Master Course – High-Performance Computing

Parallel Graph-Partitioning on HPC Architectures

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Content

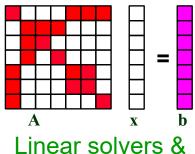
- Motivation for graph partitioning
- Overview of heuristics
- Partitioning with nodal coordinates
 - Ex: In finite element models, node at point in (x, y, z) space
 Recursive Coordinate Bisection
 Inertial Partitioning
- Partitioning <u>without</u> nodal coordinates
 - Ex: In model of WWW, nodes are web pages
 Fiduccia-Matteyes
 Spectral Methods
- Multilevel acceleration
 - **BIG IDEA**, appears often in scientific computing
- Available implementations
- Beyond Graph Partitioning: Hypergraphs

Partitioning and Load Balancing

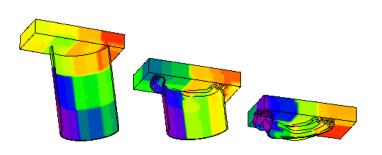
- Goal: assign data to processors to
 - minimize parallel application runtime
 - maximize utilization of computing resources

• Metrics:

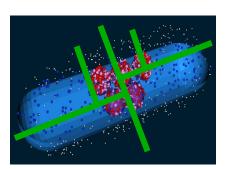
- minimize processor idle time (balance workloads)
- keep inter-processor communication costs low
- Impacts performance of a wide range of simulations



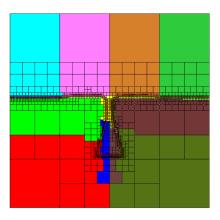
Linear solvers & preconditioners



Contact detection



Particle simulations



Adaptive mesh refinement

Graph Partitioning

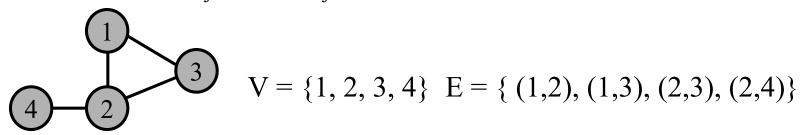
- Work-horse of load-balancing community.
- Highly successful model for PDE problems.
- Model problem as a graph:
 - vertices = work associated with data (computation)
 - edges = relationships between data/computation (communication)
- <u>Goal</u>: Evenly distribute vertex weight while minimizing weight of cut edges.

Excellent software available

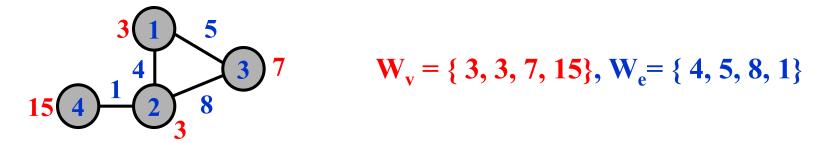
- Serial: METIS (U. Minn.), Scotch (U. Bordeaux)
- Parallel: ParMETIS (U. Minn.), PT-Sotch (U. Bordeaux)

Definition of Graph

- Given a graph G = (V, E) with
 - Vertices $V = \{ v_i | i=1,...,n \}$
 - Edges $E = \{ e_{ij} | v_i \text{ and } v_j \text{ are connected} \}$



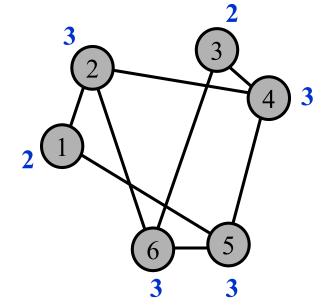
- A weighted graph G = (V, E, W_v, W_e) has node weights and edge weights
 - $W_v = \{ w_v(v_i) \mid v_i \in V \}$ (,,weight of vertices").
 - $W_e = \{ w_e(e_{ij}) \mid e_{ij} \in E \}$ (,,weight of edges").



Examples for Graphs

Symmetric sparse matrix and Graph G_A

_	1	2	3	4	5	6
1	1	1			7	
2	8	6		1		1
3			3	1		1
4		5	1	2	1	
5	2			1	5	1
6		1	5		1	1
	2 3 4 5	2 8 3 4 5 2	1 1 1 2 8 6 3 4 5 5 2	1 1 1 2 8 6 3 4 5 1 5 2	1 1 1 2 8 6 1 3 3 1 4 5 1 2 5 2 1	1 1 1 7 2 8 6 1 3 3 1 4 5 1 2 1 5 2 1 5



• $G_A = (V, E, W_V, W_E); V = \{1, 2, 3, 4, 5, 6\},$

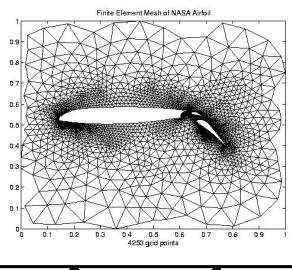
$$E = \{ (1,2), (1,5), (2,4), (2,6), (3,4), (3,6), (4,5), (5,6) \}$$

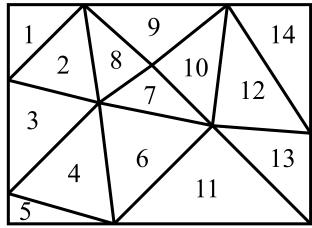
 $W_v = \{2, 3, 2, 3, 3, 3\}$ e.g. numbers of nonzeros in each row

$$W_e = \{1, 1, 1, 1, 1, 1, 1, 1\}$$

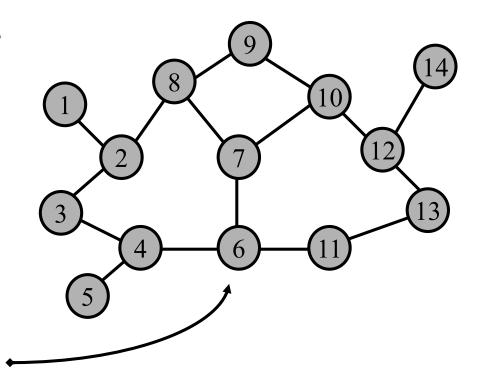
Examples for Graphs

• Finite-Element Simulations





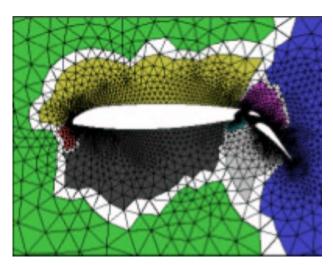
Finite-Element Mesh

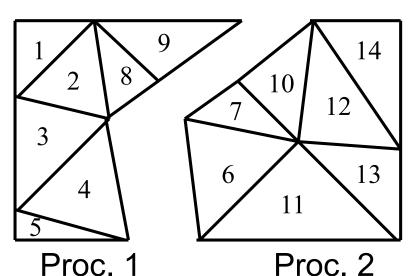


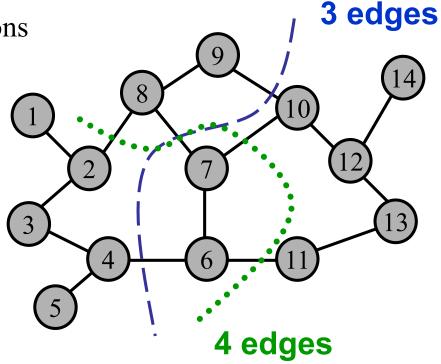
$$G_{FE} = (V, E), V = \{1, ..., 14\}$$

 $E = \{(1,2), ..., (12,14)\}$
 $W_e \equiv 1, W_v \equiv 1$

Parallel Finite-Element Simulations





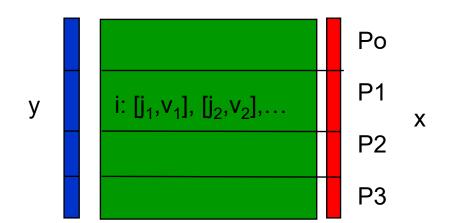


A good partitioning G_{FE} results in

- equal #elements/processor (,,load" and ,,storage balancing").
- Minimal #edges between P1 and P2 (minimal communication volume).

Sparse Matrix-Vector Multiplication:

$$y = A*x$$



communication!

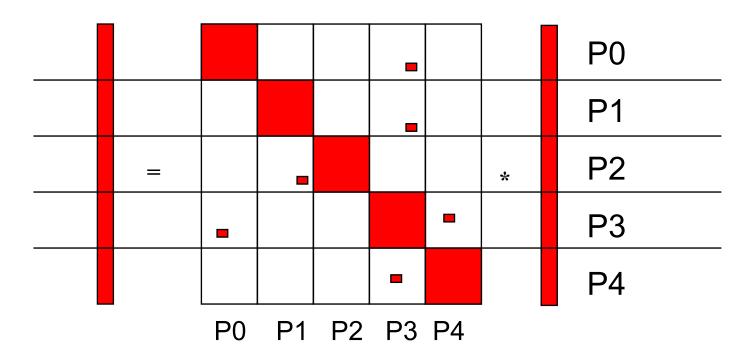
- Which processor stores the y[i], x[i] and A[i, j]?
- Which processor computes

$$y[i] = \sum (j \text{ from 1 to } n) A[i, j] * x[j]$$

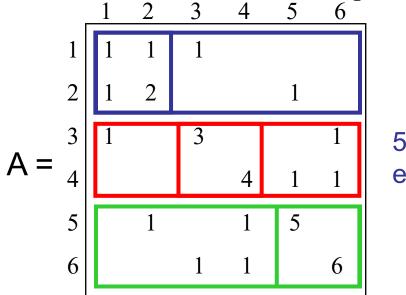
= (row i of A) * x ... sparse scalar product

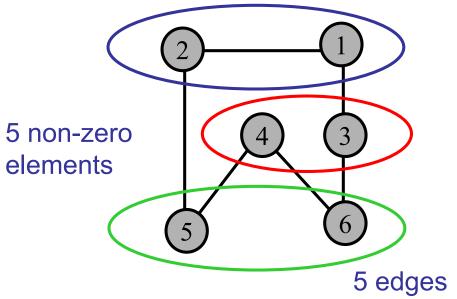
- Partitioning
 - Partition index set $\{1,...,n\} = V_1 + V_2 + ... + V_p$.
 - For each i in V_k : Proc. k stores y[i], x[i] and row i of A
 - For each i in V_k : Proc. k computes y[i] = (row i of A) * x
 - "Rule": Proc. k computes own index set y[i]'s.

