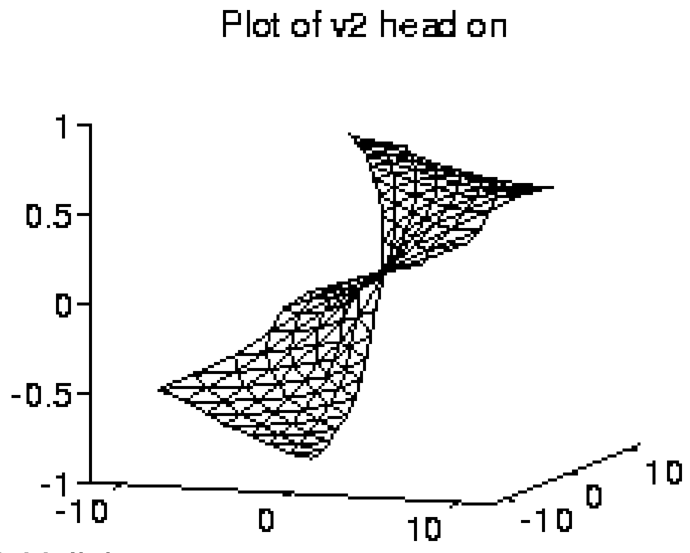


2nd eigenvector of L(planar mesh)

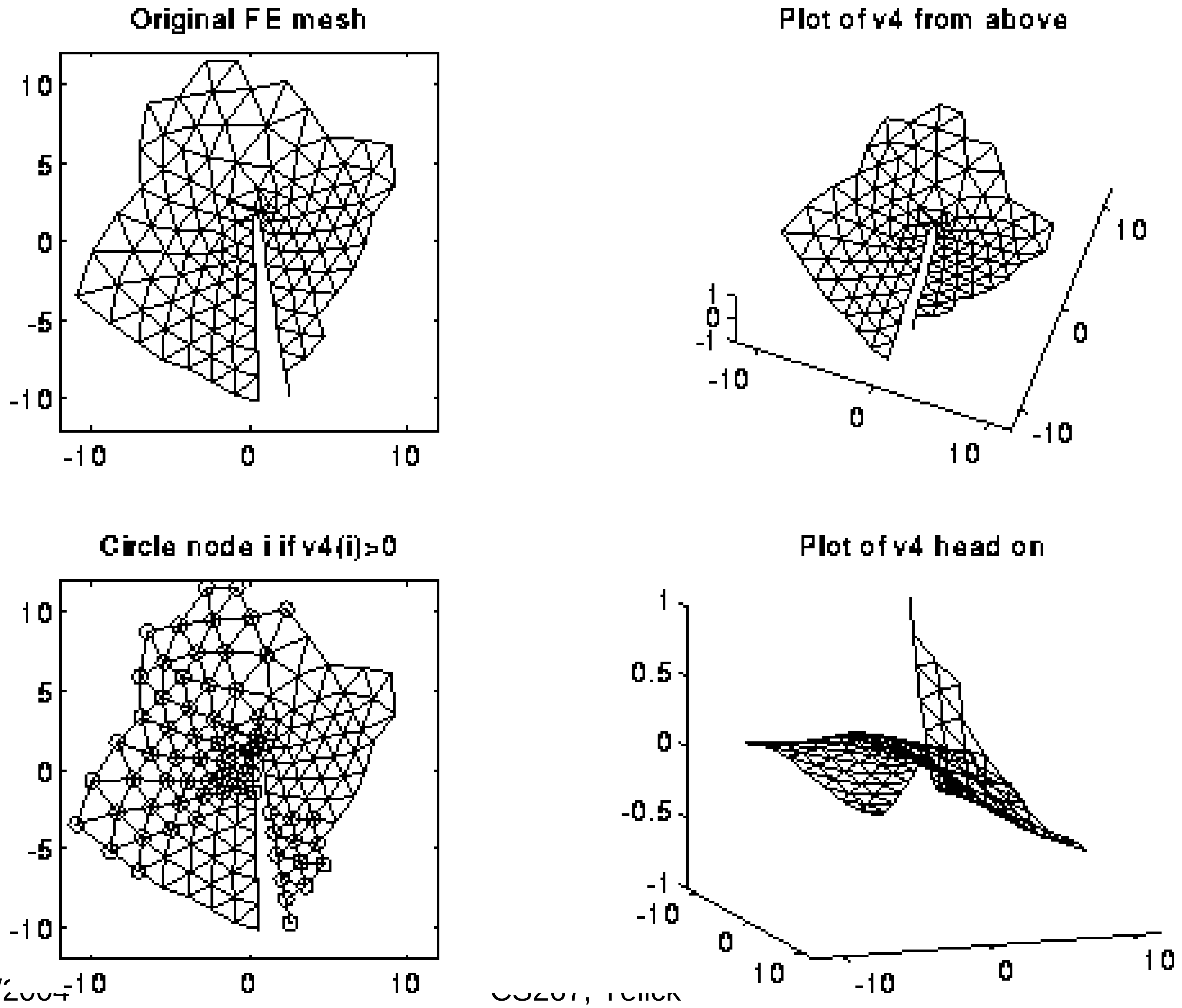








4th eigenvector of L(planar mesh)



