Minimizing communication in numerical linear algebra

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Summary

Talk thesis:

Scalable numerical algorithms and software must be designed with **a priori** consideration for **parallelism**, **communication cost**, and library **abstractions**.

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Scalable numerical algorithms and software must be designed with **a priori** consideration for **parallelism**, **communication cost**, and library **abstractions**.

Talk overview

- A cost model for a modern computer
- Quantification of algorithmic costs
- Communication lower bound techniques
- Dense linear algebra algorithms
- Sparse linear algebra methods

Cost model for a modern computer

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Such a computer has three fundamental architectural payloads

- γ - cost for a single (floating-point) computation for one processor (computation or flop cost)
- β - cost for a transfer of each byte between any pair of processors (bandwidth cost)
- α - cost for a synchronization between any pair of processors (latency or synchronization cost)

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An additional important cost, that I will not consider in this talk

- ν - cost for a transfer of each byte between fast memory (cache) and slow memory (DRAM) ($\gamma \ll \nu < \beta$)

Quantifying the cost of a parallel schedule of an algorithm

How do we quantify the execution time **T** of some schedule of some algorithm, in terms of our architectural costs (γ, β, and α)?

Traditional method: "Volume measure"

- $\bar{F}$ – the total number of (floating-point) operations done in the algorithm,
- $\bar{W}$ – the total amount of data all processors communicate,
- $\bar{S}$ – the total number of times processors synchronize.

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The "Volume measure" yields lower and upper bounds on the execution time:

$$(\gamma \cdot \bar{F} + \beta \cdot \bar{W} + \alpha \cdot \bar{S})/p \leq \mathbf{T} \leq \gamma \cdot \bar{F} + \beta \cdot \bar{W} + \alpha \cdot \bar{S}$$

where p is the number of processors.

Quantifying the cost of an schedule

How do we quantify the execution time **T** of some schedule, in terms of our architectural costs (γ, β, and α)?

Better method: "Critical path measure"

- F - longest sequence of dependent or consequently performed computations in the schedule,
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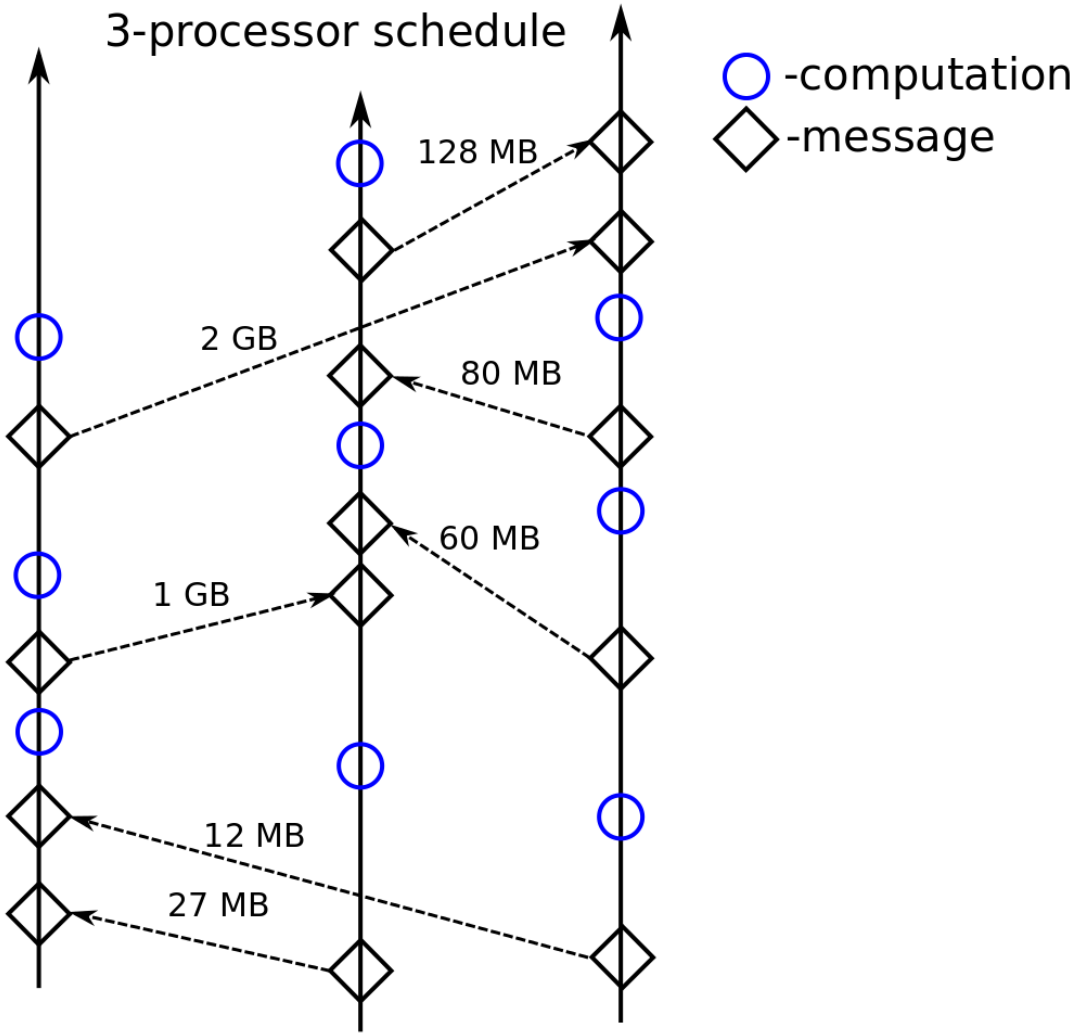
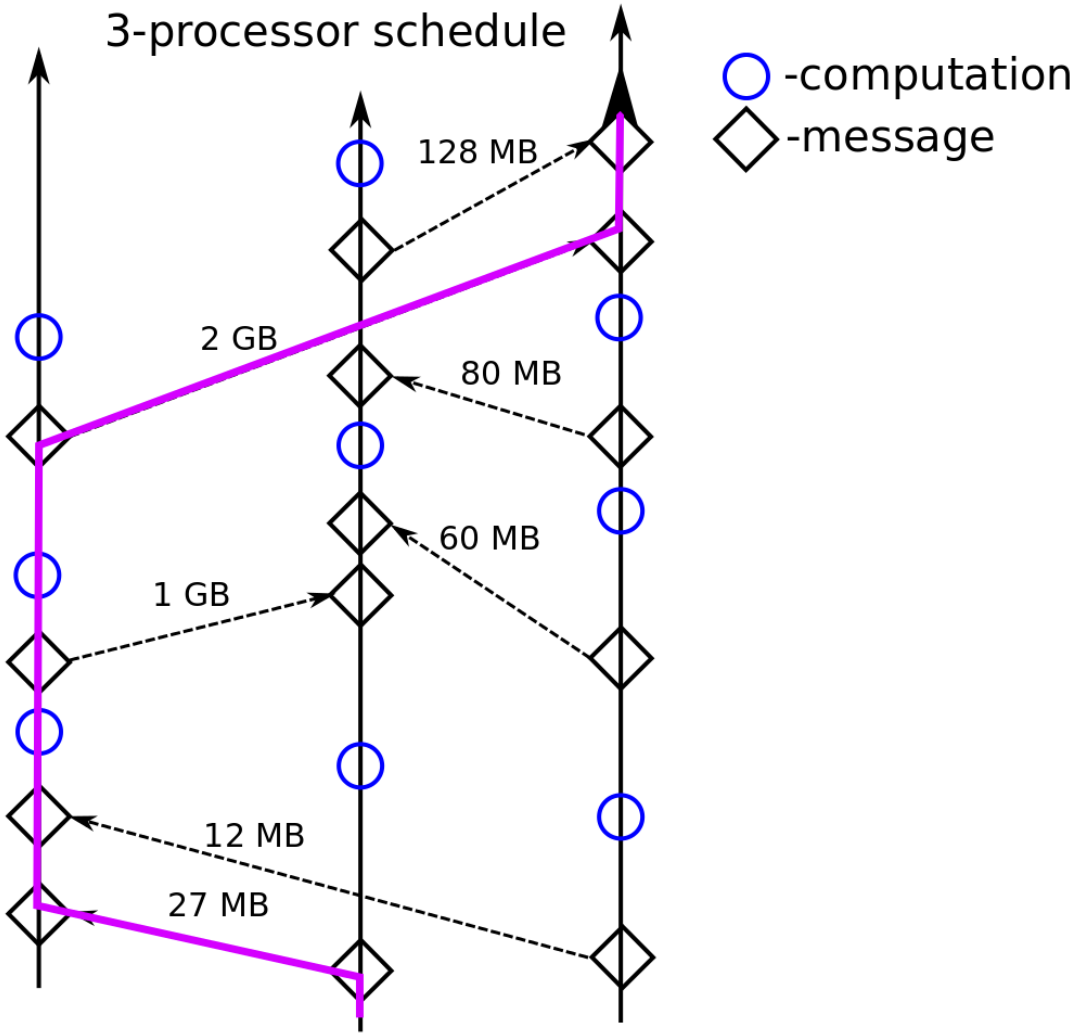
Critical path cost yields lower and upper bounds on execution time of the schedule,

