STAR-P: High Productivity Parallel Computing

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Graph Algorithms and Sparse Matrix Land

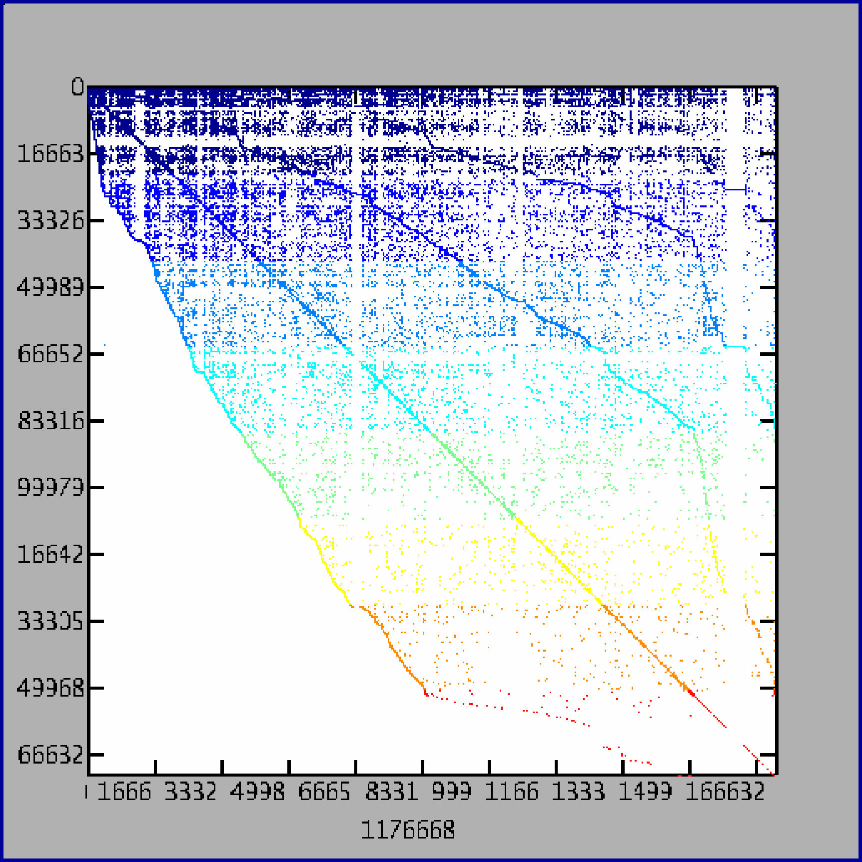
Birth of Interactive Supercomputing

- Dream of taking academic software commercial

Star-P

- Interactive Parallel Computing Environment
- Parallel Client/Server Architecture
- Main goal: parallel computing easier on the human user
- Academic Front End: MATLAB
- Four parallel approaches interacting:
  - Embarrassingly Parallel
  - Message Passing
  - Backend Support (insert *p)
  - Compiling
- Integrates several packages into one easy to use software

Page Rank Matrix



- Web crawl of 170,000 pages from mit.edu
- Matlab*P spy plot of the matrix of the graph

Clock

- c=mm(‘clock’);
- std(c);

- Simple example shows two modes interacting

Pieces of Pi

```
>> quad('4./(1+x.^2)', 0, 1);
ans = 3.14159270703219

>> a = (0:3*p) / 4
a = ddense object: 1-by-4

>> a(:)
ans =
                  0
   0.25000000000000
   0.50000000000000
   0.75000000000000

>> b = a+.25;

>> c = mm('quad','4./(1+x.^2)', a, b);   % Should be “feval”!
c = ddense object: 1-by-4

>> sum(c(:))
ans = 3.14159265358979
```

FFT2 in four lines

```
>>  A = randn(4096, 4096*p)
A = ddense object: 4096-by-4096
>> tic;

>> B = mm('fft', A);
>> C = B.';
>> D = mm('fft', C);
>> F = D.';

>> toc
elapsed_time = 73.50

>>a = A(:,:);
>>  tic; g = fft2(a); toc
elapsed_time = 202.95
```

… we have FFTW installed as well!