Computing v_2 and λ_2 of L(G) using Lanczos

- Given any n-by-n symmetric matrix A (such as L(G)) Lanczos computes a k-by-k "approximation" T by doing k matrix-vector products, k << n

```
Choose an arbitrary starting vector r
b(0) = ||r||
j=0
repeat
    j=j+1
    q(j) = r/b(j-1)             … scale a vector
    r = A*q(j)                  … matrix vector multiplication, the most expensive step
    r = r - b(j-1)*v(j-1)       …  "saxpy", or scalar*vector + vector
   a(j) = v(j)^T * r            … dot product
   r = r - a(j)*v(j)            … "saxpy"
   b(j) = ||r||                 … compute vector norm
until convergence               … details omitted
```

$$T = \begin{pmatrix} a(1) & b(1) & & & & \bigcirc \\ b(1) & a(2) & b(2) & & & \\ & b(2) & a(3) & b(3) & & \\ & & \cdots & \cdots & \cdots & \\ \bigcirc & & & b(k-2) & a(k-1) & b(k-1) \\ & & & & b(k-1) & a(k) \end{pmatrix}$$

- Approximate A's eigenvalues/vectors using T's

Spectral Bisection: Summary

- Laplacian matrix represents graph connectivity
- Second eigenvector gives a graph bisection
  - Roughly equal “weights” in two parts
  - Weak connection in the graph will be separator
- Implementation via the Lanczos Algorithm
  - To optimize sparse-matrix-vector multiply, we graph partition
  - To graph partition, we find an eigenvector of a matrix associated with the graph
  - To find an eigenvector, we do sparse-matrix vector multiply

  - Have we made progress?
    - The first matrix-vector multiplies are slow, but use them to learn how to make the rest faster

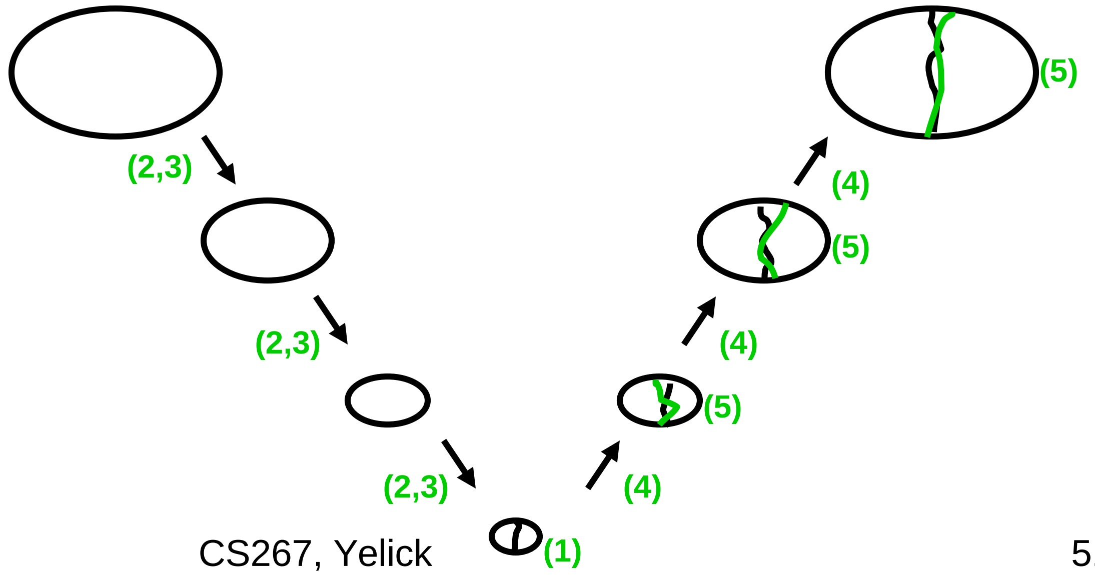
Introduction to Multilevel Partitioning

- If we want to partition G(N,E), but it is too big to do efficiently, what can we do?
  - 1) Replace G(N,E) by a coarse approximation $G_C(N_C,E_C)$, and partition G_C instead
  - 2) Use partition of G_C to get a rough partitioning of G, and then iteratively improve it
- What if G_C still too big?
  - Apply same idea recursively

Multilevel Partitioning - High Level Algorithm

```
    (N+,N- ) = Multilevel_Partition( N, E )
         … recursive partitioning routine returns N+ and N- where N = N+ U N-
         if |N| is small
(1)          Partition G = (N,E)  directly to get N = N+ U N-
             Return (N+, N- )
         else
(2)          Coarsen G to get an approximation $G_C = (N_C, E_C)$
(3)          $(N_C+ , N_C- )$ = Multilevel_Partition( $N_C, E_C$ )
(4)          Expand $(N_C+ , N_C- )$ to a partition  (N+ , N- ) of N
(5)          Improve the partition ( N+ , N- )
             Return ( N+ , N- )
         endif
```

"V - cycle:"



How do we
- Coarsen?
- Expand?
- Improve?

