Interactive Tools for Combinatorial Supercomputing

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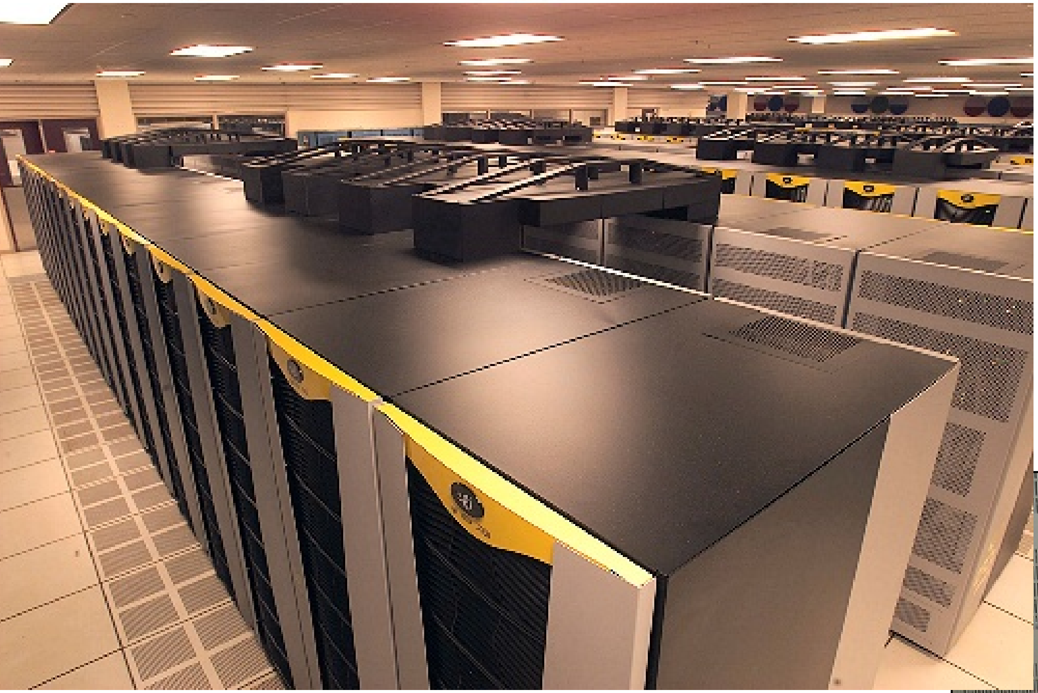
Parallel Computing Today



Columbia,
NASA Ames Research Center

Departmental Beowulf cluster

But!

How do you program it?

C with MPI

```
#include <stdio.h>
#include <stdlib.h>
#include <math.h>
#include "mpi.h"
#define A(i,j)  ( 1.0/((1.0*(i)+(j))*(1.0*(i)+(j)+1)/2 + (1.0*(i)+1)) )
void errorExit(void);
double normalize(double* x, int mat_size);
int main(int argc, char **argv)
{
  int num_procs;
  int rank;
  int mat_size = 64000;
  int num_components;
  double *x = NULL;
  double *y_local = NULL;
  double norm_old = 1;
  double norm = 0;
  int i,j;
  int count;
  if (MPI_SUCCESS != MPI_Init(&argc, &argv)) exit(1);
  if (MPI_SUCCESS != MPI_Comm_size(MPI_COMM_WORLD,&num_procs)) errorExit();
```

C with MPI (2)

```
if (0 == mat_size % num_procs) num_components = mat_size/num_procs;
else num_components = (mat_size/num_procs + 1);
mat_size = num_components * num_procs;
if (0 == rank) printf("Matrix Size = %d\n", mat_size);
if (0 == rank) printf("Num Components = %d\n", num_components);
if (0 == rank) printf("Num Processes = %d\n", num_procs);
x = (double*) malloc(mat_size * sizeof(double));
y_local = (double*) malloc(num_components * sizeof(double));
if ( (NULL == x) || (NULL == y_local) )
{
  free(x);
  free(y_local);
  errorExit();
}
if (0 == rank)
{
  for (i=0; i<mat_size; i++)
  {
    x[i] = rand();
  }
  norm = normalize(x,mat_size);
}
```

C with MPI (3)

```
if (MPI_SUCCESS !=
    MPI_Bcast(x, mat_size, MPI_DOUBLE, 0, MPI_COMM_WORLD)) errorExit();
count = 0;
while (fabs(norm-norm_old) > TOL) {
  count++;
  norm_old = norm;
  for (i=0; i<num_components; i++)
  {
    y_local[i] = 0;
  }
  for (i=0; i<num_components && (i+num_components*rank)<mat_size; i++)
  {
    for (j=mat_size-1; j>=0; j--)
    {
      y_local[i] += A(i+rank*num_components,j) * x[j];
    }
  }
  if (MPI_SUCCESS != MPI_Allgather(y_local, num_components, MPI_DOUBLE, x,
       num_components, MPI_DOUBLE, MPI_COMM_WORLD)) errorExit();
```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C with MPI (4)

```
    norm = normalize(x, mat_size);
  }
  if (0 == rank)
  {
    printf("result = %16.15e\n", norm);
  }
  free(x);
  free(y_local);

  MPI_Finalize();
  exit(0);
}
void errorExit(void)
{
  int rank;
  MPI_Comm_rank(MPI_COMM_WORLD,&rank);
  printf("%d died\n",rank);
  MPI_Finalize();
  exit(1);
}
```

C with MPI (5)

```
double normalize(double* x, int mat_size)
{
  int i;
  double norm = 0;
  for (i=mat_size-1; i>=0; i--)
  {
    norm += x[i] * x[i];
  }
  norm = sqrt(norm);
  for (i=0; i<mat_size; i++)
  {
    x[i] /= norm;
  }
  return norm;
}
```

