CS 267: Applications of Parallel Computers

Graph Partitioning

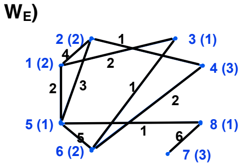
James Demmel
www.cs.berkeley.edu/~demmel/cs267_Spr16

Outline of Graph Partitioning Lecture

- Review definition of Graph Partitioning problem
- Overview of heuristics
- Partitioning with Nodal Coordinates
  - Ex: In finite element models, node at point in (x,y) or (x,y,z) space
- Partitioning without Nodal Coordinates
  - Ex: In model of WWW, nodes are web pages
- Multilevel Acceleration
  - BIG IDEA, appears often in scientific computing
- Comparison of Methods and Applications
- Beyond Graph Partitioning: Hypergraphs

Definition of Graph Partitioning

- Given a graph G = (N, E, W_N, W_E)
  - N = nodes (or vertices),
  - W_N = node weights
  - E = edges
  - 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 U N_2 U … U 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 U N_2: Graph Bisection

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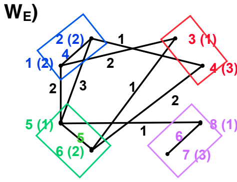

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  - The sum of the node weights in each N_j is "about the same"
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- Ex: balance the work load, while minimizing communication
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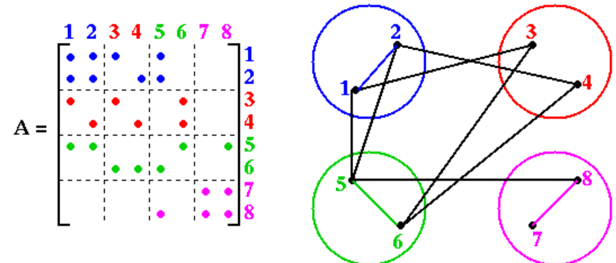
Some Applications

- Telephone network design
  - Original application, algorithm due to Kernighan
- Load Balancing while Minimizing Communication
- Sparse Matrix times Vector Multiplication (SpMV)
  - 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
- Image Segmentation

Sparse Matrix Vector Multiplication y = y +A*x

Partitioning a Sparse Symmetric Matrix

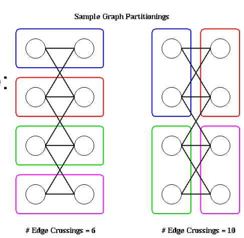



```
… declare A_local, A_remote(1:num_procs), x_local, x_remote, y_local
y_local = y_local + A_local * x_local
for all procs P that need part of x_local
        send(needed part of x_local, P)
for all procs P owning needed part of x_remote
        receive(x_remote, P)
        y_local = y_local + A_remote(P)*x_remote
```


Cost of Graph Partitioning

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

  n choose n/2 = $n!/((n/2)!)^2 \sim (2/(n\pi))^{1/2} * 2^n$ 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

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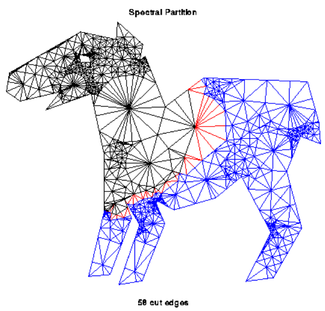
First Heuristic: Repeated Graph Bisection

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



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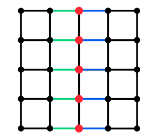
Edge Separators vs. Vertex Separators

- 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
  - $|N_s| \le |E_s|$
- Making an E_s from an N_s: pick all edges incident on N_s
  - $|E_s| \le d * |N_s|$ where d is the maximum degree of the graph
- We will find Edge or Vertex Separators, as convenient

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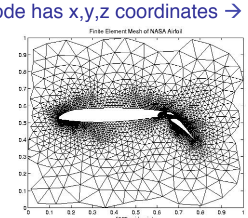
Overview of Bisection Heuristics

- 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

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  - **Ex: In model of WWW, nodes are web pages**
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- **Comparison of Methods and Applications**
- **Beyond Graph Partitioning: Hypergraphs**

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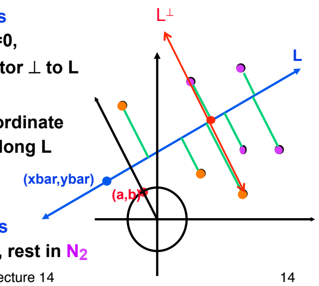
Nodal Coordinates: How Well Can We Do?

