Designing sparse direct solvers for multicore architectures

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Outline of talk

How to efficiently solve $A\mathbf{x} = \mathbf{b}$ on multicore machines

(A symmetric)

- Dense positive-definite systems
- Large sparse positive-definite systems
- Large sparse indefinite systems

Dense positive-definite systems

Factorize $A = LL^T$ using simple block algorithm:

For $k = 1, 2, \dots$:

- $A_{kk} = L_{kk} L_{kk}^T$ (Factor)
- For $i > k$: $L_{ik} = A_{ik} L_{kk}^{-T}$ (Triangular Solve)
- For $i, j > k$: $A_{ij} \leftarrow A_{ij} - L_{ik} L_{jk}^T$ (Update)

Dense positive-definite systems

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Dense positive-definite systems

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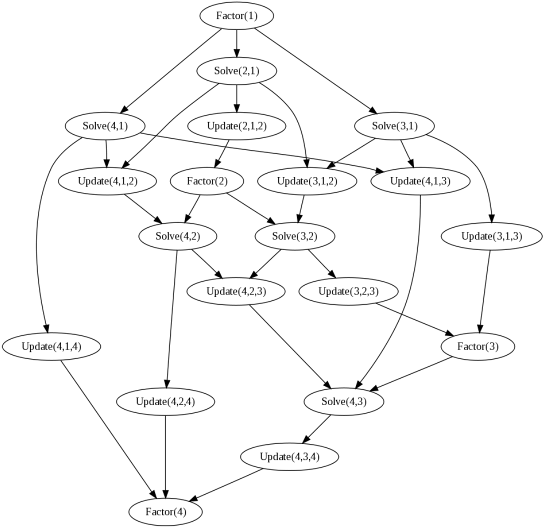
What do we need to synchronise?

Consider each block operation as a task.

Tasks have dependencies.
Represent implicitly as a Directed Acyclic Graph (DAG).

Approach of Buttari, Dongarra, Kurzak, Langou, Luszczek, Tomov '06

Task DAG (4 blocks)



Speedup for dense case

Results on machine with 2 Intel E5420 quad core processors.

n	Speedup
500	3.2
2500	5.7
10000	7.2
20000	7.4

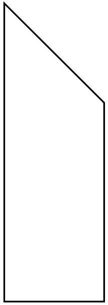
Dense DAG code `HSL_MP54` available in HSL 2007.

Sparse case?

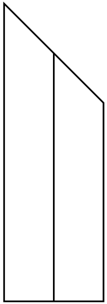
How to generalise to sparse factorizations?

Nodal matrix

Hold set of contiguous cols of sparse L with (nearly) same pattern as a dense trapezoidal matrix, referred to as nodal matrix.

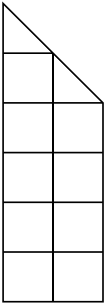


Nodal matrix



Divide nodal matrix into block columns

Nodal matrix



Divide each block column into (square) dense blocks

- Basic operation unit is the block.
- Tasks are performed using these blocks

Tasks in sparse positive-definite case

Express sparse Cholesky factorization using 4 basic operations

factor_block. Computes dense Cholesky factor L_{diag} of block on diagonal.

Tasks in sparse positive-definite case

Express sparse Cholesky factorization using 4 basic operations

factor_block. Computes dense Cholesky factor L_{diag} of block on diagonal.

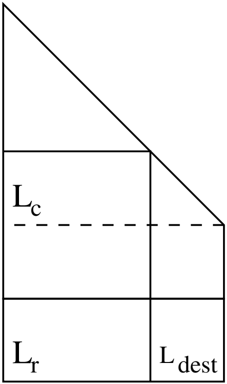
solve_block. Performs triangular solve of off-diagonal block L_{dest} by Cholesky factor L_{diag} of block on its diagonal.

$$L_{dest} \Leftarrow L_{dest} L_{diag}^{-T}$$

Tasks in sparse positive-definite case

update_internal

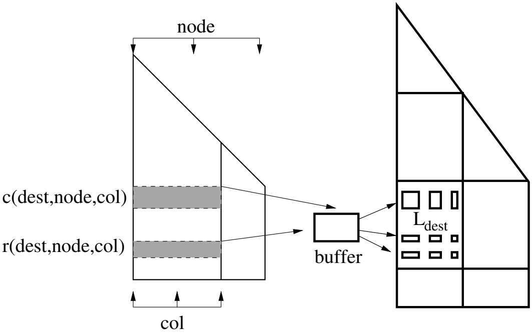
Within *node*, performs update



$$L_{dest} \Leftarrow L_{dest} - L_r L_c^T$$

Tasks in sparse DAG

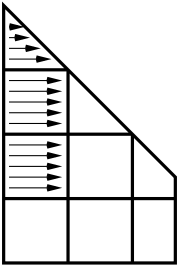
update_between



1. Form outer product $L_r L_c^T$ into a buffer.
2. Distribute results into destination block L_{dest}.

Storage of nodal matrix

- Use full storage on diagonal to allow use of efficicent BLAS and LAPACK
- Store each block by rows contiguously … removes discontinuities at row block boundaries and facilitates update tasks.



