2.5D algorithms for parallel dense linear algebra

Edgar Solomonik and James Demmel

UC Berkeley

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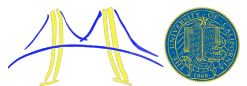


Outline

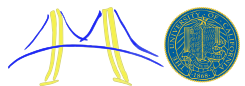
Introduction
- Strong scaling

Matrix multiplication
- 2D and 3D algorithms
- 2.5D matrix multiplication

LU factorization
- 2.5D LU without pivoting
- 2.5D LU with pivoting

QR factorization
- 2.5D QR using Givens rotations
- 2.5D QR using Householder transformations

Conclusion



Solving science problems faster

Parallel computers can solve bigger problems

- **weak scaling**

Parallel computers can also solve a fixed problem faster

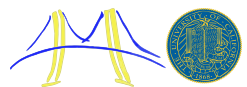
- **strong scaling**

Obstacles to strong scaling

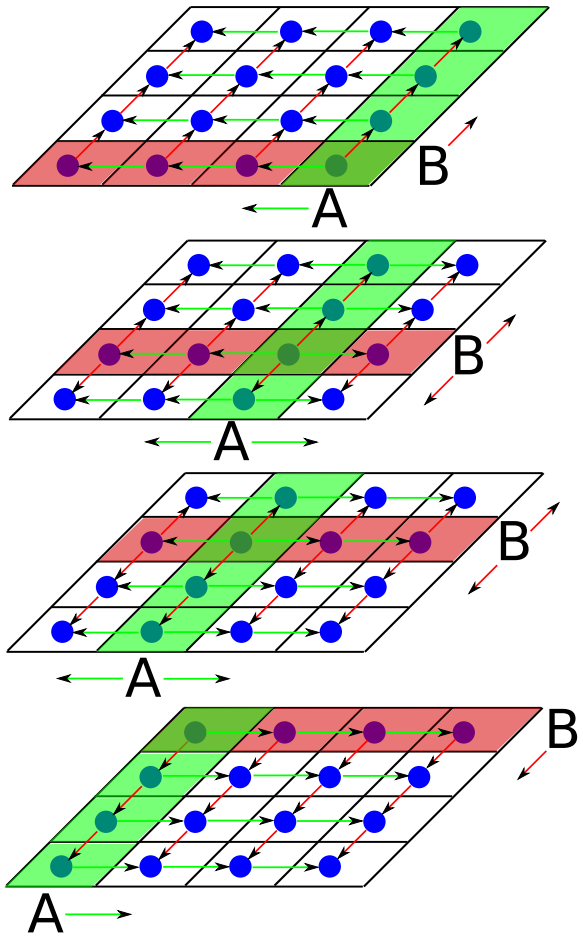
- may increase relative cost of **communication**
- may hurt **load balance**

How to reduce communication and maintain load balance?

- reduce (minimize) communication along the **critical path**
- exploit the **network topology**

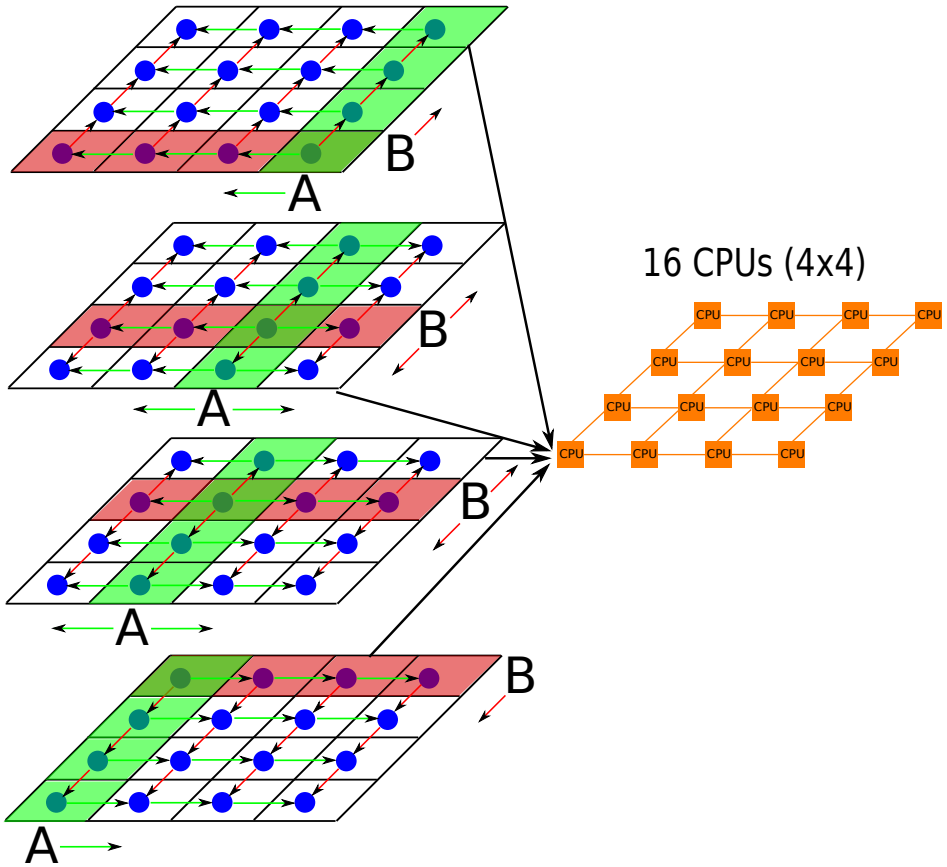


Blocking matrix multiplication



2D matrix multiplication

[Cannon 69],
[Van De Geijn and Watts 97]

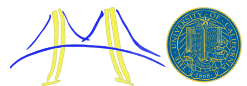


$O(n^3/p)$ flops

$O(n^2/\sqrt{p})$ words moved

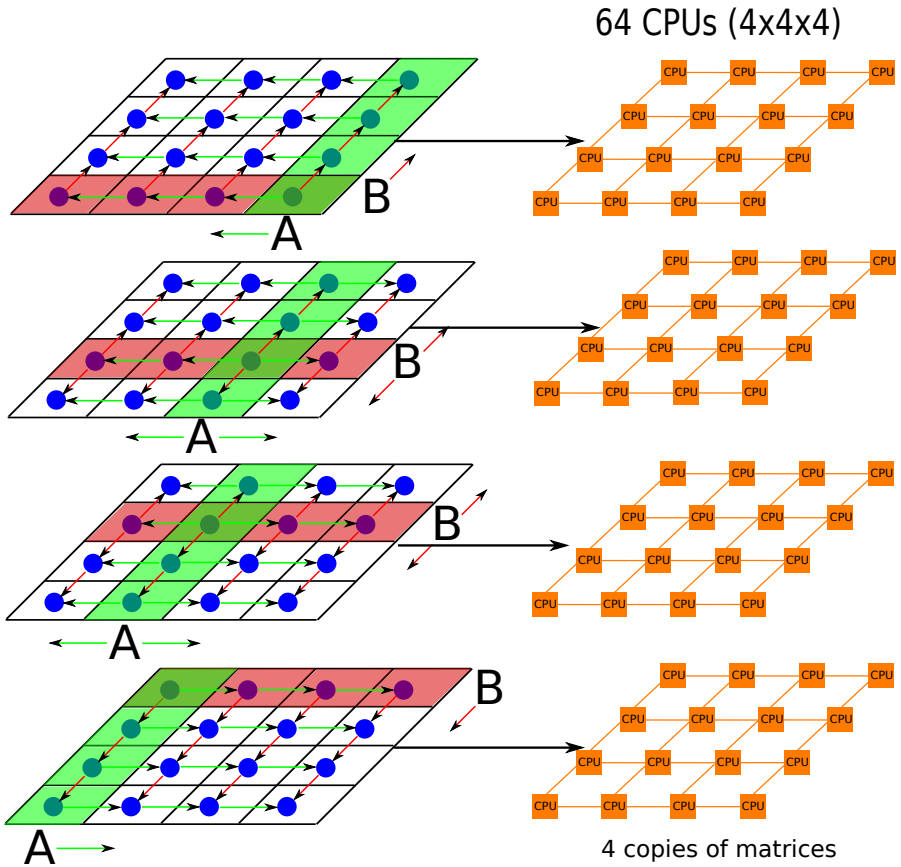
$O(\sqrt{p})$ messages

$O(n^2/p)$ bytes of memory



3D matrix multiplication

[Agarwal et al 95],
[Aggarwal, Chandra, and Snir 90],
[Bernsten 89], [McColl and Tiskin 99]

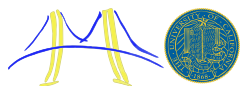


$O(n^3/p)$ flops

$O(n^2/p^{2/3})$ words moved

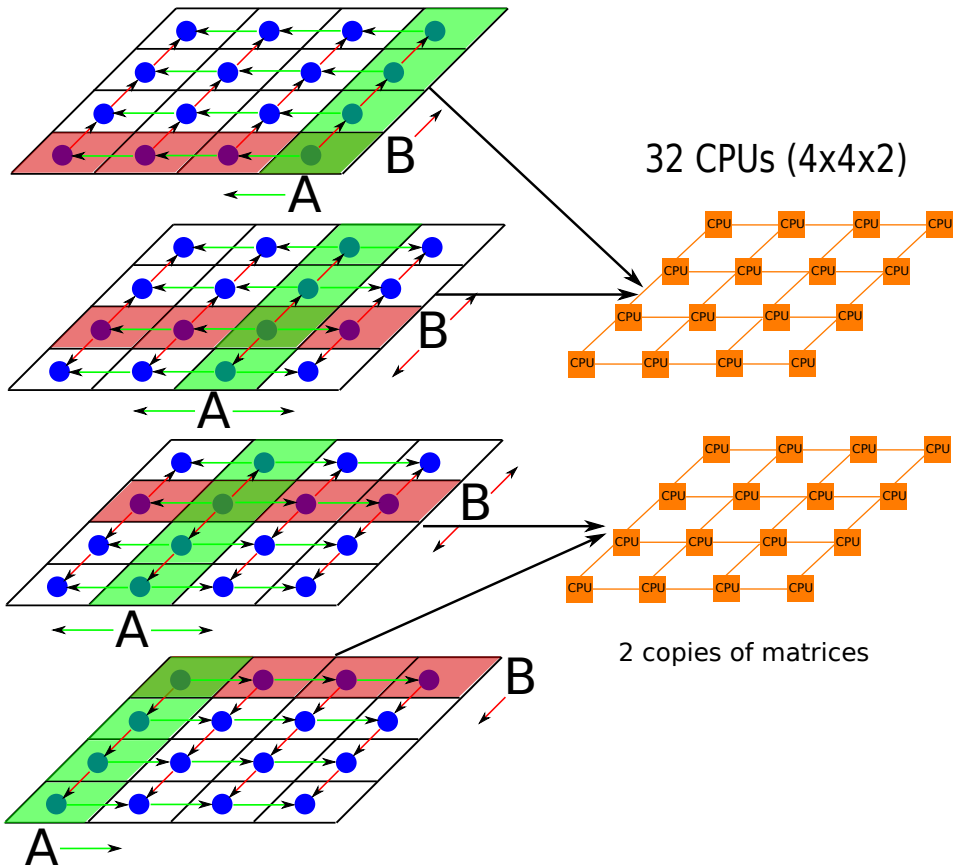
$O(1)$ messages

$O(n^2/p^{2/3})$ bytes of memory



2.5D matrix multiplication

[McColl and Tiskin 99]