Star-P

```
A = rand(4000*p, 4000*p);
x = randn(4000*p, 1);
y = zeros(size(x));
while norm(x-y) / norm(x) > 1e-11
    y = x;
    x = A*x;
    x = x / norm(x);
end;
```

Background

- Matlab*P 1.0 (1998): Edelman, Husbands, Isbell (MIT)
- Matlab*P 2.0 (2002-): MIT / UCSB / LBNL
- Star-P (2004-): Interactive Supercomputing / SGI

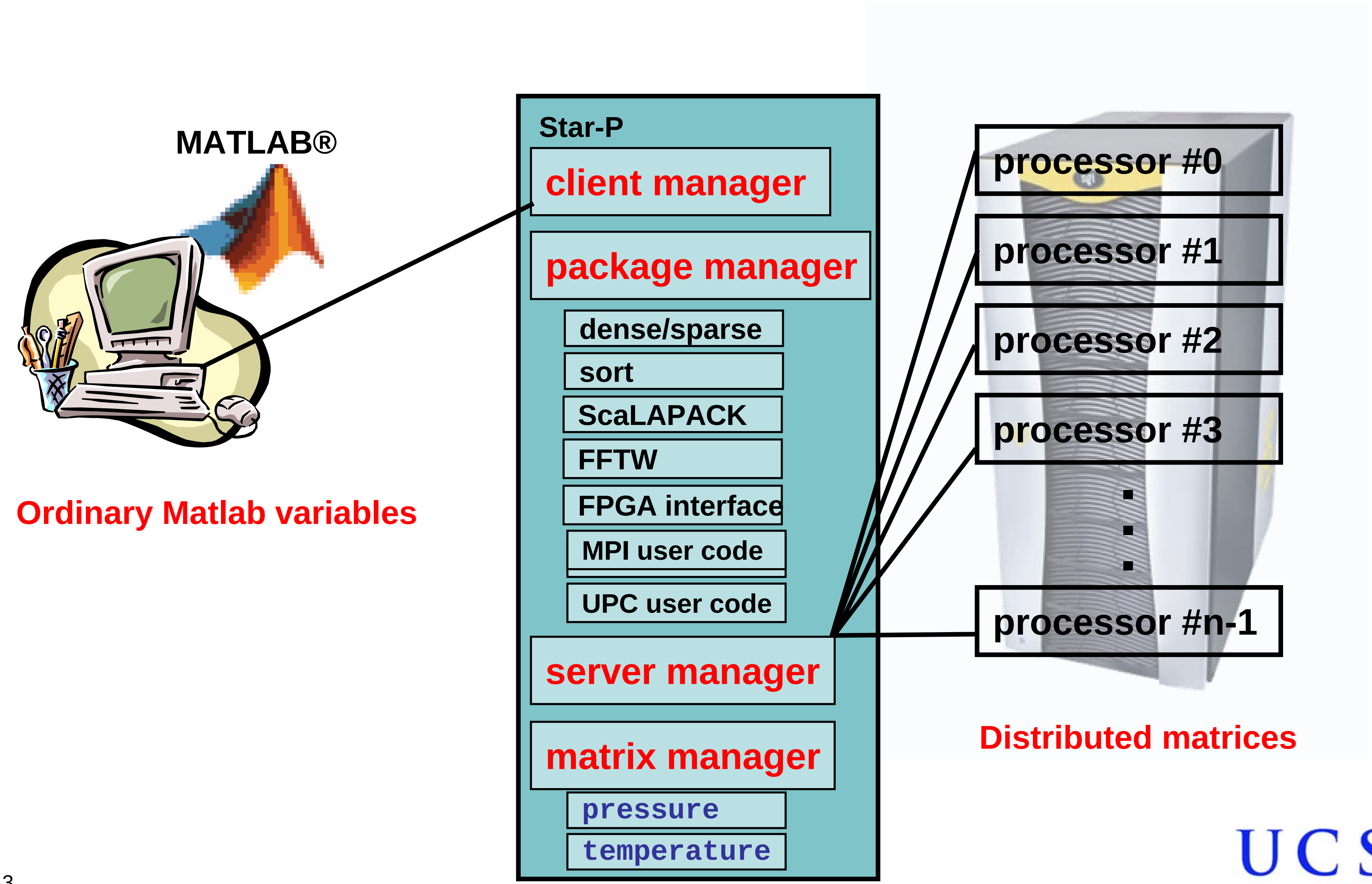
Data-Parallel Operations

```
                    < M A T L A B >
        Copyright 1984-2001 The MathWorks, Inc.
            Version 6.1.0.1989a Release 12.1

>> A = randn(500*p, 500*p)
A = ddense object: 500-by-500

>> E = eig(A);

>> E(1)
ans = -4.6711 +22.1882i

e = E(:,:);

>> ppwhos
  Name        Size              Bytes  Class
  A         500px500p             688  ddense object
  E         500px1                652  ddense object
  e         500x1                8000  double array (complex)
```