Multilevel Kernighan-Lin

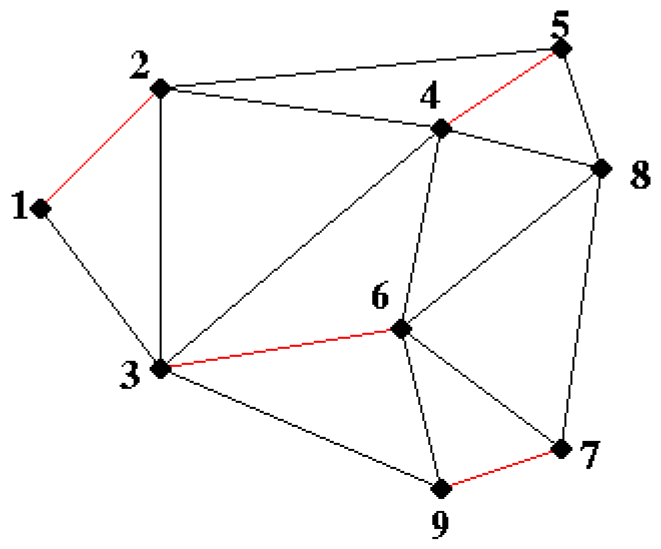
- Coarsen graph and expand partition using maximal matchings
- Improve partition using Kernighan-Lin

Maximal Matching

- *Definition*: A matching of a graph G(N,E) is a subset E_m of E such that no two edges in E_m share an endpoint
- *Definition:* A maximal matching of a graph G(N,E) is a matching E_m to which no more edges can be added and remain a matching
- A simple greedy algorithm computes a maximal matching:

```
let E_m be empty
mark all nodes in N as unmatched
for i = 1 to |N|      … visit the nodes in any order
    if i has not been matched
         mark i as matched
         if there is an edge e=(i,j)  where j is also unmatched,
             add e to E_m
             mark j as matched
         endif
    endif
endfor
```

Maximal Matching: Example



Coarsening using a maximal matching

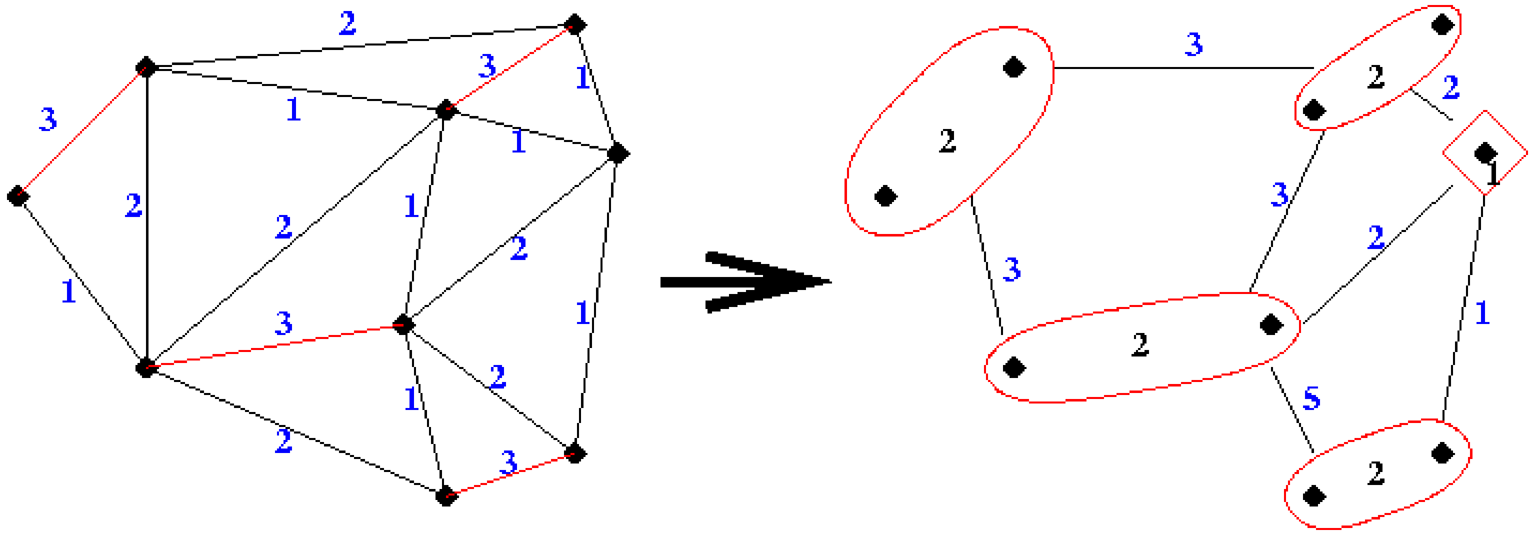
```
1) Construct a maximal matching  $E_m$ of G(N,E)
for all edges e=(j,k) in $E_m$          2) collapse matches nodes into a single one
    Put node n(e) in $N_c$
    W(n(e)) = W(j) + W(k)     … gray statements update node/edge weights
for all nodes n in N not incident on an edge in $E_m$  3) add unmatched nodes
    Put n in $N_c$      … do not change W(n)
… Now each node r in N is “inside” a unique node n(r) in $N_c$

… 4) Connect two nodes in Nc if nodes inside them are connected in E
for all edges e=(j,k) in $E_m$
    for each other edge e’=(j,r) in E incident on j
        Put edge ee = (n(e),n(r)) in $E_c$
        W(ee) = W(e’)
    for each other edge e’=(r,k) in E incident on k
        Put edge ee = (n(r),n(e)) in $E_c$
        W(ee) = W(e’)
```

