SCHEDULING SPARSE SYMMETRIC FAN-BOTH CHOLESKY FACTORIZATION

Mathias Jacquelin
mjacquelin@lbl.gov
Esmond Ng, Kathy Yelick and Yili Zheng
egng|kayelick|yzheng@lbl.gov

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Scalable Solvers Group
Computational Research Department
Lawrence Berkeley National Laboratory

OUTLINE

Background and motivation

`Fan-In`, `Fan-Out` and `Fan-Both` factorizations

Parallel distributed memory implementation, a.k.a. `symPACK`

Numerical experiments

Motivations:

- Sparse matrices arise in many applications:
  - Optimization problems
  - Discretized PDEs
  - ...
- Some sparse matrices are symmetric

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- Sparse matrices arise in many applications:
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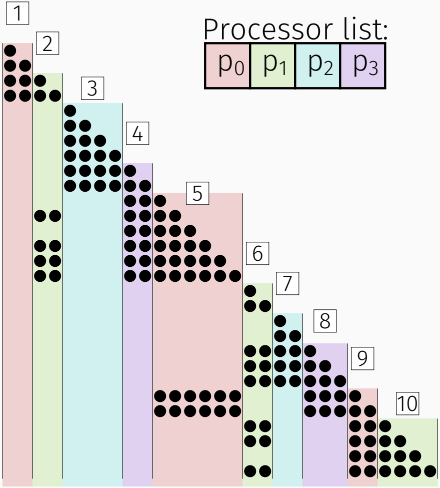
Challenges for current and future platforms:

- Higher relative communication costs
- Lower amount of memory per core

Objective:

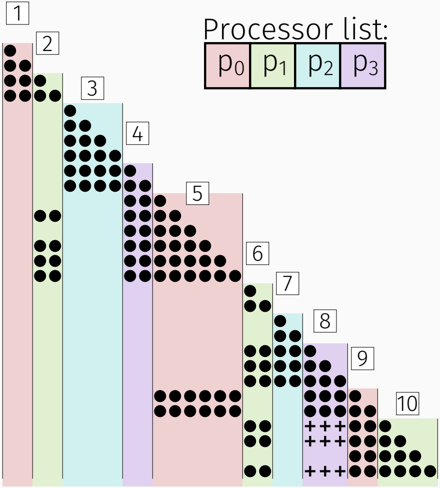
- Compute sparse $A = LL^T$ factorization
- A is sparse symmetric matrix
- A is positive definite
- Need to exploit symmetry
- L is a lower triangular matrix



$$A = LL^T$$

$\Omega(A)$ is the sparsity pattern of A

- Fill in, $\Omega(A) \subseteq \Omega(L)$



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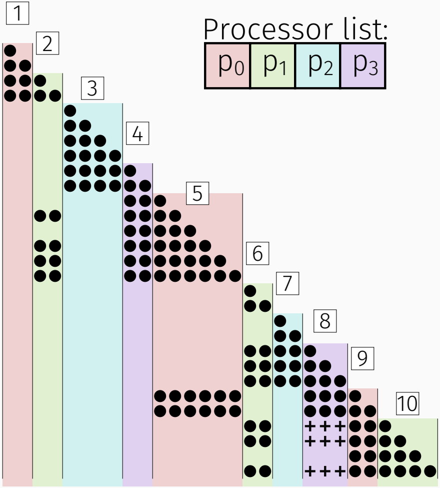

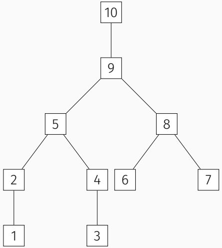

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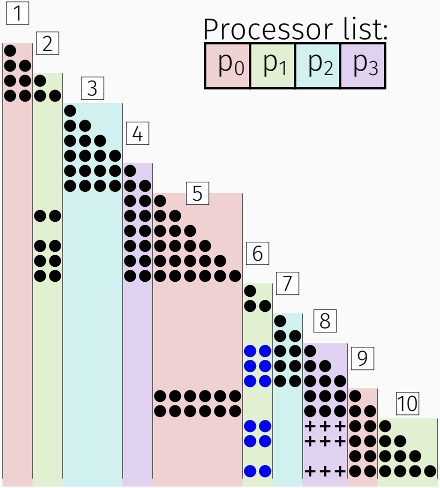