$$\max(\gamma \cdot F, \beta \cdot W, \alpha \cdot S) \leq \mathbf{T} \leq \gamma \cdot F + \beta \cdot W + \alpha \cdot S.$$

Example schedule

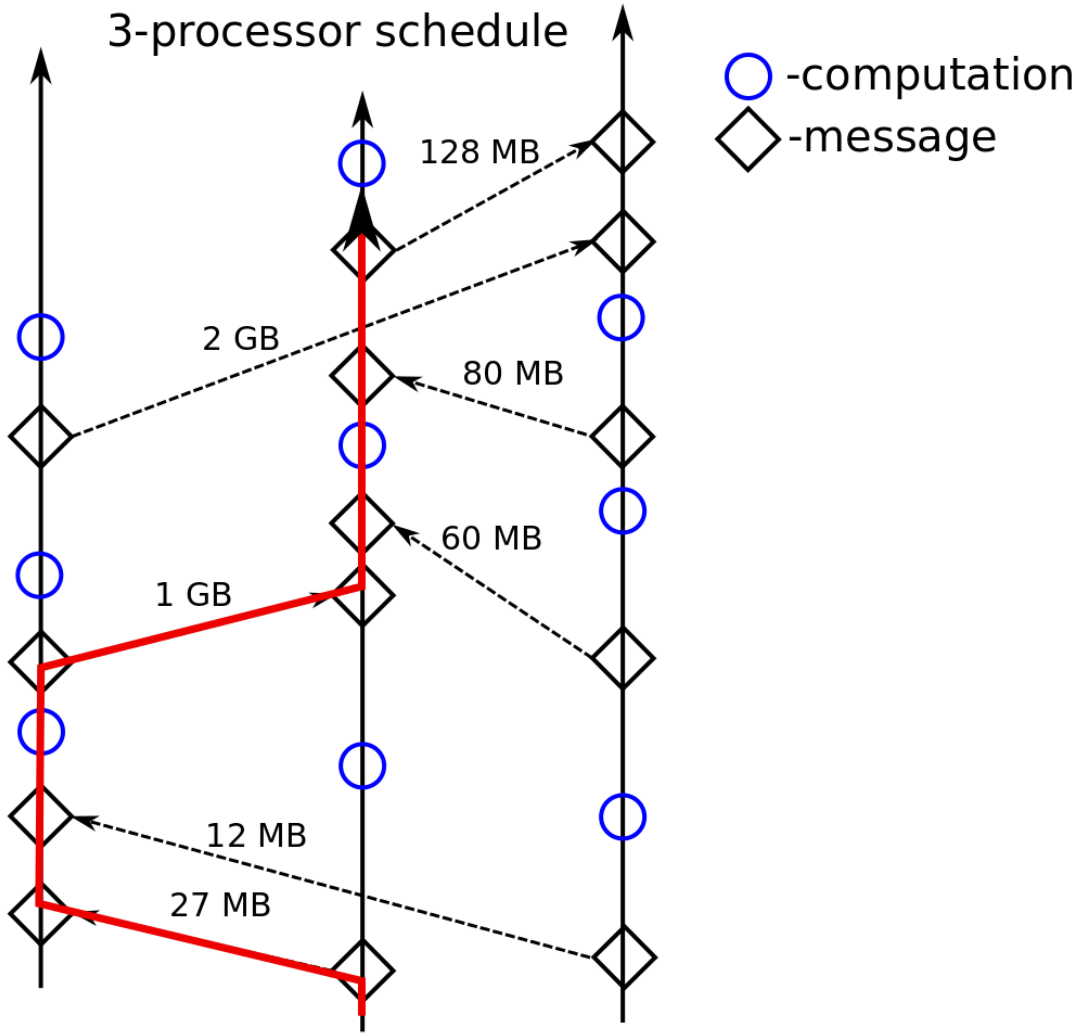


Critical path for communication cost



Critical path synchronization cost (W)