If there are multiple edges connecting two nodes in N_c, collapse them, adding edge weights

Example of Coarsening

How to coarsen a graph using a maximal matching



$G = (N, E)$

E_m is shown in red

Edge weights shown in blue

Node weights are all one

$G_c = (N_c, E_c)$

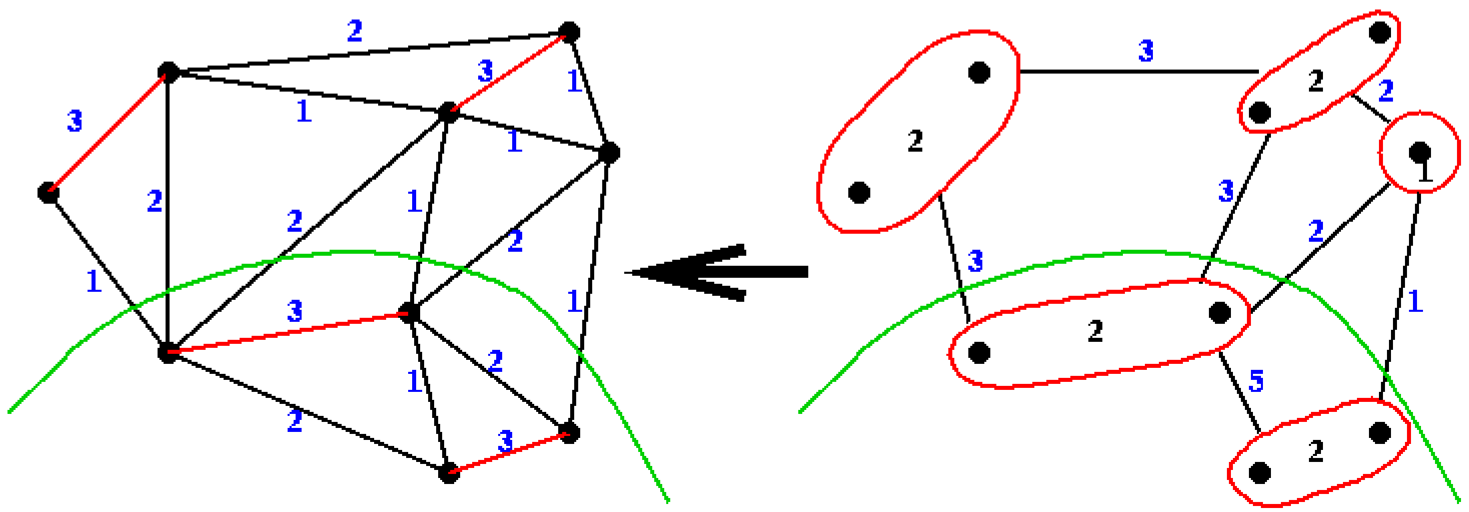
N_c is shown in red

Edge weights shown in blue

Node weights shown in black

Expanding a partition of G_C to a partition of G

Converting a coarse partition to a fine partition



Partition shown in green

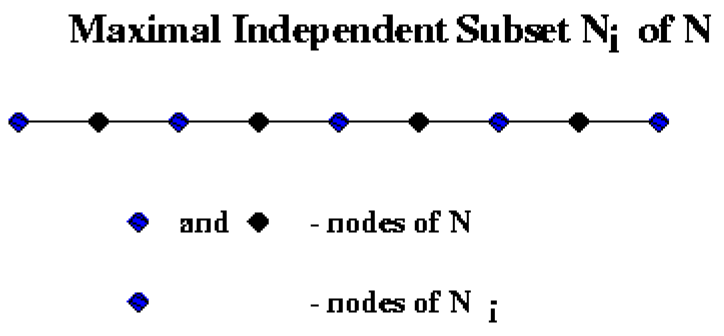
Multilevel Spectral Bisection

- Coarsen graph and expand partition using maximal independent sets
- Improve partition using Rayleigh Quotient Iteration

