Sparse Matrices and Optimized Parallel Implementations

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March 25, 2015
Topics

Projection in Scientific Computing

Sparse matrices, parallel implementations

Iterative Methods

PDEs, Numerical solution, Tools, etc.
Outline

• Part I
  – Discussion

• Part II
  – Sparse matrix computations

• Part III
  – Reordering algorithms and parallelization
Part I

Discussion
Orthogonalization

- We can orthonormalize non-orthogonal basis. **How?**

**Other approaches:** QR using Householder transformation (as in LAPACK), Cholesky, or/and SVD on normal equations (as in the homework)
What if the basis is not orthonormal?

- If we do not want to orthonormalize:
  \[ u \approx P u = c_1 x_1 + c_2 x_2 + \ldots + c_m x_m \]

  \[
  (u, x_1) = c_1 (x_1, x_1) + c_2 (x_2, x_1) + \ldots + c_m (x_m, x_1)
  \]

  \[
  \ldots
  \]

  \[
  (u, x_m) = c_1 (x_1, x_m) + c_2 (x_2, x_m) + \ldots + c_m (x_m, x_m)
  \]

- These are the so called Petrov-Galerkin conditions

- We saw examples of their use in
  * optimization, and
  * PDE discretization, e.g. FEM
What if the basis is not orthonormal?

- If we do not want to orthonormalize, e.g. in FEM

\[ u \approx P u = c_1 \phi_1 + c_2 \phi_2 + \ldots + c_7 \phi_7 \]

'Multiply' by \( \phi_1, \ldots, \phi_7 \) to get a 7x7 system

\[ a( c_1 \phi_1 + c_2 \phi_2 + \ldots + c_7 \phi_7, \phi_i) = F(\phi_i) \quad \text{for} \ i = 1, \ldots, 7 \]

- Two examples of basis functions \( \phi_i \)
- The more \( \phi_i \) overlap, the denser the resulting matrix
- Spectral element methods (high-order FEM)

Fig. 4.1B.3  Multi-basis approximations
a) piece-wise constant
b) piece-wise linear

(Image taken from http://www.urel.feec.vutbr.cz/~raida)
Stencil Computations


Part II
Sparse matrix computations
Sparse matrices

- Sparse matrix: substantial part of the coefficients is zero
- Naturally arise from PDE discretizations
  - finite differences, FEM, etc.; we saw examples in the

5-point finite difference operator

Vertices are indexed, e.g.

Row 6 will have 5 non-zero elements:
$A_{6,2}, A_{6,5}, A_{6,6}, A_{6,7},$ and $A_{6,10}$

1-D piece-wise linear FEM

Row 3, for example, will have 3 non-zeros
$A_{3,2}, A_{3,3}, A_{3,4}$
**Sparse matrices**

- **In general:**
  - Degrees of freedom (DOF), associated for ex. with vertices (or edges, faces, etc.), are indexed
  - A basis function is associated with every DOF (unknown)
  - A Petrov-Galerkin condition (equation) is derived for every basis function, representing a row in the resulting system

- Only 'a few' elements per row will be nonzero as the basis functions have local support
  - eg. row 10, using continuous piecewise linear FEM, will have 6 nonzeroes:
    \[ A_{10,10}, A_{10,35}, A_{10,100}, A_{10,332}, A_{10,115}, A_{10,201} \]
  - physical intuition behind: PDEs describe changes in physical processes;
    describing/discretizing these changes numerically, based only on local/neighbouring information, results in sparse matrices

eg. what happens at '10' is described by the physical state at '10' and the neighbouring 35, 201, 115, 100, and 332.
Sparse matrices

• Can we take advantage of this sparse structure?
  – To solve for example very large problems
  – To solve them efficiently

• Yes! There are algorithms
  – Linear solvers and preconditioners (to cover some in the last 2 lectures)
  – Efficient data storage and implementation (next ...)
Sparse matrix formats

• It pays to avoid storing the zeros!
• Common sparse storage formats:
  – AIJ
  – Compressed row/column storage (**CRS/CCS**)
  – Compressed diagonal storage (CDS)
    * for more see the 'Templates' book
      http://www.netlib.org/linalg/html_templates/node90.html#SECTION00931000000000000000
  – Blocked versions (**why?**)
**AIJ**

- Stored in 3 arrays
  - The same length
  - No order implied

<table>
<thead>
<tr>
<th>I</th>
<th>J</th>
<th>AIJ</th>
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<tr>
<td>1</td>
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<td>7</td>
</tr>
<tr>
<td>4</td>
<td>5</td>
<td>8</td>
</tr>
</tbody>
</table>

\[
\begin{bmatrix}
1 & 2 & 0 & 0 & 0 \\
3 & 0 & 4 & 0 & 0 \\
0 & 5 & 0 & 6 & 0 \\
0 & 0 & 7 & 0 & 8 \\
\end{bmatrix}
\]
CRS

- Stored in 3 arrays
  - J and AIJ the same length
  - I (representing rows) is compressed

<table>
<thead>
<tr>
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</thead>
<tbody>
<tr>
<td>1</td>
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</tr>
<tr>
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</tr>
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<td>6</td>
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<tr>
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<td></td>
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<tr>
<td>5</td>
<td>8</td>
<td></td>
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</tbody>
</table>

array I : think of it as pointers to where next row starts
CCS : similar but J is compressed
CDS

- For matrices with non-zeros along sub-diagonals

\[
A = \begin{pmatrix}
10 & -3 & 0 & 0 & 0 & 0 \\
3 & 0 & 6 & 0 & 0 & 0 \\
0 & 7 & 8 & 7 & 0 & 0 \\
0 & 0 & 8 & 7 & 5 & 0 \\
0 & 0 & 0 & 0 & 9 & 13 \\
0 & 0 & 0 & 0 & 2 & -1
\end{pmatrix}
\]
Performance (Mat-vec product)

• **Notoriously bad** for running at just a fraction of the performance peak!