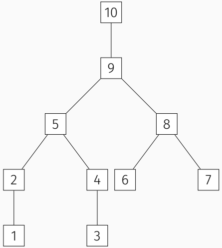

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- Fill in, $\Omega(A) \subseteq \Omega(L)$
- Supernode, same structure below diagonal block

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$\Omega(A)$ is the sparsity pattern of A

- Only lower triangular part of A is stored
- Basic algorithm:

Algorithm 1: Basic Cholesky algorithm

```
for column j = 1 to n do
    ℓ_{j,j} = sqrt(A_{j,j})
    for row i = j + 1 to n do
        ℓ_{i,j} = A_{i,j} / ℓ_{j,j}
    end

    for column k = j + 1 to n do
        for row i = k to n do
            A_{i,k} = A_{i,k} − ℓ_{i,j} · ℓ_{k,j}
        end
    end
end
```

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    $\ell_{j,j} = \sqrt{A_{j,j}}$
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    end
    (Factor column j)

    for column $k = j+1$ to n **do**
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    } Update next columns and Aggregate updates
end

CHOLESKY FACTORIZATION

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for column j = 1 to n do
    ℓ_{j,j} = √A_{j,j}                                   } Factor column j
    for row i = j + 1 to n do
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    end

    for column k = j + 1 to n do                          } Update next columns
        for row i = k to n do                               and Aggregate updates