Maximal Independent Sets

- *Definition*: An independent set of a graph G(N,E) is a subset N_i of N such that no two nodes in N_i are connected by an edge
- *Definition:* A maximal independent set of a graph G(N,E) is an independent set N_i to which no more nodes can be added and remain an independent set
- A simple greedy algorithm computes a maximal independent set:

```
let N_i be empty
for k = 1 to |N|      … visit the nodes in any order
    if  node k is not adjacent to any node already in N_i
        add k to N_i
    endif
endfor
```

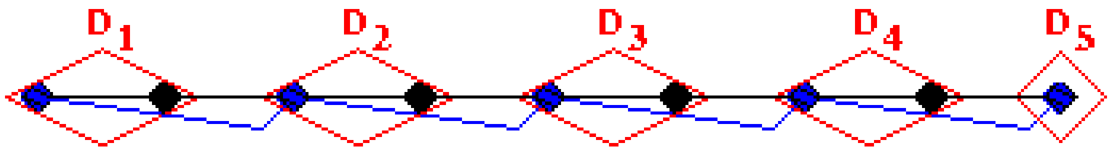


Coarsening using Maximal Independent Sets

```
… Build "domains" D(k) around each node k in $N_i$ to get nodes in $N_c$
… Add an edge to $E_c$ whenever it would connect two such domains
$E_c$ = empty set
for all nodes k in $N_i$
    D(k) = ( {k}, empty set )
    … first set contains nodes in D(k), second set contains edges in D(k)
unmark all edges in E
repeat
    choose an unmarked edge e = (k,j) from E
    if exactly one of k and j (say k) is in some D(m)
        mark e
        add j and e to D(m)
    else if k and j are in two different D(m)'s (say D(mi) and D(mj))
        mark e
        add edge (mk, mj) to $E_c$
    else if both k and j are in the same D(m)
        mark e
        add e to D(m)
    else
        leave e unmarked
    endif
until no unmarked edges
```