- A planar graph can be drawn in plane without edge crossings
- Ex: m x m grid of m^2 nodes: ∃ vertex separator N_s with $|N_s| = m = |N|^{1/2}$ (see earlier slide for m=5)
- *Theorem* (Tarjan, Lipton, 1979): If G is planar, ∃ N_s such that
  - $N = N_1 \cup N_s \cup N_2$ is a partition,
  - $|N_1| \le 2/3 |N|$ and $|N_2| \le 2/3 |N|$
  - $|N_s| \le (8 * |N|)^{1/2}$
- Theorem motivates intuition of following algorithms

Nodal Coordinates: Inertial Partitioning

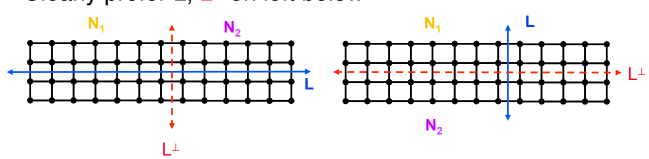
- For a graph in 2D, choose line with half the nodes on one side and half on the other
  - In 3D, choose a plane, but consider 2D for simplicity
- Choose a line L, and then choose a line L⊥ perpendicular to it, with half the nodes on either side

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 ⊥ 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

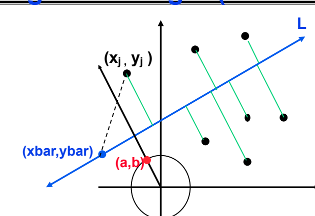
- Clearly prefer L, L⊥ on left below



- 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

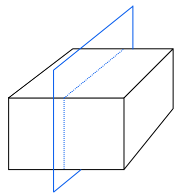


Σ_j (length of j-th green line)^2
= Σ_j [(x_j - xbar)^2 + (y_j - ybar)^2 - (-b*(x_j - xbar) + a*(y_j - ybar))^2]
… Pythagorean Theorem
= a^2 * Σ_j (x_j - xbar)^2 + 2*a*b* Σ_j (x_j - xbar)*(x_j - ybar) + b^2 Σ_j (y_j - ybar)^2
= a^2 * X1 + 2*a*b* X2 + b^2 * X3
= [a b] * $\begin{bmatrix} X1 & X2 \\ X2 & X3 \end{bmatrix}$ * $\begin{bmatrix} a \\ b \end{bmatrix}$

Minimized by choosing
(xbar , ybar) = (Σ_j x_j , Σ_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
  - Any graph can fit in 3D without edge crossings
  - Capture intuition of planar graphs of being connected to "nearest neighbors" but in higher than 2 dimensions
- For intuition, consider 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" like mesh



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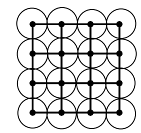
Random Spheres: Well Shaped Graphs

- 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 $\alpha \geq 1$ 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

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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 $O(\alpha * k^{1/d} * n^{(d-1)/d})$ nodes
- When d=2, similar to 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 S "randomly", so that it satisfies Theorem with high probability

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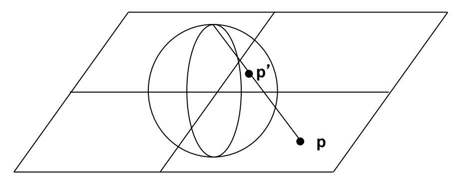
Stereographic Projection

- 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

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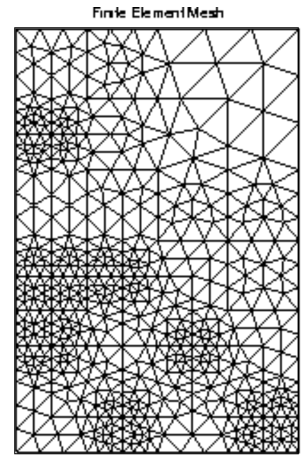
Choosing a Random Sphere

- Do stereographic projection from R^d to sphere S 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 $((1-r)/(1+r))^{1/2}$, project)
    - this maps centerpoint to origin (0,…,0), spreads points around S
- Pick a random plane through origin
  - Intersection of plane and sphere S 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)



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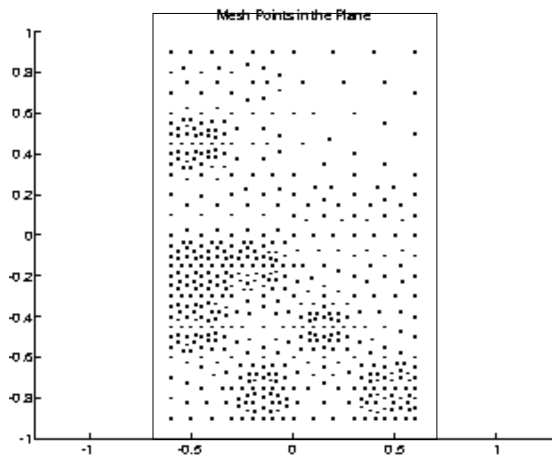