- Perfect matrix structure for parallelization: block-diagonal
 - p (# processors) blocks which can be computed locally
 - minimize non-zero elements in the off-diagonal block elements
 - Question: Can we <u>permute</u> rows and columns in such a way that the permuted matrix has a block diagonal structure



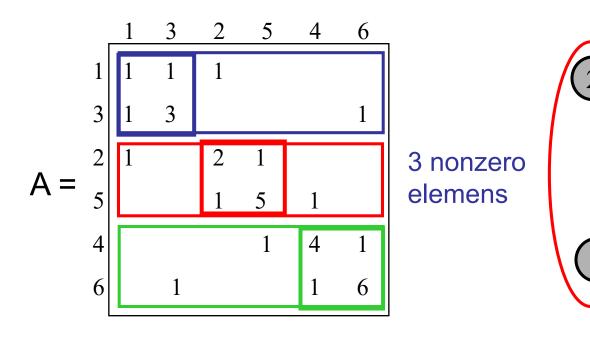
• Parallel matrix-vector multiplication y = A*x





- Good graph partitioning $G_A = (V, E, W_v)$ results in
 - Equal number of vertices on each processor (,,load" and ,,storage balancing")
 - Minimal number of edges between partitioning (minimal communication)
- Permute rows and columns according to the partitioning

• Better partitioning $y' = Py = PAP^T P^*x$



• Original system y=A*x:

$$y[0] = 1*x[0] + 1*x[1] + 1*x[2]$$

$$y[1] = 1*x[0] + 2*x[1] + 1*x[4]$$

$$y[2] = 1*x[0] + 3*x[2] + 1*x[5]$$

$$y[3] = 4*x[3] + 1*x[4] + 1*x[5]$$

• Permuted System $Py = PAP^T P*x$

3 edges

$$y[0] = 1*x[0] + 1*x[2] + 1*x[1]$$

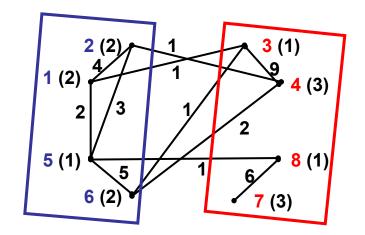
$$y[2] = 1*x[0] + 3*x[1] + 1*x[5]$$

$$y[1] = 1*x[0] + 2*x[2] + 1*x[4]$$

$$y[4] = 1*x[1] + 5*x[4] + 1*x[3]$$

Definition of Graph Partitioning: Bisection

- Given a graph $G = (V, E, W_V, W_E)$
 - V = nodes (or vertices)
 - E = edges



• Choose a partition $V = V_1 U V_2$ such that: The sum of the node in each V_i is "about the same"

$$V = V_1 \cup V_2$$
, $V_1 \cap V_2 = \emptyset$, $|V_1| = |V_2|$

The sum of edge connecting pairs V_1 and V_2 is minimized

$$min \mid \{e_{IJ} \varepsilon E \mid v_i \ \varepsilon V_1 \ und \ v_j \varepsilon \ V_2\} \mid$$

Definition of Graph Partitioning: k-Partitioning

• G = (V, E) Graph with weights W_v and W_e

Find a k-Partition $(V_1, V_2, ..., V_k)$ of V with

(1)
$$V = \bigcup_{i=1}^{k} V_i \text{ und } V_i \cap V_j = \emptyset \text{ (for all } i \neq j)$$

- (2) $\sum_{v(i) \in V_i} w_v(v_i) \text{ of equal size for all } j \in \{1, ..., k\}$
- (3) $\sum_{\substack{e_{ij} \in E \text{ und} \\ v_i \in V_p, v_j \in V_q \text{ und } p \neq q}} W_e(e_{ij}) \quad \text{minimizes over all partitionings of } V.$
- (1) and (2) is important for "load balance"
- (3) minimizes ,,edge cut"

Expected # cuts for 64-way partitioning

Question: Expected # edge cuts for 64-way partition of 2D mesh of n nodes?

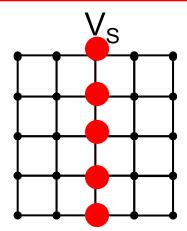
$$n^{1/2} + 2*(n/2)^{1/2} + 4*(n/4)^{1/2} + ... + 32*(n/32)^{1/2} \sim 17*n^{1/2}$$

In the printed version, the solutions can be found in the appendix

Question: Expected # edge cuts for 64-way partition of 3D mesh of n nodes?

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

In the printed version, the solutions can be found in the appendix



Heuristics — 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 V: V_1 and V_2
- Vertex Separator: V_s (subset of V) separates G if removing V_s and all incident edges leaves two ~equal-sized, disconnected components of V: V_1 and V_2

$$G = (V, E)$$
 Vertices V and Edges E

 E_s = green edges or blue edges

 $V_s = red vertices$

• Making a V_s from an E_s: pick one endpoint of each edge in E_s

Question: Given E_s - can we define an upper bound or V_s ?

$$|\mathbf{V}_{\mathbf{s}}| \leq |\mathbf{E}_{\mathbf{s}}|$$

• Making an E_s from a V_s: pick all edges incident on V_s

Question: Given V_s - can be define an upper bound or E_s ?

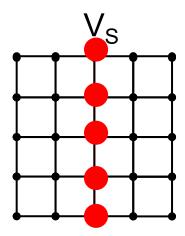
 $|E_s| \le d * |V_s|$ where d is the maximum degree of the graph

Heuristics — Graph Partitioning with Vertex Separators

Graph G = (V, E) compute partitioning with V_1, V_2, V_S such as

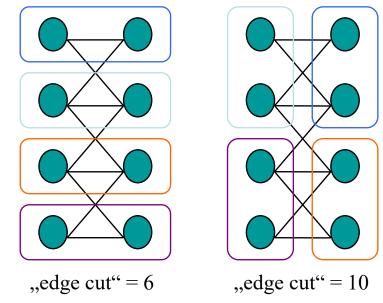
(1)
$$V = V_1 \cup V_2 \cup V_s$$
, $V_1 \cap V_2 \cap V_s = \emptyset$,

- $(2) |V_1| = |V_2|$
- (3) | V_S| small (Vertex separator)



Heuristics — Cost of Graph Partitioning

Many possible partitionings to search

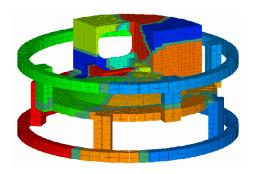


- Choosing optimal partitioning is **NP-complete**
 - Only known exact algorithms have cost = exponential(n)
- We need **good** and **fast** heuristics

Heuristics — Overview of Bisection Algorithms

• Partitioning with nodal coordinates — e.g. each node has x,y,z coordinates \rightarrow partition space

Algorithms: Recursive Coordinate Bisection Inertial Partitioning



- Partitioning <u>without</u> Nodal Coordinates e.g. indexing of web documents A(j,k) = # times keyword j appears in URL k
 Algorithms: Fiduccia-Matteyes
 Spectral Methods
- Multilevel acceleration
 - Approximate problem by "coarse graph," do so recursively

Nodal Coordinates: How Well Can We Do?