Example of Coarsening

Computing G_c from G



◆ and ◆ - nodes of N

◆ - nodes of N_i

— - edges in E

— - edges in E_c

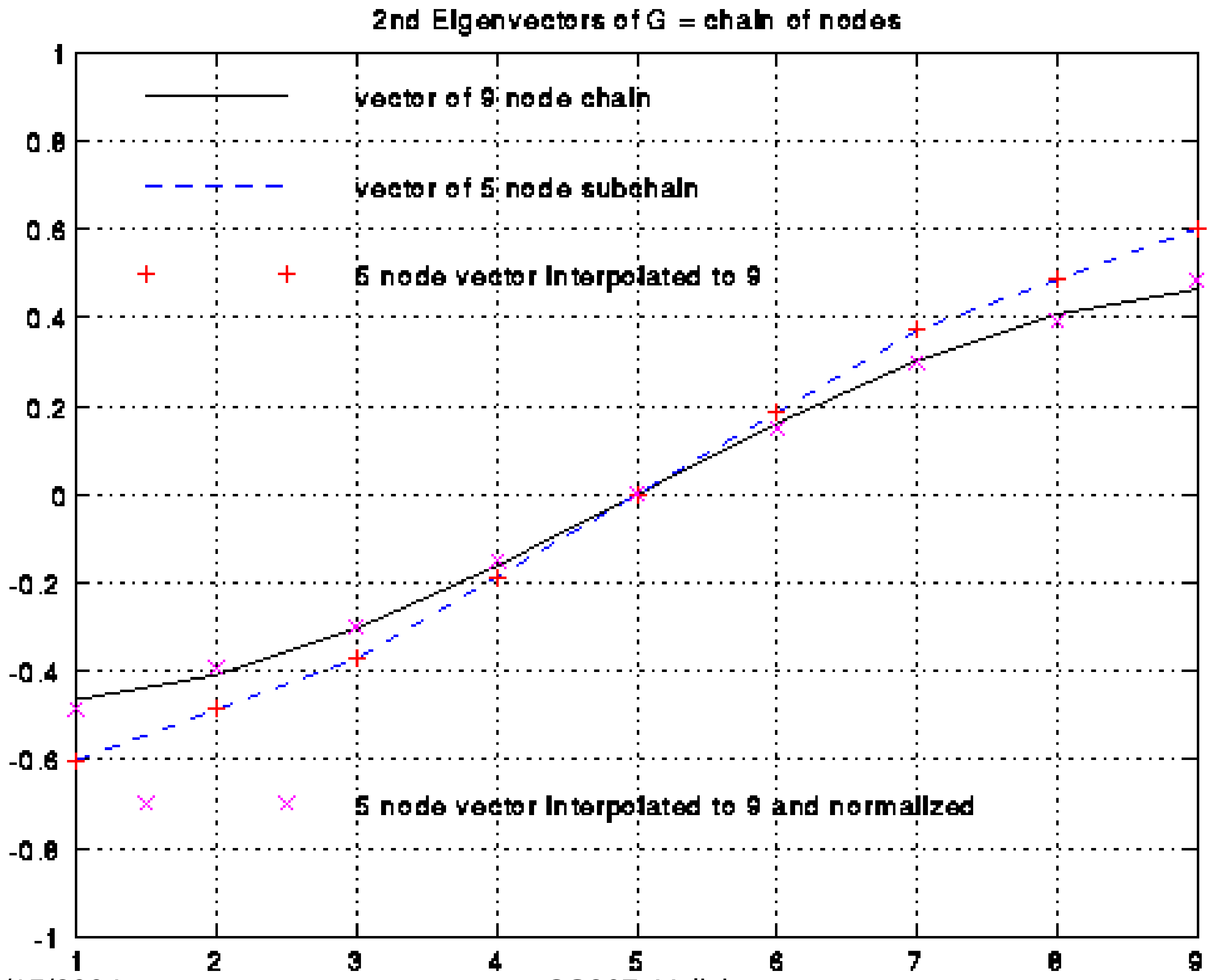
◇ - encloses domain D_k = node of N_c

Expanding a partition of G_C to a partition of G

- Need to convert an eigenvector v_C of $L(G_C)$ to an approximate eigenvector v of L(G)
- Use interpolation:

```
For each node j in N
    if j is also a node in $N_C$, then
        $v(j) = v_C(j)$    … use same eigenvector component
    else
        $v(j)$ = average of $v_C(k)$ for all neighbors k of j in $N_C$
    end if
endif
```