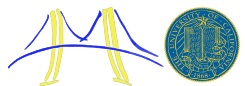


$O(n^3/p)$ flops

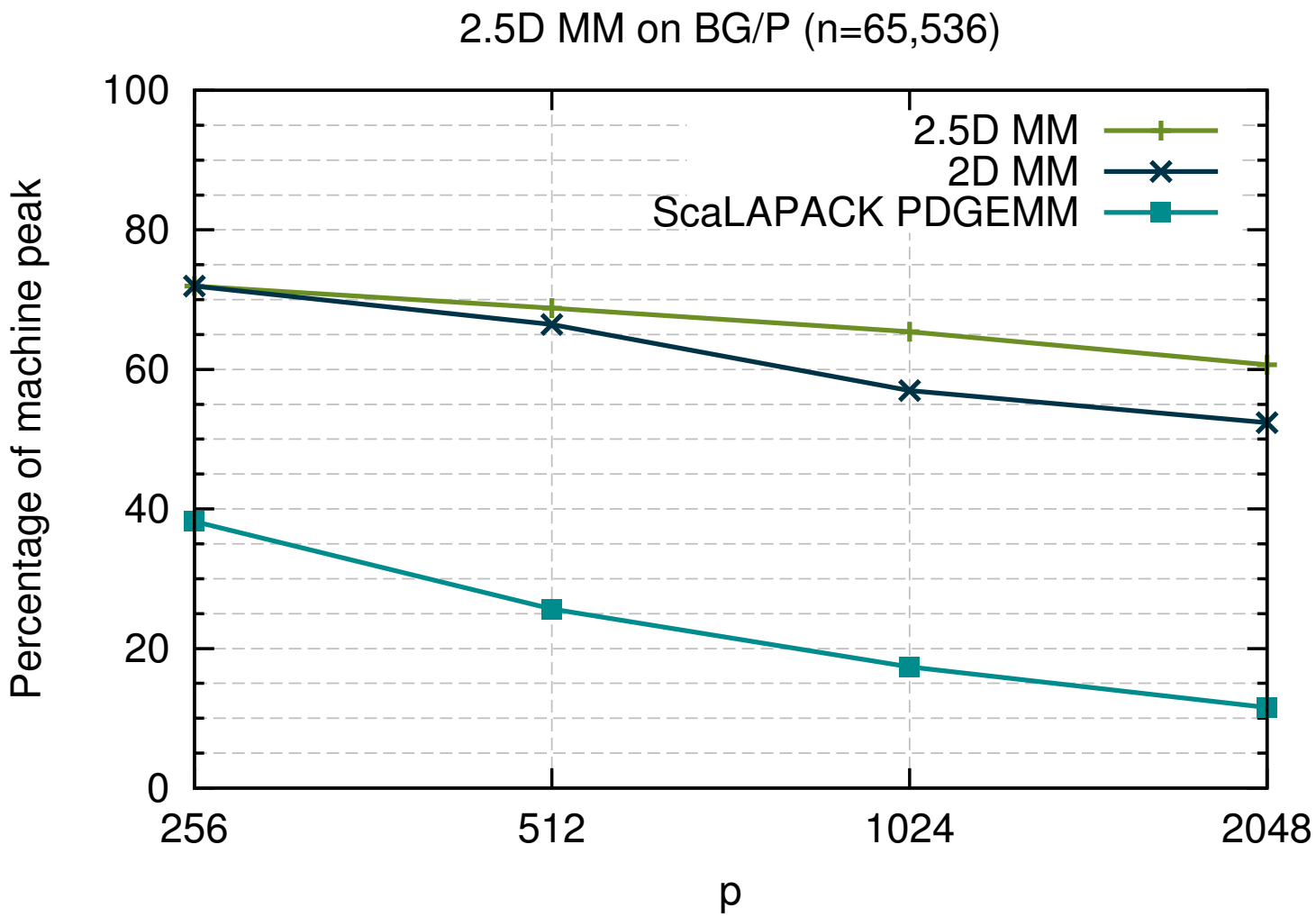
$O(n^2/\sqrt{c \cdot p})$ words moved

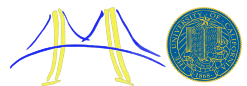
$O(\sqrt{p/c^3})$ messages

$O(c \cdot n^2/p)$ bytes of memory



Strong scaling matrix multiplication

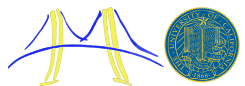




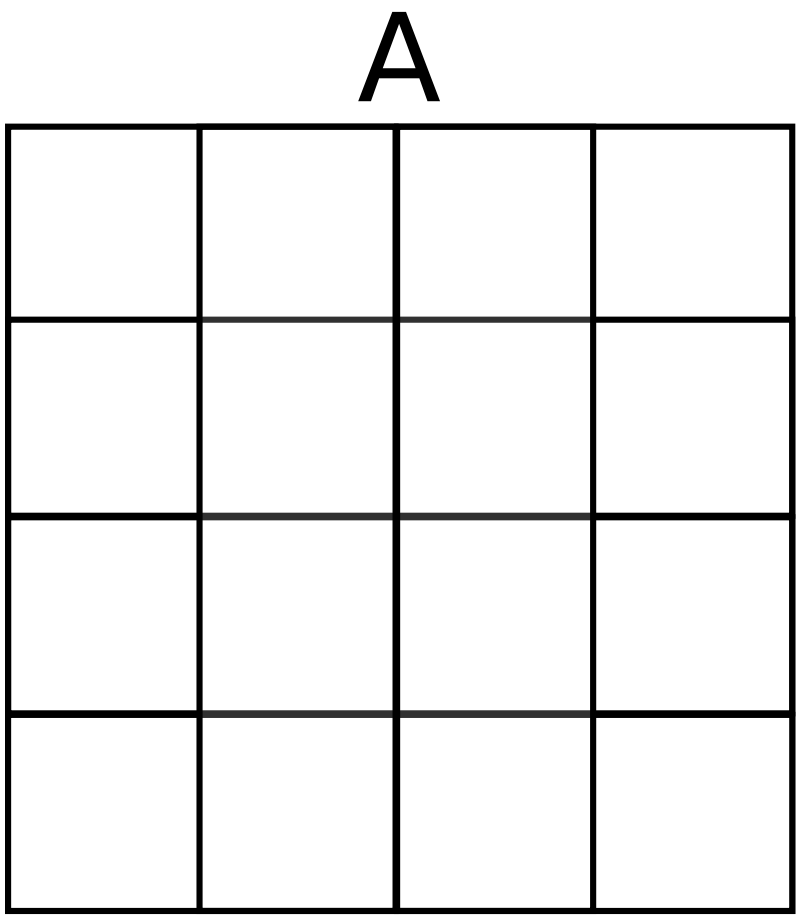
2.5D recursive LU

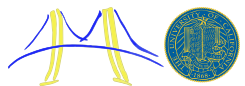
$A = L \cdot U$ where L is lower-triangular and U is upper-triangular

- A 2.5D recursive algorithm with no pivoting [A. Tiskin 2002]
- Tiskin gives algorithm under the BSP model
  - Bulk Synchronous Parallel
  - considers communication and synchronization
- We give an alternative distributed-memory adaptation and implementation
- Also, we lower-bound the latency cost