1				
4	5			
7	8	9		
10	11	12	25	
13	14	15	27	28
16	17	18	29	30
19	20	21	31	32
22	23	24	33	34

Dependency count

During analyse, calculate number of tasks to be performed for each block of L.

During factorization, keep running count of outstanding tasks for each block.

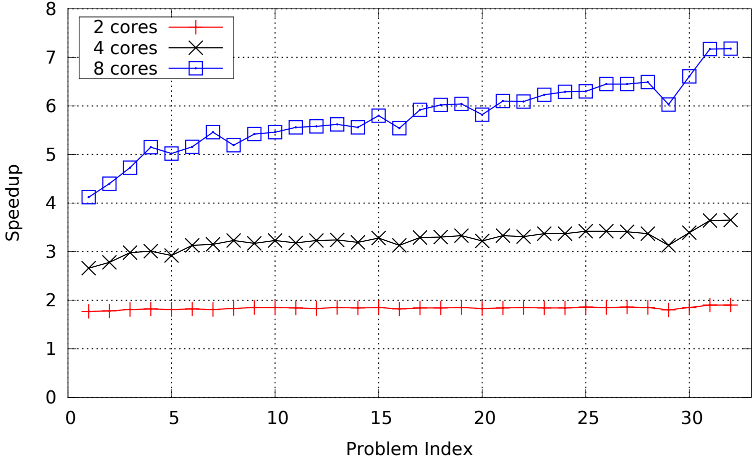
When count reaches 0, a task is stacked.

Each cache keeps small stack of tasks that are intended for use by threads sharing this cache.

Tasks added to or drawn from top of local stack. If becomes full, move bottom half to global task pool

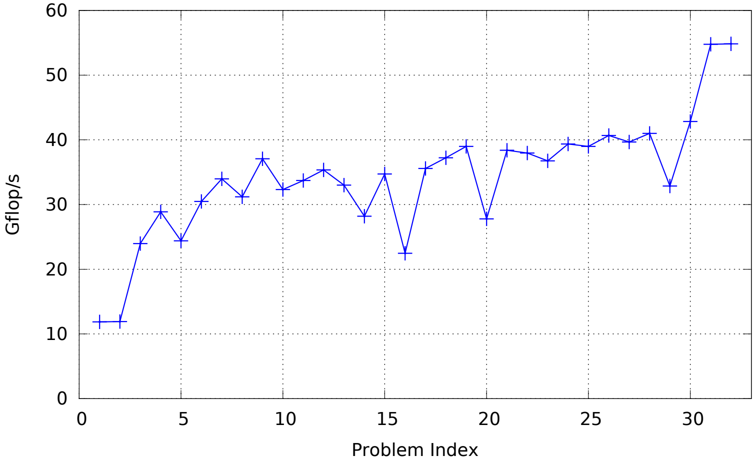
Sparse positive-definite DAG results

Speedups for factorize phase.



Sparse positive-definite DAG results

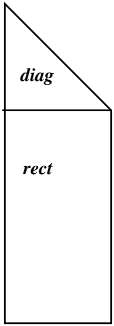
The speed of factorize phase in Gflop/s on 8 cores.
(`dgemm` peak 72.8 Gflop/s)



Sparse indefinite systems

Extra challenge: need to accommodate pivoting for stability

Do not want to restrict pivoting to within block on diagonal



Large entries in *rect* could cause problems.

Implications

- Cannot factorize the diagonal block independently of the off-diagonal blocks.
- The diagonal block and the off-diagonal blocks must all have zero dependency counts.
- Necessary to combine factor_block and **all** solve_block tasks for a block column L_{col}.
- Separate kernel code written to perform this efficiently, incorporating threshold partial pivoting with 1×1 and 2×2 pivots.

Effects

- Parallelism less fine-grained (large factorize_col task replaces smaller factor_block and solve_block tasks so we use smaller default block size)
- May need to expand storage determined during analyse

$$L_{col} \longrightarrow L_{col}^{new}$$

  (L_{col}^{new} includes delayed columns from child nodes)

- More data movement/copying
- Pivot search requires access by columns (recall: block column stored by rows)

Indefinite results: serial runs

Factorize times on single core. OOM indicates out of memory.

