Issues in the Design of Scalable Out-of-core Dense Symmetric Indefinite Factorization Algorithms

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1 Talk Outline

- introduction to (large) general dense symmetric systems factorization
- diagonal pivoting algorithms:
  - challenges for the parallel out-of-core case
  - the (exhaustive) elimination block search strategy
- left-looking parallel out-of-core algorithms:
  - blocking and data layout issues
  - a slab-based algorithm
  - memory scalability issues and a block-based algorithm
- conclusions and future work

2 Introduction to Large Symmetric Indefinite Systems Solution

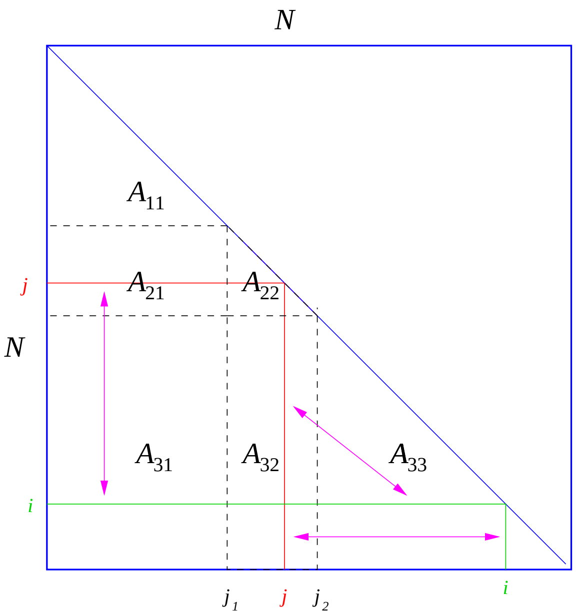
- $N \times N$ general (ie. indefinite: $x^T Ax \not> 0, ||x|| > 0$) symmetric systems of linear equations, eg. $Ax = b$, arise in:
  - incompressible flow computations, linear and non-linear optimization, electromagnetic scattering & field analysis & data mining
- a direct solution for x is the most general and accurate method
  - require $O(N^3)$ FLOPS, dominated by the fact'n of A, ie. $A \rightarrow PLDL^TP^T$
- only parallel out-of-core algorithms for LU, LL^T and QR developed so far
  - left-looking versions of blocked algorithms are preferred:
    - the number of writes to disk is only $O(N^2)$; easier to checkpoint
  - two approaches:
    - slab-based: whole block of columns being eliminated are kept in core
    - block-based: only part of the column block in core

      $\surd$ permits a wider column block $\Rightarrow$ better memory scalability

      $\times$ can't be (efficiently) applied for LU with strict partial (row) pivoting
    - seemingly harder still for LDL^T, which requires symmetric pivoting

3 Diagonal Pivoting Algorithms

- store A in lower triangular half; overwrite with L and D
- partial left-looking blocked algorithm: (A_{*1} factored, A_{*2} being factored, A_{*3} untouched)



1. apply pivots from A_{11} to $A_2 = \begin{pmatrix} A_{22} \\ \hline A_{32} \end{pmatrix}$
2. A_{22} -= $A_{21}W_{21}^T$, $W_{21} = D_{11}A_{21}$
3. A_{32} -= $A_{31}W_{21}^T$
4. eliminate block column A_2

   (applying pivots from within A_2)
5. apply pivots (row interchanges) from A_2 to $A_1 = \begin{pmatrix} A_{21} \\ \hline A_{31} \end{pmatrix}$

- diagonal pivoting methods use symmetric (row & column) interchanges based on 1×1 or 2×2 'pivots'
  - nb. interchange $i \leftrightarrow j$: $A_{i,j}$ is not moved; $A_{j,j} \leftrightarrow A_{i,i}$
- recently developed stable methods include the bounded Bunch-Kaufman and exhaustive block search methods

4 Challenges for the Parallel Out-of-core Case

- here, A is distributed over a $P \times Q$ processor grid with an $r \times r$ block-cyclic matrix distribution:
  - i.e. (storage) block (i, j) will be on processor $(i \bmod P, j \bmod Q)$
  - assume this applies to both disk and memory
  - assume storage is column-oriented for both
- in the left-looking algorithm, consider candidate pivot i lying outside A_2
  - a_i must be aligned with a_j (read a large number of remote disk blocks)
  - *all* updates from A_1 and A_2 (so far) must be applied to it (large number of disk accesses)
  - if suitable, a_i (in A_{33}) must be over-written by the *original value* of a_j
  - pivot i may not even be suitable!
- if pivot i is inside A_2, only overhead is in message exchanges . . .