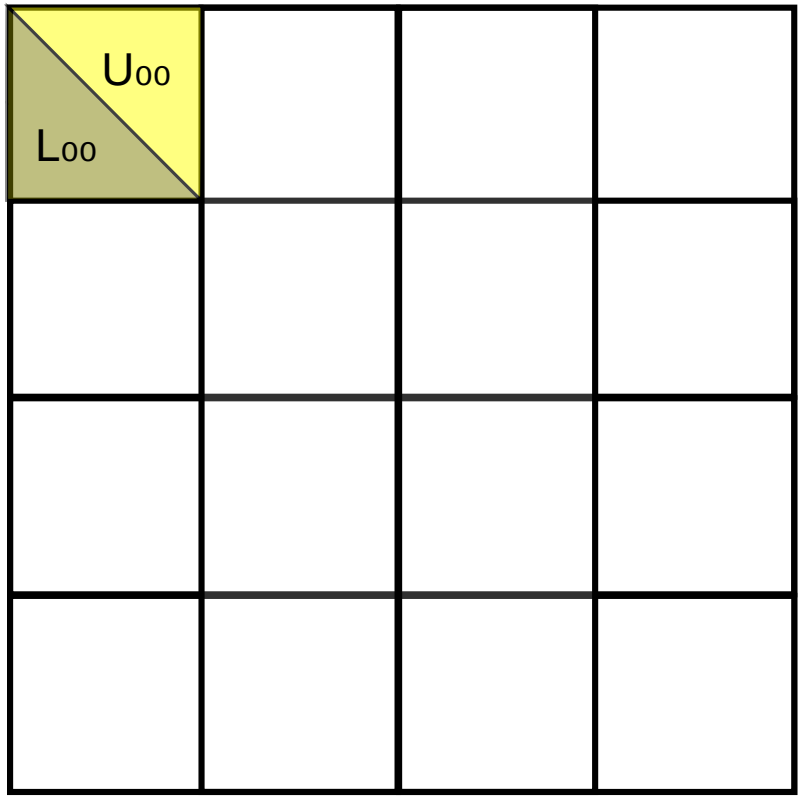


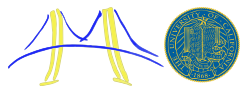
2D blocked LU factorization



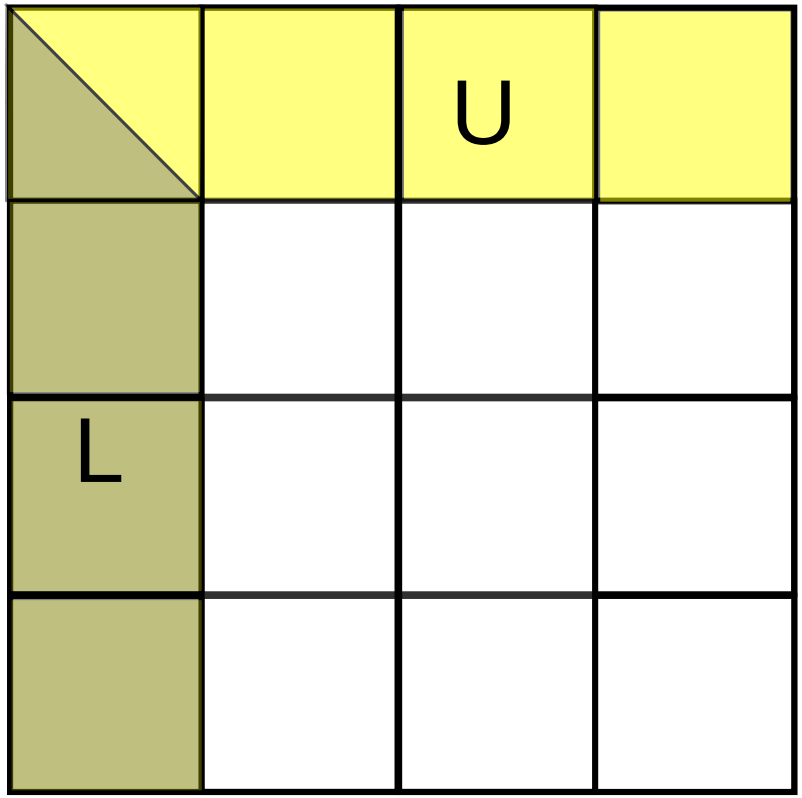


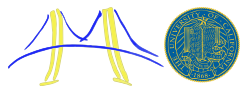
2D blocked LU factorization



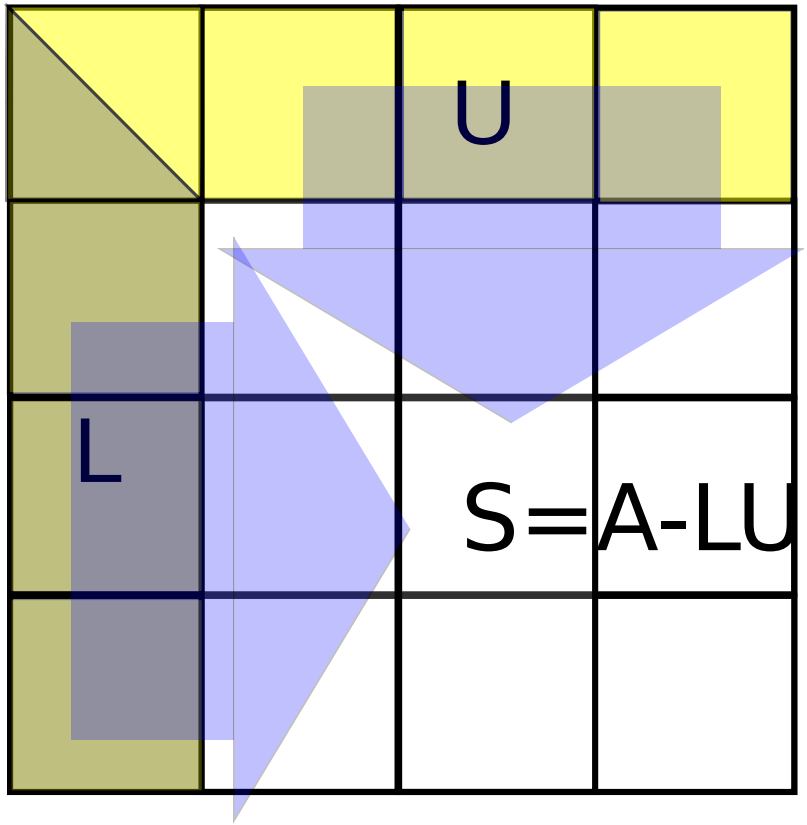


2D blocked LU factorization

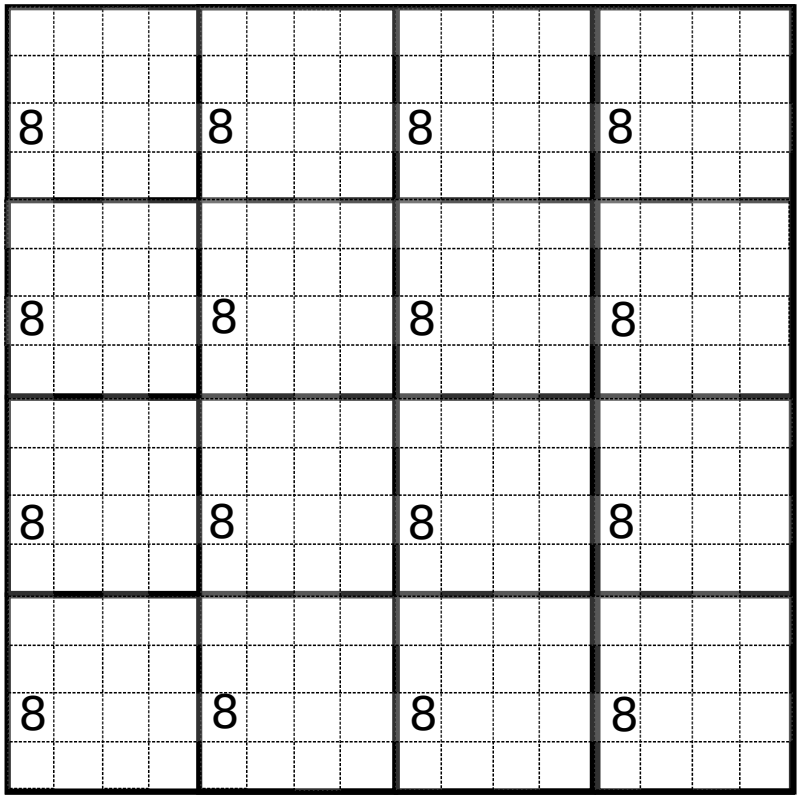


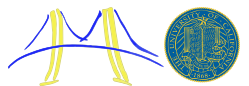


2D blocked LU factorization

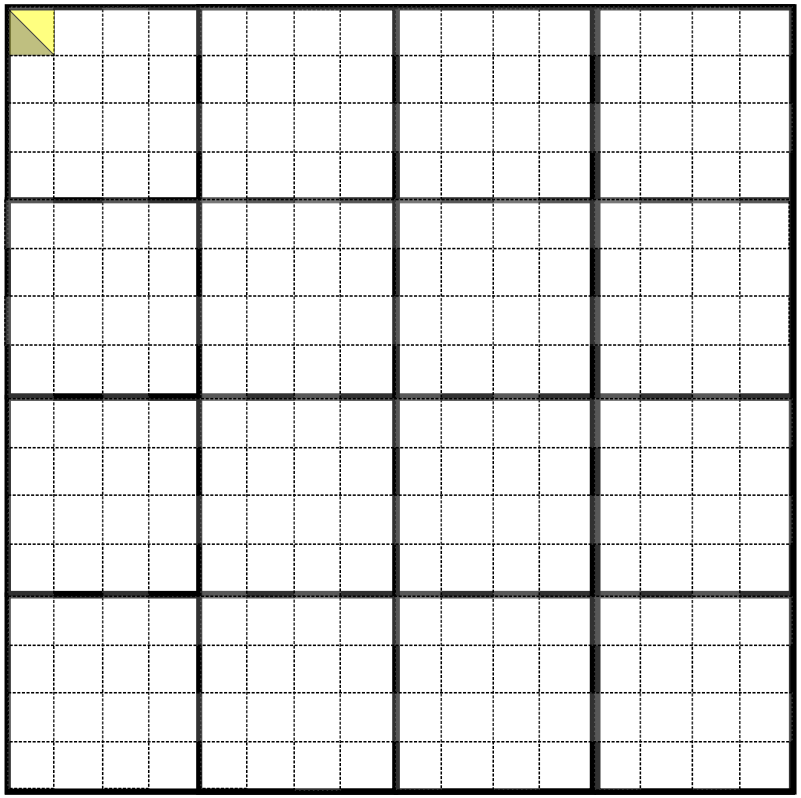


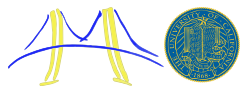
2D block-cyclic decomposition



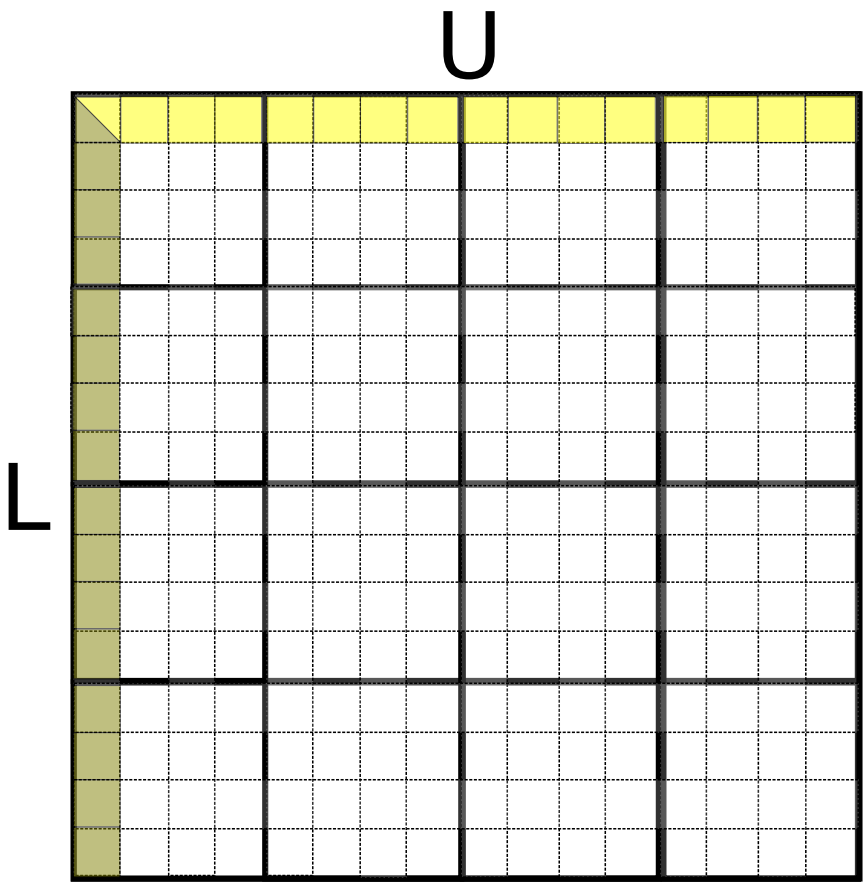


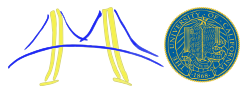
2D block-cyclic LU factorization



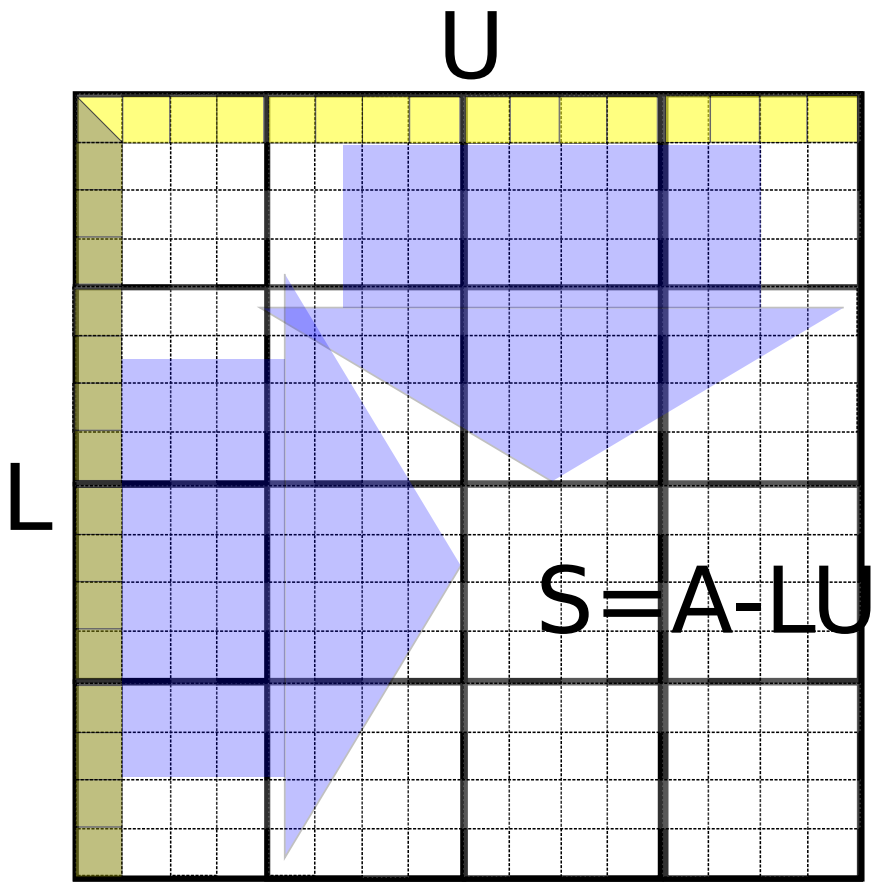