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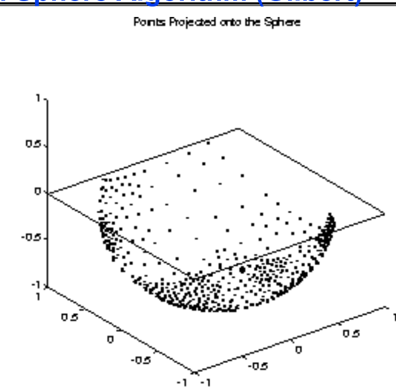
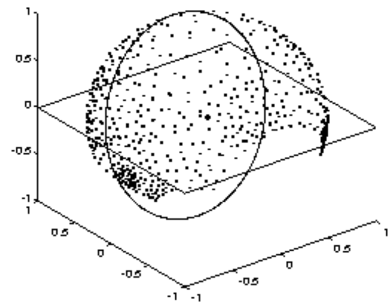


Figure 3: Projected mesh points. The large dot is the centerpoint.

Random Sphere Algorithm (Gilbert)



Random Sphere Algorithm (Gilbert)

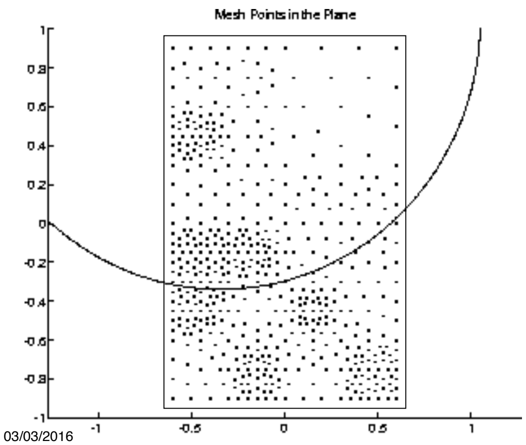


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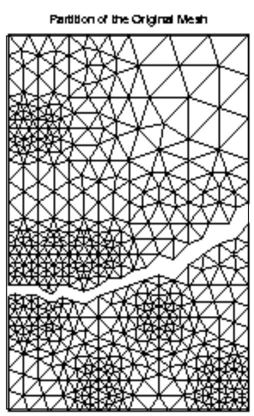
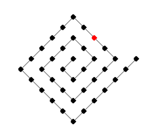
Figure 5: The separating circle projected back to the plane.



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
- Ignores edges, but can be used as good starting guess for subsequent partitioners that do examine edges
- Can do poorly if graph connectivity is not spatial:



- Details at
  - www.cs.berkeley.edu/~demmel/cs267/lecture18/lecture18.html
  - www.cs.ucsb.edu/~gilbert
  - www-bcf.usc.edu/~shanghua/

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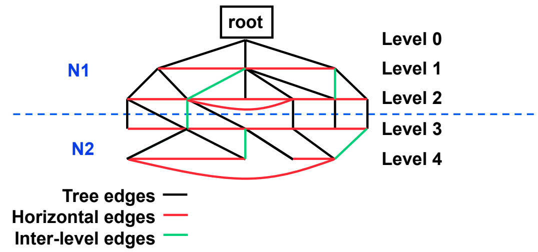
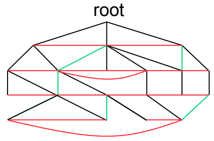
Coordinate-Free: Breadth First Search (BFS)

- 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



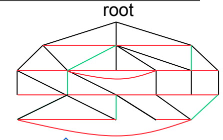
Breadth First Search (details)