5 The Exhaustive Block Search Strategy

- search for (stable) pivots in the current elimination block (A_2)
  - consider *any* 1×1 or 2×2 pivots in remaining columns $j : j_2$
  - well-known stability tests can be used
- originally developed for sparse matrices (Duff & Reid, 1983)
  - has a large payoff in preserving the sparsity
- useful in the parallel in-core case if search succeeds within the current storage block
  - $\surd$ little message overhead in searches / interchanges
  - $\times$ overhead of extra searches (finding column maximums) can outweigh
    - $\Rightarrow$ limit search to $\omega_s = 16$ columns found to be optimal
    - for highly indefinite matrices: only $0.15N$ searches outside A_2 required
    - for weakly indefinite matrices, this reduces to $< 0.05N$
  - the bounded Bunch-Kaufman algorithm used for searches outside A_2
- a successful block search can minimize the overheads in the out-of-core case

6 Parallel OOC Algorithms: Blocking and Data Layout Issues

- must consider all levels of the (parallel) memory hierarchy, exploiting locality wherever possible:
  - ω_a: the top-level algorithm's blocking factor
    - should be as large as possible, to maximize re-use at disk level
    - for slab-based algorithm, $\frac{N\omega_a}{PQ} \leq M$ (M is memory capacity)
  - ω_c: optimal blocking factor for matrix multiply
    - need $\omega_a \geq \omega_c$ to maximize re-use at cache level
  - r: the storage block size; can be chosen to minimize message overheads
    - $r = \omega_a$ best for this but may cause unacceptable load imbalance (disk and CPU)
  - ω_s: the number of columns to be searched, $\omega_s \leq \omega_a$
    - must be sufficiently large to achieve a very high success rate
  - ω_d, where ω_d^2 = disk block size
    - for block-based algorithm, $\omega_a^2 >> \omega_d^2$ to amortize disk latencies
- organization of A upon disk: could be [(ω_s or r - sized) block] row/column oriented, depending on algorithm

7 A Slab-based Algorithm Exploiting Pivoting Locality

- a modification of the left-looking algorithm:
  - the $0 \leq u_1 < \omega_a$ un-eliminated columns left over from previous stage become the 1st u_1 columns of A_2 for this stage
  - steps 1–3 only operate on last $\omega_a - u_1$ columns
  - insert step 3a: block interchange of the 1st & last $u_1' = \min(u_1, \omega_a - u_1)$ columns of A_2
  - step 4: uses the exhaustive block search (+ a non-local search to ensure ≥ 1 columns eliminated)
- provided no non-local searches were needed, step 1 is empty, and all interchanges are kept within slabs
  - as $\omega_a > r$ for other aspects of performance, this will require some communication
- column-oriented disk stage will be optimal
- performance will rely on highly successful block searches, eg. $u_i \leq 0.2\omega_a$
  - for $u_1 \approx 0$, the number of words read from disk (dominated by steps 2–3) is: $\Sigma_{i=0}^{N/\omega_a} i\omega_a(N - i\omega_a) = \frac{N^3}{6\omega_a} + O(N^2)$

8 A Block-Based Algorithm

- only for very large problems (or small processor grids) will slab-based algorithms result in a too small ω_a
- can convert the slab-based algorithm to a block-based one in which only ω_a ($\omega_c \leq \omega_s \leq \omega_a$) columns are kept in core:
  - apply a left-looking factorization internally to step 4 (factorize A_2), using a blocking factor of ω_s
    - the columns of A_2 must now be read repeatedly as they were for A_1 for the slab-based algorithm
    - the number of extra reads is given by: $\Sigma_{i=0}^{N/\omega_a}\Sigma_{j=0}^{\omega_a/\omega_s} i\omega_a \cdot j\omega_s = \frac{N^2\omega_a}{4\omega_s} + O(N)$
  - for the top-level algorithm, steps 2–3 proceed using $\omega_a \times \omega_a$ sized blocks
  - as these form the dominant accesses, a row-block disk storage is optimal

9 Conclusions

- solving general symmetric systems has an accuracy–performance trade-off
  - for the parallel out-of-core case, potentially very large disk/message overheads from non-local symmetric interchanges
- however, efficient slab- and even (a limited) block-based algorithms exist, based on applying exhaustive pivots searches in (overlapping) elimination blocks
  - seems likely that *most* searches and interchanges can be kept within these blocks
  - performance is highly dependent on overlap being small
  - block-based algorithm has better memory scalability but slab-based algorithm will normally be adequate in practice
- future (current!) work includes:
  - investigating whether the overlap can be kept small (eg. $\frac{u_1}{\omega_a} \leq 0.2$) for any indefinite matrices
  - developing and evaluating these highly complex algorithms!