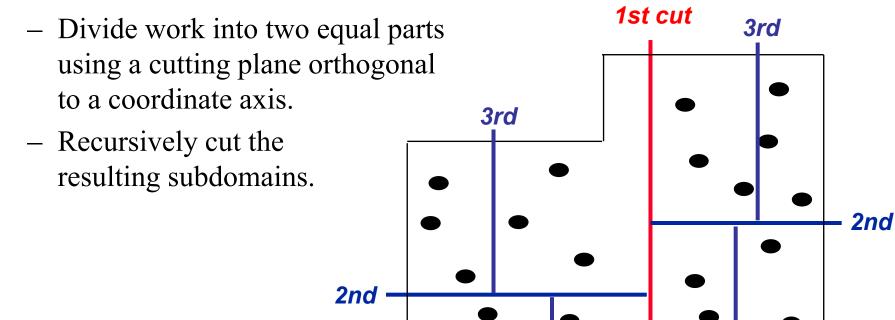
- A planar graph can be drawn in plane without edge crossings
- Example: m x m grid of m² nodes: there exists a vertex separator N_s with $|N_s| = m = |N|^{1/2}$ (see earlier slide for m=5)
- *Theorem* (Tarjan, Lipton, 1979): If G is planar, there exists N_s such that
 - $-N = N_1 U N_s U N_2$ is a partition,
 - $|N_1| \le 2/3 |N| \text{ and } |N_2| \le 2/3 |N|$
 - $|N_s| \le (8 * |N|)^{1/2}$
- Theorem motivates intuition of following algorithms

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 Fiduccia-Matteyes
 Spectral Methods
- Multilevel Acceleration
- Comparison of Methods and Applications

Nodal Coordinates — Recursive Coordinate Bisection (RCB)

- Developed by Berger & Bokhari (1987)
 - Independently discovered by others.
- Idea:

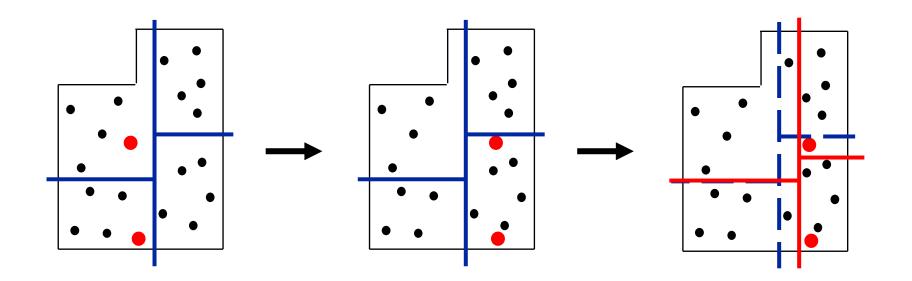


3rd

3rd

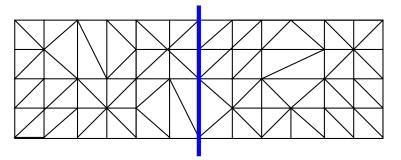
Nodal Coordinates — RCB Advantages

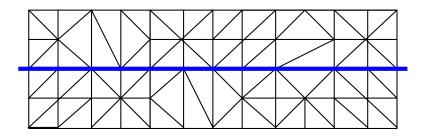
- Conceptually simple; fast and inexpensive.
- Regular subdomains.
 - Can be used for structured or unstructured applications.
- Effective when connectivity info is not available.
- Incremental, but no control of communication costs.



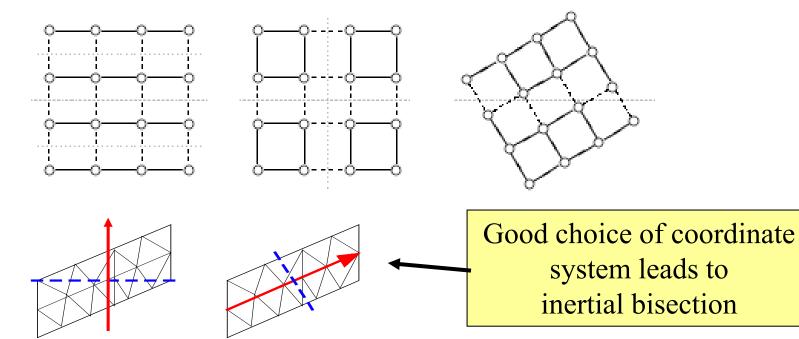
Nodal Coordinates — Coordinate Bisection

• Partition the domain along hyperplanes with node coordinates





• Change the coordinate systems



Nodal Coordinates — Inertial Partitioning

• Choose a line L, and then choose a line H orthogonal to it, with half the nodes on either side

 (x_m, y_m)

(a, b)

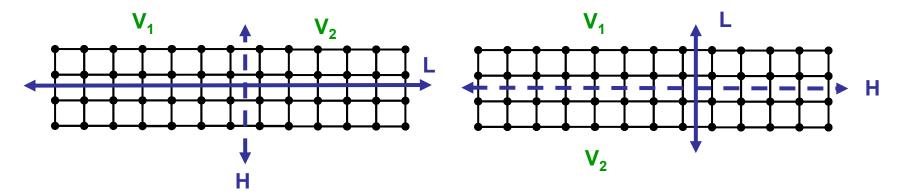
- (1) Center of mass: x_m , y_m
- (2) Choose a line L through the points: L given by a*(x-x_m)+b*(y-y_m)=0 with a²+b²=1; (a, b) is a unit vector orthogonal to L
- (3) Project each point to the line

For each $n_j = (x_j, y_j)$ compute coordinate $S_j = -b^*(x_j-x_m) + a^*(y_j-y_m)$ along L

- (4) Compute the median
 - Let $S_k = \text{median}(S_1, ..., S_n)$
- (5) Use median to partition the nodes
 - Let nodes with $S_j < S_m$ be in V_1 , rest in V_2

Nodal Coordinates — Inertial Partitioning, Choosing L

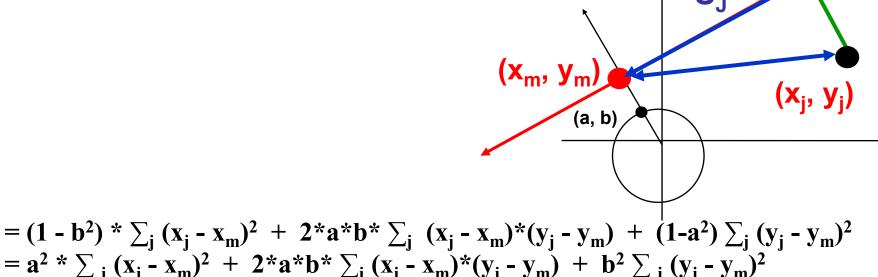
Clearly prefer L on left below



- 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

Nodal Coordinates — Inertial Partitioning, Choosing L

• \sum_{j} (length of j-th green line)² = \sum_{J} [$(x_j - x_m)^2 + (y_j - y_m)^2 - (-b*(x_j-x_m) + a*(y_j-y_m))^2$] ... Pythagorean Theorem



$$= a^{2} * \sum_{j} (x_{j} - x_{m})^{2} + 2*a*b* \sum_{j} (x_{j} - x_{m})*(y_{j} - y_{m}) + b^{2} \sum_{j} (y_{j} - y_{m})^{2}$$

$$= a^{2} * X_{1} + 2*a*b* X_{2} + b^{2} * X_{3}$$

$$= |a b| * |X1 X2| * |a| = \underline{\text{minimum}} = \lambda$$

$$|X2 X3| |b|$$

Minimized by choosing

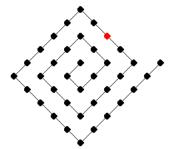
 $(x_m, y_m) = (\sum_j x_j, \sum_j y_j) / n = center of mass$

(a,b) = eigenvector of smallest eigenvalue of 2x2 matrix $M = [X1 \ X2; X2 \ X3]$

Nodal Coordinates — Summary

- Algorithms using nodal coordinates are efficient
- Rely on graphs having nodes connected (mostly) to "nearest neighbors" in space
 - algorithm does <u>not depend on where actual edges</u> 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 very poorly if graph connection is not spatial

Example (graph that is not spatial connected)



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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,WE) and a partitioning N = A U B, where |A| = |B|
 - $T = cost(A,B) = S \{W(e) \text{ where e connects nodes in A and B}\}$
 - 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)

Coordinate-Free — Fiduccia-Matteyes

- Take an **initial partition** and iteratively improve it
- Given $G = (V, E, W_E)$ and a partitioning V = A U B, where |A| = |B|
 - $T = cost(A, B) = \sum \{W(e) \text{ 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

Coordinate-Free — Fiduccia-Matteyes

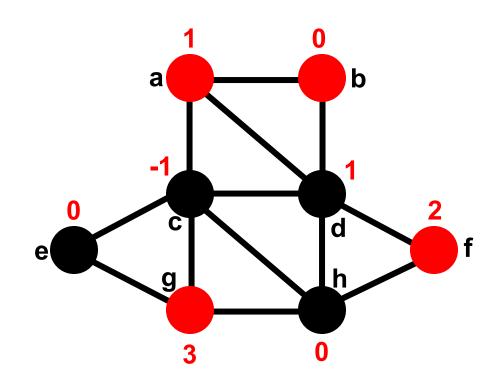
- T = cost(A, B), newT = cost(newA, newB)
- Need an efficient formula for newT; we will use
 - E(a) = external cost of a in $A = \sum \{W(a, b) \text{ for b in B}\}$
 - I(a) = internal cost of a in A = $\sum \{W(a, a') \text{ for other a' in A}\}$
 - D(a) = cost of a in A = E(a) I(a)
 - E(b), I(b) and D(b) defined analogously for b in B

Simplified Fiduccia-Mattheyses: Example (1)

Red nodes are in Part1; black nodes are in Part2.

The initial partition into two parts is arbitrary. In this case it cuts 8 edges.

The initial node gains are shown in red.



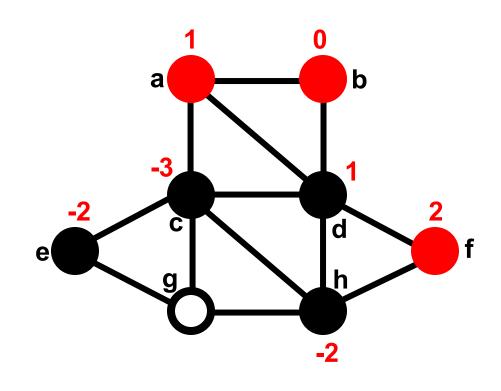
Nodes tentatively moved (and cut size after each pair):

none (8);

Simplified Fiduccia-Mattheyses: Example (2)

The node in Part1 with largest gain is g. We tentatively move it to Part2 and recompute the gains of its neighbors.