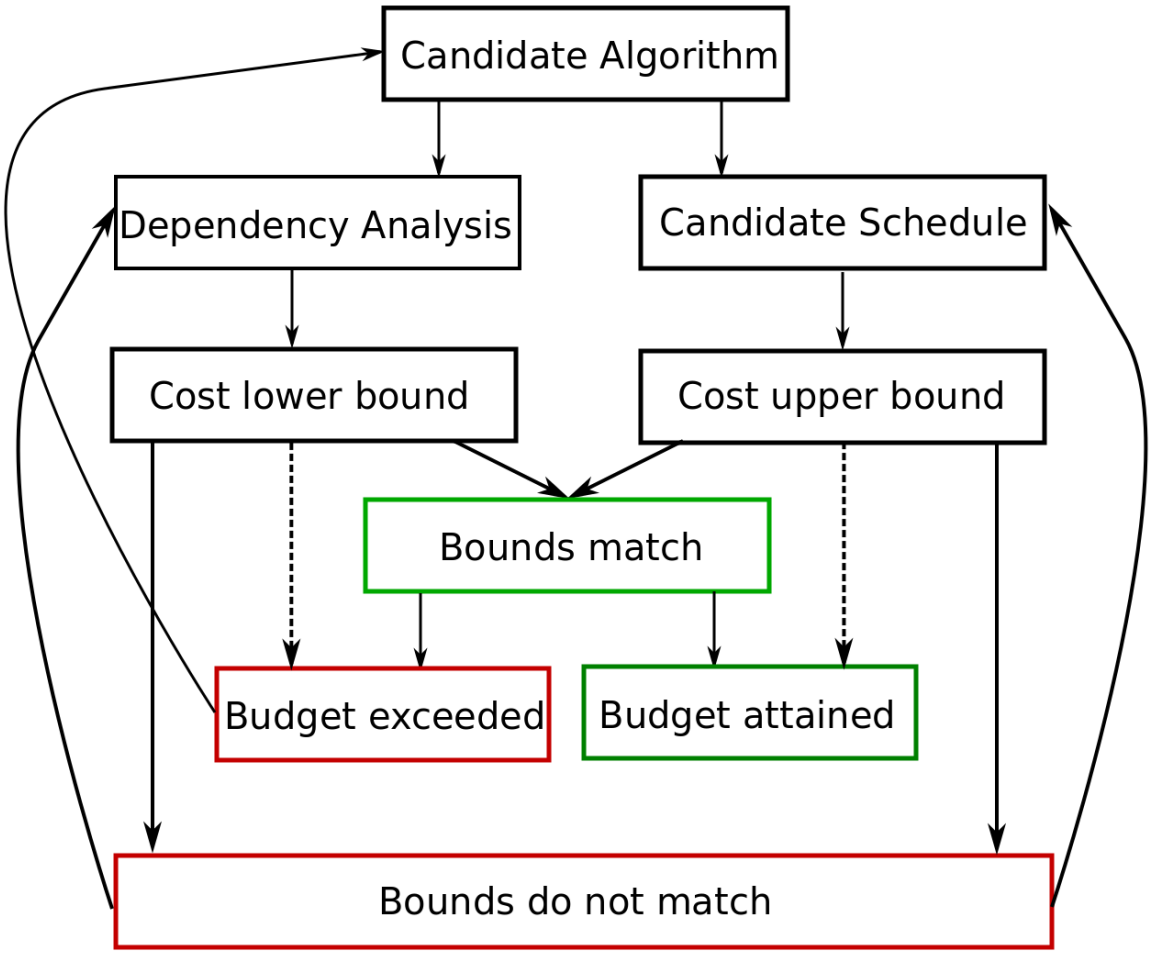
Critical path for synchronization cost



Critical path synchronization cost (S)

Designing parallel algorithms

How do we find a scalable algorithm and schedule?



Dependency graph representation of an algorithm

We can represent an algorithm as a graph $G = (V, E)$ where

- V includes the input, intermediate, and output values used by the algorithm
- E represents the dependencies between pairs of values
- e.g. to compute $c = a \cdot b$, we have $a, b, c \in V$ and $(a, c), (b, c) \in E$

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A lower bound on the computation cost F is just the length longest path in the graph, $Q \subset G$, which also bounds the amount of available parallelism as $p \leq |V|/|Q|$.

Communication bandwidth lower bounds

For some algorithm $G = (V, E)$...

we can lower bound the communication cost of the schedule, by characterizing the expansion properties of the dependency graph

- We let the vertex expansion $E(G, Z)$ of a subset vertex set $Z \subset V$ be the number of vertices in $V \setminus Z$ to which Z is adjacent
- A lower bound on the amount of communication required to parallelize G on p processors is

$$W \geq \min_{Z \subset V, |Z| = |V|/p} E(Z),$$

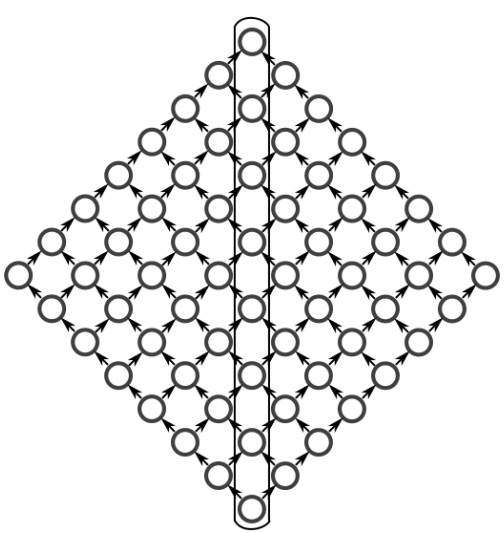
since some process must do at least $|V|/p$ work.

Path-expander graph

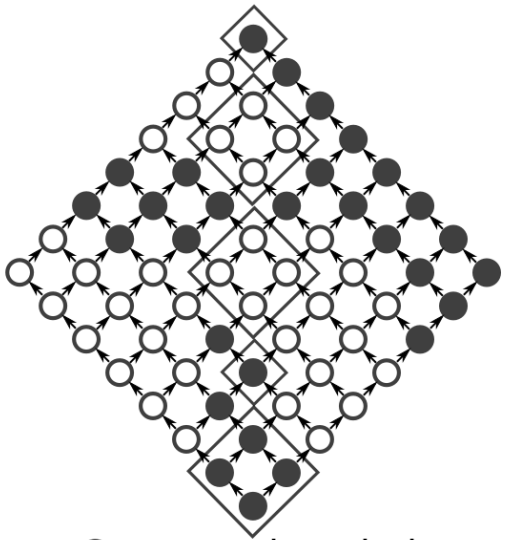
Definition (order-d-path-expander)

Graph $G = (V, E)$ is an **order-d-path-expander** if it has a path $(u_1, \ldots u_n) \subset V$, and the union of all paths between u_i and u_{i+b} for all i, b has size $\Theta(b^d)$ and a minimum cut of size $\Omega(b^{d-1})$.