Matlab sparse matrix design principles

- All operations should give the same results for sparse and full matrices (almost all)
- Sparse matrices are never created automatically, but once created they propagate
- Performance is important -- but usability, simplicity, completeness, and robustness are more important
- Storage for a sparse matrix should be O(nonzeros)
- Time for a sparse operation should be O(flops) (as nearly as possible)

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Matlab*P dsparse matrices: same principles, but some different tradeoffs

Sparse matrix operations

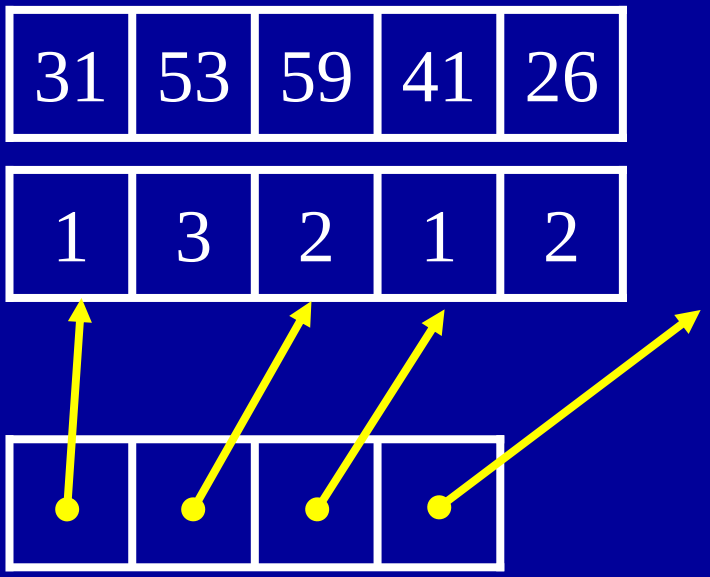
- dsparse layout, same semantics as ddense
- For now, only row distribution
- Matrix operators: +, -, max, etc.
- Matrix indexing and concatenation

  A (1:3, [4 5 2]) = [B(:, 7) C] ;