            A_{i,k} = A_{i,k} − ℓ_{i,j} · ℓ_{k,j}           for row i = k to n do
        end                                                     tmp_i = tmp_i + ℓ_{i,j} · ℓ_{k,j}
                                                            end
    end                                                     A_{*,k} = A_{*,k} − tmp_*
end
```

`fan-both` ALGORITHM

- Three families [Ashcraft'95]:
  - Fan-In: "fanning-in updates"
    - Reduce **aggregate vectors** (updates)
    - Factorize column
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Fan-In, Fan-Out $\subset$ Fan-Both

- Three families [Ashcraft'95]: **Fan-In, Fan-Out ⊂ Fan-Both**

- Task based algorithm:
  - A(i): accumulation of **aggregate vectors** (updates) to column i

    Reduces the aggregate vectors t_i^*
  - F(j): factorization of col. j

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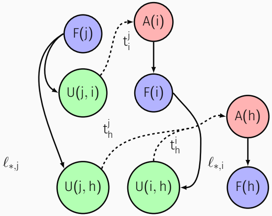
  - U(j,i): update of col. i with col. j

    Put the update in an (temporary) **aggregate vector** t_i^j



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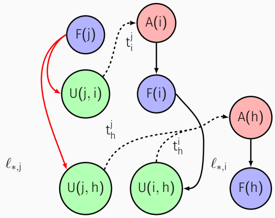

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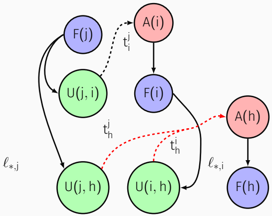

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- Use of 2D computation mapping grid $\mathcal{M}$
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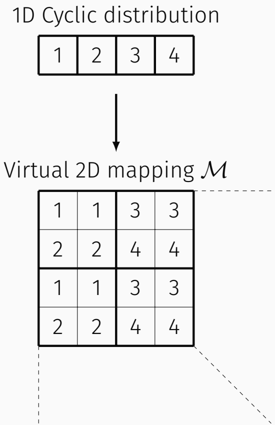