2D block-cyclic LU factorization



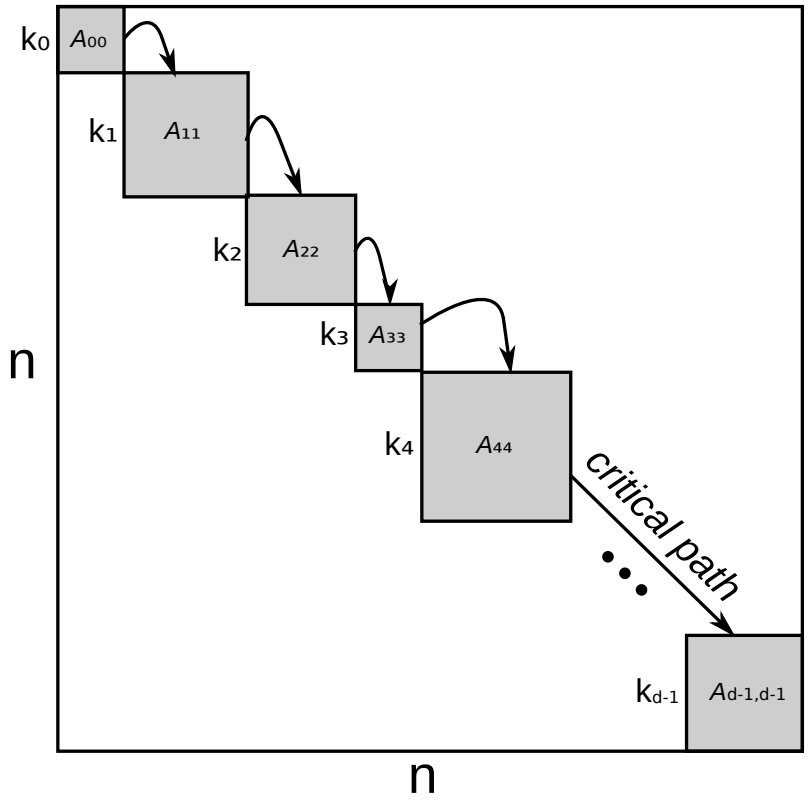


2D block-cyclic LU factorization

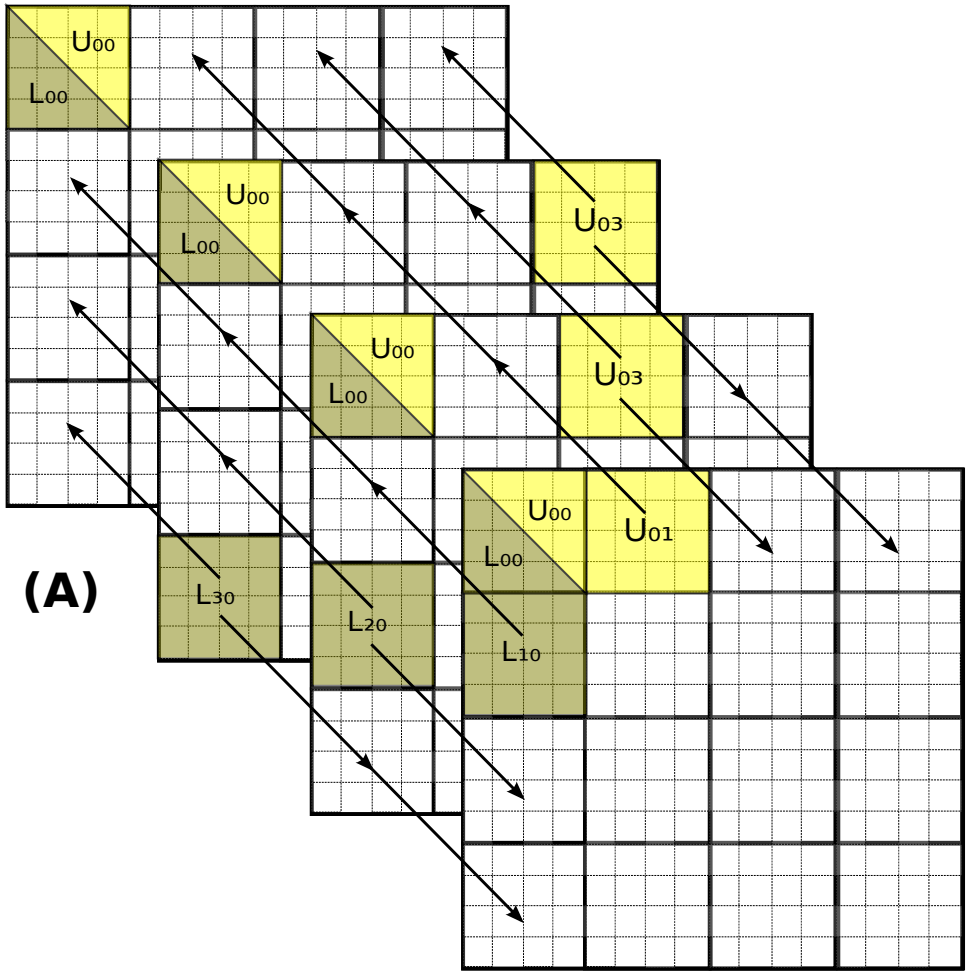


A new latency lower bound for LU

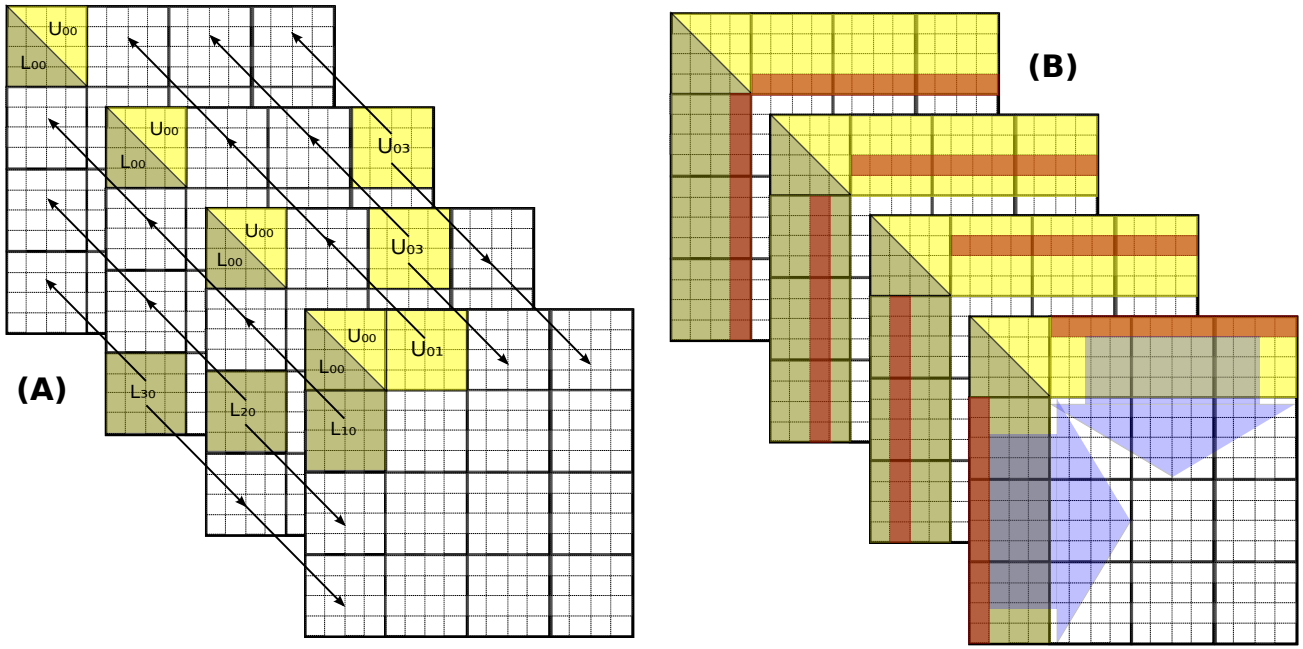
- Relate volume to surface area to diameter
- For block size $n/\mathbf{d}$ LU does
  - $\Omega(n^3/\mathbf{d^2})$ flops
  - $\Omega(n^2/\mathbf{d})$ words
  - $\Omega(\mathbf{d})$ msgs
- Now pick $\mathbf{d}$ (=latency cost)
  - $\mathbf{d} = \mathbf{\Omega}(\sqrt{\mathbf{p}})$ to minimize flops
  - $\mathbf{d} = \mathbf{\Omega}(\sqrt{\mathbf{c} \cdot \mathbf{p}})$ to minimize words
- More generally, latency $\cdot$ bandwidth $= n^2$