Tentatively moved nodes are hollow circles. After a node is tentatively moved its gain doesn't matter any more.



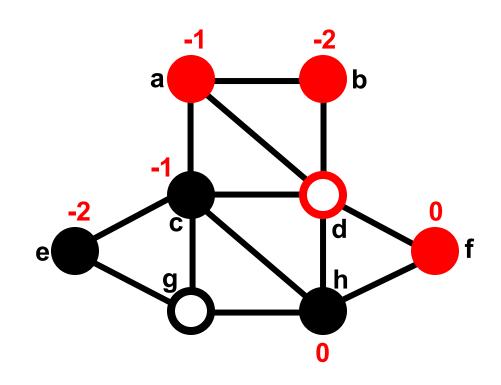
Nodes tentatively moved (and cut size after each pair):

none (8); g,

Simplified Fiduccia-Mattheyses: Example (3)

The node in Part2 with largest gain is d. We tentatively move it to Part1 and recompute the gains of its neighbors.

After this first tentative swap, the cut size is 4.

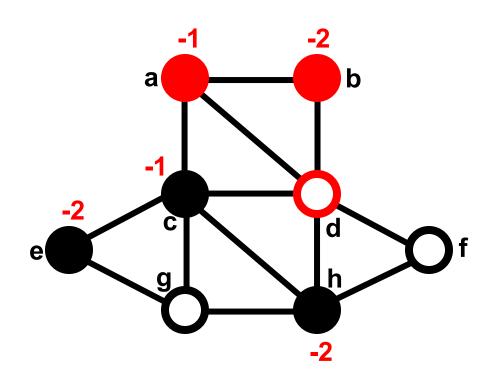


Nodes tentatively moved (and cut size after each pair):

none (8); g, d (4);

Simplified Fiduccia-Mattheyses: Example (4)

The unmoved node in Part1 with largest gain is f. We tentatively move it to Part2 and recompute the gains of its neighbors.



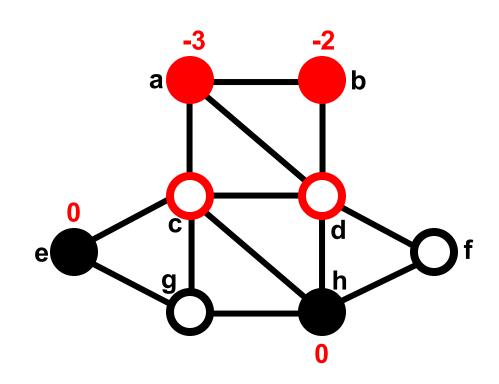
Nodes tentatively moved (and cut size after each pair):

none (8); g, d (4); f

Simplified Fiduccia-Mattheyses: Example (5)

The unmoved node in Part2 with largest gain is c. We tentatively move it to Part1 and recompute the gains of its neighbors.

After this tentative swap, the cut size is 5.

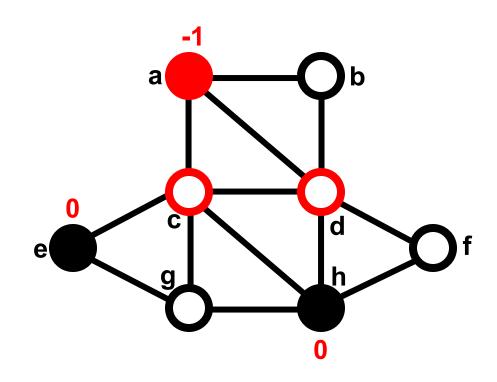


Nodes tentatively moved (and cut size after each pair):

none (8); g, d (4); f, c (5);

Simplified Fiduccia-Mattheyses: Example (6)

The unmoved node in Part1 with largest gain is b. We tentatively move it to Part2 and recompute the gains of its neighbors.

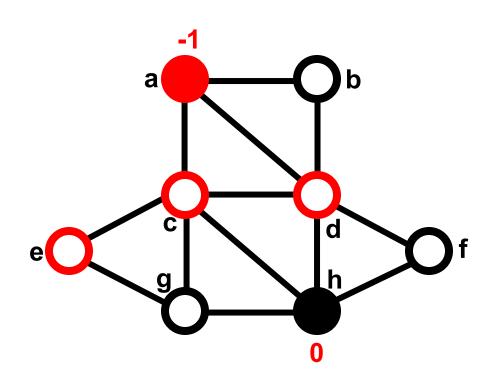


Nodes tentatively moved (and cut size after each pair):

none (8); g, d (4); f, c (5); b

Simplified Fiduccia-Mattheyses: Example (7)

There is a tie for largest gain between the two unmoved nodes in Part2. We choose one (say e) and tentatively move it to Part1. It has no unmoved neighbors so no gains are recomputed.



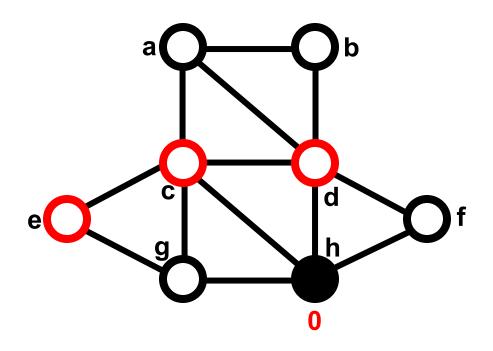
After this tentative swap the cut size is 7.

Nodes tentatively moved (and cut size after each pair):

none (8); g, d (4); f, c (5); b, e (7);

Simplified Fiduccia-Mattheyses: Example (8)

The unmoved node in Part1 with the largest gain (the only one) is a. We tentatively move it to Part2. It has no unmoved neighbors so no gains are recomputed.



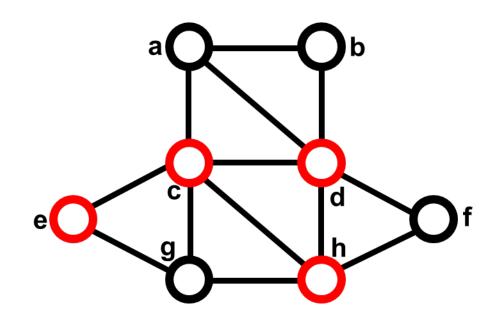
Nodes tentatively moved (and cut size after each pair):

none (8); g, d (4); f, c (5); b, e (7); a

Simplified Fiduccia-Mattheyses: Example (9)

The unmoved node in Part2 with the largest gain (the only one) is h. We tentatively move it to Part1.

The cut size after the final tentative swap is 8, the same as it was before any tentative moves.

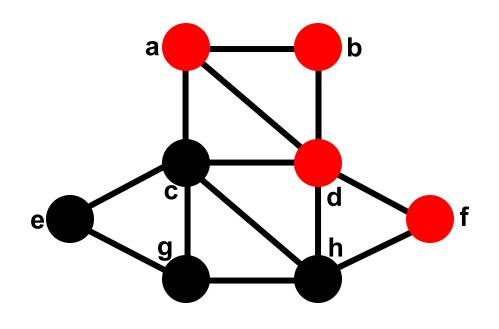


Nodes tentatively moved (and cut size after each pair):

none (8); g, d (4); f, c (5); b, e (7); a, h (8)

Simplified Fiduccia-Mattheyses: Example (10)

After every node has been tentatively moved, we look back at the sequence and see that the smallest cut was 4, after swapping g and d. We make that swap permanent and undo all the later tentative swaps.



This is the end of the first improvement step.

Nodes tentatively moved (and cut size after each pair):

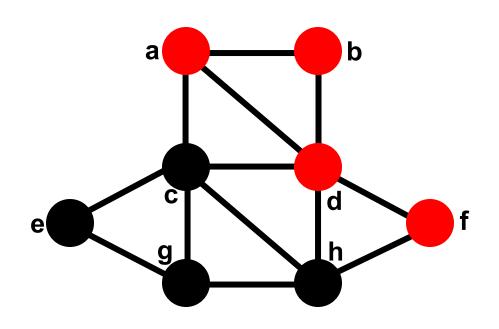
none (8); **g, d (4)**; f, c (5); b, e (7); a, h (8)

Simplified Fiduccia-Mattheyses: Example (11)

Now we recompute the gains and do another improvement step starting from the new size-4 cut. The details are not shown.

The second improvement step doesn't change the cut size, so the algorithm ends with a cut of size 4.

In general, we keep doing improvement steps as long as the cut size keeps getting smaller.