- 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 $T(N_T,E_T)$

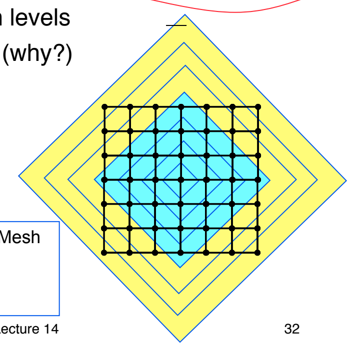



```
NT = {(r,0)}, ET = empty set          ... Initially T = root r, which is at level 0
Enqueue((r,0),Q)                      ... Put root on initially empty Queue Q
Mark r                                ... Mark root as having been processed
While Q not empty                     ... While nodes remain to be processed
    (n,level) = Dequeue(Q)            ... Get a node to process
    For all unmarked children c of n
        NT = NT U (c,level+1)         ... Add child c to NT
        ET = ET U (n,c)               ... Add edge (n,c) to ET
        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
  - $N = N_1 \cup N_2$, 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 U B, where |A| = |B|
  - T = cost(A,B) = Σ {W(e) where e connects nodes in A and B}
  - Find subsets X of A and Y of B with |X| = |Y|
  - Consider swapping X and Y if it decreases cost:
    - newA = (A – X) U Y and newB = (B – Y) U X
    - newT = cost(newA , newB) < T = cost(A,B)
- Need to compute newT efficiently for many possible X and Y, choose smallest (best)

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 = Σ {W(a,b) for b in B}
  - I(a) = internal cost of a in A = Σ {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 = Σk=1 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

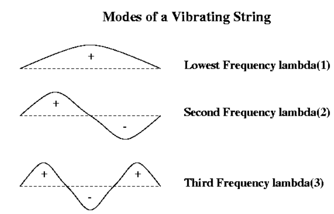
- Most expensive line shown in red, $O(n^3)$
- Some gain(k) may be negative, but if later gains are large, then final Gain may be positive
  - can escape "local minima" where switching no pair helps
- How many times do we Repeat?
  - K/L tested on very small graphs (|N|<=360) and got convergence after 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

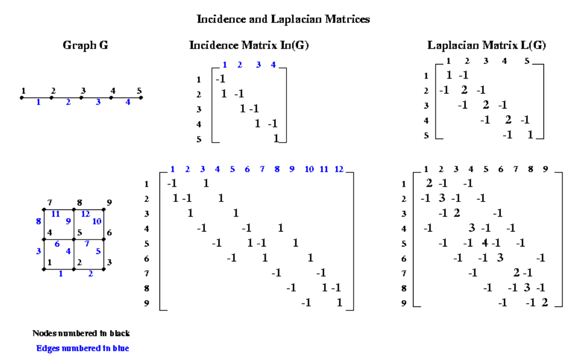
- Vibrating string
- Think of G = 1D mesh as masses (nodes) connected by springs (edges), i.e. a string that can vibrate
- Vibrating string has modes of vibration, or harmonics
- Label nodes by whether mode - or + to partition into N- and N+
- Same idea for other graphs (eg planar graph ~ trampoline)



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



Properties of Laplacian Matrix

- *Theorem 1:* Given G, L(G) has the following properties
  (proof on 1996 CS267 web page)
  - L(G) is symmetric.
    - This means the eigenvalues of L(G) are real and its eigenvectors are real and orthogonal.
  - In(G) * $(In(G))^T$ = L(G)
  - The eigenvalues of L(G) are nonnegative:
    - $0 = \lambda_1 \le \lambda_2 \le \ldots \le \lambda_n$
  - 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, $\lambda_2 \neq 0$ if and only if G is connected.

Spectral Bisection Algorithm

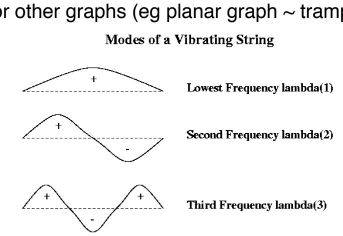
- Spectral Bisection Algorithm:
  - Compute eigenvector v_2 corresponding to $\lambda_2(L(G))$
  - For each node n of G
    - if $v_2(n) < 0$ put node n in partition N-
    - else put node n in partition N+
- Why does this make sense? First reasons...
  - *Theorem 2 (Fiedler, 1975):* Let G be connected, and N- and N+ defined as above. Then N- is connected. If no $v_2(n) = 0$, then N+ is also connected. (proof on 1996 CS267 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 $\lambda_2(L(G_1)) \le \lambda_2(L(G))$, i.e. the algebraic connectivity of G_1 is less than or equal to the algebraic connectivity of G. (proof on 1996 CS267 web page)

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? More reasons...
  - *Theorem 4 (Fiedler, 1975):* Let G be connected, and N1 and N2 be any partition into part of equal size |N|/2. Then the number of edges connecting N1 and N2 is at least .25 * |N| * $\lambda_2(L(G))$.
    (proof on 1996 CS267 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)



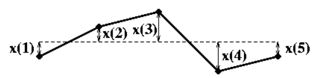
Details for Vibrating String Analogy

- 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

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

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

Vibrating Mass Spring System



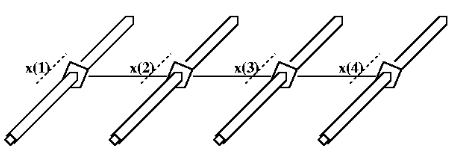
Details for Vibrating String (continued)

- $-(m/k)\, x'' = L*x$, where $x = [x_1, x_2, \dots, x_n]^T$
- Seek solution of form $x(t) = \sin(\alpha * t) * x_0$
  - $L*x_0 = (m/k)*\alpha^2 * x_0 = \lambda * x_0$
  - For each integer i, get $\lambda = 2*(1-\cos(i*\pi/(n+1)))$, $x_0 = \begin{pmatrix} \sin(1*i*\pi/(n+1)) \\ \sin(2*i*\pi/(n+1)) \\ \dots \\ \sin(n*i*\pi/(n+1)) \end{pmatrix}$
  - Thus x_0 is a sine curve with frequency proportional to i
  - Thus $\alpha^2 = 2*k/m *(1-\cos(i*\pi/(n+1)))$ or $\alpha \sim (k/m)^{1/2} * \pi * i/(n+1)$
- $L = \begin{pmatrix} 2 & -1 & & \\ -1 & 2 & -1 & \\ & \dots & & \\ & & -1 & 2 \end{pmatrix}$ not quite Laplacian of 1D mesh, but we can fix that ...

Details for Vibrating String (continued)

- Write down F=ma for "vibrating string" below
- Get Graph Laplacian of 1D mesh

"Vibrating String" for Spectral Bisection

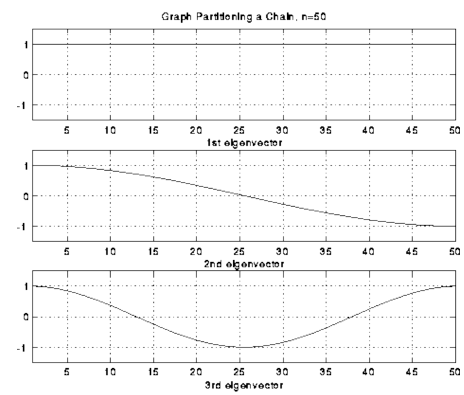


Eigenvectors of L(1D mesh)

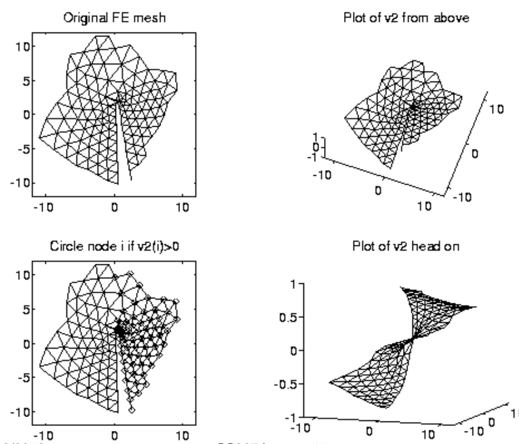
Eigenvector 1 (all ones)

Eigenvector 2

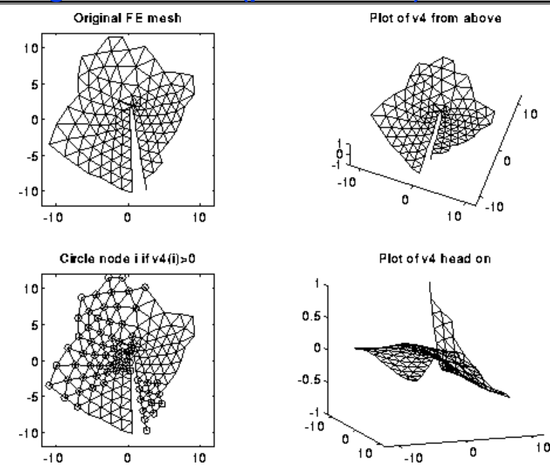
Eigenvector 3



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 (BLAS1)
    r = A*q(j)               … matrix vector multiplication, the most expensive step
    r = r - b(j-1)*v(j-1)    … "axpy", or scalar*vector + vector (BLAS1)
    a(j) = v(j)^T * r        … dot product (BLAS1)
    r = r - a(j)*v(j)        … "axpy" (BLAS1)
    b(j) = ||r||             … compute vector norm (BLAS1)
until convergence            … details omitted
```