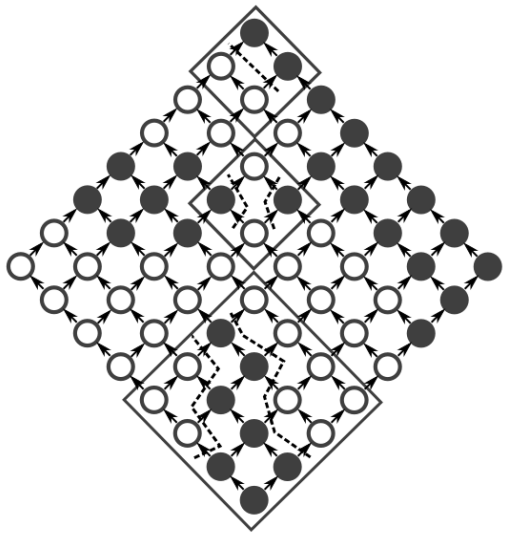
An example of a order-2-path-expander



Dependency path P



Computation chain



Communication chain

Scheduling tradeoffs of path-expander graphs

Theorem (Path-expander communication lower bound)

Any schedule of an algorithm with an **order-d-path-expander** *dependency graph about a path of length n for some $b \in [1, n]$ incurs computation (F), bandwidth (W), and latency (S) costs:*

$$F = \Omega\left(n \cdot b^{d-1}\right), \quad W = \Omega\left(n \cdot b^{d-2}\right), \quad S = \Omega\left(n/b\right),$$

which implies the following tradeoffs:

$$F \cdot S^{d-1} = \Omega\left(n^d\right), \quad W \cdot S^{d-2} = \Omega\left(n^{d-1}\right).$$

Cholesky factorization

The Cholesky factorization of a symmetric positive definite matrix $\mathbf{A}$ of dimension n into a lower-triangular matrix $\mathbf{L}$ is

$$\mathbf{A} = \mathbf{L} \cdot \mathbf{L}^T,$$

and has dependency graph $G_{\text{Ch}} = (V_{\text{Ch}}, E_{\text{Ch}})$.

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[Tiskin 2002] and [S., Demmel 2011] achieve the costs

- computation: $F_{\text{Ch}} = \Theta(n^3/p)$
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Algorithms with the same costs exist for LU, QR, SVD, etc.

Algorithms for dense matrix factorizations

Standard algorithms for LU, QR, and SVD factorization have communication costs

$$W = O(n^2/\sqrt{p}) \quad S = O(n).$$

The algorithms from the previous slide achieved, for $c \in [1, p^{1/3}]$,

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What is necessary to achieve this?

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- For SVD and the symmetric eigenproblem: *change of algorithm*: successive band reduction

Krylov subspace methods

We 'formally' consider the s-step Krylov subspace basis computation

$$\mathbf{x}^{(l)} = \mathbf{A} \cdot \mathbf{x}^{(l-1)},$$

for $l \in \{1, \ldots, s\}$ where the graph of the symmetric sparse matrix $\mathbf{A}$ is a $(2m+1)^d$-point stencil.

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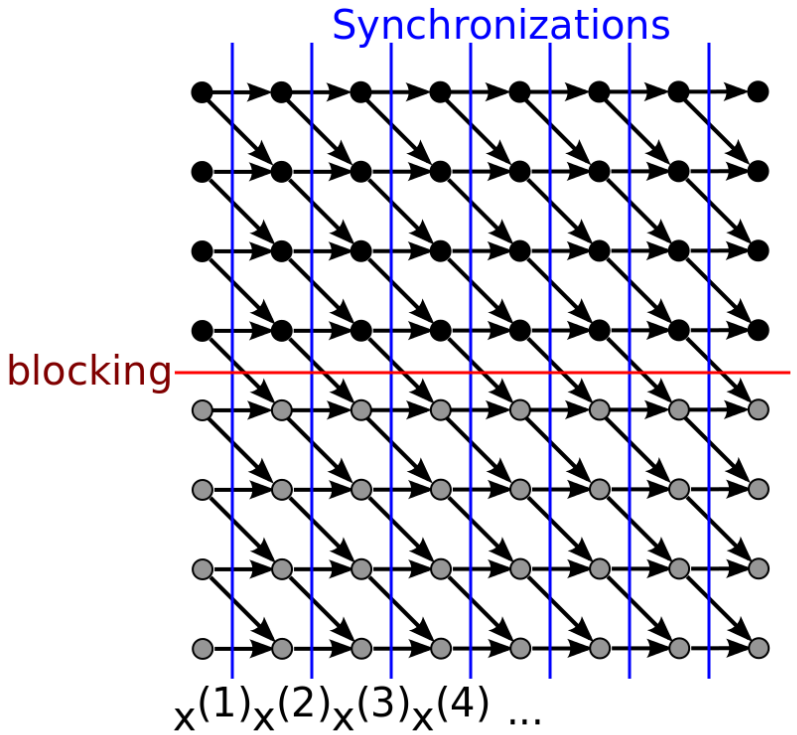
We 'informally' consider an s-step iterative method where nodes (mesh points, particles, ...), in d-dimensional space, interact at each step with all other nodes that are within distance m.

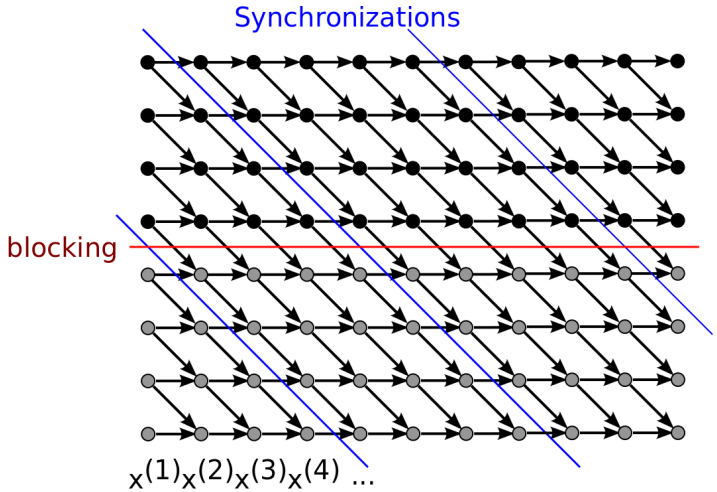
The standard algorithm (1D 2-pt stencil diagram)

