A DAG-based sparse Cholesky solver for multicore architectures

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Outline of talk

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

- Introduction
- Dense systems
- Sparse systems
- Future directions and conclusions

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Solving systems in parallel

Haven't we been solving linear systems in parallel for years?
Yes — large problems on distributed memory machines

We want to solve

- Medium and large problems (more than 10^{10} flops)
- On desktop machines
- Shared memory, complex cache-based architectures
- 2–6 cores now in all new machines.
- Soon 16–64 cores will be standard.

Traditional MPI methods work, but not well.

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Faster

I have an 8-core machine...

...I want to go (nearly) 8 times faster

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The dense problem

Solve

$$A\mathbf{x} = \mathbf{b}$$

with A

- Symmetric and dense
- Positive definite (indefinite problems require pivoting)
- Not small (order at least a few hundred)

Pen and paper approach

Factorize $A = LL^T$ then solve $A\mathbf{x} = \mathbf{b}$ as

$$\begin{aligned} L\mathbf{y} &= \mathbf{b} \\ L^T\mathbf{x} &= \mathbf{y} \end{aligned}$$

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Algorithm:

- For each column k:
  - $L_{kk} = \sqrt{A_{kk}}$ (Calculate diagonal element)
  - For rows $i > k$: $L_{ik} = A_{ik}L_{kk}^{-1}$ (Divide column by diagonal)
  - Update trailing submatrix
    $A_{(k+1:n)(k+1:n)} \leftarrow A_{(k+1:n)(k+1:n)} - L_{(k+1:n)k}L_{(k+1:n)k}^T$

Serial approach

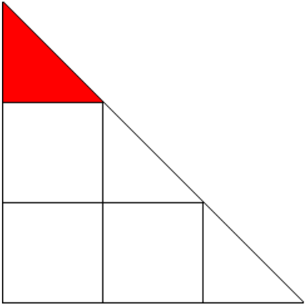
Exploit caches

Use algorithm by blocks

- Same algorithm, but submatrices not elements
- $10\times$ faster than a naive implementation
- Built using Basic Linear Algebra Subroutines (BLAS)

Cholesky by blocks

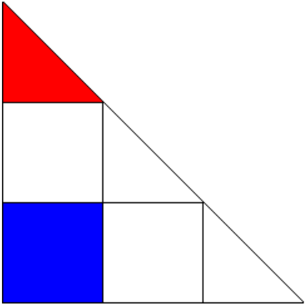
Factorize diagonal



Factor(col)

Cholesky by blocks

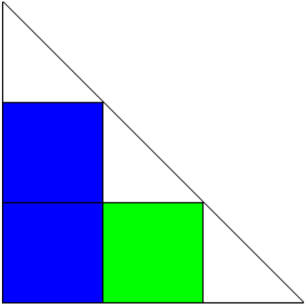
Solve column block



Solve(row, col)

Cholesky by blocks

Update block



Update(row, source col, target col)

Parallelism mechanisms

MPI	Designed for distributed memory, requires substantial changes
OpenMP	Designed for shared memory
pthreads	POSIX threads, no Fortran API
ITBB	Intel Thread Building Blocks, no Fortran API
Coarrays	Not yet widely supported

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Traditional approach

Just parallelise the operations

Solve(row,col) Can do the solve in parallel

Update(row,scol,tcol) Easily split as well

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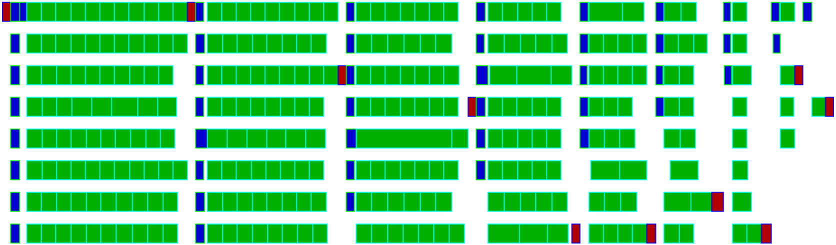
What does this look like...