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

- 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

Outline of Graph Partitioning Lectures

- Review definition of Graph Partitioning problem
- Overview of heuristics
- Partitioning with Nodal Coordinates
  - Ex: In finite element models, node at point in (x,y) or (x,y,z) space
- Partitioning without Nodal Coordinates
  - Ex: In model of WWW, nodes are web pages
- Multilevel Acceleration
  - BIG IDEA, appears often in scientific computing
- Comparison of Methods and Applications
- Beyond Graph Partitioning: Hypergraphs

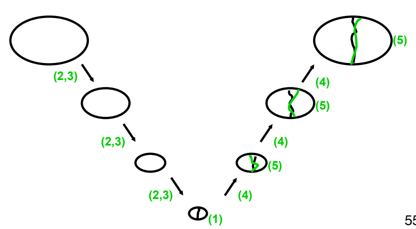
Introduction to Multilevel Partitioning

- 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

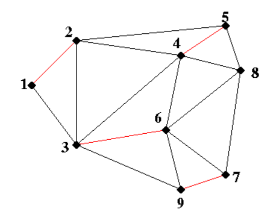
- Coarsen graph and expand partition using maximal matchings
- Improve partition using Kernighan-Lin

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:

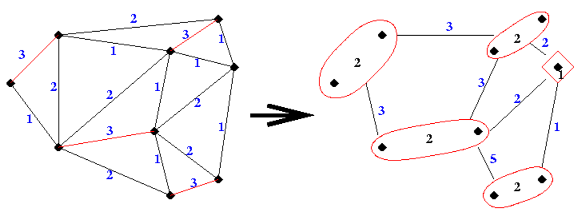
```
let Em be empty
mark all nodes in N as unmatched
for i = 1 to |N|      ... visit the nodes in any order
    if i has not been matched
        mark i as matched
        if there is an edge e=(i,j)  where j is also unmatched,
            add e to Em
            mark j as matched
        endif
    endif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


Maximal Matching: Example



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

Coarsening using a maximal matching (details)

1) Construct a maximal matching E_m of G(N,E)

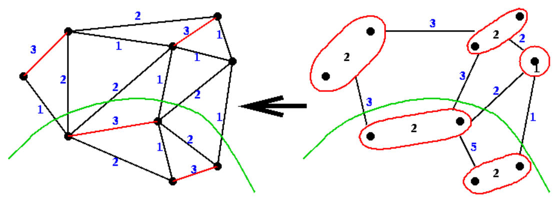
```
for all edges e=(j,k) in Em          2) collapse matched nodes into a single one
    Put node n(e) in Nc
    W(n(e)) = W(j) + W(k)    ... gray statements update node/edge weights
for all nodes n in N not incident on an edge in Em   3) add unmatched nodes
    Put n in Nc     ... do not change W(n)
... Now each node r in N is "inside" a unique node n(r) in Nc

... 4) Connect two nodes in Nc if nodes inside them are connected in E
for all edges e=(j,k) in Em
    for each other edge e'=(j,r) or (k,r) in E
        Put edge ee = (n(e),n(r)) in Ec
        W(ee) = W(e')
```

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

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

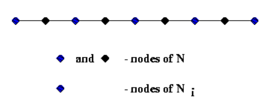
- Coarsen graph and expand partition using maximal independent sets
- Improve partition using Rayleigh Quotient Iteration

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:

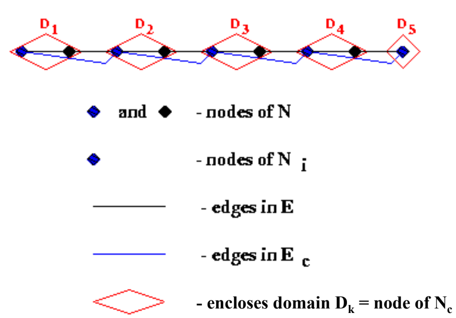
```
let Ni be empty
for k = 1 to |N|      … visit the nodes in any order
    if  node k is not adjacent to any node already in Ni
        add k to Ni
    endif
endfor
```

Maximal Independent Subset N_i of N



Example of Coarsening

Computing G_c from G



Coarsening using Maximal Independent Sets (details)

... 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

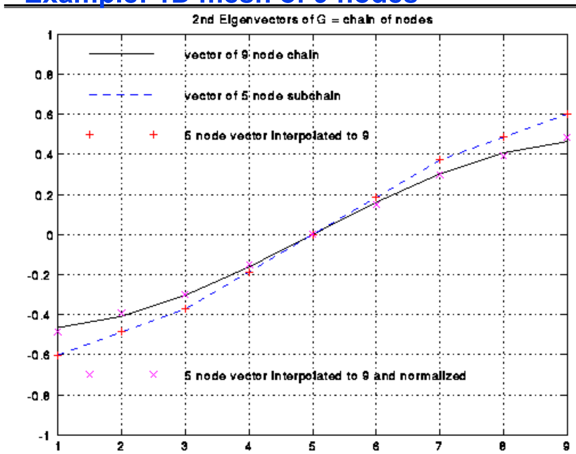
```
Ec = empty set
for all nodes k in Ni
    D(k) = ( {k}, empty set )
    … first set contains nodes in D(k), second set contains edges in D(k)
unmark all edges in E
repeat
    choose an unmarked edge e = (k,j) from E
    if exactly one of k and j (say k) is in some D(m)
        mark e
        add j and e to D(m)
    else if k and j are in two different D(m)'s (say D(mk) and D(mj))
        mark e
        add edge (mk, mj) to Ec
    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
```


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 NC, then
        v(j) = vC(j)   … use same eigenvector component
    else
        v(j) = average of vC(k) for all neighbors k of j in NC
    end if
endif
```