• **Why?**

  Consider mat-vec product for matrix in CRS:

  ```
  for i = 1, n
      for j = I[i], I[i+1]-1
          y[i] += AIJ[j] * x[J[j]]
  ```
Performance (Mat-vec product)

- **Notoriously bad** for running at just a fraction of the performance peak!

- **Why?**
  Consider mat-vec product for matrix in CRS:

  ```
  for i = 1, n
  for j = I[i], I[i+1]-1
  y[i] += A[I][j] * x[J[j]]
  ```

  * Irregular indirect memory access for x
  - result in cache trashing
  * performance often <10% peak
Performance (Mat-vec product)

* Performance of mat-vec products of various sizes on a 2.4 GHz Pentium 4
* An example from Gahvari et.al.:

(a) Untuned SpMV performance
Performance (Mat-vec product)

• How to improve the performance?
  – A common technique
    (as done for dense linear algebra)
    is **blocking** (register, cache: next ... )
  – **Index reordering** (in Part II)
  – Exploit special matrix structure (e.g., symmetry, bands, other structures)
Block Compressed Row Storage (BCRS)

- Example of using 2x2 blocks

<table>
<thead>
<tr>
<th>BI</th>
<th>BJ</th>
<th>AIJ</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
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</tr>
<tr>
<td>4</td>
<td>3</td>
<td>0</td>
</tr>
</tbody>
</table>

\[
\begin{bmatrix}
1 & 0 & 2 & 3 & 0 & 0 \\
0 & 4 & 5 & 0 & 0 & 0 \\
0 & 0 & 0 & 6 & 7 \\
0 & 0 & 0 & 0 & 8 & 9
\end{bmatrix}
\]

- Reduced storage for indexes
- Drawback: add 0s
- What block size to choose?
- BCRS for register blocking
- Discussion?
BCRS

(a) Untuned SpMV performance

(b) Speedups obtained from tuning
Cache blocking

• Improve cache reuse for $x$ in $Ax$ by splitting $A$ into a set of sparse matrices, e.g.

Sparse matrix and its splitting

For more info check:
Eun-Jin Im, K. Yelick, R. Vuduc
Part III
Reordering algorithms and Parallelization
Reorder to preserve locality

e.g., Cuthill-McKee Ordering: start from arbitrary node, say '10' and reorder
* '10' becomes 0
* neighbours are ordered next to become 1, 2, 3, 4, 5, denote this as level 1
* neighbours to level 1 nodes are next consecutively reordered, and so on until end
Cuthill-McKee Ordering

• Reversing the ordering (RCM) results in ordering that is better for sparse LU
• Reduces matrix bandwidth (see example)
• Improves cache performance
• Can be used as partitioner (*parallelization*) but in general does not reduce edge cut
Self-Avoiding Walks (SAW)

- Enumeration of mesh elements through 'consecutive elements' (sharing face, edge, vertex, etc.)
  - similar to space-filling curves but for unstructured meshes
  - improves cache reuse
  - can be used as partitioner with good load balance but in general does not reduce edge cut
Graph partitioning

- Refer back to Lecture #9, Part II: Mesh Generation and Load Balancing
- Can be used for reordering
- Metis/ParMetis:
  - multilevel partitioning
  - Good load balance and minimize edge cut
Parallel Mat-Vec Product

- Easiest way:
  - 1D partitioning
  - May lead to load unbalance (why?)
  - May need a lot of communication for $x$

- Can use any of the just mentioned techniques

- Most promising seems to be spectral multilevel methods (as in Metis/ParMetis)
Possible optimizations

• Block communication
  – To send the min. required part of $x$
  – e.g., pre-compute blocks of interfaces
• Load balance, minimize edge cut
  – e.g., a good partitioner would do it
• Reordering
• Advantage of additional structure (symmetry, bands, etc)
Comparison

Distributed memory implementation
(by X. Li, L. Oliker, G. Heber, R. Biswas)

- ORIG ordering has large edge cut (interprocessor comm) and poor locality (high number of cache misses)
- MeTiS minimizes edge cut, while SAW minimizes cache misses

<table>
<thead>
<tr>
<th>P</th>
<th>ORIG (10^6)</th>
<th>MeTiS (10^6)</th>
<th>RCM (10^6)</th>
<th>SAW (10^6)</th>
<th>ORIG (10^6 bvtes)</th>
<th>MeTiS (10^6 bvtes)</th>
<th>RCM (10^6 bvtes)</th>
<th>SAW (10^6 bvtes)</th>
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<tbody>
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<td>8</td>
<td>3.684</td>
<td>3.034</td>
<td>3.749</td>
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<td>16</td>
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<td>1.017</td>
<td>0.507</td>
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<tr>
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<td>0.358</td>
<td>0.515</td>
<td>0.290</td>
<td>0.828</td>
<td>0.008</td>
<td>0.032</td>
<td>0.023</td>
</tr>
</tbody>
</table>
Learning Goals

• Efficient sparse computations are challenging!

• Computational challenges and issues related to sparse matrices
  – Data formats
  – Optimization
    • Blocking
    • Reordering
    • Other

• Parallel sparse Mat-Vec product
  – Code optimization opportunities