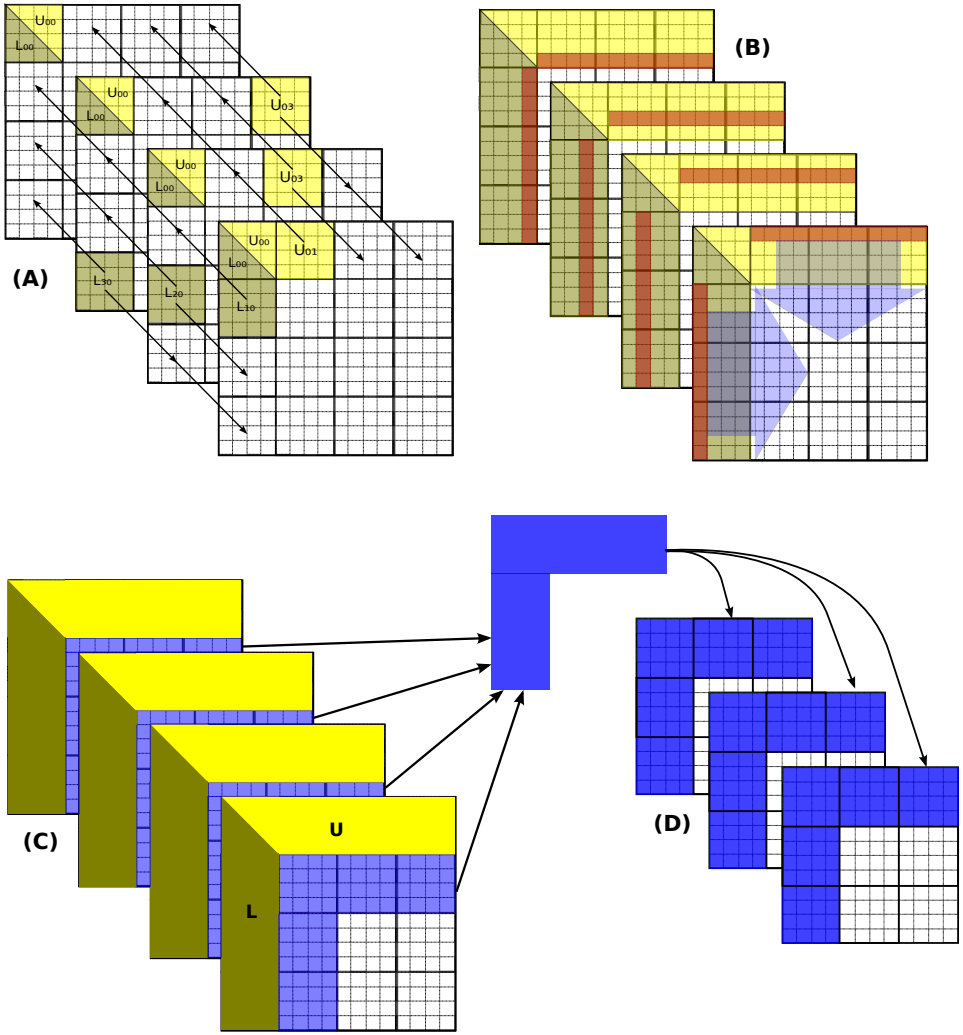
2.5D LU factorization



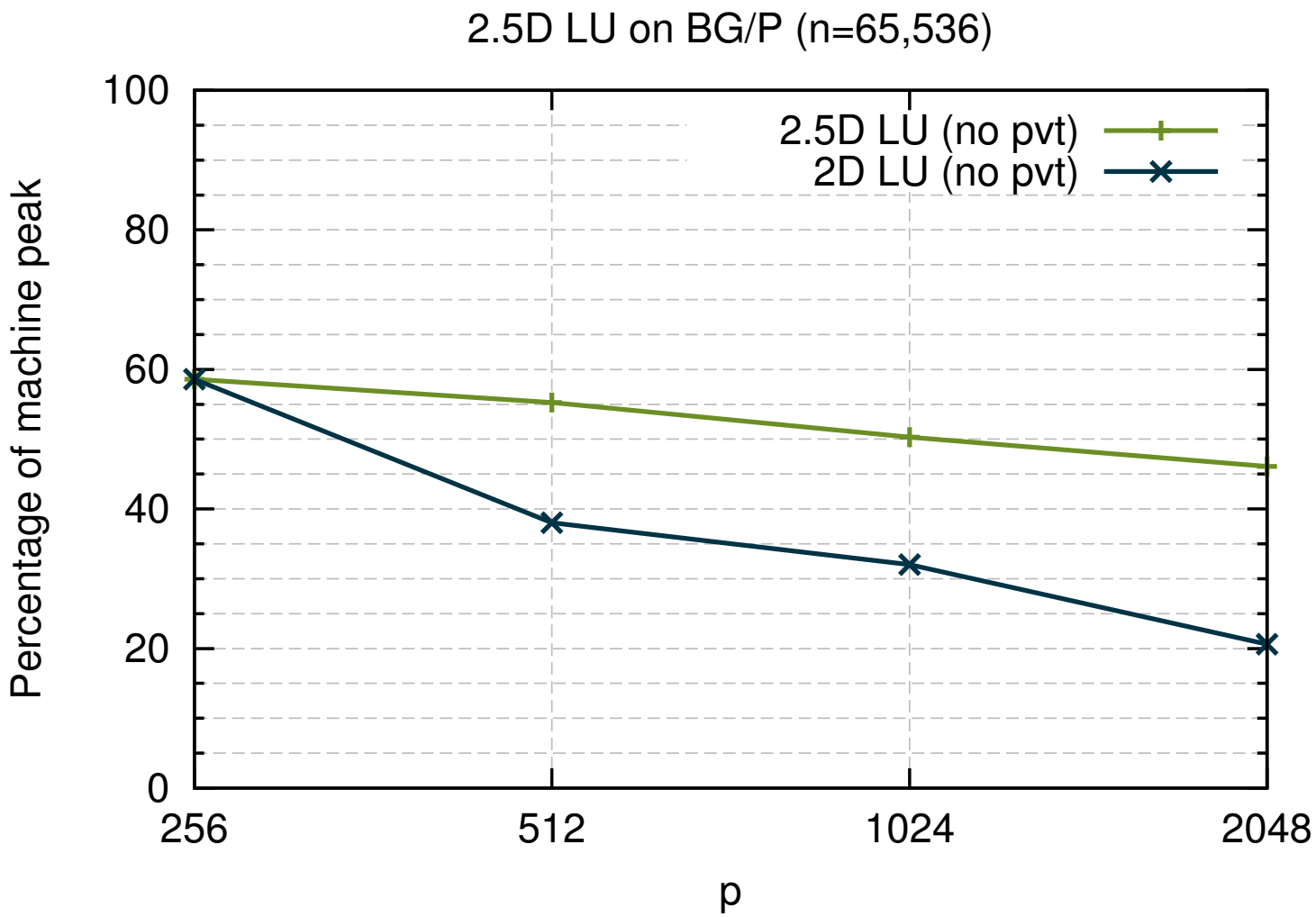
2.5D LU factorization

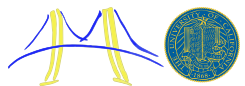


2.5D LU factorization



2.5D LU strong scaling (without pivoting)

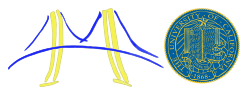




2.5D LU with pivoting

$A = P \cdot L \cdot U$, where P is a permutation matrix

- 2.5D generic pairwise elimination (neighbor/pairwise pivoting or Givens rotations (QR)) [A. Tiskin 2007]
  - pairwise pivoting does not produce an explicit L
  - pairwise pivoting may have stability issues for large matrices
- Our approach uses tournament pivoting, which is more stable than pairwise pivoting and gives L explicitly
  - pass up rows of A instead of U to avoid error accumulation