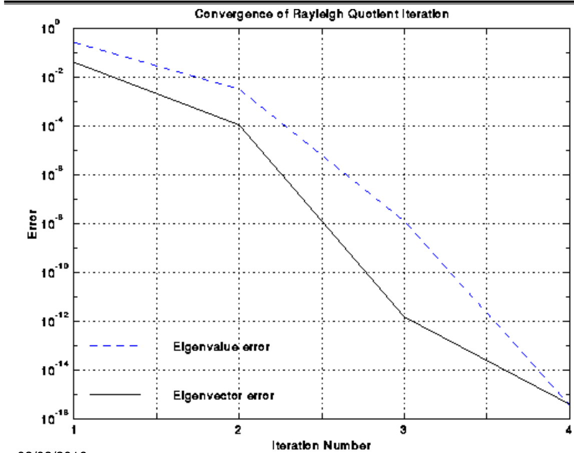

Example: 1D mesh of 9 nodes



Improve eigenvector: Rayleigh Quotient Iteration

```
j = 0
pick starting vector v(0)   … from expanding vC
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 cubic convergence for 1D mesh



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Outline of Graph Partitioning Lectures

- Review definition of Graph Partitioning problem
- Overview of heuristics
- Partitioning with Nodal Coordinates
  - Ex: In finite element models, node at point in (x,y) or (x,y,z) space
- Partitioning without Nodal Coordinates
  - Ex: In model of WWW, nodes are web pages
- Multilevel Acceleration
  - BIG IDEA, appears often in scientific computing
- **Comparison of Methods and Applications**
- Beyond Graph Partitioning: Hypergraphs

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Available Implementations

- **Multilevel Kernighan/Lin**
  - **METIS and ParMETIS (glaros.dtc.umn.edu/gkhome/views/metis)**
  - **SCOTCH and PT-SCOTCH (www.labri.fr/perso/pelegrin/scotch/)**
- **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/~bahendr/chaco.html)**
- **Hybrids possible**
  - **Ex: Using Kernighan/Lin to improve a partition from spectral bisection**
- **Recent package, collection of techniques**
  - **Zoltan (www.cs.sandia.gov/Zoltan)**
- **See www.cs.sandia.gov/~bahendr/partitioning.html**

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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/main.html
  - Spectral give much better cuts for some applications
    - Ex: image segmentation
    - See "Normalized Cuts and Image Segmentation" by J. Malik, J. Shi

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Number of edges cut for a 64-way partition, by METIS

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!

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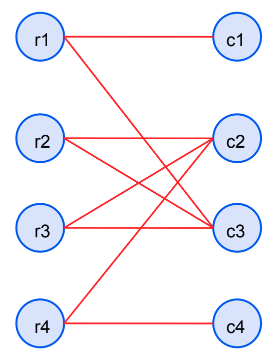
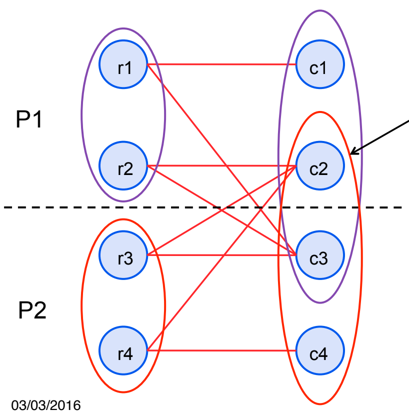
- **Beyond Graph Partitioning: Hypergraphs**

Beyond simple graph partitioning: Representing a sparse matrix as a hypergraph

$$\begin{bmatrix} \times & 0 & \times & 0 \\ 0 & \times & \times & 0 \\ 0 & \times & \times & 0 \\ 0 & \times & 0 & \times \end{bmatrix}$$



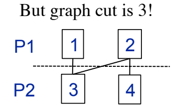
Using a graph to partition, versus a hypergraph



Source vector entries corresponding to c2 and c3 are needed by both partitions – so total volume of communication is 2

$$\begin{bmatrix} \times & 0 & \times & 0 \\ 0 & \times & \times & 0 \\ 0 & \times & \times & 0 \\ 0 & \times & 0 & \times \end{bmatrix}$$

But graph cut is 3!



⇒ Cut size of graph partition may not accurately count communication volume