- A \ b by direct methods
- Conjugate gradients

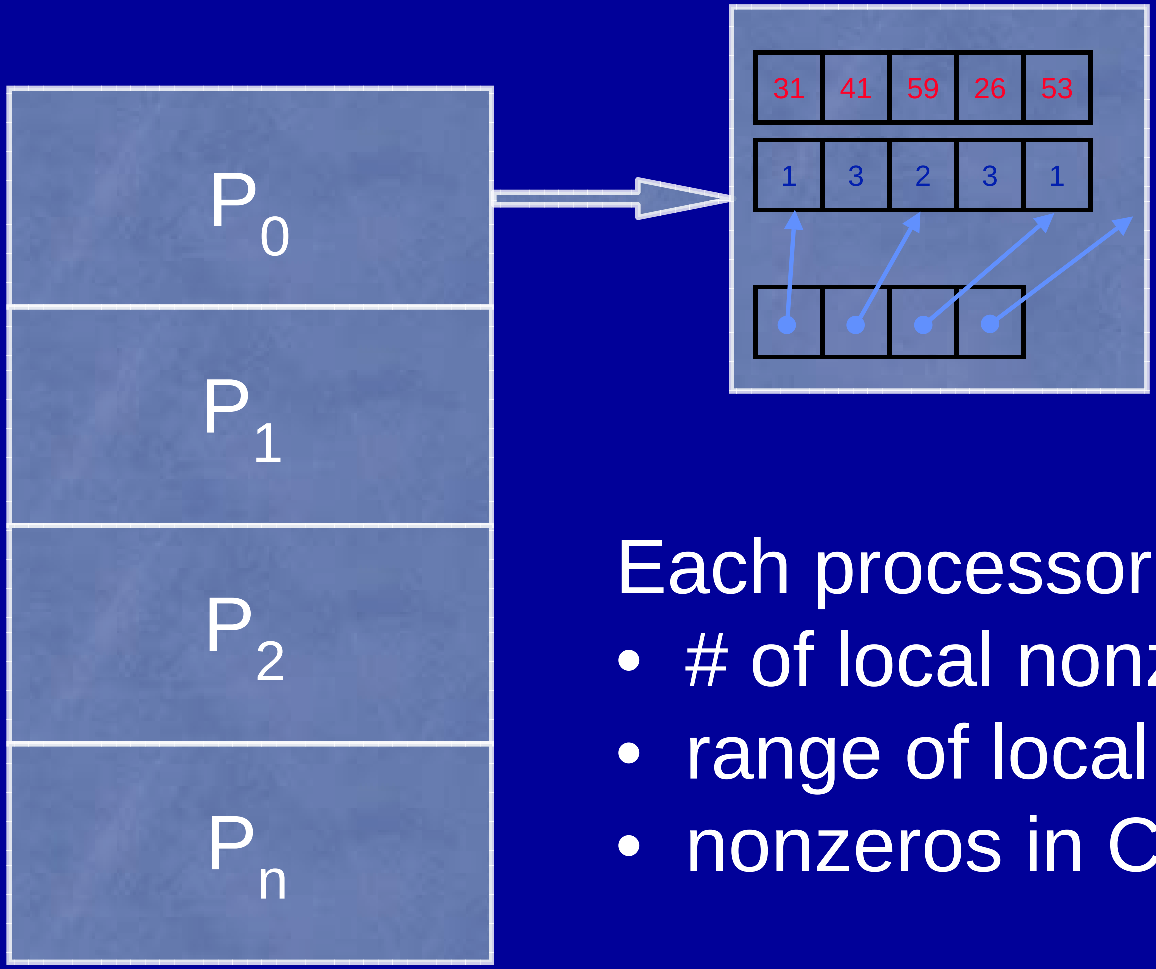
Sparse data structure

31	0	53
0	59	0
41	26	0



- Full:
  - 2-dimensional array of real or complex numbers
  - (nrows*ncols) memory
- Sparse:
  - compressed row storage
  - about (1.5*nzs + .5*nrows) memory

Distributed sparse data structure



Each processor stores:

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

Sparse matrix times dense vector

- y = A * x
- The first call to matvec caches a communication schedule for matrix A. Later calls to multiply any vector by A use the cached schedule.
- Communication and computation overlap.
- Can use a tuned sequential matvec kernel on each processor.

Sparse linear systems

- x = A \ b
- Matrix division uses MPI-based direct solvers:
  - SuperLU_dist: nonsymmetric static pivoting
  - MUMPS: nonsymmetric multifrontal
  - PSPASES: Cholesky

```
ppsetoption('SparseDirectSolver','SUPERLU')
```

- Iterative solvers implemented in Matlab*P
- Some preconditioners; ongoing work

Application: Fluid dynamics

- Modeling density-driven instabilities in miscible fluids (Goyal, Meiburg)
- Groundwater modeling, oil recovery, etc.
- Mixed finite difference & spectral method
- Large sparse generalized eigenvalue problem

```
function lambda = peigs (A, B,
  sigma, iter, tol)

  [m n] = size (A);
  C = A - sigma * B;
  y = rand (m, 1);

  for k = 1:iter
    q = y ./ norm (y);
    v = B * q;
    y = C \ v;
    theta = dot (q, y);
    res = norm (y - theta*q);
    if res <= tol
      break;
    end;
  end;

  lambda = 1 / theta;
```

Combinatorial algorithms in Matlab*P

- Sparse matrices are a good start on primitives for combinatorial scientific computing.
  - Random-access indexing: `A(i,j)`
  - Neighbor sequencing: `find (A(i,:))`
  - Sparse table construction: `sparse (I, J, V)`
- What else do we need?

Sorting in Matlab*P

- **`[V, perm] = sort (V)`**

- Common primitive for many sparse matrix and array algorithms: sparse(), indexing, transpose

- Matlab*P uses a parallel sample sort

Sample sort

- (Perform a random permutation)
- Select p-1 “splitters” to form p buckets
- Route each element to the correct bucket
- Sort each bucket locally
- “Starch” the result to match the distribution of the input vector

Sample sort example

Initial data (after randomizing)

3	6	8	1	5	4	7	2	9

Choose splitters (2 and 6)