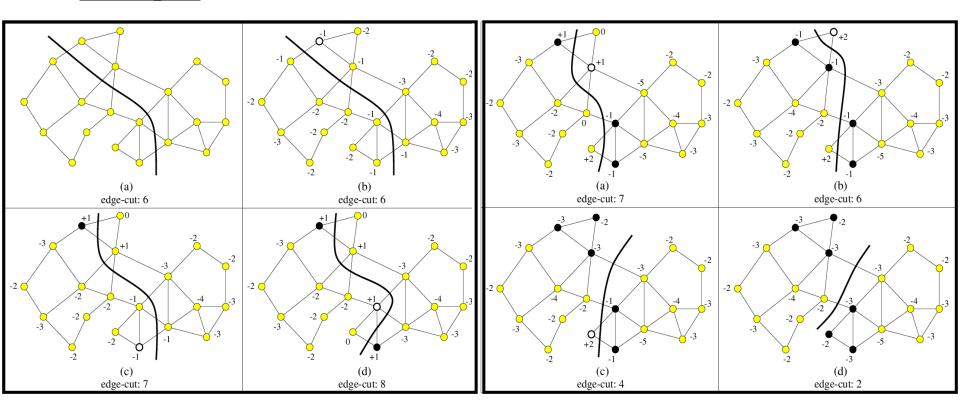
• Algorithm:

```
Repeat
   Compute edge-cut T = cost(A, B) for initial A, B
                                                                          ...O( |E| )
   Compute D(v) for initial A, B with V = A \cup B
                                                                          ...O( |E| )
   Initialize two queues (Q<sub>A</sub>, Q<sub>B</sub>) with highest D(v) on top
                                                                          ...O( |V| log |V| )
   Unmark all nodes in V
                                                                          ...O( |V| )
   While there are nodes v in queue Q_A, Q_B that can be moved
                                                                          ... |V| iterations
          v = TopNode (Q_A, Q_B) (see next slide)
                                                                          ...0(|1|)
          Mark node v and move it in the other subgraph
                                                                          ...0( |1| )
          Remove node v from selected queue Q<sub>A</sub> or Q<sub>B</sub>
                                                                          ...0( |1| )
          // v has d neighbours
          Update gains of adjacent vertices v
                                                                          ...O( |d| )
          Order priority queue Q_A and Q_B
                                                                          ...O( |d| )
   Update T = T - D(v)
                                                                          ...0( |1| )
   Endwhile
Until T <= 0
                                                     Total Complexity ...|V|^*|d| = |E|
```

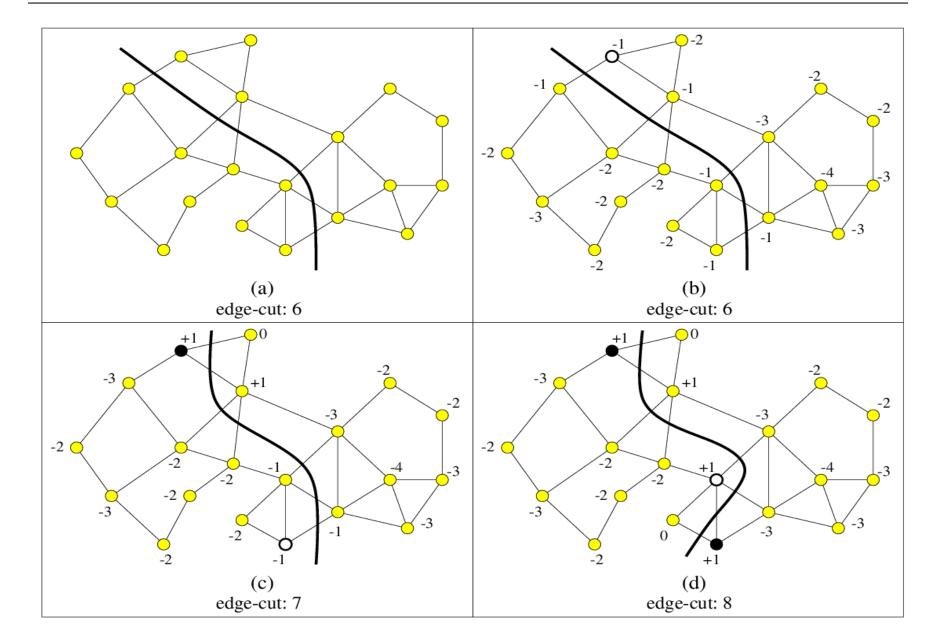
• FM allows a small load imbalance and swaps only one vertex in each iteration

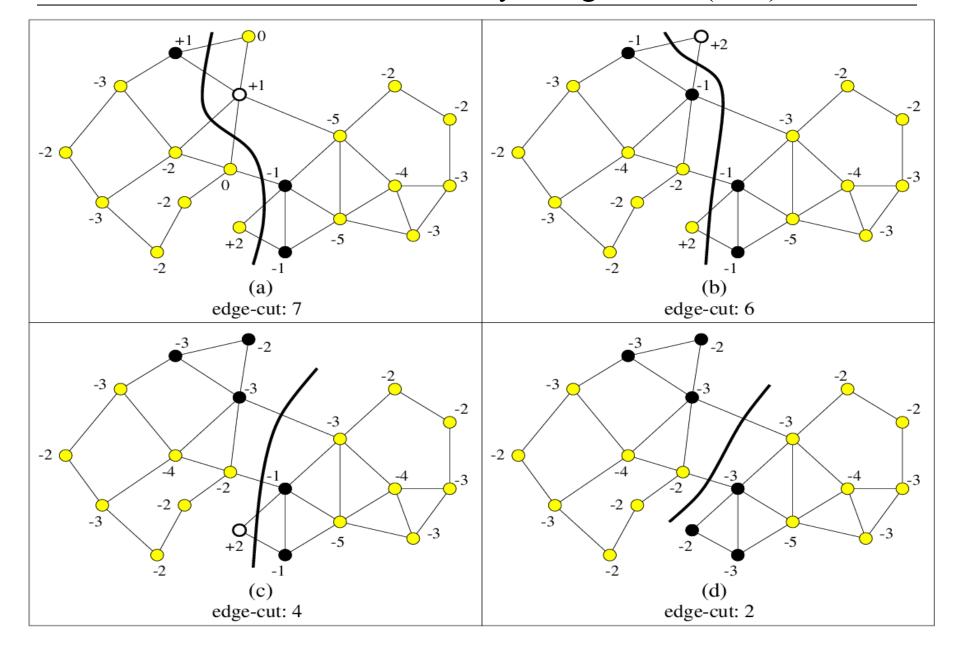
```
node v = TopNode(Q_{\Delta}, Q_{R})
   ... selection of vertex v from Q_{\Delta} or Q_{R}
   a := top node in queue Q_A, b:= top node queue Q_B
   // if one domain is (1+eps) larger than the other domain,
   // select the vertex from the smaller domain
   if ( (|A| > (1+eps)|B|) \text{ or } (|B| > (1+eps)|A|) )
          select the node v from larger domain
   else
          if (D(a) < D(b))
                    select node b to move
          if (D(a) > D(b))
                    select node a to move
          if (D(a) = D(b))
          select node from larger domain
```

• Example:



- All vertices v are marked with D(v) Reduction of edge-cut.
- Load imbalance: 10% therefore in iteration (c) the vertex marked with D(v) = +1 can not move into other domain.



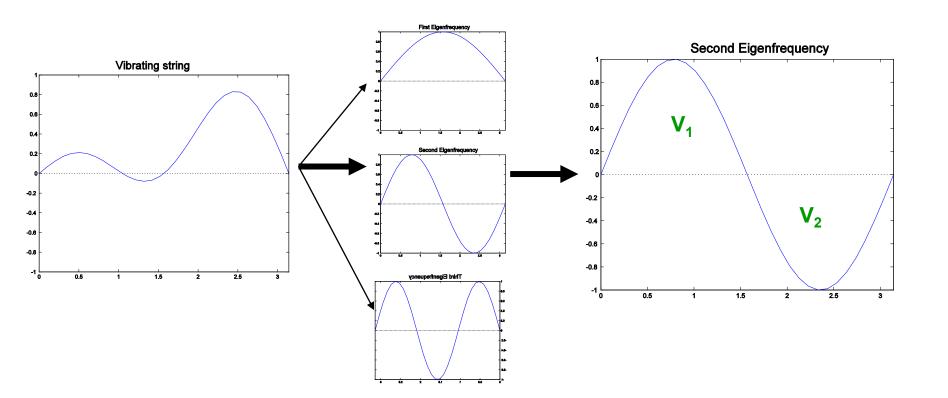


Coordinate-Free — Spectral Methods

- Spectral methods as an example for global partitioning algorithms
- Heavily use of Eigenvalue/Eigenvector analysis

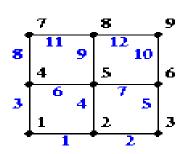
Coordinate-Free — Spectral Methods

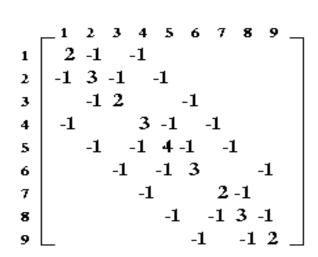
- Based on theory of Fiedler (1970s), popularized by Horst Simon (1995)
- First motivation with vibrating string
- Label nodes by whether mode or + to partition into V₁ and V₂



Coordinate-Free — Spectral Methods, Basic Definitions

- <u>Definition</u>: The Laplacian matrix L(G) of a graph G(V, E) is a |V| by |V| 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





Properties of Laplacian matrices

- Theorem: Given a graph G, L(G) has the following properties
 - L(G) is symmetric this means the eigenvalues of L(G) are real and its eigenvectors are real and orthogonal.
 - Let $e = [1,...,1]^T$, i.e. the column vector of all ones. Then L(G)*e=0*e=0
 - The eigenvalues of L(G) are **nonnegative**:

$$0 = \lambda_1 \le \lambda_2 \le \dots \le \lambda_n$$

- The number of connected components of G is equal to the number of l_i equal to 0.
- **Definition**: λ_2 (L(G)) is the **algebraic connectivity** of G
 - The magnitude of λ_2 measures connectivity
 - In particular, $\lambda_2 != 0$ if and only if G is connected

• Theorem (Fiedler, 1975):

Let G be connected, L(G) the Laplace matrix, and N₊ and N₋ a partitioning with

$$x(i) = +1$$
 if v_i in N_+
 $x(i) = -1$ if v_i in N_- .