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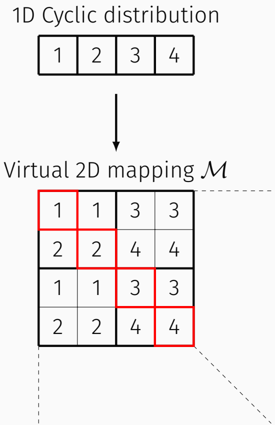

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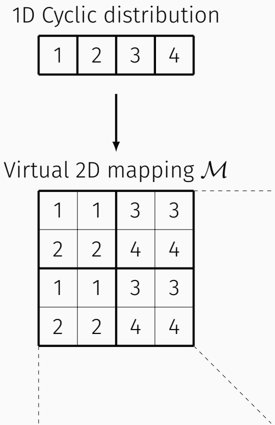

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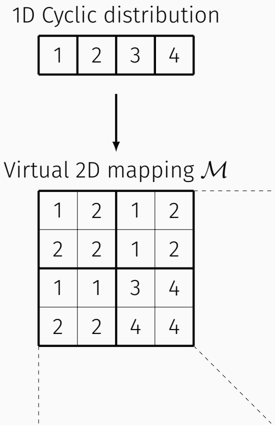

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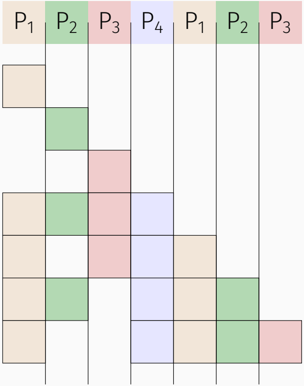

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P_1	P_1	P_3	P_3	P_1	P_1	P_3
P_1	P_2	P_4	P_4	P_2	P_2	P_4
P_3	P_4	P_3	P_3	P_1	P_1	P_3
P_3	P_4	P_3	P_4	P_2	P_2	P_4
P_1	P_2	P_1	P_2	P_1	P_1	P_3
P_1	P_2	P_1	P_2	P_1	P_2	P_4
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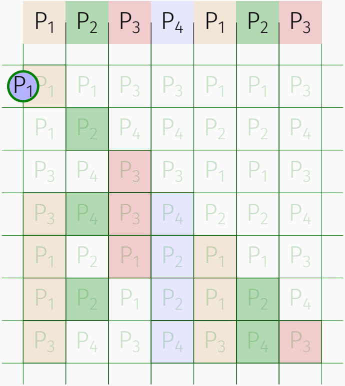

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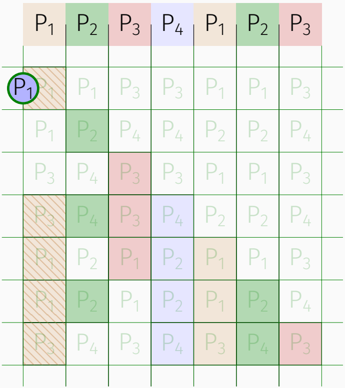

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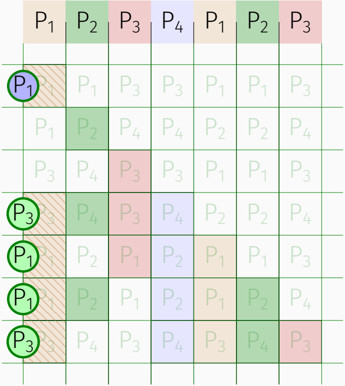

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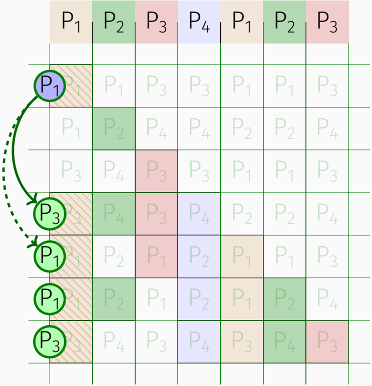

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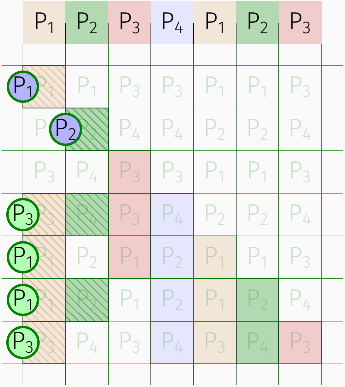

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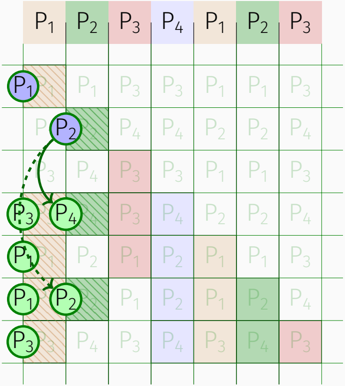

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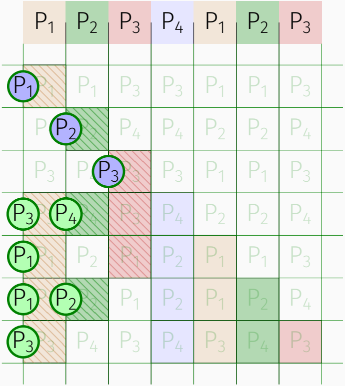

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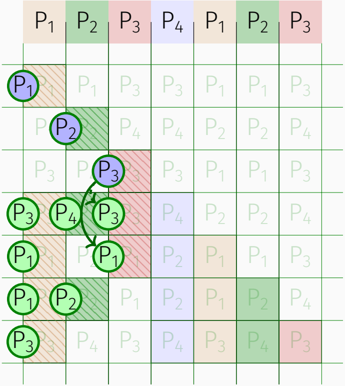