Task-Parallel Operations

```
>> 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 = ppeval('quad','4./(1+x.^2)', a, b);
c = ddense object: 1-by-4

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

Star-P Architecture



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)

Star-P dsparse matrices: same principles, but some different tradeoffs

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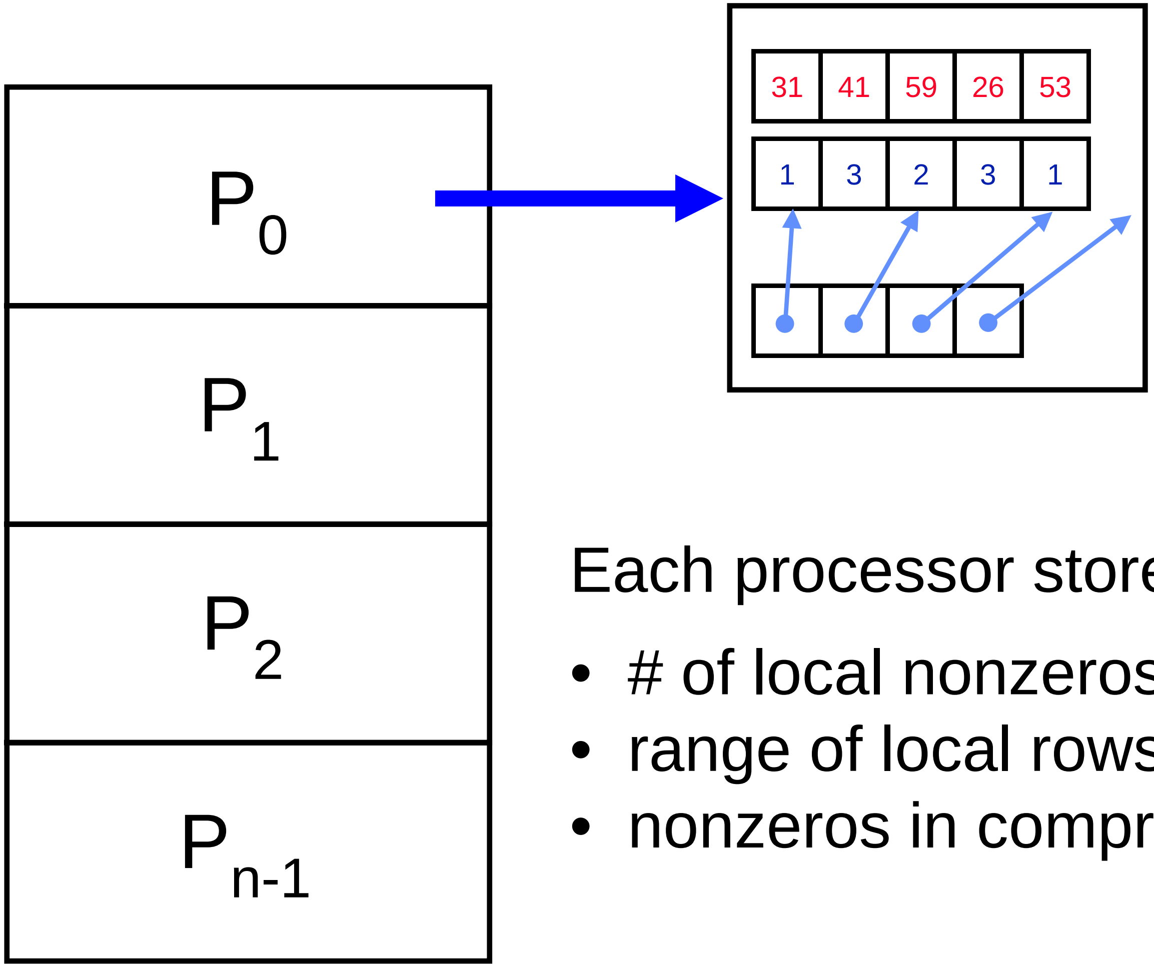
Distributed sparse data structure



Each processor stores:

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

The sparse( ) constructor

- `A = sparse (I, J, V, nr, nc)`
- Input: ddense vectors **I**, **J**, **V**, dimensions **nr**, **nc**
- Output: **A**(**I**(k), **J**(k)) = **V**(k)
- Sort triples **<** i, j, v **>** by **<** i, j **>**
- Locally convert to compressed row indices
- Sum values with duplicate indices

Sparse array and matrix operations

- dsparse layout, same semantics as ddense
- Data distribution by rows only, for now
- Matrix arithmetic: +, *, max, sum, etc.
- Matrix indexing and concatenation

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

- Linear solvers: x = A \ b; using SuperLU (MPI)
- Eigensolvers: [V, D] = eigs(A); using PARPACK (MPI)

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Sorting in Star-P

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