Perform one matrix vector multiplication at a time, and synchronize each time



The matrix-powers kernel

Avoid synchronization by blocking across matrix-vector multiplies



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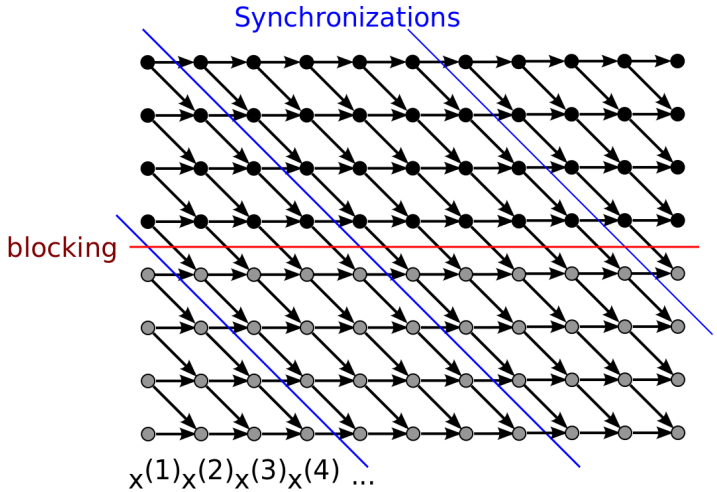
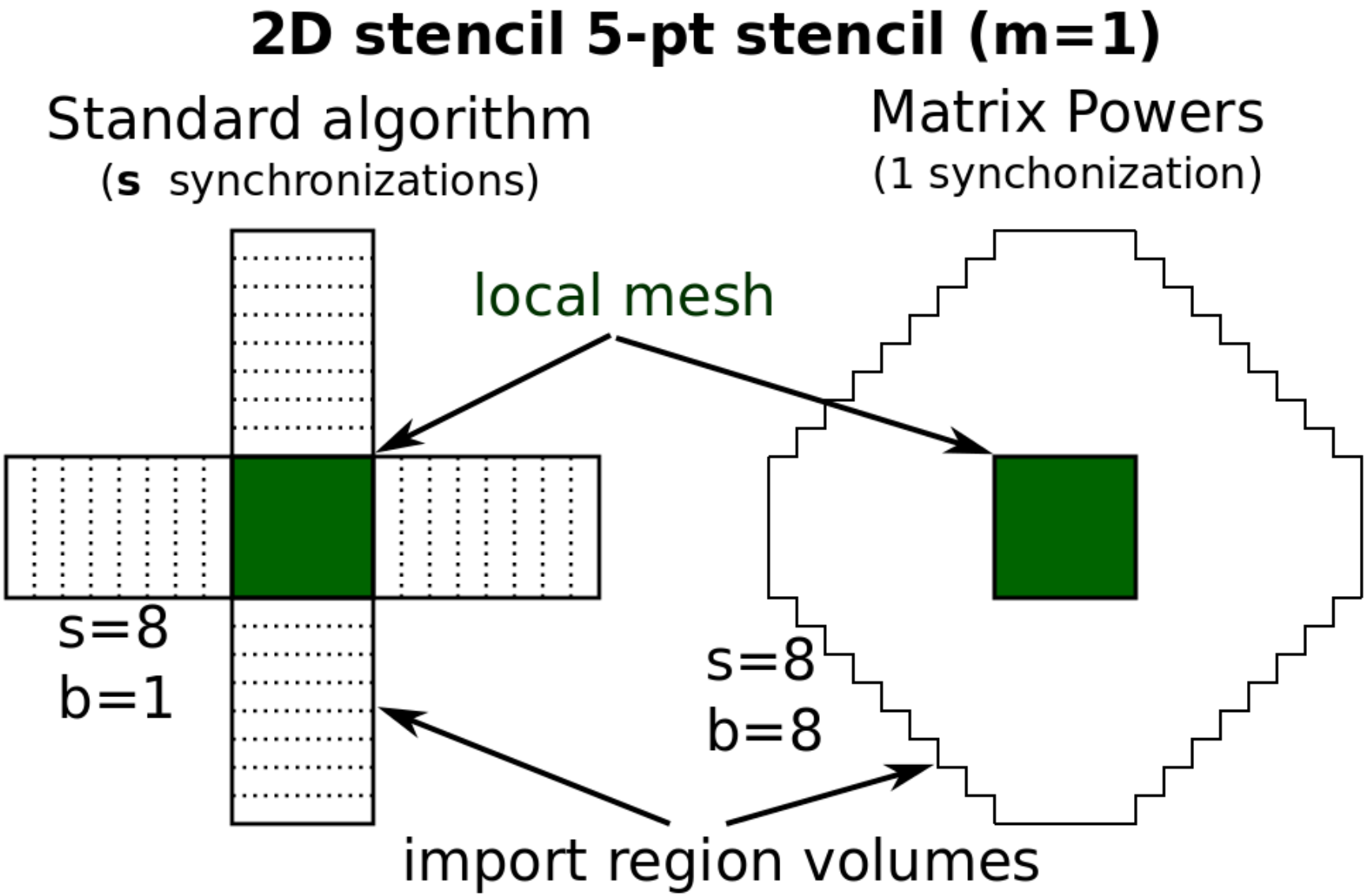


In general for a $(2m+1)^d$-point stencil, s/b invocations of the matrix-powers kernel compute an s-dimensional Krylov subspace basis with cost

$$F_{\mathrm{Kr}} = \Theta\left(m^d \cdot b^d \cdot s\right), W_{\mathrm{Kr}} = \Theta\left(m^d \cdot b^{d-1} \cdot s\right), S_{\mathrm{Kr}} = \Theta\left(s/b\right).$$

Optimal since the dependency graph of a s-step $(2m+1)^d$-point stencil is a **order-(d+1)-path-expander** with a prefactor of m^d.

Illustration of import region of the matrix-powers kernel



Summary and conclusion

High-level points summary:

- Communication cost should be the pervasive factor in the design of new numerical algorithms
- Lower bound are useful for understanding whether a better parallelization is possible or a different algorithm is necessary
- Communication cost of algorithms is dictated by dependency graph expansion properties

Collaborators and acknowledgements

Collaborators on presented work:

- Nicholas Knight, Erin Carson, James Demmel (UC Berkeley)
- Grey Ballard (formerly UC Berkeley, now Sandia National Lab)

Major collaborators on other parts of thesis work:

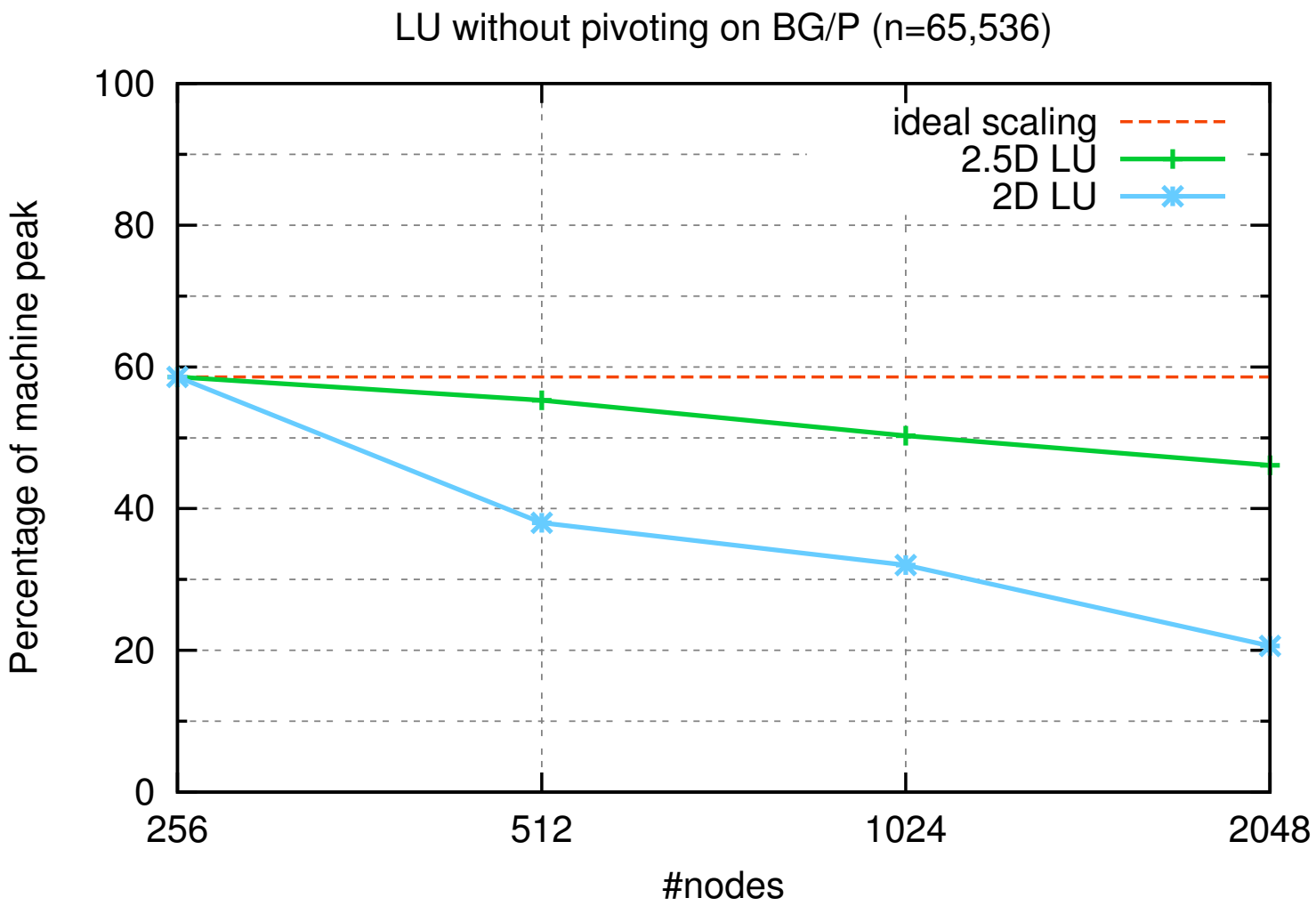
- Devin Matthews (UT Austin, CSGF fellow)
- Jeff Hammond (formerly Argonne National Lab, now Intel, CSGF alumni)
- Erik Draeger (Lawrence Livermore National Lab)
- Kathy Yelick (UC Berkeley, Lawrence Berkeley National Lab)

Support:

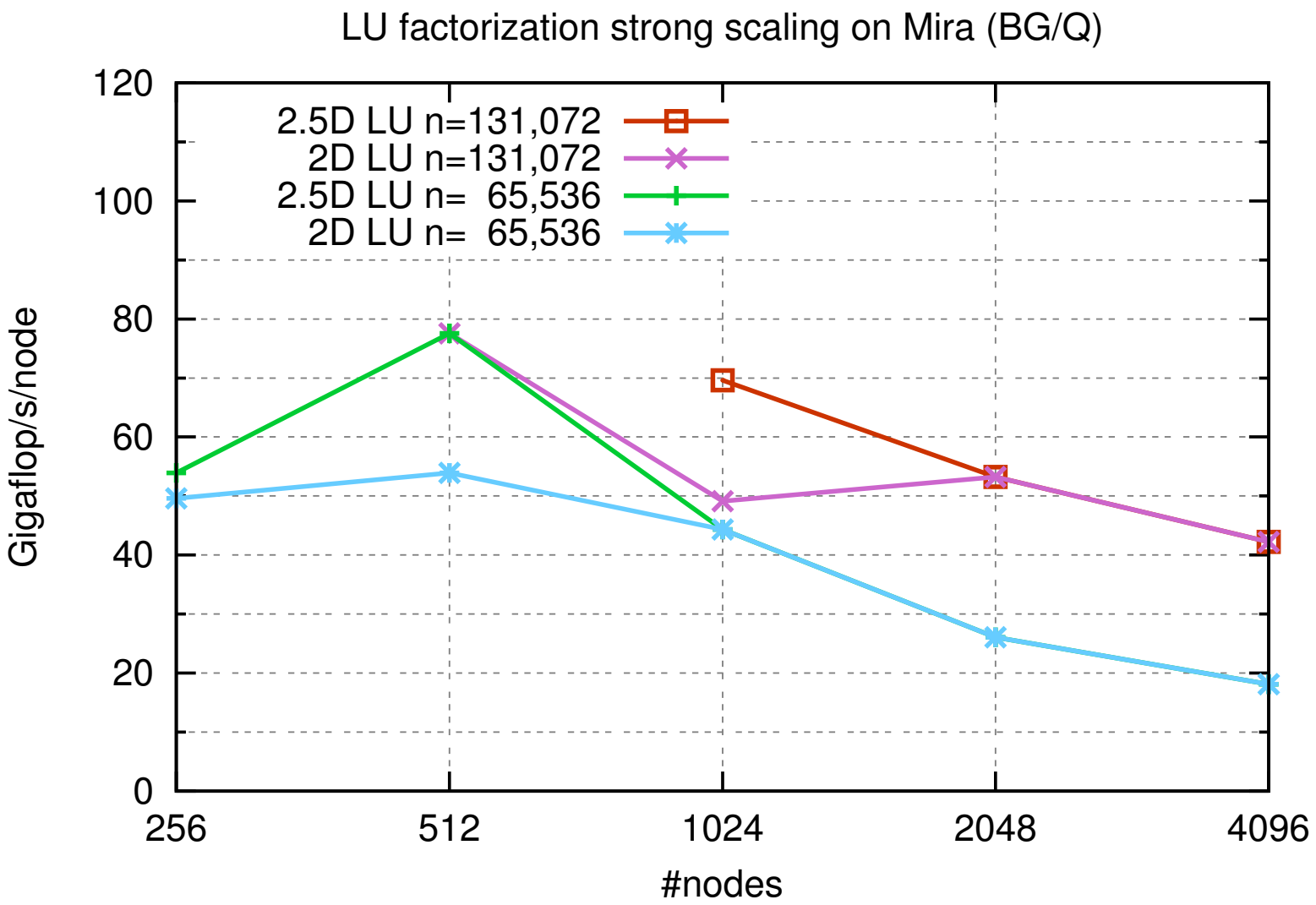
- Krell DOE Computational Science Graduate Fellowship