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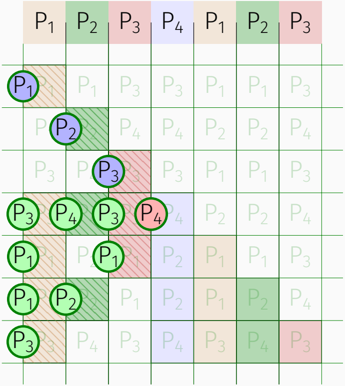

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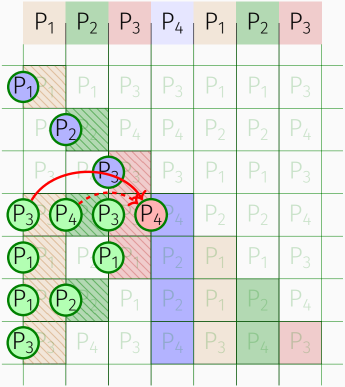

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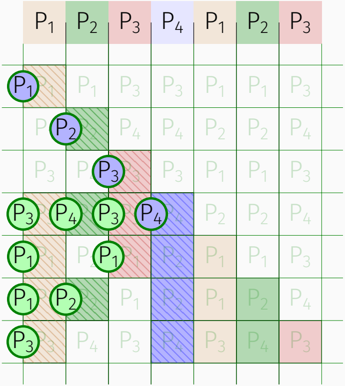

0	1	2	3	0	1
0	1	2	3	0	1
0	1	2	3	0	1
0	1	2	3	0	1
0	1	2	3	0	1
0	1	2	3	0	1

Fan-In

$\mathcal{M}_{i,j} = \text{mod}(i, P)$

0	0	0	0	0	0
1	1	1	1	1	1
2	2	2	2	2	2
3	3	3	3	3	3
0	0	0	0	0	0
1	1	1	1	1	1

Fan-Out

$\mathcal{M}_{i,j} = \text{mod}(j, P)$

0	0	2	2	0	0
1	1	3	3	1	1
0	0	2	2	0	0
1	1	3	3	1	1
0	0	2	2	0	0
1	1	3	3	1	1

Fan-Both

$\mathcal{M}_{i,j} = \begin{array}{l}\text{mod}(\min(i,j), P)+ \\ P\lfloor \text{mod}(\max(i,j), P)/P \rfloor\end{array}$

Three different computation maps, corresponding to `Fan-In`, `Fan-Out` and `Fan-Both`

DESIGN PRINCIPLES

- Remove synchronization points
  - Asynchronous point to point send
  - Group communication:
    (MPI) Collectives probably not the way to go
    - Requires too many communicators
    - Efficient non blocking collectives needed
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- Minimize memory operations
  - Row-major layout
  - Avoid making extra copies when sending data

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- All operations described by task $T_{src \to tgt}$
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  - Total order in operations/messages

    (Also observed by Amestoy et al.)