Parallel right looking



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Jack says...

Jack Dongarra's suggested aims for multicore:

Low granularity Many many more tasks than cores.

Asyncronicity Don't use tight coupling, only enforce necessary ordering.

Dynamic Scheduling Static (precomputed) scheduling is easily upset.

Locality of reference Cache/performance ratios will only get worse, try not to upset them.

DAGs

What do we really need to synchronise?

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Represent each block operation (Factor, Solve, Update) as a task.

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- Tasks are vertices
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It is acyclic — hence have a Directed Acyclic Graph (DAG)

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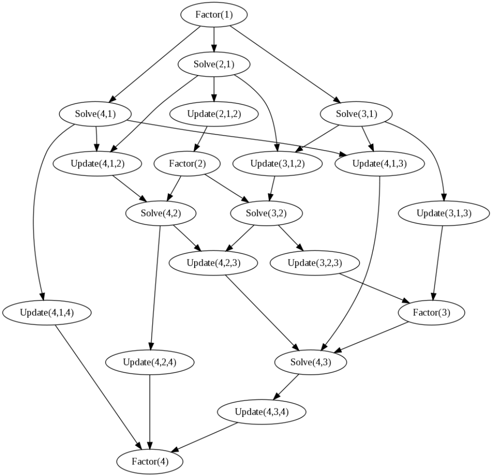
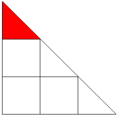
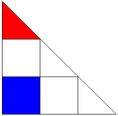
Task DAG



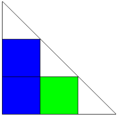
Factor(col) $A_{kk} = L_{kk} L_{kk}^T$



Solve(row, col) $L_{ik} = A_{ik} L_{kk}^{-T}$



Update(row, scol, tcol)
$A_{ij} \leftarrow A_{ij} - L_{ik} L_{jk}^T$



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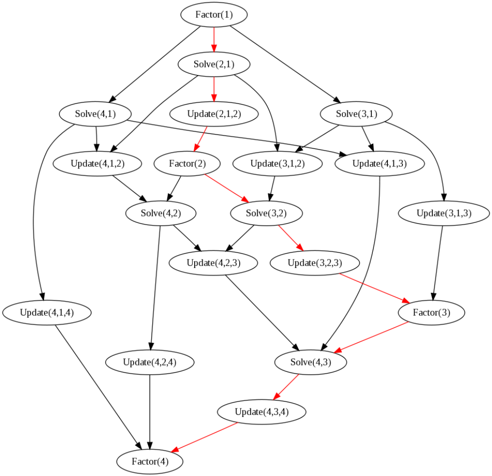
Task DAG



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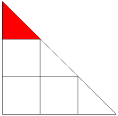

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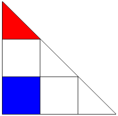

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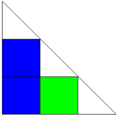

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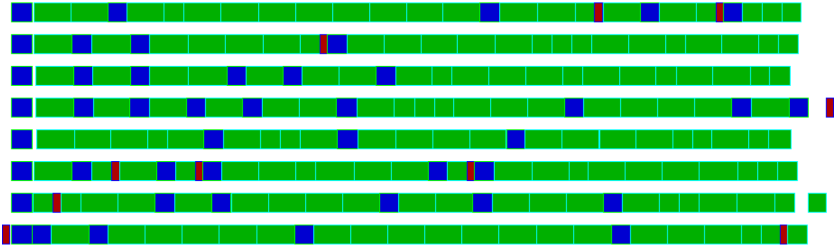
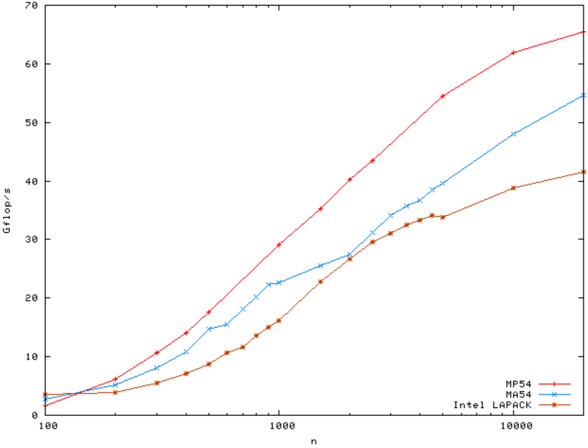
Profile