Then we have the following property:

#edge-cut between
$$N_+$$
 and N_-

$$= \frac{\frac{1}{4} * x^T * L(G) * x}{}$$

Proof: (next slide)

$$\begin{array}{ll} x^T \cdot L(G) \cdot x &=& \displaystyle \sum_{j} \sum_{i} L(G)_{(i,j)} \cdot x_i \cdot x_j \\ &=& \displaystyle \sum_{i=j} L(G)_{(i,i)} \cdot x_i^2 + \sum_{i \neq j} L(G)_{(i,j)} \cdot x_i \cdot x_j \\ &=& \displaystyle \sum_{i=j} L(G)_{(i,i)} \cdot x_i^2 \\ &+& \displaystyle \sum_{i \neq j; \ i, j \in N^+} L(G)_{(i,j)} \cdot x_i \cdot x_j + \sum_{i \neq j; \ i, j \in N^-} L(G)_{(i,j)} \cdot x_i \cdot x_j \\ &+& \displaystyle \sum_{i \neq j; \ i \in N^+, \ j \in N^-} L(G)_{(i,j)} L(G)_{(i,j)} \cdot x_i \cdot x_j \\ &=& \displaystyle \sum_{i \neq j; \ i \in N^+, \ j \in N^-} L(G)_{(i,j)} L(G)_{(i,j)} \cdot x_i \cdot x_j \\ &+& \displaystyle \sum_{i \neq j; \ i, j \in N^+} (-1) \cdot (+1) \cdot (+1) + \sum_{i \neq j; \ i, j \in N^-} (-1) \cdot (-1) \cdot (-1) \\ &+& \displaystyle \sum_{i \neq j; \ i \in N^+, \ j \in N^-} (-1) \cdot (+1) \cdot (-1) \end{array}$$

$$\begin{array}{ll} x^T \cdot L(G) \cdot x &=& \sum_{j} \sum_{i} L(G)_{(i,j)} \cdot x_i \cdot x_j \\ &=& \sum_{i=j} L(G)_{(i,i)} \cdot x_i^2 + \sum_{i \neq j} L(G)_{(i,j)} \cdot x_i \cdot x_j \\ &=& \sum_{i=j} L(G)_{(i,i)} \cdot x_i^2 \\ &+& \sum_{i \neq j; \ i, j \in N^+} L(G)_{(i,j)} \cdot x_i \cdot x_j + \sum_{i \neq j; \ i, j \in N^-} L(G)_{(i,j)} \cdot x_i \cdot x_j \\ &+& \sum_{i \neq j; \ i \in N^+, \ j \in N^-} L(G)_{(i,j)} L(G)_{(i,j)} \cdot x_i \cdot x_j \\ &=& \sum_{i \neq j; \ i \in N^+, \ j \in N^-} L(G)_{(i,j)} L(G)_{(i,j)} \cdot x_i \cdot x_j \\ &+& \sum_{i \neq j; \ i, j \in N^+} (-1) \cdot (+1) \cdot (+1) + \sum_{i \neq j; \ i, j \in N^-} (-1) \cdot (-1) \cdot (-1) \\ &+& \sum_{i \neq j; \ i \in N^+, \ j \in N^-} (-1) \cdot (+1) \cdot (-1) \end{array}$$

$$x^T \cdot L(G) \cdot x = \sum_{i,j} L(G)_{(i,j)} \cdot x_i \cdot x_j$$

$$= \sum_{i \neq j} degree(i)$$

$$+ \sum_{i \neq j; \ i,j \in N^+} (-1) \cdot (+1) \cdot (+1) + \sum_{i \neq j; \ i,j \in N^-} (-1) \cdot (-1) \cdot (-1)$$

$$+ \sum_{i \neq j; \ i \in N^+, \ j \in N^-} (-1) \cdot (+1) \cdot (-1)$$

$$= 2 \cdot \#edges \ in \ G$$

$$-2 \cdot (\#edges \ connecting \ node \ in \ N^+ \ to \ nodes \ in \ N^+)$$

$$-2 \cdot (\#edges \ connecting \ node \ in \ N^- \ to \ nodes \ in \ N^-)$$

$$+2 \cdot (\#edges \ connecting \ node \ in \ N^+ \ to \ nodes \ in \ N^-)$$

=
$$4 \cdot (\# edges connecting node in N^+ to nodes in N^-)$$

With the theorem we can formulate the **graph bisection** as a discrete optimization problem

1.
$$|V_1| = |V_2|$$
 $\Leftrightarrow \sum_i x(i) = 0$
2. min #cut edges between V_1 and V_2 \Leftrightarrow min $x^T *L(G)*x$

or

min
$$f(x) = \frac{1}{4} x^{T} * L(G) * x$$
 constraints
$$x_{I} = \{+/-1\}, \quad x^{T}*x = n$$

$$x^{T}*e = 0 \text{ with } e=[1, 1, ..., 1]^{T}$$

The discrete combinatorial problem is NP-hard \rightarrow use a continuous problem

min
$$f(z) = \frac{1}{4} z^{T} * L(G) * z$$
constraints
$$z^{T*}z = n, z \text{ real vector}$$

$$z^{T*}e = 0 \text{ with } e=[1,1,...,1]^{T}$$

• Let' try to solve the continuous graph bisection problem

- Minimal solution of $z^T * L(G) * z$ is easy to find.
- L(G) is symmetric \rightarrow L(G) has n orthonormal eigenvectors $u_1, ..., u_n$ with eigenvalues $0 = \lambda_1 \le ... \le \lambda_n$ and $u_1 = \operatorname{sqrt}(n) * e, e = [1, 1, ..., 1]^T$.
- A vector z is a linear combination of eigenvectors u_i : $z = \sum \alpha_i u_i = \alpha_1 u_1 + \alpha_2 u_2 + ... + \alpha_n u_n.$
- First constrained: $z^{T*}e = 0$ or $z^{T*}u_1 = 0$ it is necessary that $z^{T*}u_1 = (\sum \alpha_i u_i)^{T*}u_1 = \alpha_1 u_1^{T*}u_1 = \alpha_1 = 0$
- Second constrained: $z^{T*}z = n$ it is necessary that $z^{T*}z = (\sum \alpha_i u_i)^{T*}(\sum \alpha_j u_j) = \sum \sum \alpha_i \alpha_j u_i^{T*} u_i = \sum \alpha_i^2 = n$
- Minimize $4*f(z)=z^T*L(G)*z$

$$\frac{\mathbf{z}^{T*}\mathbf{L}(\mathbf{G})^{*}\mathbf{z}}{\sum \sum \alpha_{i} \alpha_{i} \lambda_{j} u_{i}^{T*}\mathbf{u}_{i}} = \sum \alpha_{i}^{2} \lambda_{j} \sum \lambda_{j}^{2} \sum \alpha_{i}^{2} \alpha_{i}^{2} \sum \alpha_{i}^{$$

• Minimize $4*f(z)=z^T*L(G)*z$

$$z^{T*}L(G)^*z = (\sum \alpha_i u_i) *L^*(\sum \alpha_j u_j) = (\sum \alpha_i u_i)^{T*}(\sum \alpha_j \lambda_j u_j) =$$

$$\sum \sum \alpha_i \alpha_i \lambda_i u_i^{T*}u_i = \sum \alpha_i^2 \lambda_j$$

$$\geq \lambda_2 \sum \alpha_i^2 = \lambda_2 * \mathbf{n}$$

• Minimum is at $z = sqrt(n) * u_2$

• **Spectral Bisection Algorithm:**

- Compute eigenvector u_2 corresponding to $\lambda_2(L(G))$
- For each vertex v of G
 - if $u_2(v) < 0$ put node v in partition V_1
 - else put vertex v in partition V₂
- The second eigenvector u₂ is called **Fiedler Eigenvector** of the Graph Partitioning problem.

Content

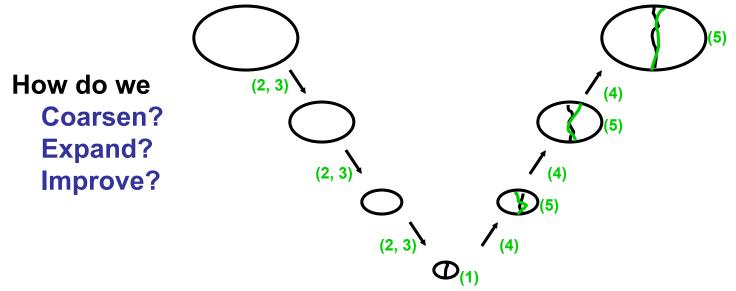
- Motivation for graph partitioning
- Overview of heuristics
- Partitioning with nodal coordinates
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 Inertial Partitioning
- Partitioning <u>without</u> nodal coordinates
 - Ex: In model of WWW, nodes are web pages
 Fiduccia-Matteyes
 Spectral Methods
- Multilevel Acceleration
 - **BIG IDEA**, appears often in scientific computing
- Available Implementations
- Beyond Graph Partitioning: Hypergraphs