  - Order by non decreasing tgt, then src:

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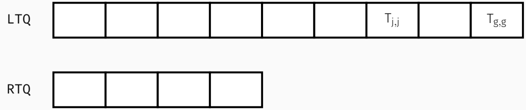
    Potential over-synchronization
- "Pull" strategy (one sided communications)
  - Signal data when available
  - Receiver gets data when ready

TASK SCHEDULING IN sympack

- Tasks $T_{src \to tgt}$
- Tasks currently mapped statically
- Processor manages local task queue LTQ



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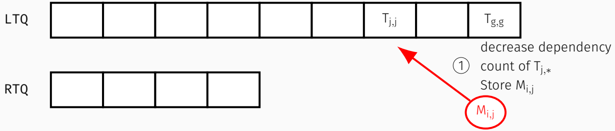

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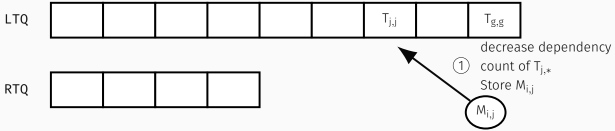

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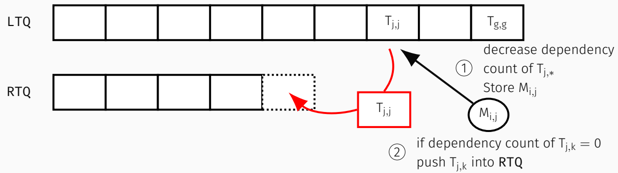

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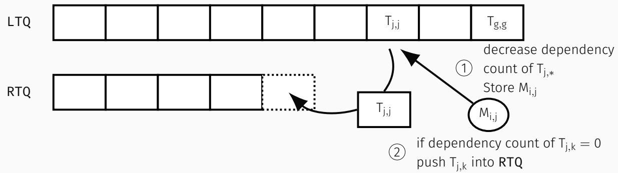

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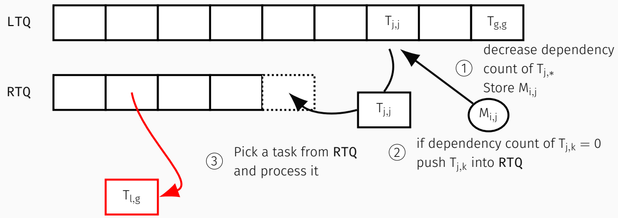

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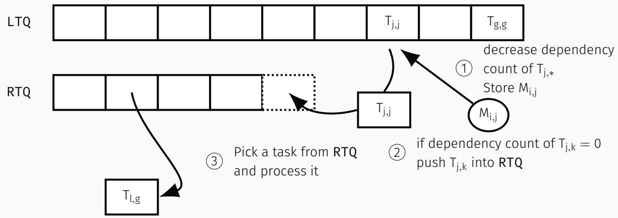

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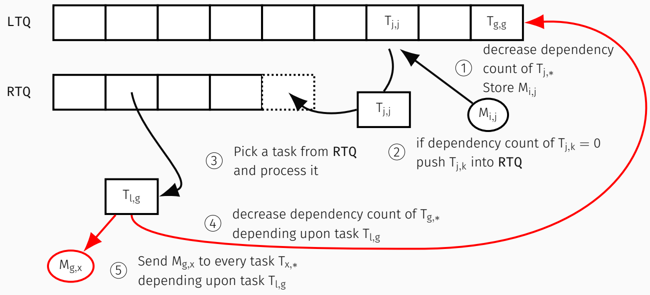

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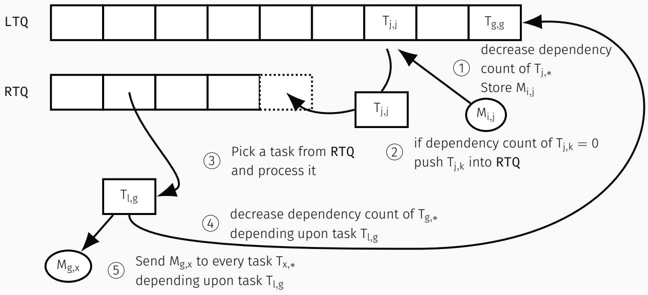

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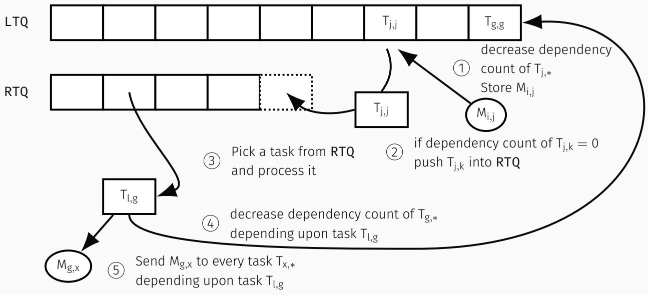
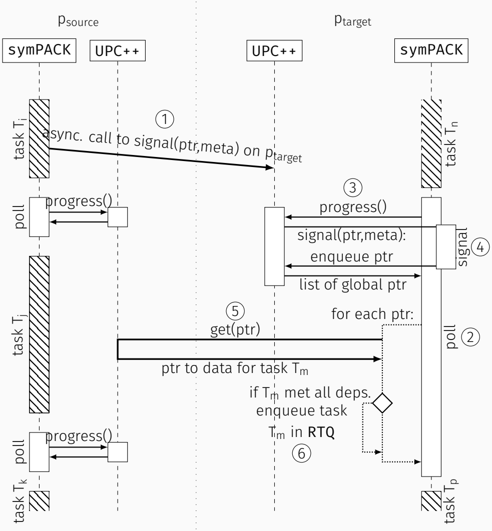
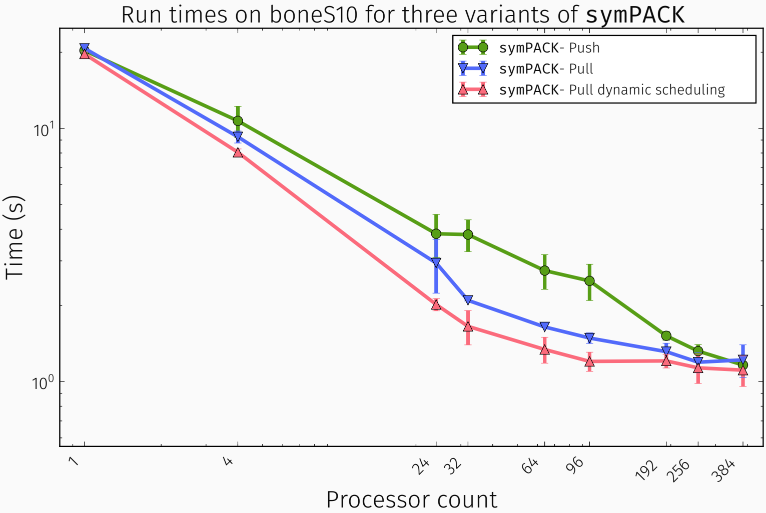


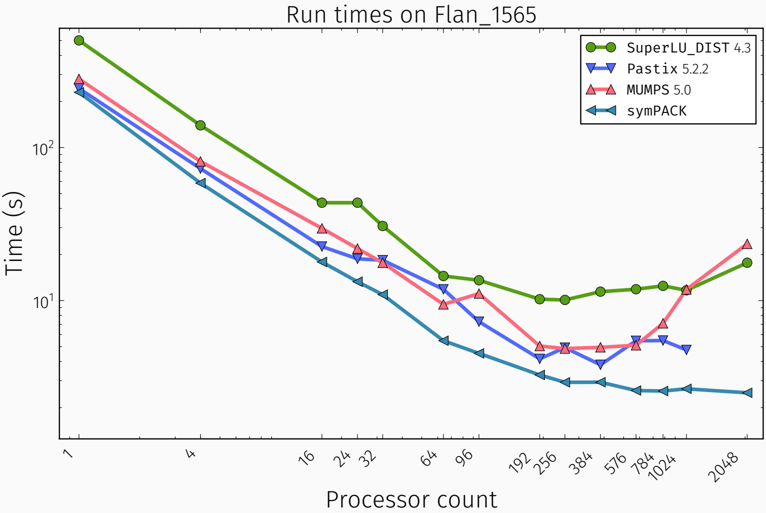
