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

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

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

>> a(:)
an =
     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(:))
an = 3.14159265358979
```
FFT2 in four lines

```matlab
>> 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 $O(\text{nonzeros})$

• Time for a sparse operation should be $O(\text{flops})$ (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
  
  \[
  A \ (1:3, \ [4 \ 5 \ 2]) = \ [ B(:, \ 7) \ C ];
  \]

- \( A \ \backslash \ b \) by direct methods
- Conjugate gradients
Sparse data structure

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<td>41</td>
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- **Full:**
  - 2-dimensional array of real or complex numbers
  - (nrows*ncols) memory

- **Sparse:**
  - compressed row storage
  - about \((1.5*\text{nzs} + .5*\text{nrows})\) memory
Distributed sparse data structure

Each processor stores:
- # of local nonzeros
- range of local rows
- nonzeros in CSR form
Sparse matrix times dense vector

- $y = A \times x$

- 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

- \( x = A \backslash b \)

- Matrix division uses MPI-based direct solvers:
  - SuperLU_dist: nonsymmetric static pivoting
  - MUMPS: nonsymmetric multifrontal
  - PSPASES: Cholesky
    
    \texttt{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

```matlab
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: \( \text{find} \ (A(i,:)) \)
  - Sparse table construction: \( \text{sparse} \ (I, J, V) \)

- What else do we need?
Sorting in Matlab*P

- \([V, \text{perm}] = \text{sort} (V)\)

- Common primitive for many sparse matrix and array algorithms: \text{sparse()}, \text{indexing}, \text{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

• \( A = \text{sparse} \ (I, \ J, \ V) \)

• 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 $\mathbb{R}^d$ to $\mathbb{R}^{d+1}$
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:**
  - \([p, q, r] = \text{dmperm}(A)\);
  - \(A(p,q)\) is block upper triangular with nonzero diagonal
  - also, strongly connected components of a directed graph
  - also, connected components of an undirected graph

- **Arbitrary A:**
  - \([p, q, r, s] = \text{dmperm}(A)\);
  - 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 (\texttt{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
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