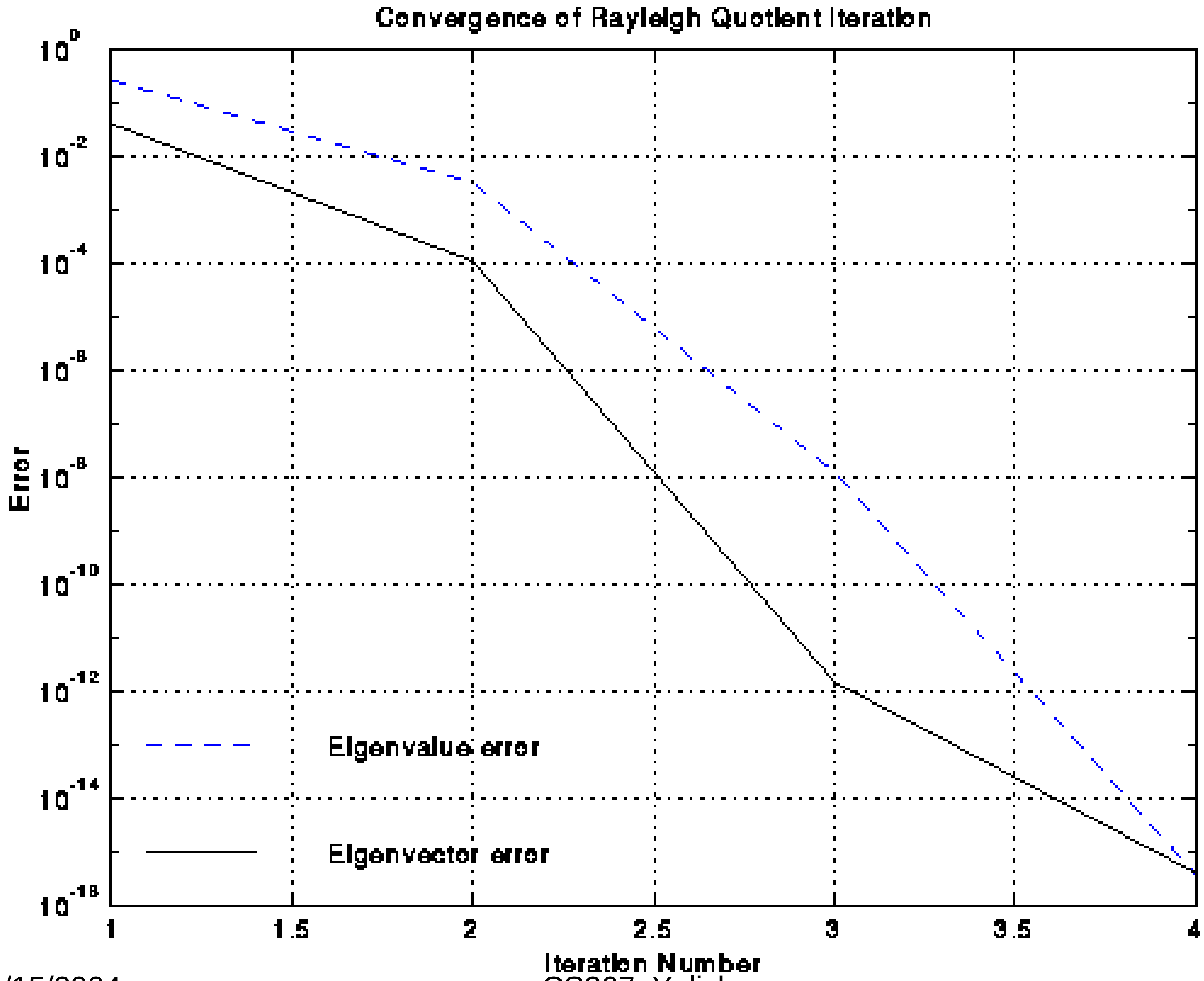
Example: 1D mesh of 9 nodes



Improve eigenvector: Rayleigh Quotient Iteration

```
j = 0
pick starting vector v(0)   … from expanding $v_c$
repeat
    j=j+1
    r(j) = $v^T$(j-1) * L(G) * v(j-1)
    …  r(j) = *Rayleigh Quotient* of v(j-1)
    …         = good approximate eigenvalue
    v(j) = (L(G) - r(j)*I)$^{-1}$ * v(j-1)
    … expensive to do exactly, so solve approximately
    … using an iteration called SYMMLQ,
    … which uses matrix-vector multiply (no surprise)
    v(j) = v(j) / || v(j) ||     … normalize v(j)
until v(j) converges
… Convergence is very fast: cubic
```

Example of convergence for 1D mesh



Available Implementations

- Multilevel Kernighan/Lin
  - METIS (www.cs.umn.edu/~metis)
  - ParMETIS - parallel version
- Multilevel Spectral Bisection
  - S. Barnard and H. Simon, “A fast multilevel implementation of recursive spectral bisection …”, Proc. 6th SIAM Conf. On Parallel Processing, 1993
  - Chaco (www.cs.sandia.gov/CRF/papers_chaco.html)
- Hybrids possible
  - Ex: Using Kernighan/Lin to improve a partition from spectral bisection

Comparison of methods

- Compare only methods that use edges, not nodal coordinates
  - CS267 webpage and KK95a (see below) have other comparisons
- Metrics
  - Speed of partitioning
  - Number of edge cuts
  - Other application dependent metrics
- Summary
  - No one method best
  - Multi-level Kernighan/Lin fastest by far, comparable to Spectral in the number of edge cuts
    - www-users.cs.umn.edu/~karypis/metis/publications/mail.html
    - see publications KK95a and KK95b
  - Spectral give much better cuts for some applications
    - Ex: image segmentation
    - www.cs.berkeley.edu/~jshi/Grouping/overview.html
    - see “Normalized Cuts and Image Segmentation”

Number of edges cut for a 64-way partition

For Multilevel Kernighan/Lin, as implemented in METIS (see KK95a)

Graph	# of Nodes	# of Edges	# Edges cut for 64-way partition	Expected # cuts for 2D mesh	Expected # cuts for 3D mesh	Description
144	144649	1074393	88806	6427	31805	3D FE Mesh
4ELT	15606	45878	2965	2111	7208	2D FE Mesh
ADD32	4960	9462	675	1190	3357	32 bit adder
AUTO	448695	3314611	194436	11320	67647	3D FE Mesh
BBMAT	38744	993481	55753	3326	13215	2D Stiffness M.
FINAN512	74752	261120	11388	4620	20481	Lin. Prog.
LHR10	10672	209093	58784	1746	5595	Chem. Eng.
MAP1	267241	334931	1388	8736	47887	Highway Net.
MEMPLUS	17758	54196	17894	2252	7856	Memory circuit
SHYY161	76480	152002	4365	4674	20796	Navier-Stokes
TORSO	201142	1479989	117997	7579	39623	3D FE Mesh

Expected # cuts for 64-way partition of 2D mesh of n nodes

$$n^{1/2} + 2*(n/2)^{1/2} + 4*(n/4)^{1/2} + \ldots + 32*(n/32)^{1/2} \sim 17 * n^{1/2}$$

Expected # cuts for 64-way partition of 3D mesh of n nodes =

$$n^{2/3} + 2*(n/2)^{2/3} + 4*(n/4)^{2/3} + \ldots + 32*(n/32)^{2/3} \sim 11.5 * n^{2/3}$$