Results



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Speedup for dense case

n	Speedup
500	3.2
2500	5.7
10000	7.2
20000	7.4

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New dense DAG code HSL_MP54 available in HSL2007.

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Sparse case?

So far, so dense. What about sparse factorizations?

Sparse matrices

- Sparse matrix is mostly zero — only track non-zeros.
- Factor L is denser than A.
- Extra entries are known as fill-in.
- Reduce fill-in by preordering A.

Direct methods

Generally comprise four phases:

- **Reorder** Symmetric permutation P to reduce fill-in.
- **Analyse** Predict non-zero pattern. Build elimination tree.
- **Factorize** Using data structures built in analyse phase perform the numerical factorization.
- **Solve** Using the factors solve $A\mathbf{x} = \mathbf{b}$.

Aim: Organise computations to use dense kernels on submatrices.

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Elimination and assembly tree

The elimination tree provides partial ordering for operations.

If U is a descendant of V then we must factorize U first.

To exploit BLAS, combine adjacent nodes whose cols have same (or similar) sparsity structure.

Condensed tree is assembly tree.

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Factorize phase

Existing parallel approaches usually rely on two levels of parallelism

Tree-level parallelism: assembly tree specifies only partial ordering (parent processed after its children). Independent subtrees processed in parallel.

Node-level parallelism: parallelism within operations at a node. Normally used near the root.

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Tree-level parallelism: assembly tree specifies only partial ordering (parent processed after its children). Independent subtrees processed in parallel.

Node-level parallelism: parallelism within operations at a node. Normally used near the root.

Our experience: speedups less than ideal on multicore machines.

Sparse DAG

Basic idea: Extend DAG-based approach to the sparse case by adding new type of task to perform sparse update operations.

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

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Sparse DAG

Basic idea: Extend DAG-based approach to the sparse case by adding new type of task to perform sparse update operations.

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

Divide the nodal matrix into blocks and perform tasks on the blocks.

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Tasks in sparse DAG

factorize(`diag`) Computes dense Cholesky factor L_{triang} of the triangular part of block `diag` on diagonal. If block trapezoidal, perform triangular solve of rectangular part

$$L_{rect} \Leftarrow L_{rect} L_{triang}^{-T}$$

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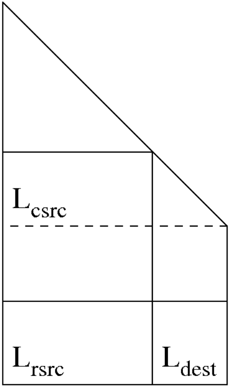
solve(`dest, diag`) Performs triangular solve of off-diagonal block `dest` by Cholesky factor L_{triang} of block `diag` on its diagonal.

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

Tasks in sparse DAG

update_internal(dest, rsrc, csrc)

Within nodal matrix, performs update



$$L_{dest} \Leftarrow L_{dest} - L_{rsrc} L_{csrc}^T$$

Tasks in sparse DAG

update_between(dest, snode, scol)
Performs update

$$L_{dest} \Leftarrow L_{dest} - L_{rsrc} L_{csrc}^T$$

- where L_{dest} is a submatrix of the block dest of an ancestor of node snode
- L_{rsrc} and L_{csrc} are submatrices of contiguous rows of block column scol of snode.