Backup slides

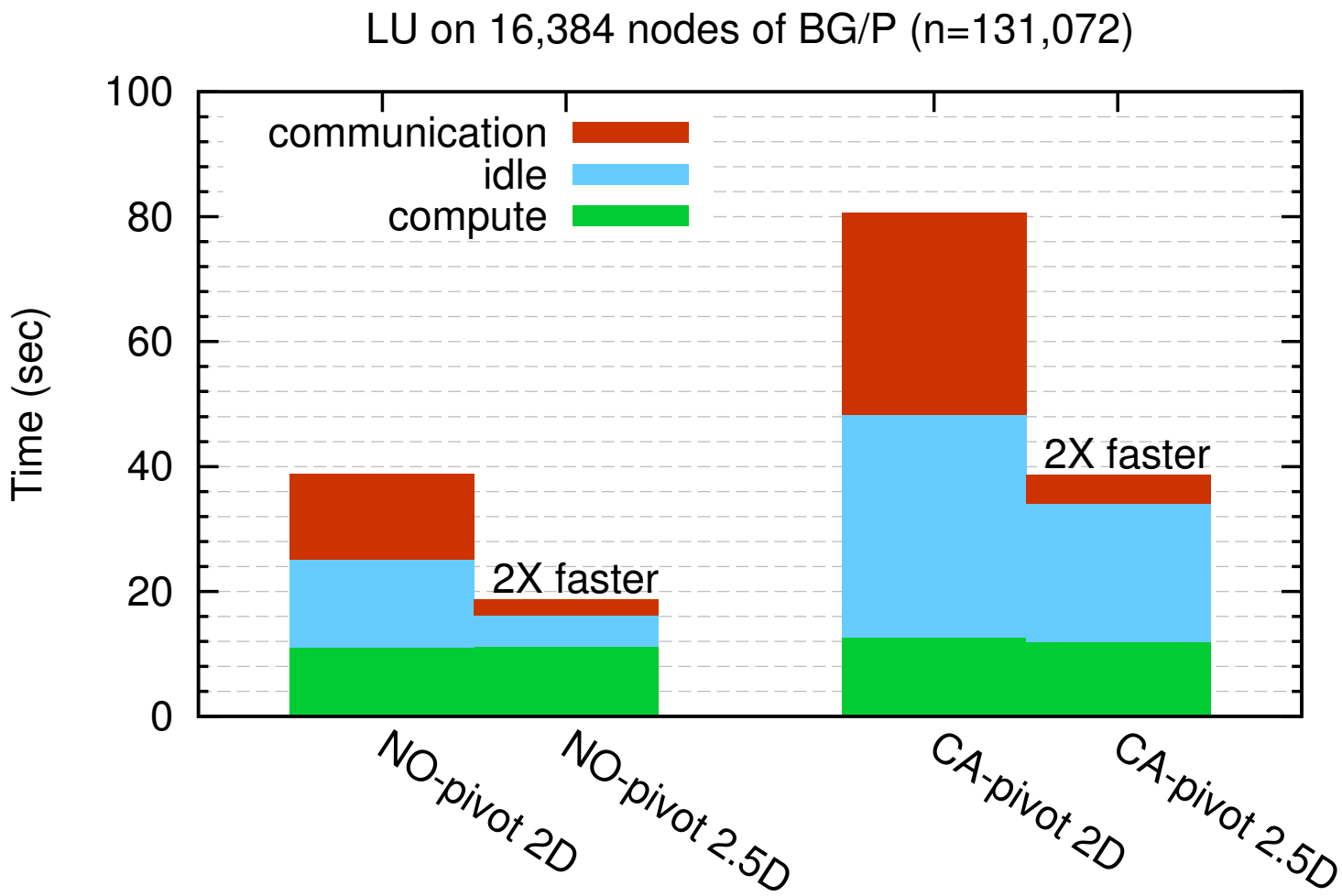
2.5D LU strong scaling (without pivoting)



Benefit of replication on BG/Q



2.5D LU on 65,536 cores



Parallel costs of Gauss-Jordan elimination

The floating point cost of Gauss-Jordan elimination is $F = \Theta(n^3/p)$. Our lower bounds may be applied since the computation has the same structure as Gaussian Elimination, so

$$F \cdot S^2 = \Omega(n^3), \quad W \cdot S = \Omega(n^2).$$

These costs are achieved for $W = O(n^2/p^{2/3})$ by schedules in

- Aggarwal, Chandra, and Snir 1990
- Tiskin 2007
- Solomonik, Buluc, and Demmel 2012

Lower synchronization cost via path doubling

We can compute the tropical semiring closure

$$\mathbf{A}^* = \mathbf{I} \oplus \mathbf{A} \oplus \mathbf{A}^2 \oplus \ldots \oplus \mathbf{A}^n = (\mathbf{I} \oplus \mathbf{A})^n,$$

directly via repeated squaring (path-doubling)

$$(\mathbf{I} \oplus \mathbf{A})^{2k} = (\mathbf{I} \oplus \mathbf{A})^k \otimes (\mathbf{I} \oplus \mathbf{A})^k$$

with a total of $\log(n)$ matrix-matrix multiplications, with

$$F = O(n^3 \log(n)/p)$$

operations and $O(\log(n))$ synchronizations, which can be less than the $O(p^{1/2})$ required by Floyd-Warshall.