Scheduling policy ? FIFO, close to diagonal, etc.

- UPC++ and GASNet for communications
- global pointer to remote memory
- one-sided communications
- asynchronous remote functions calls

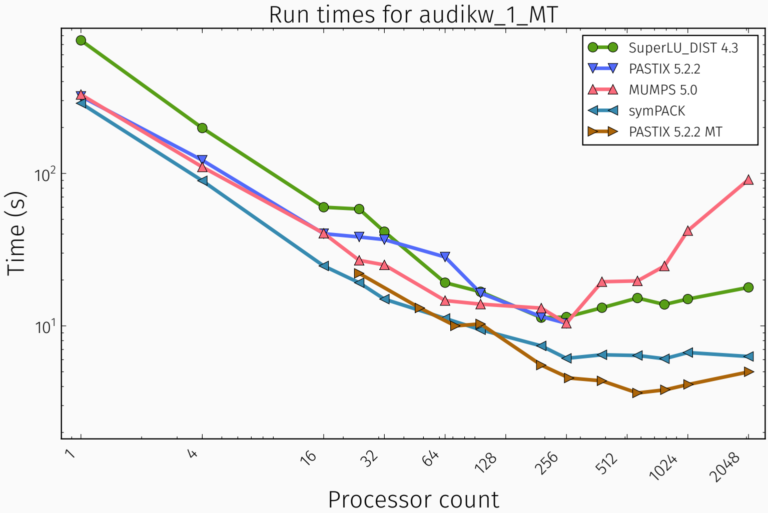




n=914,898 nnz(A)=20,896,803 nnz(L)=318,019,434



n=1,564,794 nnz(A)=57,865,083 nnz(L)=1,574,541,576



n=943,695 nnz(A)=39,297,771 nnz(L)=1,221,674,796

CONCLUSIONS

- Reduces communication cost in theory [Ashcraft'95]
- Increases parallelism during updates

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- Reduces communication cost in theory [Ashcraft'95]
- Increases parallelism during updates
- Avoiding deadlocks is challenging (Similar to observation by Larkar et al.)
- New symmetric solver `symPACK`
  - implements `Fan-Both`
  - Task based Cholesky requires fine / dynamic scheduling
  - One sided approach using UPC++
  - Asynchronous task execution model
  - dynamic scheduling

ONGOING AND FUTURE WORK

- 2D wrap mapping performance
- Hybrid parallelism (UPC++/OpenMP, UPC++ / UPC++)
- Conflict with load balancing (proportional mapping) ?

- Tree-based group communications

- Data distribution (2D, block based ?)
- Scheduling strategies
- New task mapping policies

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Async. model important for scalability and to tolerate variability

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`www.sympack.org`