1	2	3	6	5	4	8	7	9

Sort local data

1	2	3	4	5	6	7	8	9

Starch

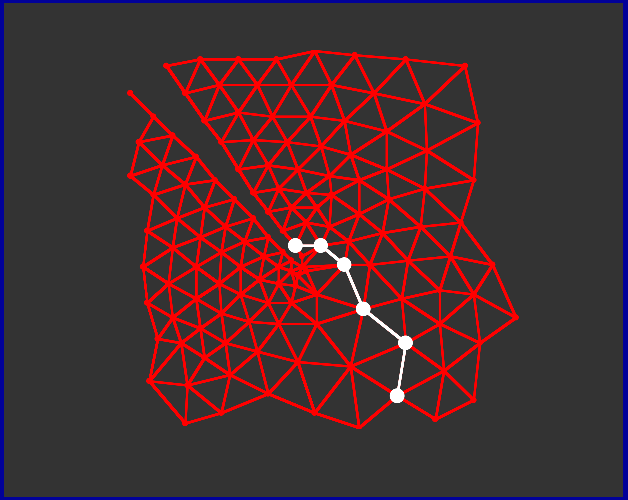
1	2	3	4	5	6	7	8	9

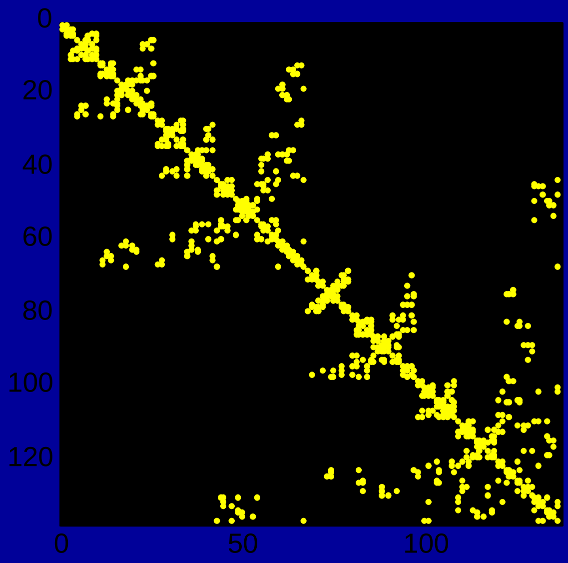
How sparse( ) works

- **`A = sparse (I, J, V)`**
- Input: ddense vectors I, J, V (optionally, also dimensions and distribution info)
- Sort triples (i, j, v) by (i, j)
- Starch the vectors for desired row distribution
- Locally convert to compressed row indices
- Sum values with duplicate indices

Graph / mesh partitioning

- Reduce communication in matvec and other parallel computations
- Reordering for sparse GE
- PARMETIS
- Parts of G/Teng Matlab meshpart toolbox