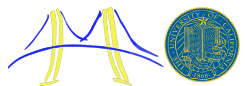
Tournament pivoting

Partial pivoting is not communication-optimal on a blocked matrix

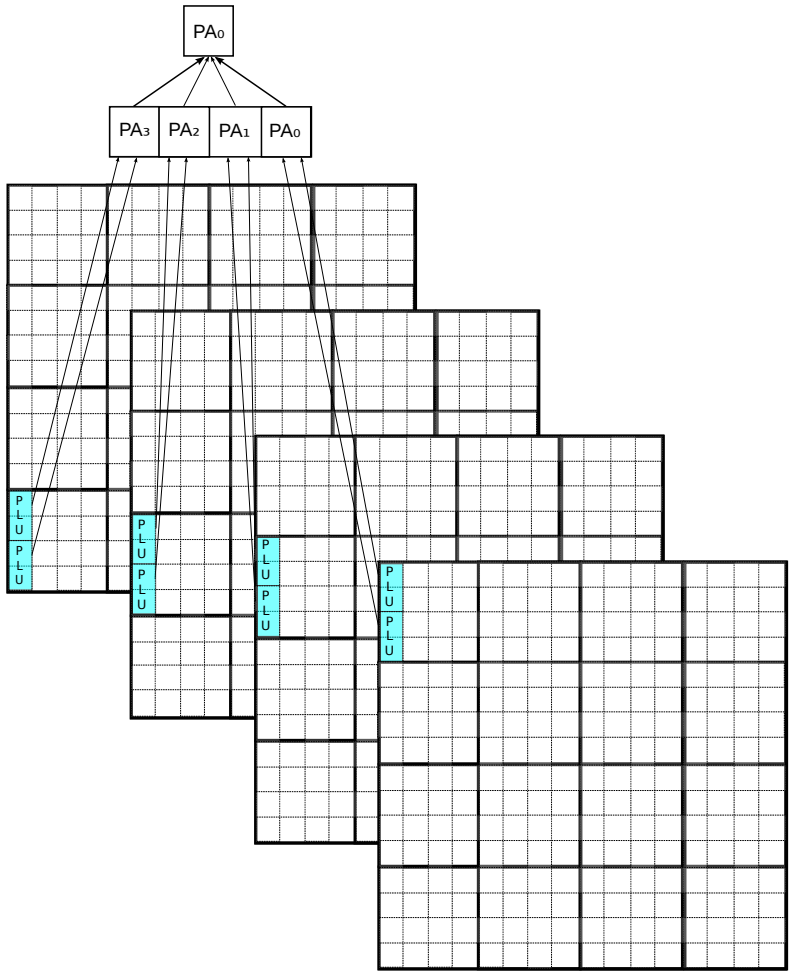
- requires message/synchronization for each column
- $O(n)$ messages needed

Tournament pivoting is communication-optimal

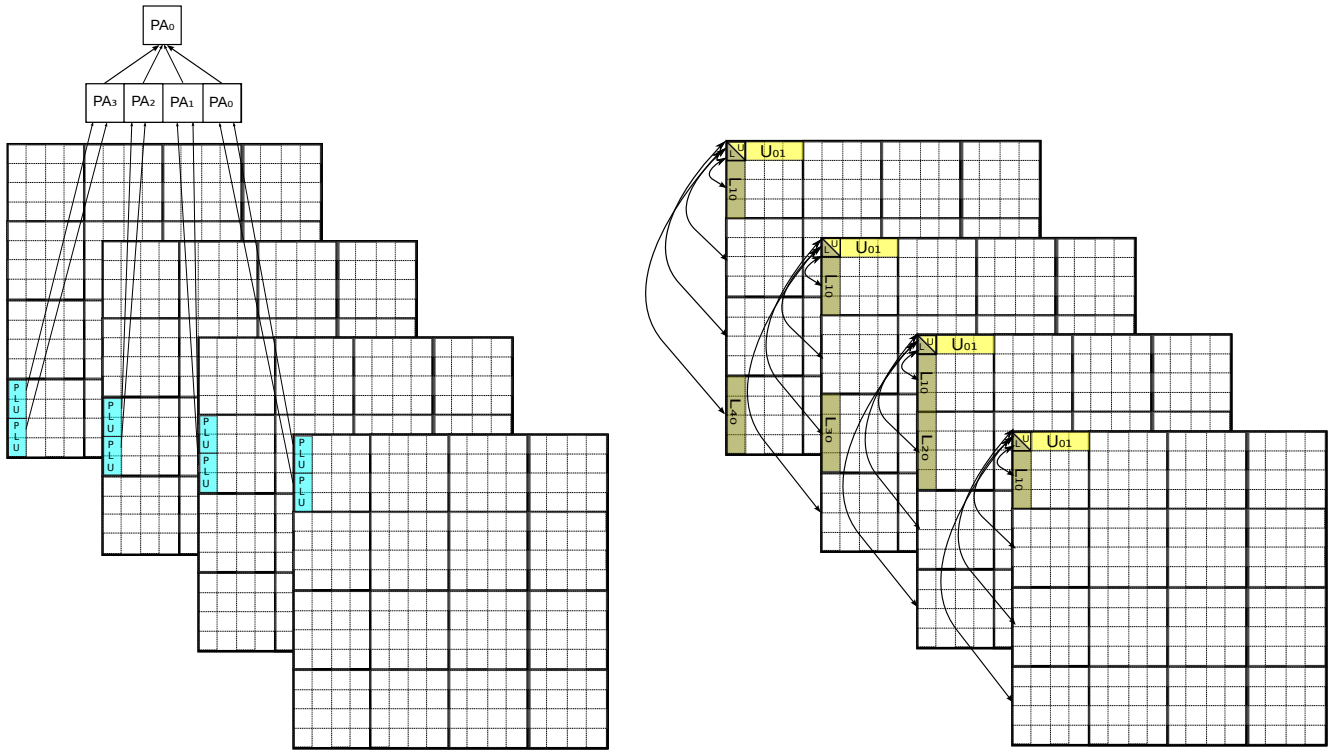
- performs a tournament to determine best pivot row candidates
- passes up 'best rows' of A



2.5D LU factorization with tournament pivoting



2.5D LU factorization with tournament pivoting



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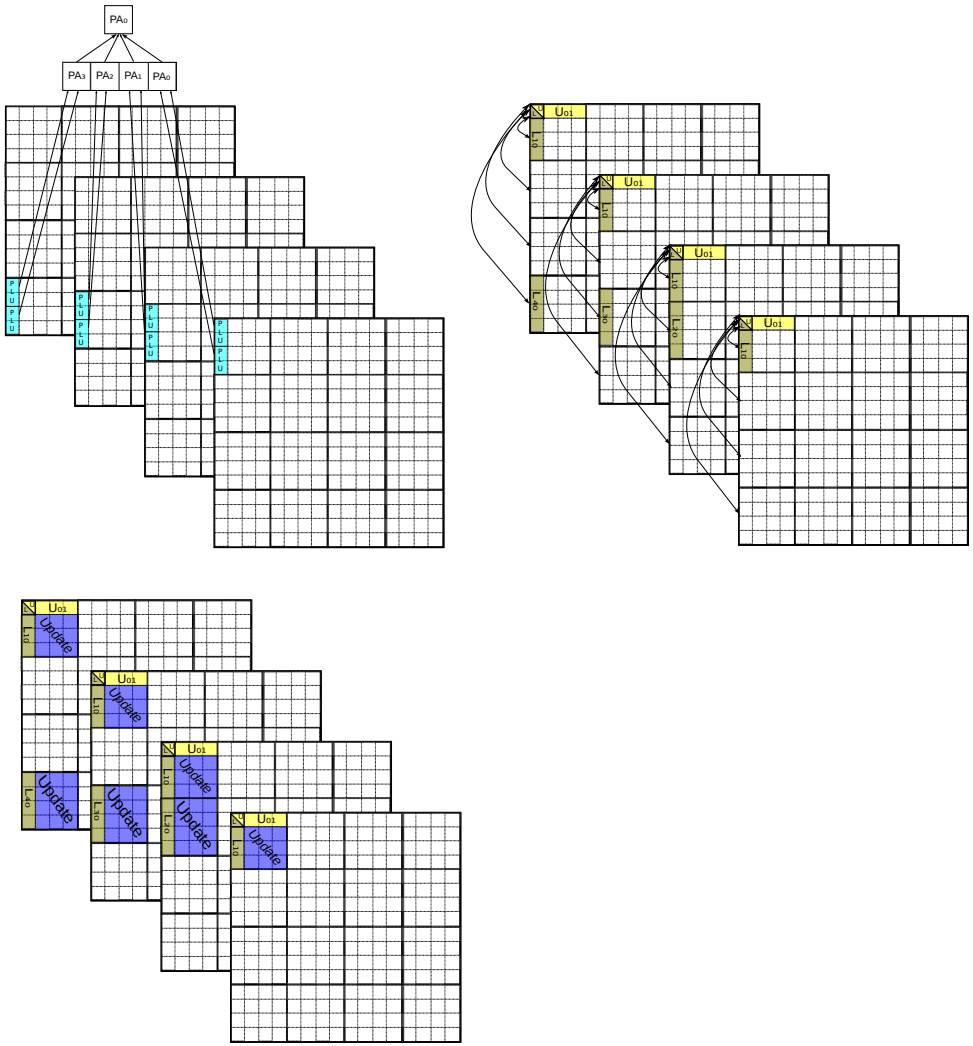
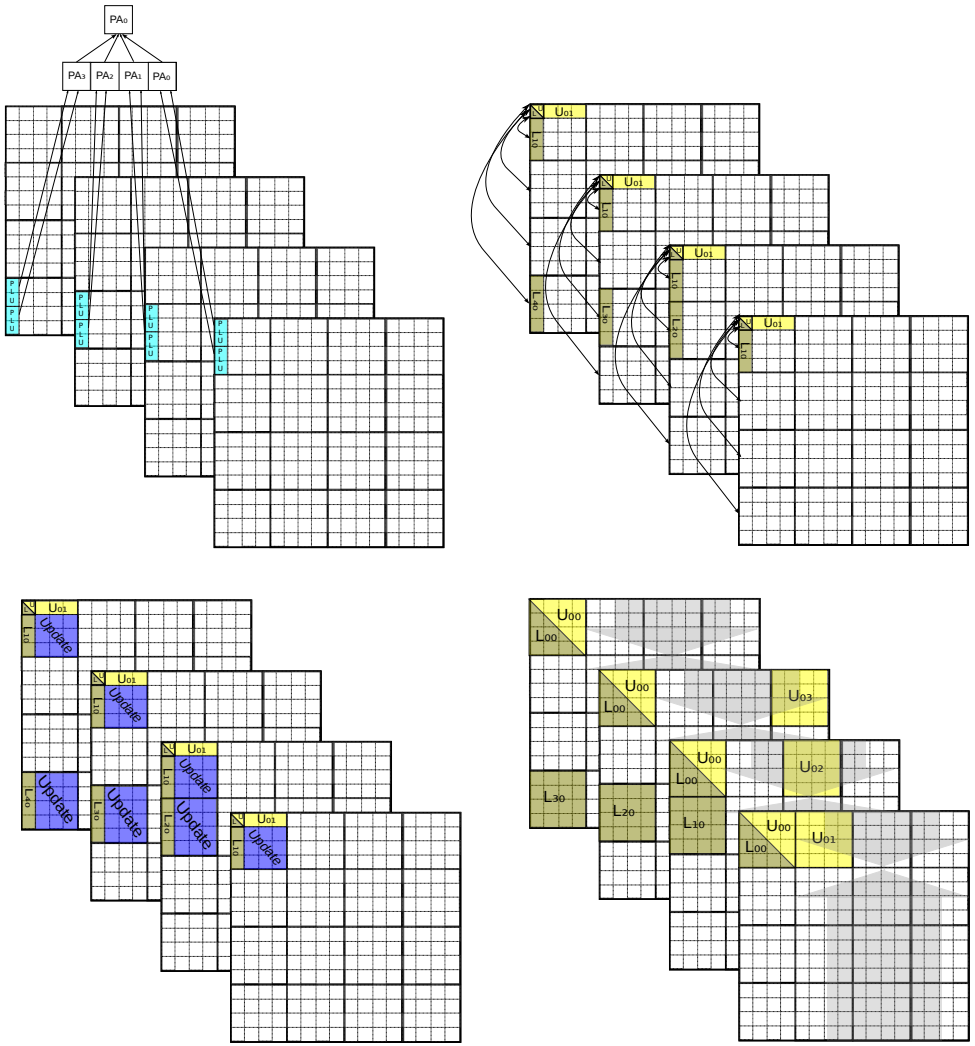
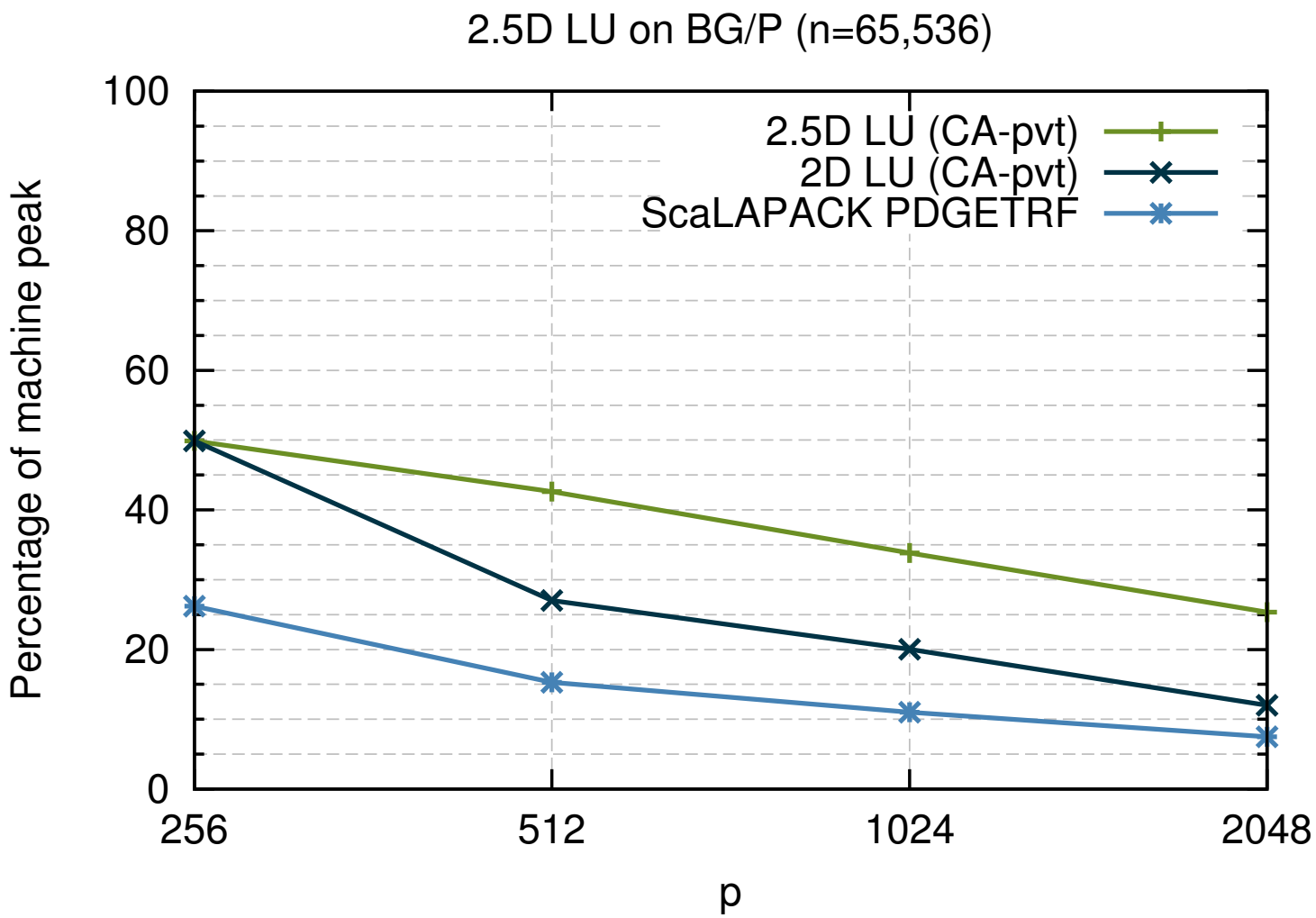