Tiskin's path doubling algorithm

Tiskin gives a way to do path-doubling in $F = O(n^3/p)$ operations. We can partition each $\mathbf{A}^k$ by path size (number of edges)

$$\mathbf{A}^k = \mathbf{I} \oplus \mathbf{A}^k(1) \oplus \mathbf{A}^k(2) \oplus \ldots \oplus \mathbf{A}^k(k)$$

where each $\mathbf{A}^k(l)$ contains the shortest paths of up to $k \geq l$ edges, which have exactly l edges. We can see that

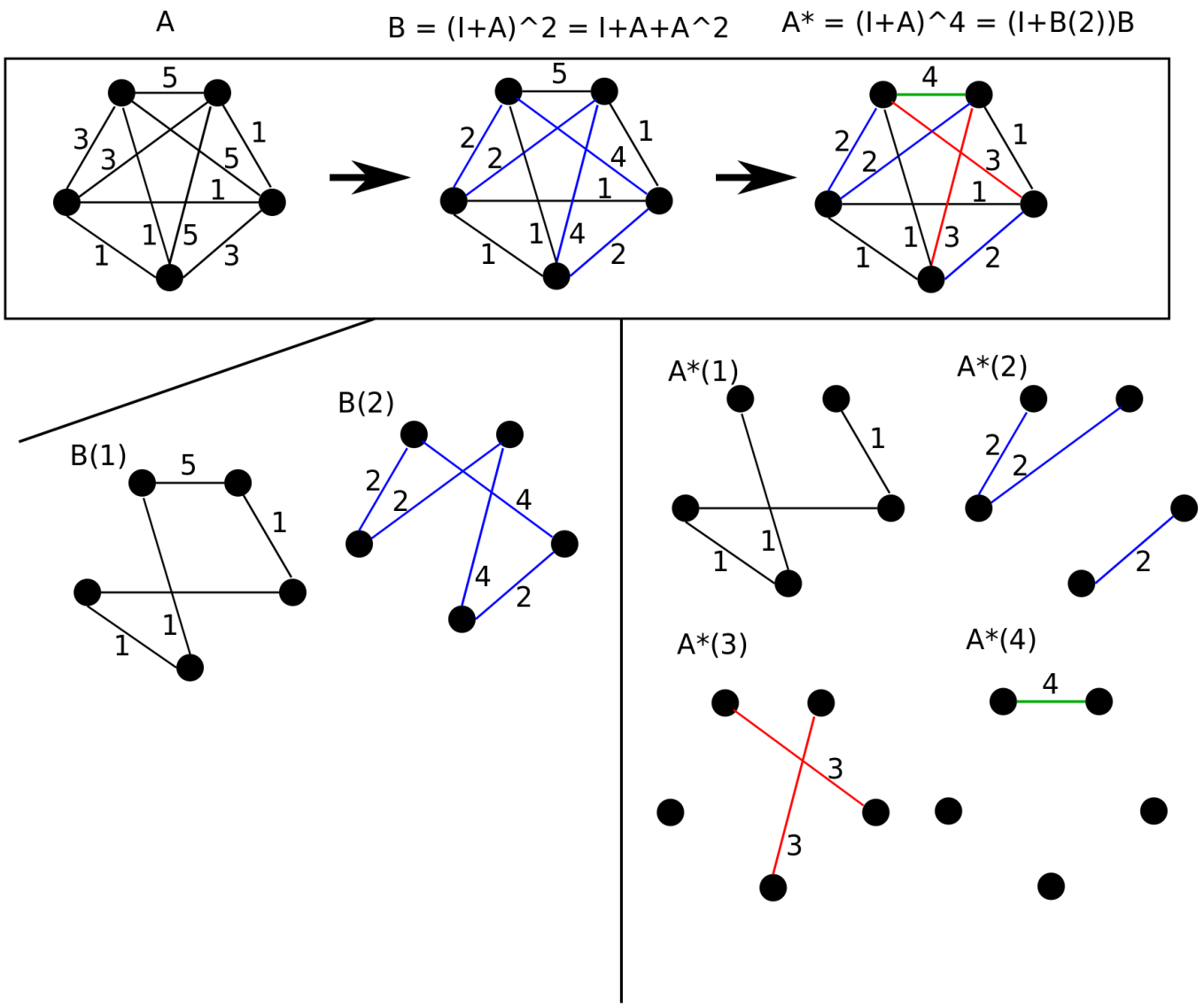
$$\mathbf{A}^l(l) \leq \mathbf{A}^{l+1}(l) \leq \ldots \leq \mathbf{A}^n(l) = \mathbf{A}^*(l),$$

in particular $\mathbf{A}^*(l)$ corresponds to a sparse subset of $\mathbf{A}^l(l)$. The algorithm works by picking $l \in [k/2, k]$ and computing

$$(\mathbf{I} \oplus \mathbf{A})^{3k/2} \leq (\mathbf{I} \oplus \mathbf{A}^k(l)) \otimes \mathbf{A}^k,$$

which finds all paths of size up to $3k/2$ by taking all paths of size exactly $l \geq k/2$ followed by all paths of size up to k.

Path-doubling (Tiskin's algorithm)



Path-doubling

Earlier caveat:

$$(\mathbf{I} \oplus \mathbf{A})^{3k/2} \leq (\mathbf{I} \oplus \mathbf{A}^k(l)) \otimes \mathbf{A}^k,$$

does not hold in general. The fundamental property used by the algorithm is really

$$\mathbf{A}^*(l) \otimes \mathbf{A}^*(k) = \mathbf{A}^*(l + k).$$

All shortest paths of up to any length are composible (factorizable), but not paths up to a limited length. However, the algorithm is correct because $\mathbf{A}^l \leq \mathbf{A}^k(l) \leq \mathbf{A}^*(k)$.

Cost of Tiskin's algorithm

Since the decomposition by path size is disjoint, one can pick $\mathbf{A}^k(l)$ for $l \in [k/2, k]$ to have size

$$|\mathbf{A}^k(l)| \geq 2n^2/k.$$

Each round of path doubling becomes cheaper than the previous, so the cost is dominated by the first matrix multiplication,

$$F = O(n^3/p) \quad W = O(n^2/p^{2/3}) \quad S = O(\log(n)),$$

solving the APSP problem with no $F \cdot S^2$ or $W \cdot S$ tradeoff and optimal flops.

More on Tiskin's APSP algorithms

Tiskin gives a way to lower the synchronization from $S = O(\log(n))$ to $O(\log(p))$. For nonnegative edge lengths it is straightforward

- compute $\mathbf{A}^p$ via path-doubling
- pick a small $\mathbf{A}^p(l)$ for $l \in [p/2, p]$
- replicate $\mathbf{A}^p(l)$ and compute Dijkstra's algorithm for n/p nodes with each process, obtaining $(\mathbf{A}^p(l))^*$
- compute by matrix multiplication

$$\mathbf{A}^* = (\mathbf{A}^p(l))^* \otimes \mathbf{A}^p$$

since all shortest paths are composed of a path of size that is a multiple of $l \leq p$, followed by a shortest path of size up to p