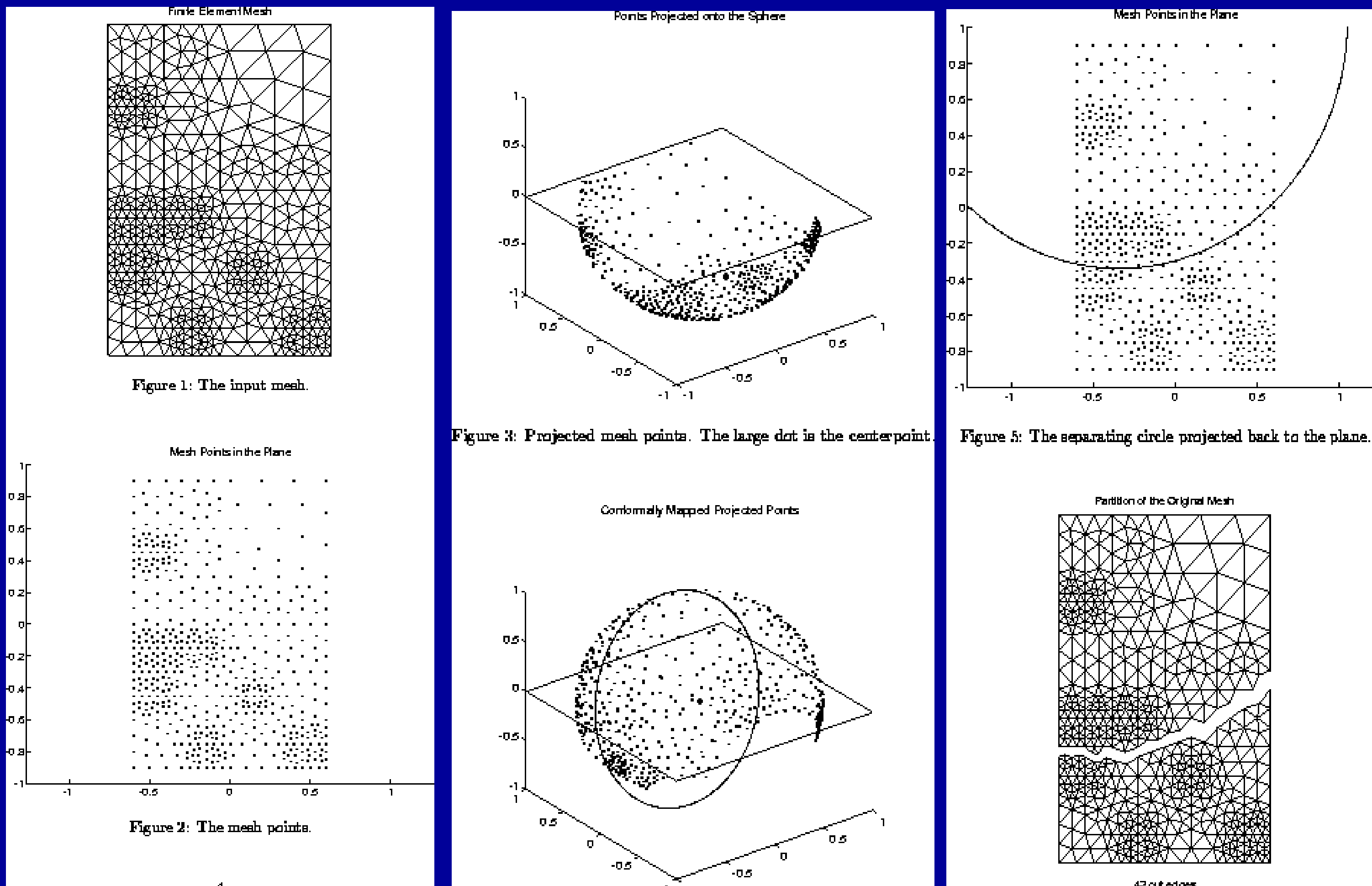
Geometric mesh partitioning

- Algorithm of Miller, Teng, Thurston, Vavasis
- Partitions irregular finite element meshes into equal-size pieces with few connecting edges
- Guaranteed quality partitions for well-shaped meshes, often very good results in practice
- Existing implementation in sequential Matlab
- Code runs in Matlab*P with very minor changes

Outline of algorithm

1. Project points stereographically from R^d to R^{d+1}
2. Find "centerpoint" (generalized median)
3. Conformal map: Rotate and dilate
4. Find great circle
5. Unmap and project down
6. Convert circle to separator

Geometric mesh partitioning



Matching and depth-first search in Matlab

- dmperm: Dulmage-Mendelsohn decomposition

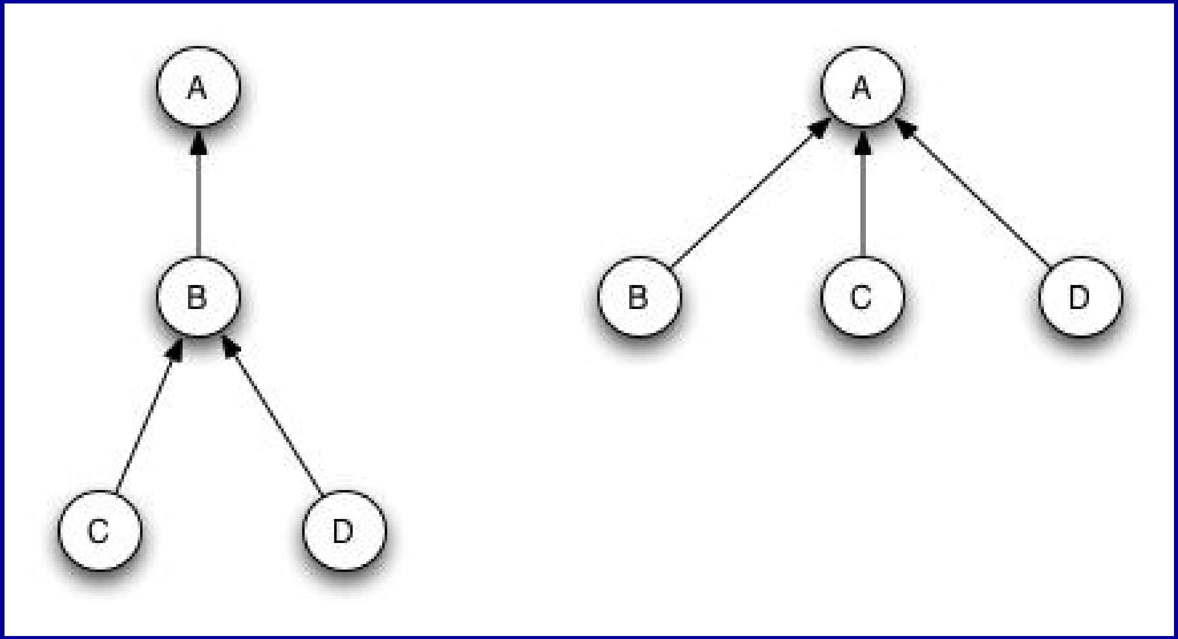
- Square, full rank A:
  - [p, q, r] = dmperm(A);
  - A(p,q) is block upper triangular with nonzero diagonal
  - also, strongly connected components of a directed graph
  - also, connected components of an undirected graph