- Common primitive for several sparse array algorithms, including the sparse constructor

- Star-P uses a parallel sample sort

Sparse matrix times dense vector

- y = A * x

- First matvec with A caches a communication schedule
- Later matvecs with A use the cached schedule
- Communication and computation overlap

Combinatorial Scientific Computing

- Sparse matrix methods
- Knowledge discovery
- Web search and information retrieval
- Graph matching
- Machine learning
- Geometric modeling
- Computational biology
- Bioinformatics
- . . .

How will combinatorial methods be used by nonexperts?

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Analogy: Matrix division in Matlab

x = A \ b;

- Works for either full or sparse A
- Is A square?

  no => use QR to solve least squares problem
- Is A triangular or permuted triangular?

  yes => sparse triangular solve
- Is A symmetric with positive diagonal elements?

  yes => attempt Cholesky after symmetric minimum degree
- Otherwise

  => use LU on A(:, colamd(A))

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Combinatorics in Star-P

- Represent a graph as a sparse adjacency matrix

- A sparse matrix language is a good start on primitives for computing with graphs

  - Random-access indexing: `A(i,j)`
  - Neighbor sequencing: `find (A(i,:))`
  - Sparse table construction: `sparse (I, J, V)`
  - Breadth-first search step : `A * v`

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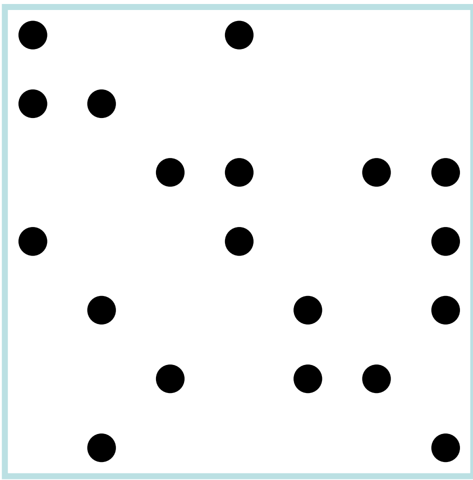
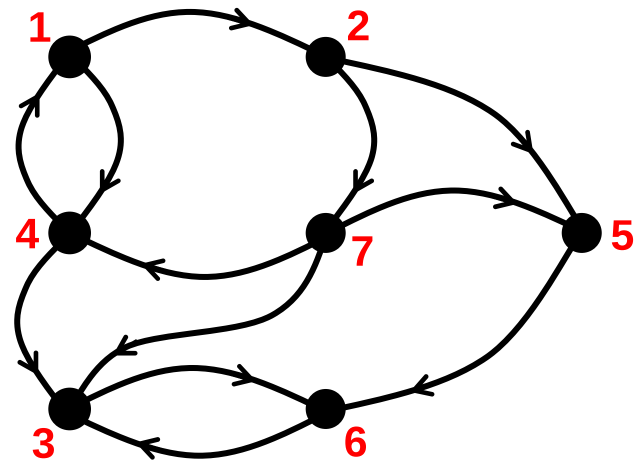
Sparse adjacency matrix and graph

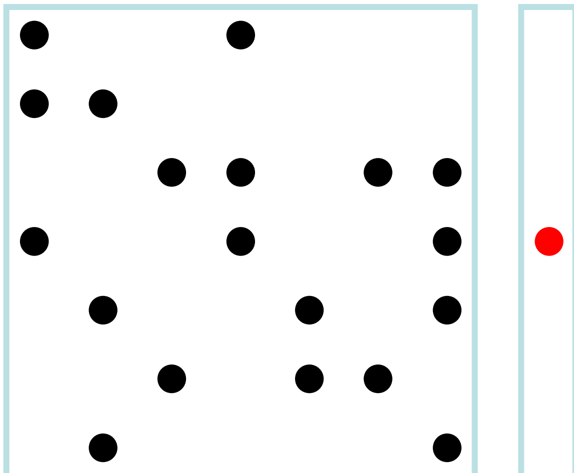


A^T

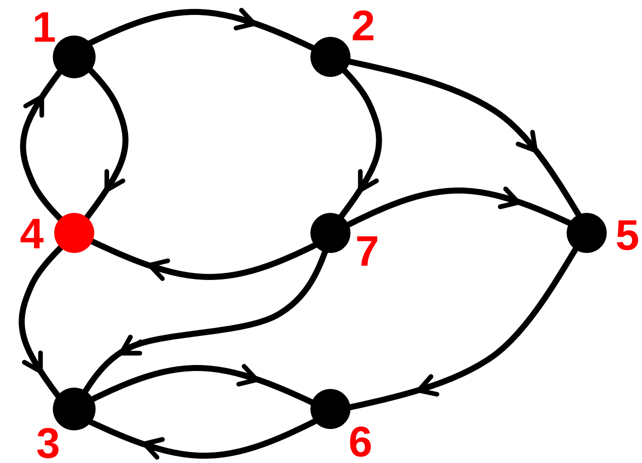


- Adjacency matrix: sparse array w/ nonzeros for graph edges
- Storage-efficient implementation from sparse data structures

Breadth-first search: sparse mat * vec

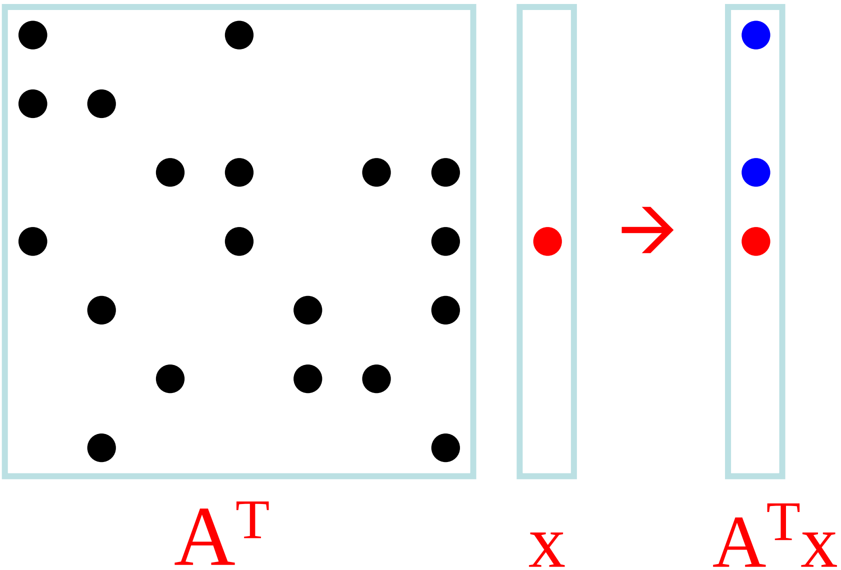


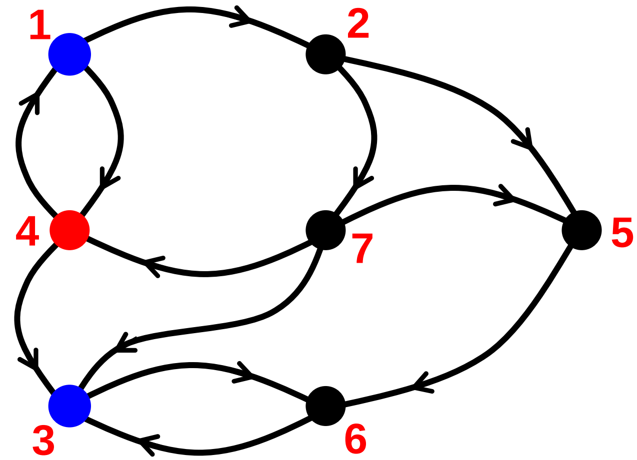
A^T x



- Multiply by adjacency matrix → step to neighbor vertices
- Efficient implementation from sparse data structures

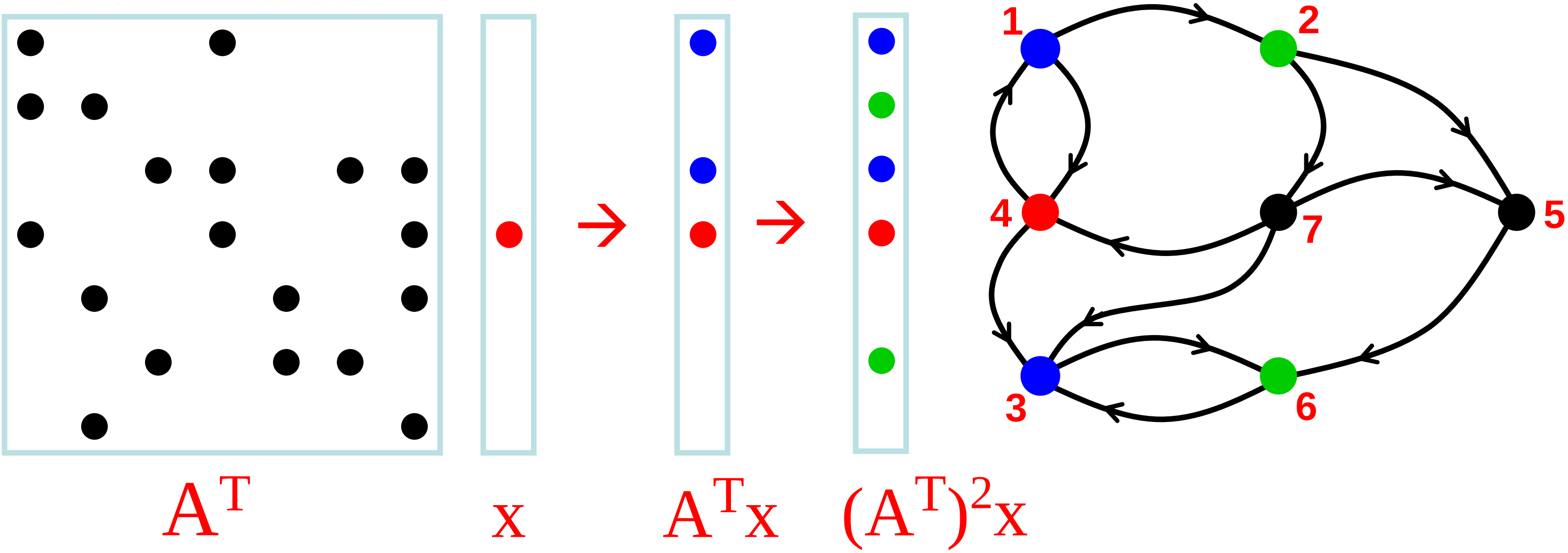
Breadth-first search: sparse mat * vec





- Multiply by adjacency matrix → step to neighbor vertices
- Efficient implementation from sparse data structures

Breadth-first search: sparse mat * vec



- Multiply by adjacency matrix → step to neighbor vertices
- Efficient implementation from sparse data structures

Connected components of a graph

- Sequential Matlab uses depth-first search (**`dmperm`**), which doesn't parallelize well
- Pointer-jumping algorithms (Shiloach/Vishkin & descendants)
  - repeat
    - Link every (super)vertex to a neighbor
    - Shrink each tree to a supervertex by pointer jumping
  - until no further change