Problem	MA57	HSL_MA77	New code
Schenk_IBMNA/c-56	0.404	0.130	0.163
Simon/olafu	0.559	0.234	0.244
Koutsovasilis/F2	4.48	2.42	2.57
Oberwolfach/t3dh	20.2	11.7	12.1
Schenk_AFE/af_shell10	100	76.2	72.8
Oberwolfach/bone010	877	637	590
PARSEC/Ga41As41H72	OOM	9241	7290

Indefinite results: good news

Factorize times on 1 and 8 cores.

Problem	1	8	speedup
Boeing/crystk03	1.29	0.36	3.58
Koutsovasilis/F2	2.57	0.57	4.51
Cunningham/qa8fk	4.23	0.88	4.79
Oberwolfach/t3dh	12.1	2.17	5.58
Schenk_AFE/af_shell10	72.8	11.7	6.22
Oberwolfach/bone010	590	88.3	6.68
PARSEC/Ga41As41H72	7290	1141	6.39

Conclude: very good results for some large problems

Indefinite results: tough problems

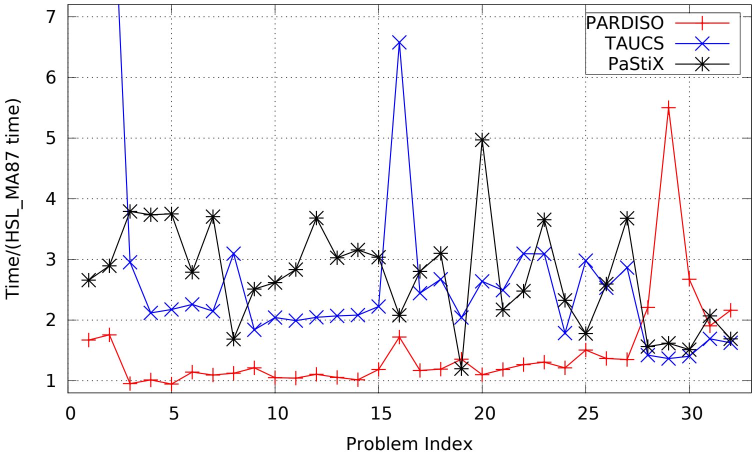
Many delayed pivots cause performance hit.

Problem	num_delay	1	8	speedup
GHS_indef/sparsine	16	250	44.4	5.65
Schenk_IBMA/c-62	28728	9.07	4.93	1.84
GHS_indef/aug3d	144955	36.5	25.9	1.41

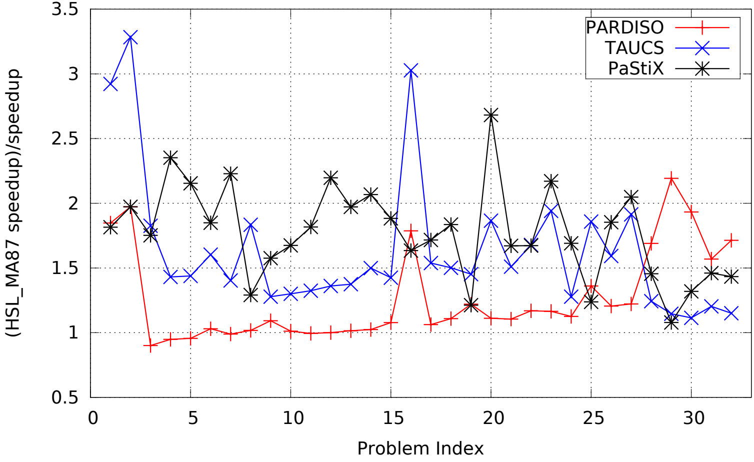
Concluding remarks

- Extended DAG approach from dense positive-definite systems to sparse systems
- Very good results for factorizing positive-definite matrices on our 8-core machine
- Also good results for large indefinite problems provided there are few delayed pivots
- For some tough indefinite problems, further work needed to improve performance while maintaining stability.

Positive-definite case: comparison with other solvers



Positive-definite case: speedup ratios



Indefinite case: comparison with PARDISO

Wall-clock times for factorization phase on 8 cores.

Problem	PARDISO	New code
Schenk_IBMNA/c-56	0.055	0.152
Boeing/crystk03	0.269	0.359
Cunningham/qa8fk	0.704	0.882
Schenk_AFE/af_shell10	13.2	11.7
Oberwolfach/bone010	174	88.3
GSH_indef/sparsine	159	44.4
PARSEC/Ga41As41H72	3020	1141