Sparse Matrices and Optimized Parallel Implementations

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Topics
Projection in Scientific Computing

Sparse matrices, parallel implementations

PDEs, Numerical solution, Tools, etc.

Iterative Methods
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 homeworks 9 and 10)

Hybrid CPU-GPU (NVIDIA Quadro FX 5600)
computation as in Homework #9

128 vectors

CPU computation

AMD Opteron (tm), Processor 265 (1.8 Ghz, 1 GB cache)
What if the basis is not orthonormal?

- If we do not want to orthonormalize:
  \[ u \approx P u = c_1 x_1 + c_2 x_2 + \ldots + c_m x_m \]
  / 'Multiply' by \( x_1, \ldots, x_m \) to get

\[
\begin{align*}
(u, x_1) &= c_1 (x_1, x_1) + c_2 (x_2, x_1) + \ldots + c_m (x_m, x_1) \\
\ldots \\
(u, x_m) &= c_1 (x_1, x_m) + c_2 (x_2, x_m) + \ldots + c_m (x_m, x_m)
\end{align*}
\]

- 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
  \[ \mathbf{u} \approx \mathbf{P} \mathbf{u} = c_1 \phi_1 + c_2 \phi_2 + \ldots + c_7 \phi_7 \]

  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

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

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 nonzeros:
      \[ A_{10,10}, A_{10,35}, A_{10,100}, A_{10,332}, A_{10,115}, A_{10,201} \]
    - 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#SECTION009310000000000000000
  – Blocked versions (why?)
- **Stored in 3 arrays**
  - The same length
  - No order implied

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CRS

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

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

I | J | AIJ
---|---|---
1 | 1 | 1
3 | 2 | 2
5 | 1 | 3
7 | 3 | 4
9 | 2 | 5
4 | 6
3 | 7
5 | 8

array I: think of it as pointers to where next row starts
CCS: similar but J is compressed
• For matrices with non-zeros along sub-diagonals

\[ A = \begin{pmatrix}
10 & -3 & 0 & 0 & 0 & 0 \\
3 & 9 & 6 & 0 & 0 & 0 \\
0 & 7 & 8 & 7 & 0 & 0 \\
0 & 0 & 8 & 7 & 5 & 0 \\
0 & 0 & 0 & 0 & 9 & 13 \\
0 & 0 & 0 & 0 & 2 & -1 \\
\end{pmatrix} \]
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]
  ```
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] ]
  ```

  * 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

(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

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<th>BJ</th>
<th>AIJ</th>
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<td>0</td>
<td>6</td>
</tr>
<tr>
<td>8</td>
<td>9</td>
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</tr>
</tbody>
</table>
```

- 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](image)

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
  – eg. 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>Avd. Cache Misses ($10^6$)</th>
<th>Avd. Comm ($10^6$ bytes)</th>
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<tr>
<td>64</td>
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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