- Other coming graph kernels:
  - Shortest-path search (after Husbands, LBNL)
  - Bipartite matching (after Riedy, UCB)
  - Strongly connected components (after Pinar, LBNL)

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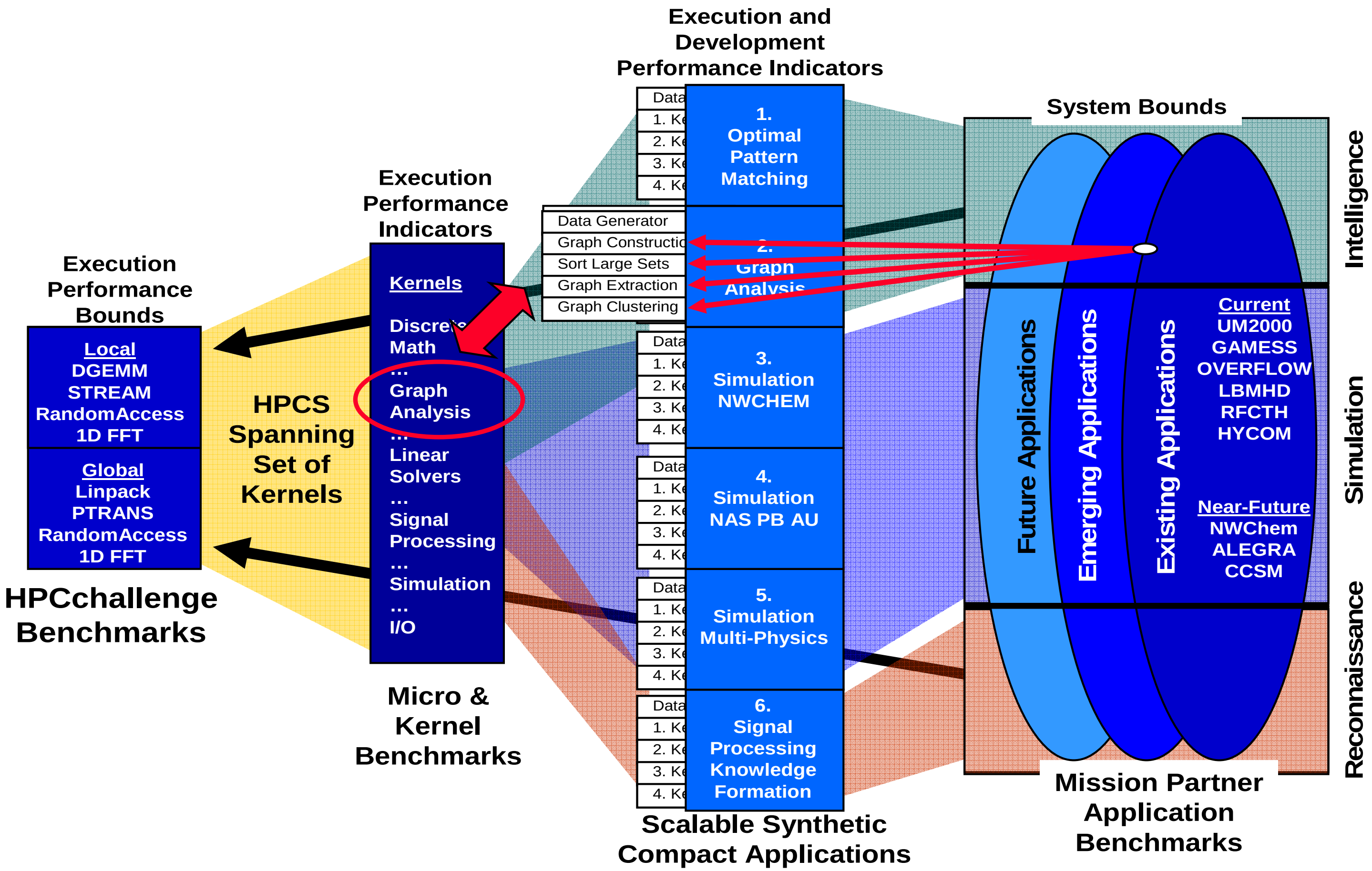
HPCS Scalable Synthetic Compact Apps

SSCA#1: Bioinformatics / Pattern Matching

SSCA#2: Graph Analysis

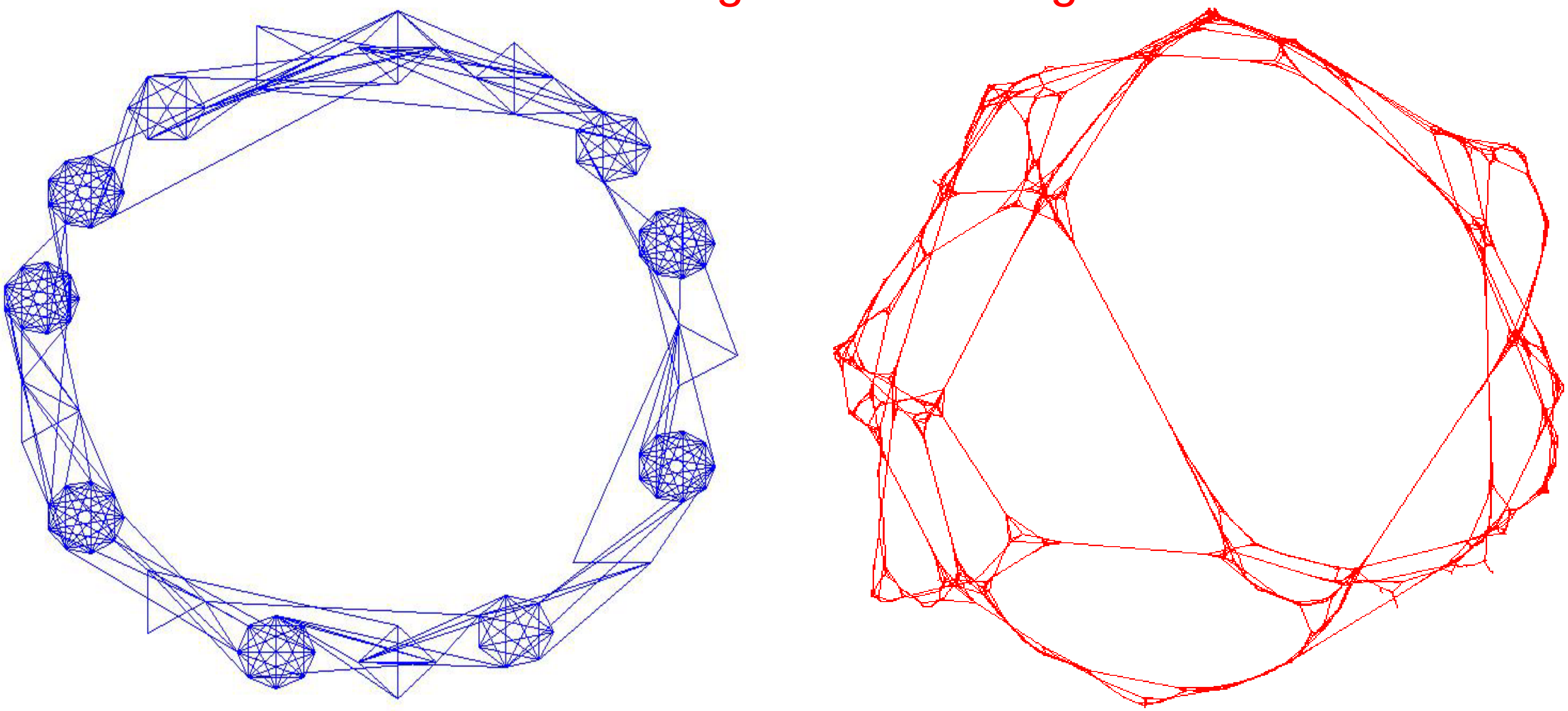
SSCA#3: Sensor Processing / Imaging



SSCA#2: “Graph Analysis”

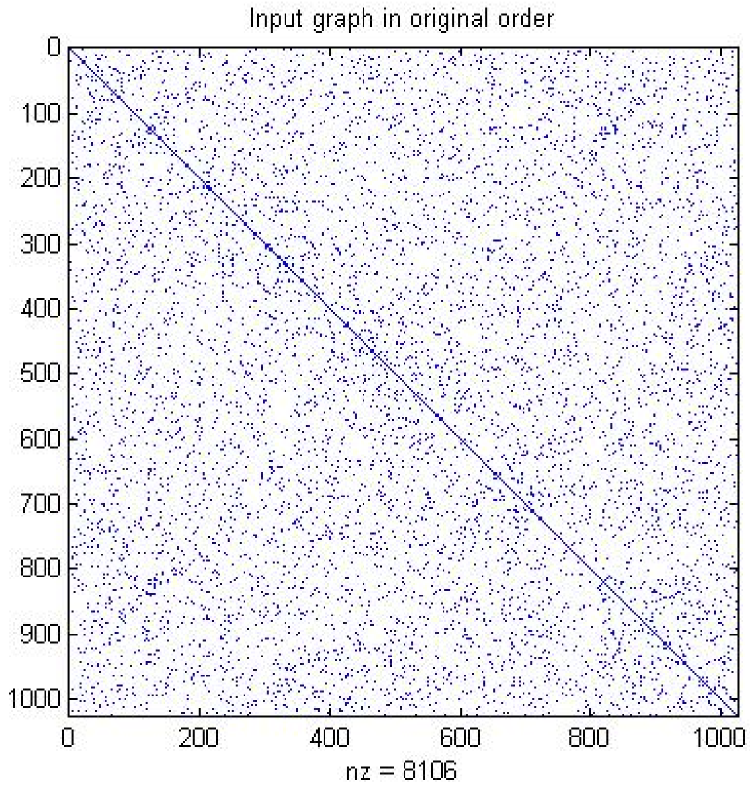
Fine-grained, irregular data access

Searching and clustering



- Many tight clusters, loosely interconnected
- Input data is edge triples < i, j, label(i,j) >
- Vertices and edges permuted randomly

Concise SSCA#2 in Star-P



Kernel 1: Construct graph data structures

- Graphs are dsparse matrices, created by sparse( )

Kernels 2 and 3

Kernel 2: Search by edge labels

- About 12 lines of executable Matlab or Star-P

Kernel 3: Extract subgraphs

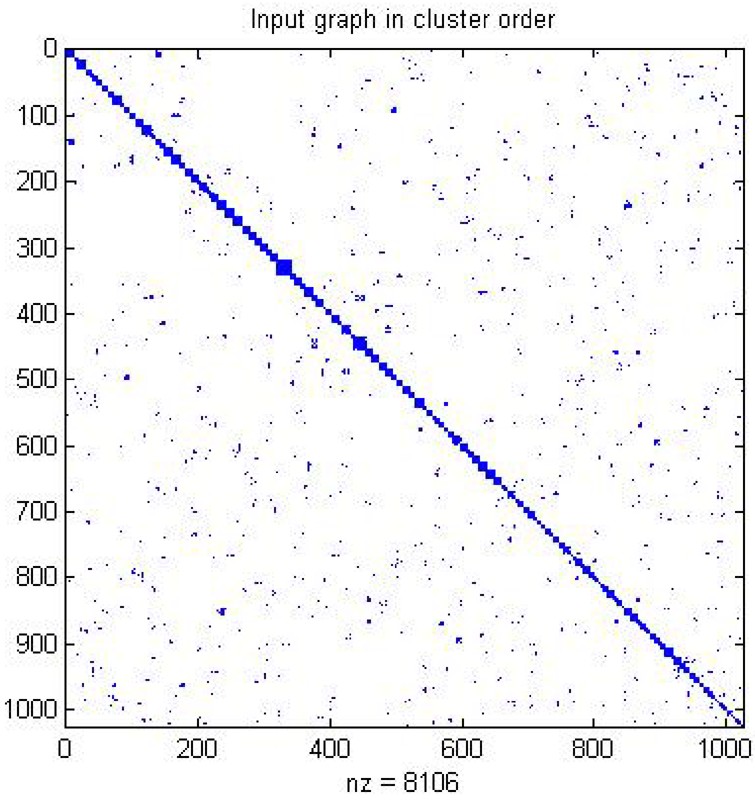
- Returns subgraphs consisting of vertices and edges within fixed distance of given starting vertices
- Sparse matrix-vector product for breadth-first search
- About 25 lines of executable Matlab or Star-P

Kernel 4: Vertex clustering

- Grow local clusters from many seeds in parallel
- Breadth-first search by sparse matrix * matrix