Multilevel Partitioning — Introduction

- If we want to partition G(V, E), but it is too big to do efficiently, what can we do?
 - 1) Replace G(V, E) by a **coarse approximation** $G_{\mathbf{C}}(V_{\mathbf{C}}, E_{\mathbf{C}})$, and partition $G_{\mathbf{C}}$ 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

```
(V+, V-) = Multilevel Partition(V, E)
        // recursive partitioning routine returns V+ and V- where V = V+ U V-
        if |V| is small
            Partition G = (V, E) directly to get V = V+ U V-
(1)
           Return (V+, V-)
        else
            Coarsen G to get an approximation G_C = (V_C, E_C)
(2)
            (V_C + , V_{C^-}) = Multilevel_Partition(V_C, E_C)
(3)
            Expand (V_C+, V_{C-}) to a partition (V+, V-) of V
(4)
(5)
            Improve the partition (V+, V-)
           Return (V+, V-)
        endif
```



Multilevel Partitioning — Multilevel Fiduccia-Matteyes

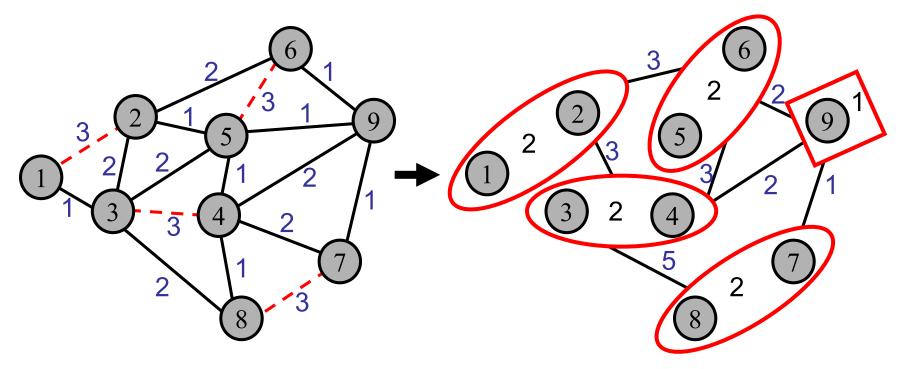
- Coarsen graph and expand partition using maximal matchings
- Improve partition using Fiduccia-Matteyes

Multilevel Partitioning — Maximal Matching

- Definition: A matching of a graph G(V, 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(V, 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<sub>m</sub> be empty
mark all nodes in V as unmatched
for vertex i = 1 to |V| // visit the nodes in any order
  if i has not been matched
      mark vertex i as matched
      if there is an edge e=(i, j) where vertex j is also unmatched
         add e to E<sub>m</sub>
         mark vertex j as matched
      endif
  endif
end
```

Multilevel Partitioning — Coarsening



G=(V, E)

Matching E_m is red

Edge weights are blue

Vertex weights all 1

 $G_c = (V_c, E_c)$

Vertices V_c are red

Edge weights are blue

Vertex weights are black

Multilevel Partitioning — Coarsening with maximal matchings

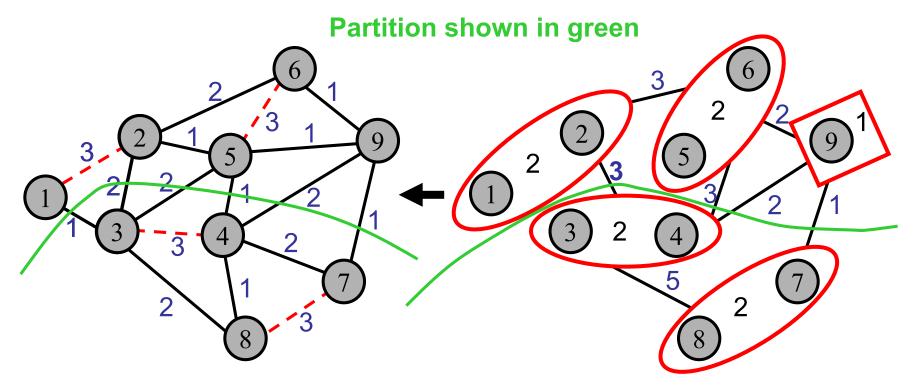
- 1) Construct a maximal matching E_m of G(V, E)
- 2) Collapse matched nodes into a single one for all edges e= (j, k) in E_m
 Put vertex v(e) in V_c
 W(v(e)) = W(j) + W(k) // update vertex weights
- 3) Add unmatched vertices

```
for all vertices v in V not incident on an edge in E<sub>m</sub>
Put v in V<sub>c</sub> // do not change W(n)
// Now each vertex r in V is "inside" a unique node v(r) in V<sub>c</sub>
// Compute now the edges and edge weights of the coarse graph
```

4) Connect two vertices in V_c if vertices inside them are connected in C for all edges e= (j, k) in E_m for each other edge e'= (j, r) or (k, r) in E Put edge ee = (v(e), v(r)) in E_c W(ee) = W(e')

If there are multiple edges connecting two vertices in C_c, collapse them, adding edge weights

Multilevel Partitioning — Expanding a partitioning of G_c to G



Matching E_m is red

Edge weights are blue

Vertex weights all 1

$$G_c = (V_c, E_c)$$

Vertices V_c are red

Edge weights are blue

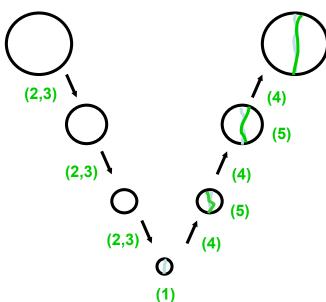
Vertex weights are black

Multilevel Spectral Bisection