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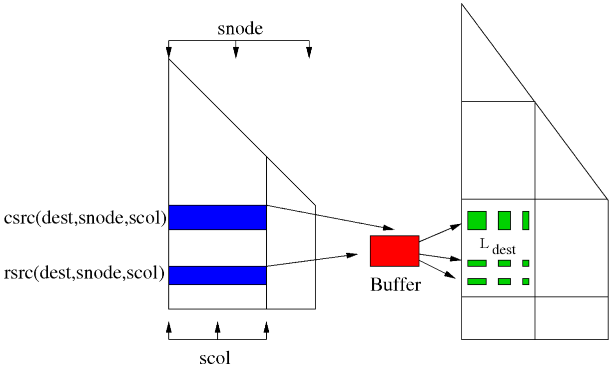
update_between(dest, snode, scol)



1. Form outer product $L_{rsrc}L_{csrc}^T$ into Buffer.
2. Distribute the results into the destination block L_{dest}.

Dependency count

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

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When count reaches 0 for block on the diagonal, store factorize task and decrement count for each off-diagonal block in its block column by one.

When count reaches 0 for off-diagonal block, store solve task and decrement count for blocks awaiting the solve by one. Update tasks may then be spawned.

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Task pool

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 task pool.

Tasks in pool given priorities:

1.	**factorize**	Highest priority
2.	**solve**	
3.	**update_internal**	
4.	**update_between**	Lowest priority

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Sparse DAG results

Results on machine with 2 Intel E5420 quad core processors.

Problem	Time		Speedup
cores	1	8	
DNVS/thread	5.25	0.98	5.36
GHS_psdef/apache2	30.1	5.07	5.94
Koutsovasilis/F1	37.8	6.05	6.24
JGD_Trefethen/Trefethen_20000b	102	16.5	6.18
ND/nd24k	335	53.7	6.23

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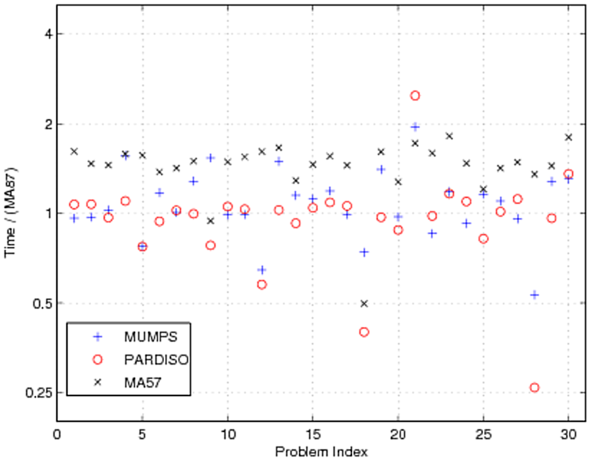
Comparisons with other solvers, one thread



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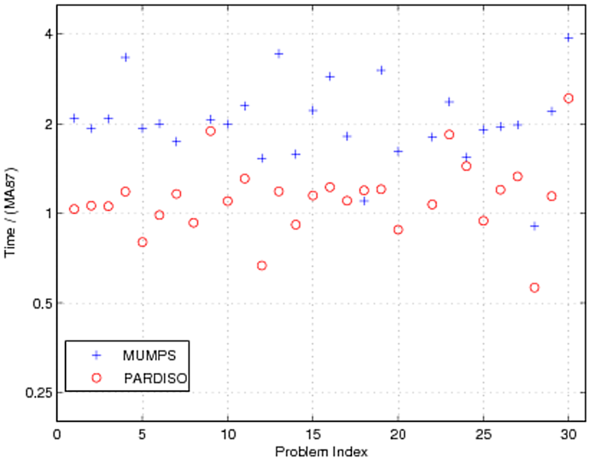
Comparisons with other solvers, 8 threads



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Indefinite case

Sparse DAG approach very encouraging for multicore architectures.

Indefinite case

Sparse DAG approach very encouraging for multicore architectures.

BUT

- So far, only considered positive definite case.
- Indefinite case is harder because of pivoting.
- Currently looking at block column dependency counts and combining factor and solve tasks.
- Anticipate speed ups will not be quite so good.

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Code availability

New sparse DAG code is HSL_MA87.

Will shortly be available as part of HSL.

If you want to try it out, let us know.

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