```
% Grow each seed to vertices
%    reached by at least two
%    paths of length 1 or 2

 C = sparse(seeds, 1:ns, 1, n, ns);
 C = A * C;
 C = C + A * C;
 C = C > 1;
```



Expressive Power: SSCA#2 Kernel 3

Star-P (25 lines)

```
A = spones(G.edgeWeights{1});
nv = max(size(A));
npar = length(G.edgeWeights);
nstarts = length(starts);
for i = 1:nstarts
    v = starts(i);
    % x will be a vector whose nonzeros
    % are the vertices reached so far
    x = zeros(nv,1);
    x(v) = 1;
    for k = 1:pathlen
        x = A*x;
        x = (x ~= 0);
    end;
    vtxmap = find(x);
    S.edgeWeights{1} = G.edgeWeights{1}(v
    for j = 2:npar
        sg = G.edgeWeights{j}(vtxmap,vtxm
        if nnz(sg) == 0
            break;
        end;
        S.edgeWeights{j} = sg;
    end;
    S.vtxmap = vtxmap;
    subgraphs{i} = S;
end
```

MATLABmpi (91 lines)

```
declareGlobals;


intSubgraphs = subgraphs(G, pathLength, startSetInt);
strSubgraphs = subgraphs(G, pathLength, startSetStr);