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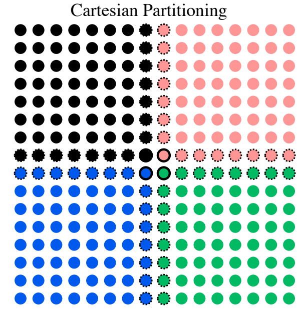
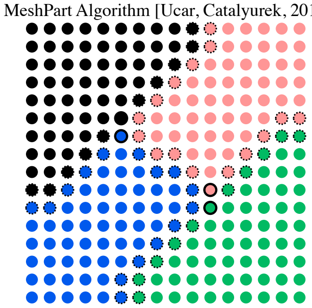
Two Different 2D Mesh Partitioning Strategies

Graph:
Cartesian Partitioning



Hypergraph:
MeshPart Algorithm [Ucar, Catalyurek, 2010]



Total SpMV communication volume = 64

Total SpMV communication volume = 58

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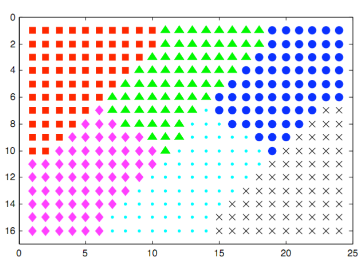
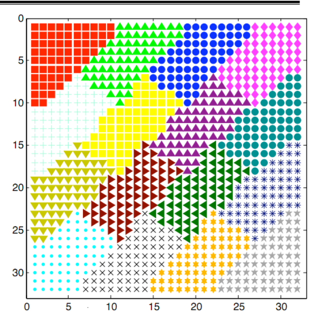
Generalization of the MeshPart Algorithm



vol = 102 boundary−1 = 86 boundary−2 = 8

(a) 2 × 3-way partitioning of the 16 × 24 mesh



vol = 354 boundary−1 = 282 boundary−2 = 36

(c) 16-way partitioning of the 32 × 32 mesh

For NxN mesh on PxP processor grid:
Usual Cartesian partitioning costs ~4NP words moved
MeshPart costs ~3NP words moved, 25% savings

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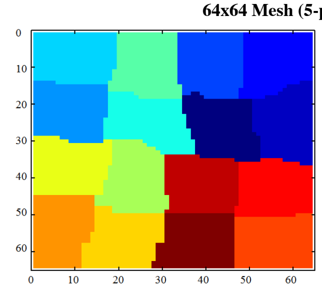
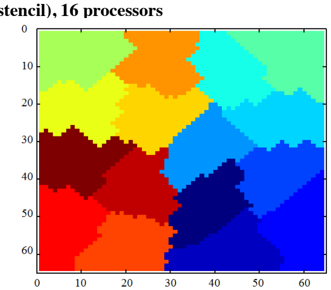
Source: Ucar and Catalyruk, 2010

Experimental Results: Hypergraph vs. Graph Partitioning

64x64 Mesh (5-pt stencil), 16 processors



Graph Partitioning (Metis)
Total Comm. Vol = 777
Max Vol per Proc = 69



Hypergraph Partitioning (PaToH)
Total Comm. Vol = 719
Max Vol per Proc = 59

~8% reduction in total communication volume using hypergraph partitioning (PaToH) versus graph partitioning (METIS)

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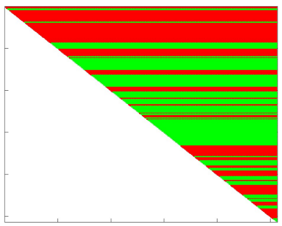
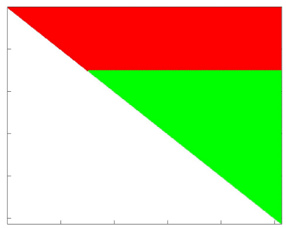
Further Benefits of Hypergraph Model: Nonsymmetric Matrices

- Graph model of matrix has edge (i,j) if either A(i,j) or A(j,i) nonzero
- Same graph for A as $|A| + |A^T|$
- Ok for symmetric matrices, what about nonsymmetric?
  - Try A upper triangular



Graph Partitioning (Metis)
Total Communication Volume= 254
Load imbalance ratio = 6%



Hypergraph Partitioning (PaToH)
Total Communication Volume= 181
Load imbalance ratio = 0.1%

Summary: Graphs versus Hypergraphs

- Pros and cons
  - When matrix is non-symmetric, the graph partitioning model (using $A+A^T$) loses information, resulting in suboptimal partitioning in terms of communication and load balance.
  - Even when matrix is symmetric, graph cut size is not an accurate measurement of communication volume
  - Hypergraph partitioning model solves both these problems
  - However, hypergraph partitioning (PaToH) can be much more expensive than graph partitioning (METIS)
- Hypergraph partitioners: PaToH, HMETIS, ZOLTAN
- For more see Bruce Hendrickson's web page
  - www.cs.sandia.gov/~bahendr/partitioning.html
  - "Load Balancing Fictions, Falsehoods and Fallacies"