- Arbitrary A:
  - [p, q, r, s] = dmperm(A);
  - maximum-size matching in a bipartite graph
  - minimum-size vertex cover in a bipartite graph
  - decomposition into strong Hall blocks

Connected components

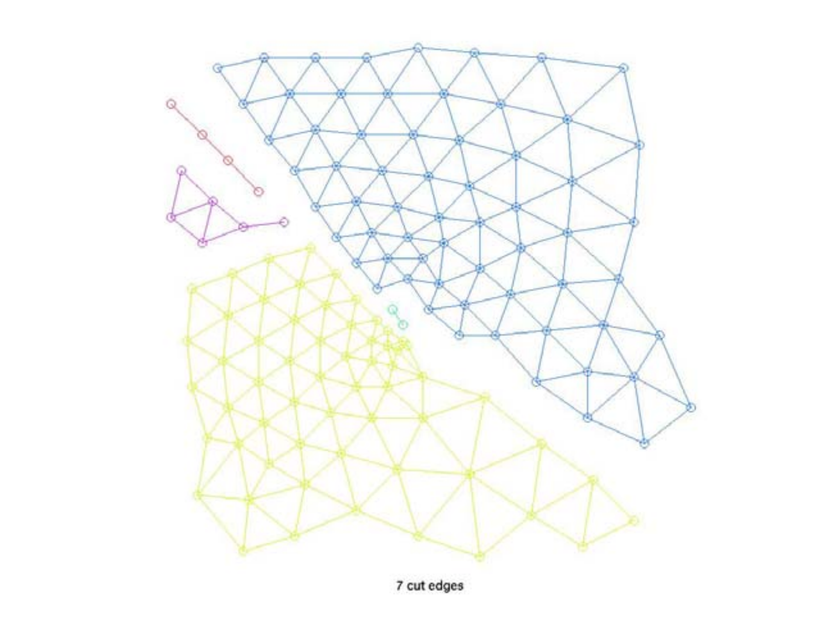
- Sequential Matlab uses depth-first search (`dmperm`), which doesn't parallelize well
- Shiloach-Vishkin algorithm:
  - repeat
    - Link every (super)vertex to a random neighbor
    - Shrink each tree to a supervertex by pointer jumping
  - until no further change
- Originally a processor-efficient PRAM algorithm
- Matlab*P code looks much like the PRAM code