%| Finish helping other processors.
if P.Ncpus > 1
  if P.myRank == 0                % if we are the leader
    for unused = 1:P.Ncpus-1
      [src tag] = probeSubgraphs(G, [P.tag.K3.results]);
      [isg ssg] = MPI_Recv(src, tag, P.comm);
      intSubgraphs = [intSubgraphs isg];
      strSubgraphs = [strSubgraphs ssg];
    end
    for dest = 1:P.Ncpus-1
      MPI_Send(dest, P.tag.K3.done, P.comm);
    end
  else
    MPI_Send(0, P.tag.K3.results, P.comm, ...
        intSubgraphs, strSubgraphs);
    [src tag] = probeSubgraphs(G, [P.tag.K3.done]);
    MPI_Recv(src, tag, P.comm);
  end
```

```
      % Wait for a response for each request we sent out.
      for unused = 1:numRqst
        [src tag] = probeSubgraphs(G, [P.tag.K3.dataResp]);
        [starts newEdges] = MPI_Recv(src, tag, P.comm);
        subg.edgeWeights{1}(:, starts) = newEdges;
        [newEnds unused] = find(newEdges);
        allNewEnds = [allNewEnds; newEnds];
      end
    end % of if ~P.paral

    % Eliminate any new ends already in the all starts list.
    newStarts = setdiff(allNewEnds.', allStarts);
    allStarts = [allStarts newStarts];

    if ENABLE_PLOT_K3DB
      plotEdges(subg.edgeWeights{1}, startVertex, endVertex, k);
    end % of ENABLE_PLOT_K3DB

    if isempty(newStarts)          % if empty we can quit early.
      break;
    end
  end
```

Lines of code	Star-P cSSCA2	MATLABmpi spec	C/Pthreads/ SIMPLE
Kernel 1	29	68	256
Kernel 2	12	44	121
Kernel 3	25	91	297
Kernel 4	44	295	241

```
% For each processor which has any of the vertices we need:
startDests = floor((newStarts - 1) / P.myV);
uniqDests = unique(startDests);
for dest = uniqDests
  starts = newStarts(startDests == dest);

  if dest == P.myRank
    newEdges = G.edgeWeights{1}(:, starts - P.myBase);
    subg.edgeWeights{1}(:, starts) = newEdges;
    [allNewEnds unused] = find(newEdges);
  elseif ~isempty(starts)
    MPI_Send(dest, P.tag.K3.dataReq, P.comm, starts);
    numRqst = numRqst + 1;
```

Scaling up

Early results on SGI Altix (up to 64 processors):

- Have run cSSCA2 on graphs with 2^{27} = 134 million vertices
- Have manipulated graphs with 400 million vertices and 4 billion edges
- Timings scale well – for large graphs,
  - 2x problem size → 2x time
  - 2x problem size & 2x processors → same time

Using this benchmark to tune lots of infrastructure

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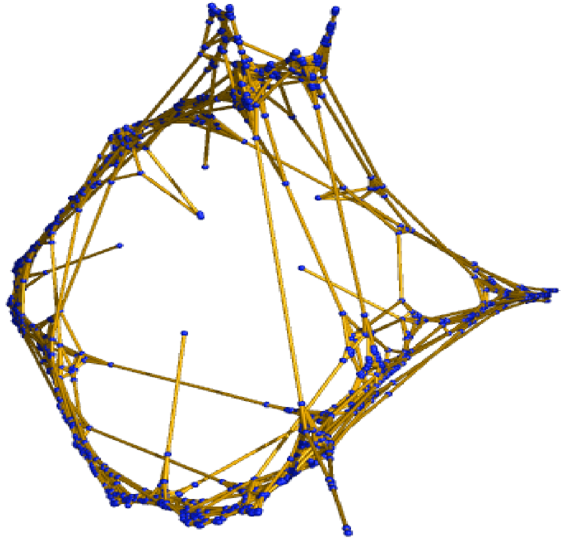
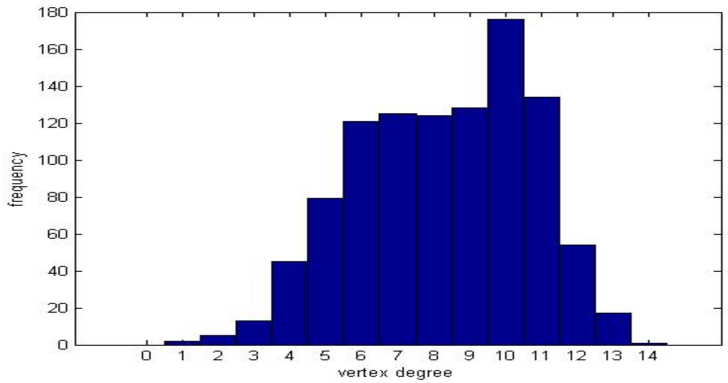
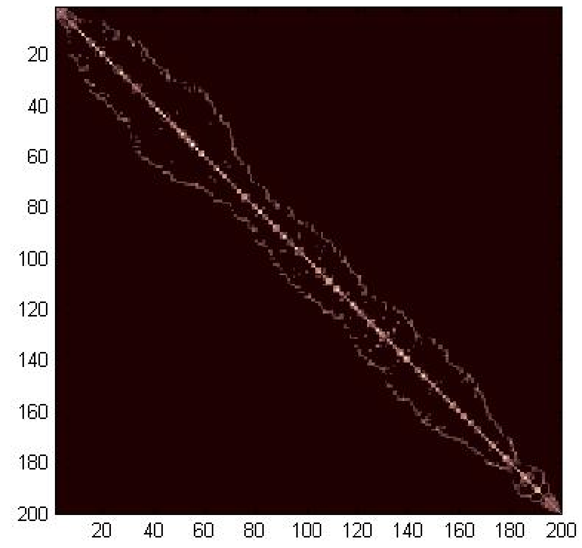
Work in progress: Toolbox for Graph Analysis and Pattern Discovery



Layer 1: Graph Theoretic Tools

- Graph operations
- Global structure of graphs
- Graph partitioning and clustering
- Graph generators
- Visualization and graphics
- Scan and combining operations
- Utilities





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