Speed of 256-way partitioning (from KK95a)

Partitioning time in seconds

Graph	# of Nodes	# of Edges	Multilevel Spectral Bisection	Multilevel Kernighan/ Lin	Description
144	144649	1074393	607.3	48.1	3D FE Mesh
4ELT	15606	45878	25.0	3.1	2D FE Mesh
ADD32	4960	9462	18.7	1.6	32 bit adder
AUTO	448695	3314611	2214.2	179.2	3D FE Mesh
BBMAT	38744	993481	474.2	25.5	2D Stiffness M.
FINAN512	74752	261120	311.0	18.0	Lin. Prog.
LHR10	10672	209093	142.6	8.1	Chem. Eng.
MAP1	267241	334931	850.2	44.8	Highway Net.
MEMPLUS	17758	54196	117.9	4.3	Memory circuit
SHYY161	76480	152002	130.0	10.1	Navier-Stokes
TORSO	201142	1479989	1053.4	63.9	3D FE Mesh

Kernighan/Lin much faster than Spectral Bisection!

Coordinate-Free Partitioning: Summary

- Several techniques for partitioning without coordinates
    - Breadth-First Search – simple, but not great partition
    - Kernighan-Lin – good corrector given reasonable partition
    - Spectral Method – good partitions, but slow
- Multilevel methods
    - Used to speed up problems that are too large/slow
    - Coarsen, partition, expand, improve
    - Can be used with K-L and Spectral methods and others
- Speed/quality
    - For load balancing of grids, multi-level K-L probably best
    - For other partitioning problems (vision, clustering, etc.) spectral may be better
    - Good software available

Is Graph Partitioning a Solved Problem?

- Myths of partitioning due to Bruce Hendrickson
  1. ➡ Edge cut = communication cost
  2. ➡ Simple graphs are sufficient
  3. ➡ Edge cut is the right metric
  4. Existing tools solve the problem
  5. Key is finding the right partition
  6. Graph partitioning is a solved problem

- Slides and myths based on Bruce Hendrickson's:
  "Load Balancing Myths, Fictions & Legends"

Myth 1: Edge Cut = Communication Cost

- Myth1: The edge-cut deceit

  edge-cut = communication cost

- Not quite true:
  - #vertices on boundary is actual communication volume
    - Do not communicate same node value twice
  - Cost of communication depends on # of messages too (α term)
  - Congestion may also affect communication cost

- Why is this OK for most applications?
  - Mesh-based problems match the model: cost is ~ edge cuts
  - Other problems (data mining, etc.) do not

Myth 2: Simple Graphs are Sufficient

- Graphs often used to encode data dependencies
  - Do X before doing Y
- Graph partitioning determines data partitioning
  - Assumes graph nodes can be evaluated in parallel
  - Communication on edges can also be done in parallel
  - Only dependence is between sweeps over the graph
- More general graph models include:
  - Hypergraph: nodes are computation, edges are communication, but connected to a set (>= 2) of nodes
  - Bipartite model: use bipartite graph for directed graph
  - Multi-object, Multi-Constraint model: use when single structure may involve multiple computations with differing costs

Myth 3: Partition Quality is Paramount

- When structure are changing dynamically during a simulation, need to partition dynamically
  - Speed may be more important than quality
  - Partitioner must run fast in parallel
  - Partition should be incremental
    - Change minimally relative to prior one
  - Must not use too much memory
- Example from Touheed, Selwood, Jimack and Bersins
  - 1 M elements with adaptive refinement on SGI Origin
  - Timing data for different partitioning algorithms:
    - Repartition time from 3.0 to 15.2 secs
    - Migration time : 17.8 to 37.8 secs
    - Solve time: 2.54 to 3.11 secs

References

- Details of all proofs on Jim Demmel's 267 web page
- A. Pothen, H. Simon, K.-P. Liou, "Partitioning sparse matrices with eigenvectors of graphs", SIAM J. Mat. Anal. Appl. 11:430-452 (1990)
- M. Fiedler, "Algebraic Connectivity of Graphs", Czech. Math. J., 23:298-305 (1973)
- M. Fiedler, Czech. Math. J., 25:619-637 (1975)
- B. Parlett, "The Symmetric Eigenproblem", Prentice-Hall, 1980
- www.cs.berkeley.edu/~ruhe/lantplht/lantplht.html
- www.netlib.org/laso

Summary

- Partitioning with nodal coordinates:
  - Inertial method
  - Projection onto a sphere
  - Algorithms are efficient
  - Rely on graphs having nodes connected (mostly) to “nearest neighbors” in space
- Partitioning without nodal coordinates:
  - Breadth-First Search – simple, but not great partition
  - Kernighan-Lin – good corrector given reasonable partition
  - Spectral Method – good partitions, but slow
- Today:
  - Spectral methods revisited
  - Multilevel methods