Pointer jumping



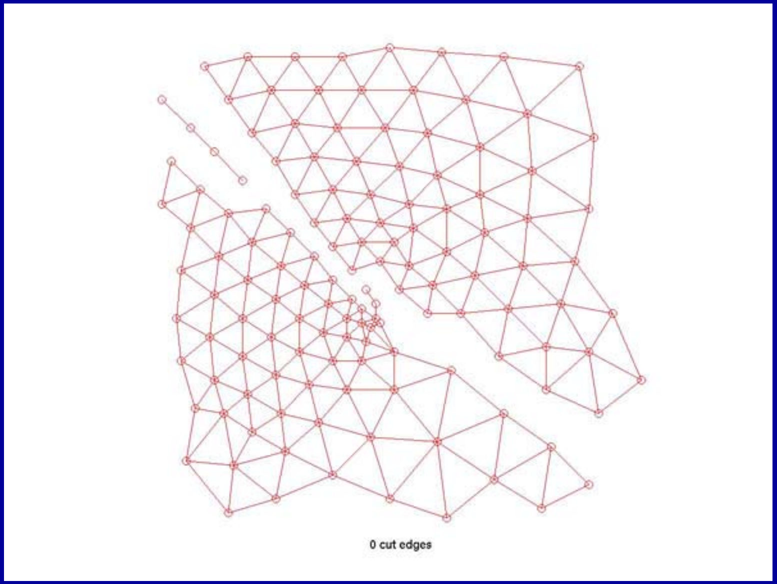

```
while ~all( C(myrows) == C(C(myrows)) )
  C(myrows) = C(C(myrows));
end
C(myrows) = min (C(myrows), C(C(myrows)));
```

Example of execution



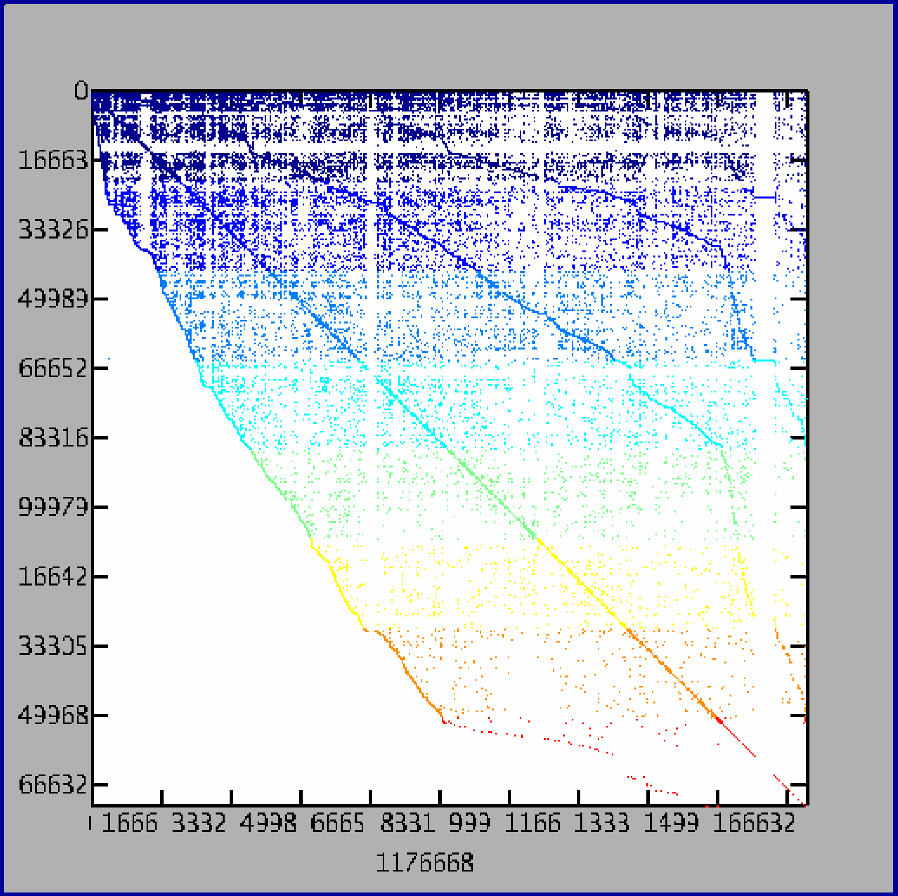
After first iteration

Final components



Page Rank

- Importance ranking of web pages
- Stationary distribution of a Markov chain
- Power method: matvec and vector arithmetic
- Matlab*P page ranking demo (from SC’03) on a web crawl of mit.edu (170,000 pages)



Remarks

- Easy-to-use interactive programming environment
- Interface to existing parallel packages
- Combinatorial methods toolbox being built on parallel sparse matrix infrastructure
  - Much to be done: spanning trees, searches, etc.
- A few issues for ongoing work
  - Dynamic resource management
  - Fault management
  - Programming in the large