2.5D LU factorization with tournament pivoting



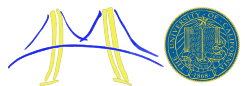
Strong scaling of 2.5D LU with tournament pivoting



2.5D QR factorization

$A = Q \cdot R$ where Q is orthogonal R is upper-triangular

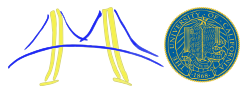
- 2.5D QR using Givens rotations (generic pairwise elimination) is given by [A. Tiskin 2007]
- Tiskin minimizes latency and bandwidth by working on slanted panels
- 2.5D QR cannot be done with right-looking updates as 2.5D LU due to non-commutativity of orthogonalization updates



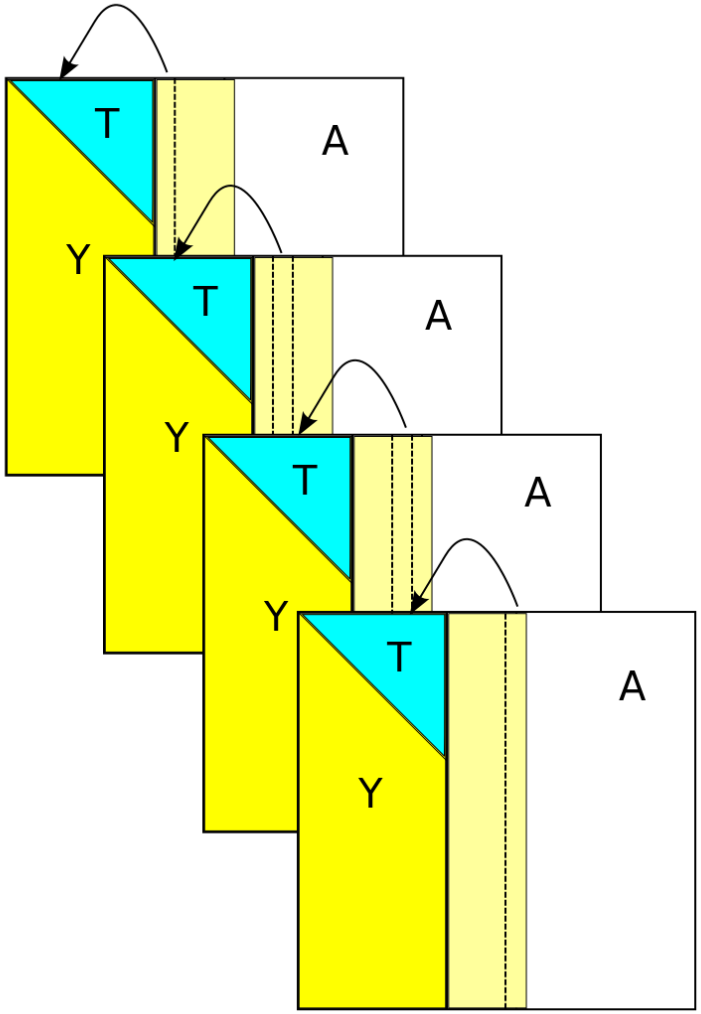
2.5D QR factorization using the YT representation

The YT representation of Householder QR factorization is more work efficient when computing only R

- We give an algorithm that performs 2.5D QR using the YT representation
- The algorithm performs left-looking updates on Y
- Householder with YT needs fewer computation (roughly 2x) than Givens rotations
- Our approach achieves optimal bandwidth cost, but has $O(n)$ latency



2.5D QR using YT representation



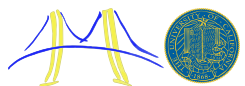
Conclusion

Our contributions:

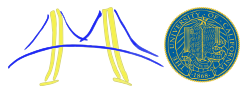
- 2.5D mapping of matrix multiplication
  - Optimal according to lower bounds [Irony, Tiskin, Toledo 04] and [Aggarwal, Chandra, and Snir 90]
- A new latency lower bound for LU
- Communication-optimal 2.5D LU and QR
  - Both are bandwidth-optimal according to general lower bound [Ballard, Demmel, Holtz, Schwartz 10]
  - LU is latency-optimal according to new lower bound

Reflections:

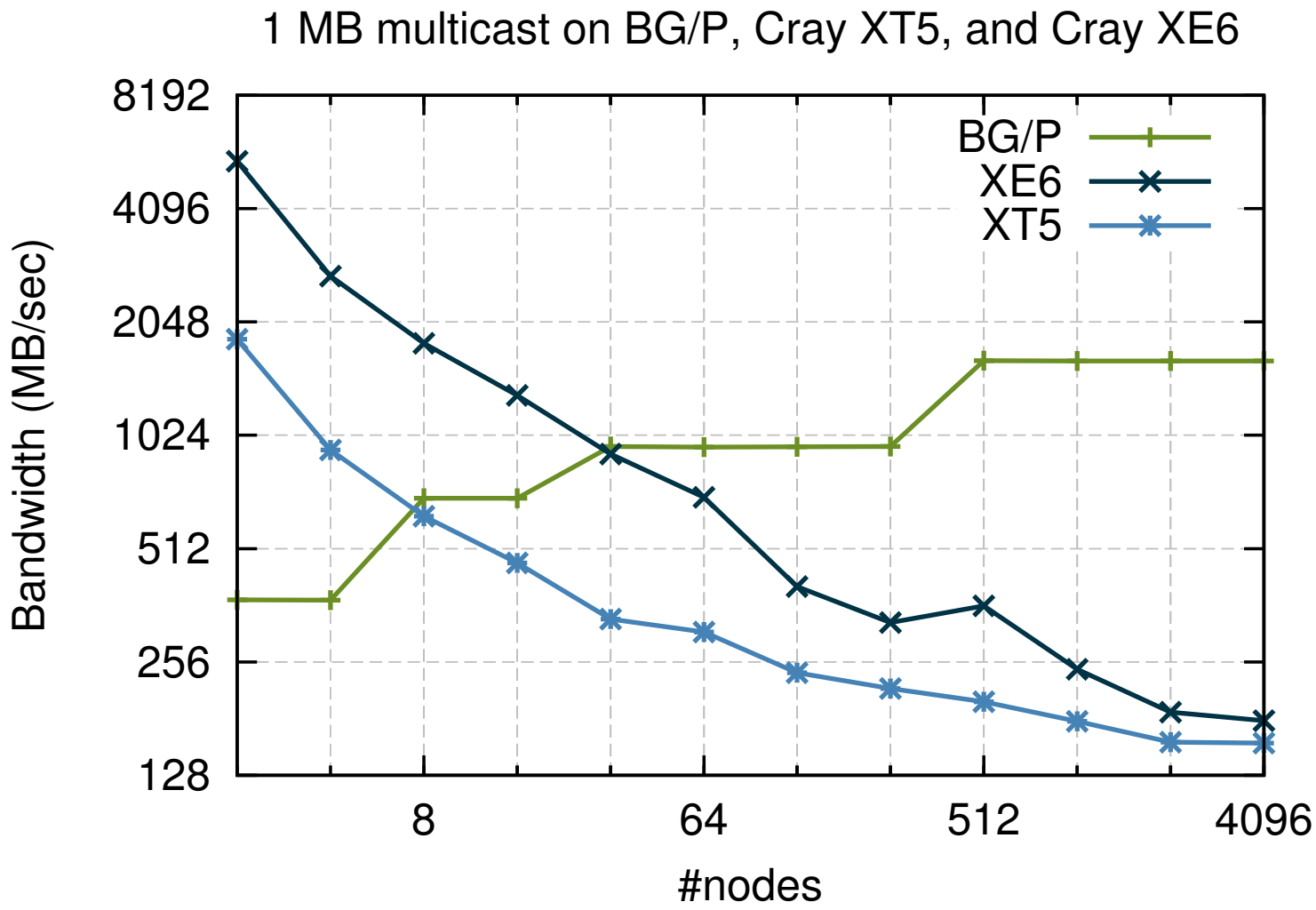
- Replication allows better strong scaling
- Topology-aware mapping cuts communication costs



Backup slides

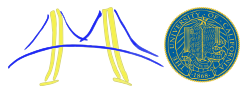


Performance of multicast (BG/P vs Cray)

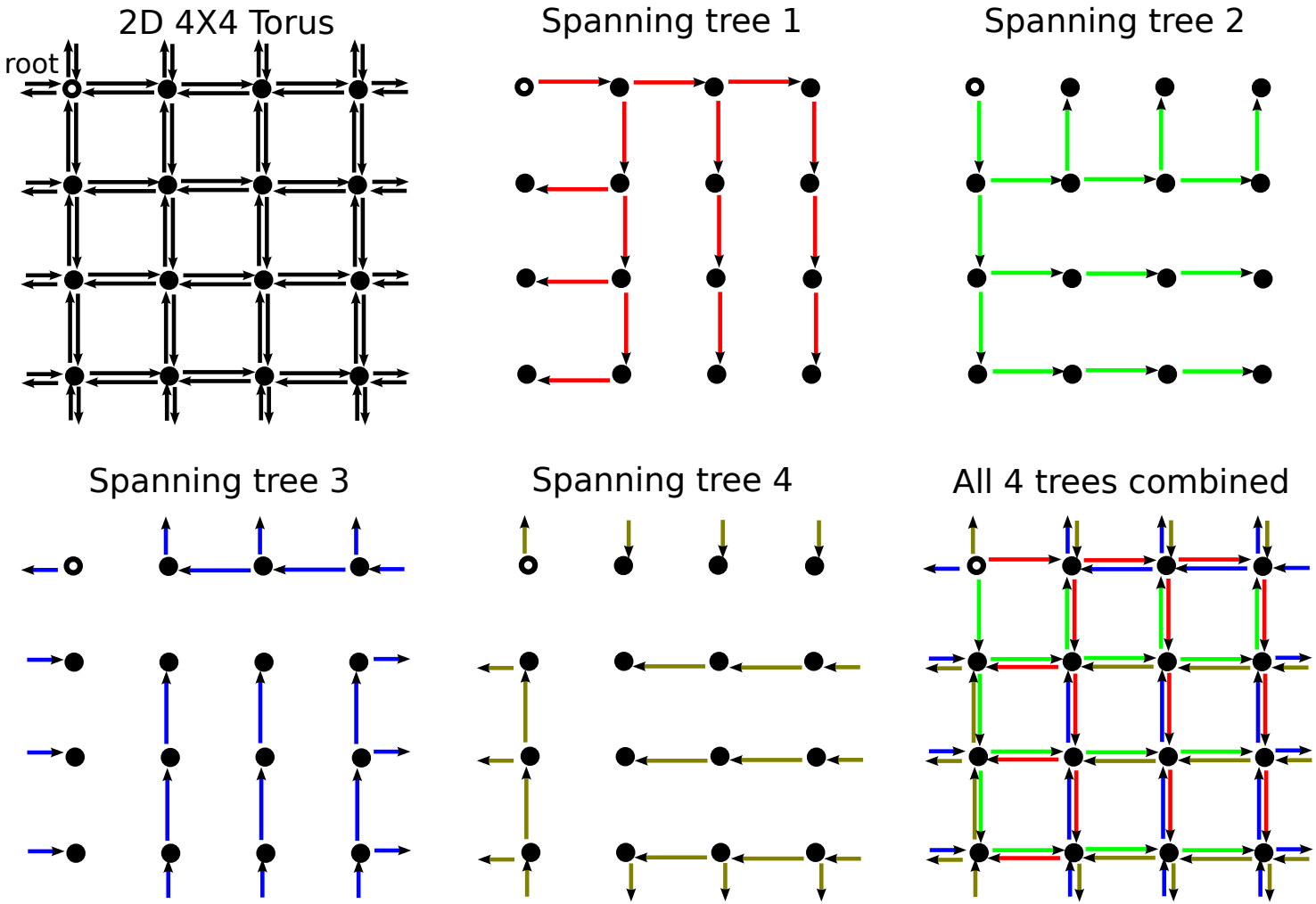


Why the performance discrepancy in multicasts?

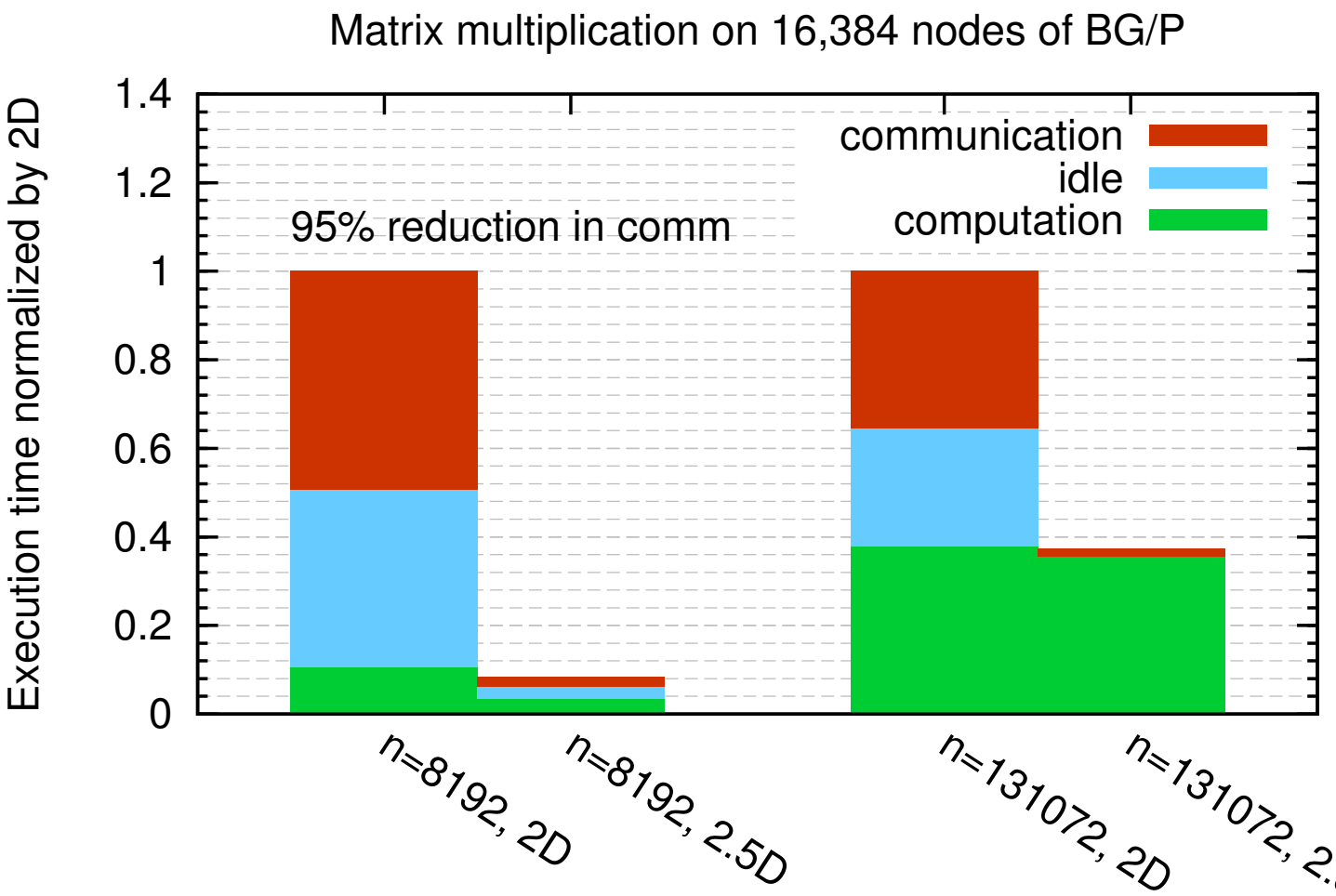
- Cray machines use **binomial multicasts**
  - Form spanning tree from a list of nodes
  - Route copies of message down each branch
  - Network contention degrades utilization on a 3D torus
- BG/P uses **rectangular multicasts**
  - Require network topology to be a k-ary n-cube
  - Form $2n$ edge-disjoint spanning trees
    - Route in different dimensional order
    - Use both directions of bidirectional network



2D rectangular multicasts trees



Cost breakdown of MM on 65,536 cores



2.5D LU on 65,536 cores