```
f = Fiedler (V, E)
        ... Recursive computation of Fiedler Vector of Laplacian L(G)
        if |V| is small
            Calculate f=u<sub>2</sub> using eigenvalue/eigenvector algorithms
(1)
            Return f
        else
            Coarsen G to get an approximation G_c = (V_c, E_c)
(2)
            f' = Fiedler(V_c, E_c)
(3)
            Use f 'to find an inital guess for f (0)
(4)
(5)
            improve f from the initial guess f (0)
            Return f
        endif
```

How do we

Coarsen?
use initial guess?
improve the initial guess?



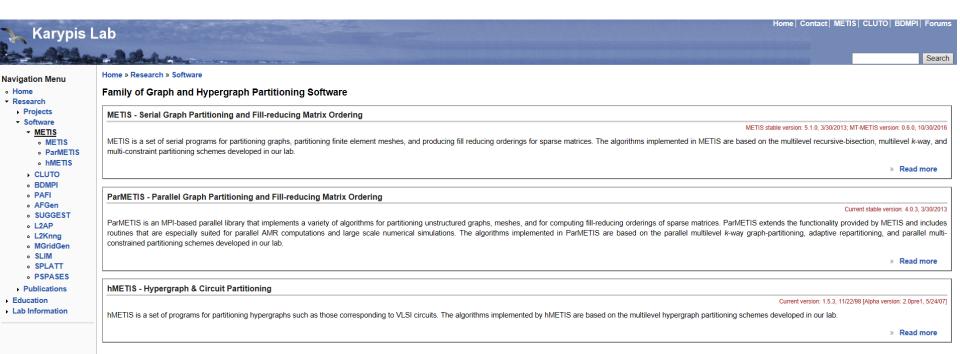
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Available Implementations

- 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 ...", 1993
 - Chaco (SC'14 Test of Time Award)
- Hybrids possible
 - Ex: Use Kernighan/Lin to improve a partition from spectral bisection
- Recent packages with collection of techniques
 - Zoltan (<u>www.cs.sandia.gov/Zoltan</u>)
 - KaHIP (http://algo2.iti.kit.edu/kahip/)

METIS - Family of Graph and Hypergraph Partitioning Software



Copyright 2006-2015, George Karypis

http://glaros.dtc.umn.edu/gkhome/views/metis

KaHyPar - Karlsruhe Hypergraph Partitioning

KaHyPar -Karlsruhe Hypergraph Partitioning

A multilevel hypergraph partitioning framework providing direct k-way and recursive bisection based partitioning algorithms that compute solutions of very high quality.

View the Project on GitHub

This project is maintained by SebastianSchlag

Hosted on GitHub Pages — Theme by orderedlist

KaHyPar - Karlsruhe Hypergraph Partitioning

License	Linux & macOS Build	Windows Build	Code Coverage	Coverity Scan	SonarQube	Fossa
License GPL v3	build passing	build passing	codecov 80%	coverity passed	Qualit	Scene can passing

What is a Hypergraph? What is Hypergraph Partitioning?

Hypergraphs are a generalization of graphs, where each (hyper)edge (also called net) can connect more than two vertices. The k-way hypergraph partitioning problem is the generalization of the well-known graph partitioning problem: partition the vertex set into k disjoint blocks of bounded size (at most 1 + ϵ times the average block size), while minimizing an objective function defined on the nets.

The two most prominent objective functions are the cut-net and the connectivity (or λ – 1) metrics. Cut-net is a straightforward generalization of the edge-cut objective in graph partitioning (i.e., minimizing the sum of the

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

	# of	# of	# Edges cut	Expected	Expected	
Graph	Nodes	Edges	for 64-way	# cuts for	# cuts for	Description
			partition	2D mesh	3D mesh	
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 $n^{1/2} + 2*(n/2)^{1/2} + 4*(n/4)^{1/2} + ... + 32*(n/32)^{1/2} \sim 17 * n^{1/2}$

Expected # cuts for 64-way partition of 3D mesh of n nodes = $n^{2/3} + 2*(n/2)^{2/3} + 4*(n/4)^{2/3} + ... + 32*(n/32)^{2/3} \sim 11.5 * n^{2/3}$

Speed of 256-way partitioning (from KK95a)

Partitioning time in seconds

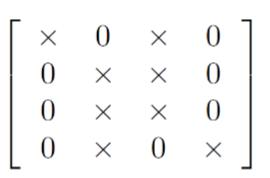
	# of	# of	Multilevel	Multilevel	
Graph	Nodes	Edges	Spectral	Kernighan/	Description
			Bisection	Lin	_
144	144649	1074393	607.3	48.1	3D FE Mesh
4ELT	15606	45878	25.0	3.1	2D FE Mesh
ADD32	4960	9462	18.7	1.6	32 bit adder
AUTO	448695	3314611	2214.2	179.2	3D FE Mesh
BBMAT	38744	993481	474.2	25.5	2D Stiffness 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

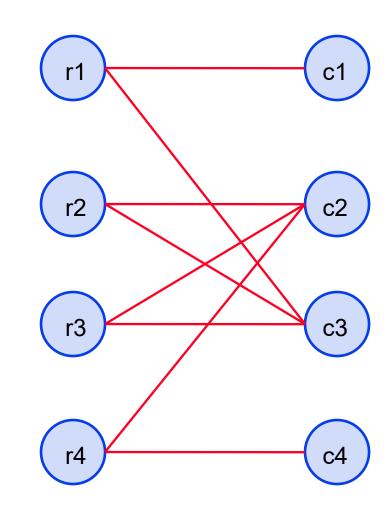
Kernighan/Lin much faster than Spectral Bisection!

Content

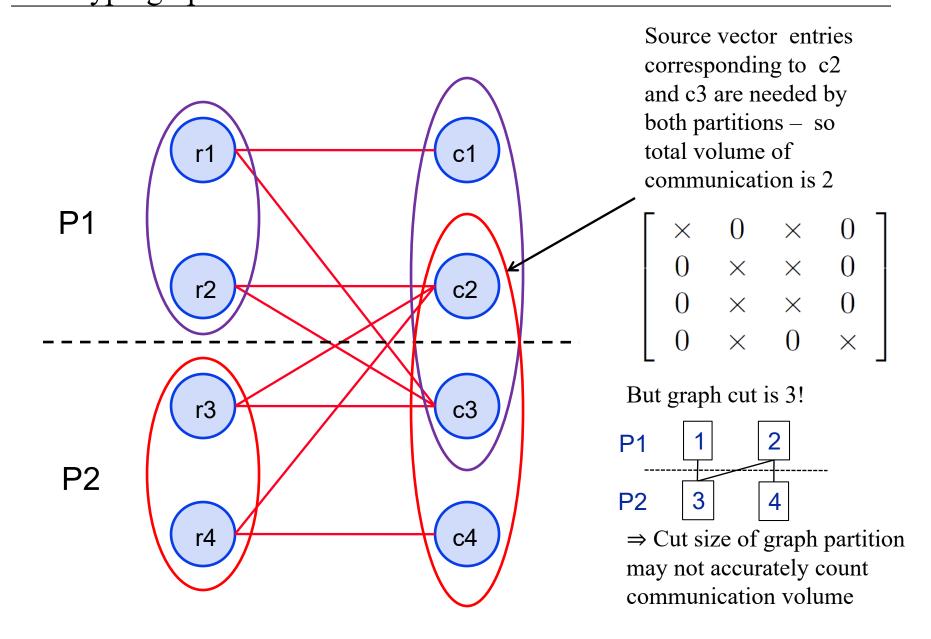
- Motivation for graph partitioning
- Overview of heuristics
- Partitioning with nodal coordinates
 - Ex: In finite element models, node at point in (x, y, z) space
 Recursive Coordinate Bisection
 Inertial Partitioning
- Partitioning <u>without</u> nodal coordinates
 - Ex: In model of WWW, nodes are web pages
 Fiduccia-Matteyes
 Spectral Methods
- Multilevel Acceleration
 - BIG IDEA, appears often in scientific computing
- Available Implementations
- Beyond Graph Partitioning: Hypergraphs

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

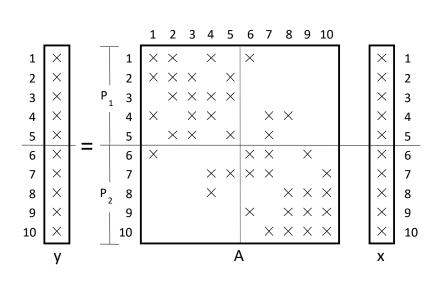


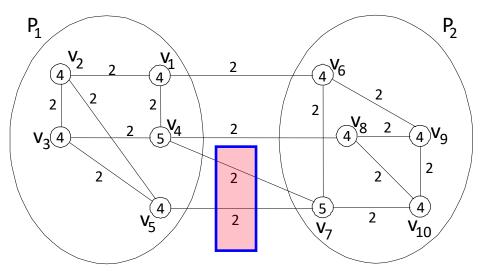


Beyond simple graph partitioning: Representing a sparse matrix as a hypergraph



A sparse matrix in the graph model





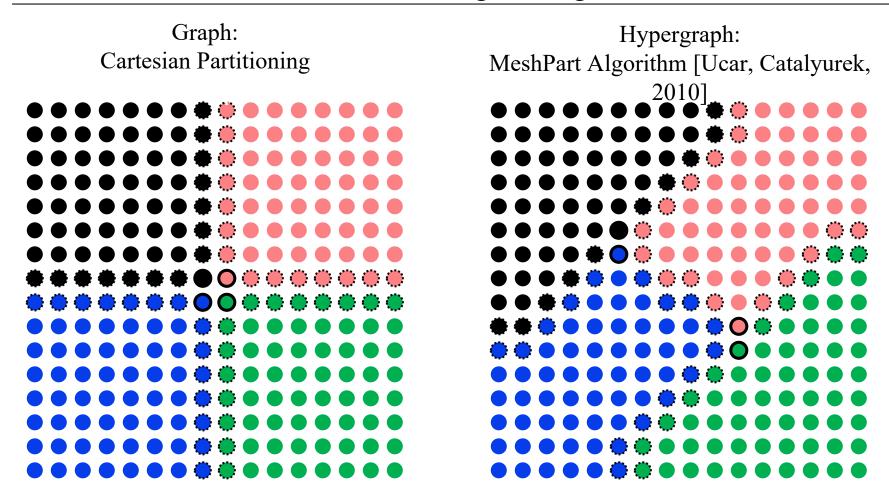
edge
$$(v_i, v_j) \in E \Rightarrow$$

 $y(i) \leftarrow y(i) + A(i,j) x(j)$ and $y(j) \leftarrow y(j) + A(j,i) x(i)$

P₁ performs:
$$y(4) \leftarrow y(4) + A(4,7) x(7)$$
 and $y(5) \leftarrow y(5) + A(5,7) x(7)$

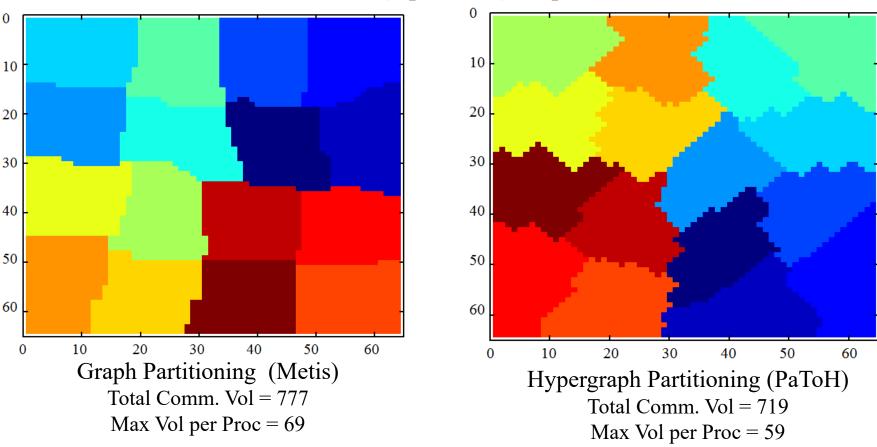
x(7) only needs to be communicated **once!**

Two Different 2D Mesh Partitioning Strategies



Experimental Results: Hypergraph vs. Graph Partitioning

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



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

Coordinate-Free — Summary

- Several techniques for partitioning without coordinates
 - Fiduccia-Matteyes good corrector given reasonable partition
 - Spectral Method good partitions, but slow

Multilevel methods

- Used to speed up problems that are too large/slow
- Can be used with FM and Spectral methods and others

Speed/quality

- For load balancing of grids, multi-level FM probably best
- For other partitioning problems (www, circuit, ...) spectral may be better
- Good software available: (METIS, KaHyPar)

Coordinate-Free – Local/Global Partitioning Algorithms

- Fiduccia-Matteyes are **local** partitioning algorithms:
 - both need an initial partitioning.
 - improve partitioning based on local partitioning decisions.
- Multi-level methods and spectral methods are **global** partitioning methods based on information that take all edges into account.

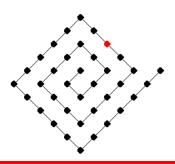
The combination of both methods typically form a very efficient partitioning method.

Appendix

Example 1:

- $-|V_s| \leq |E_s|$
- $-|E_s| \le d * |V_s|$ where d is the maximum degree of the graph

Example (graph that is not spatial connected)



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

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

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

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

Inertial Partitioning: $M u = \lambda u \leftrightarrow u^T M u = u^T \lambda u = \lambda u^T u = \lambda$