

Communication-Avoiding Algorithms for Linear Algebra, ML and Beyond

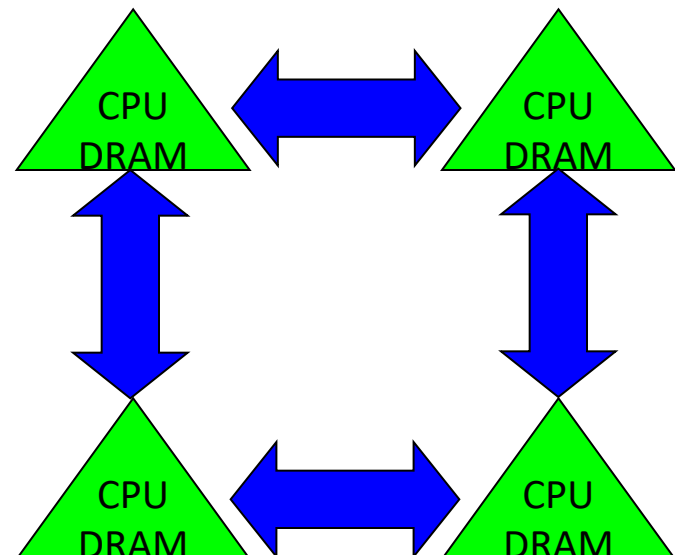
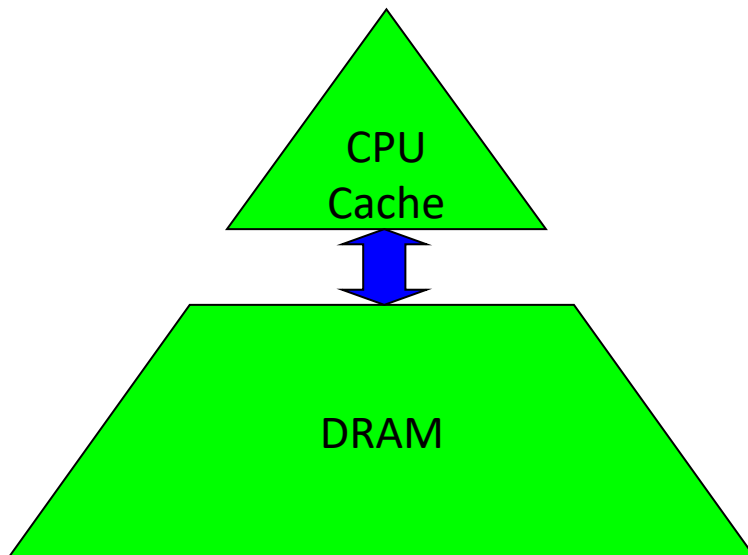
Jim Demmel, EECS & Math Depts., UC Berkeley

And many, many others ...

Why avoid communication? (1/3)

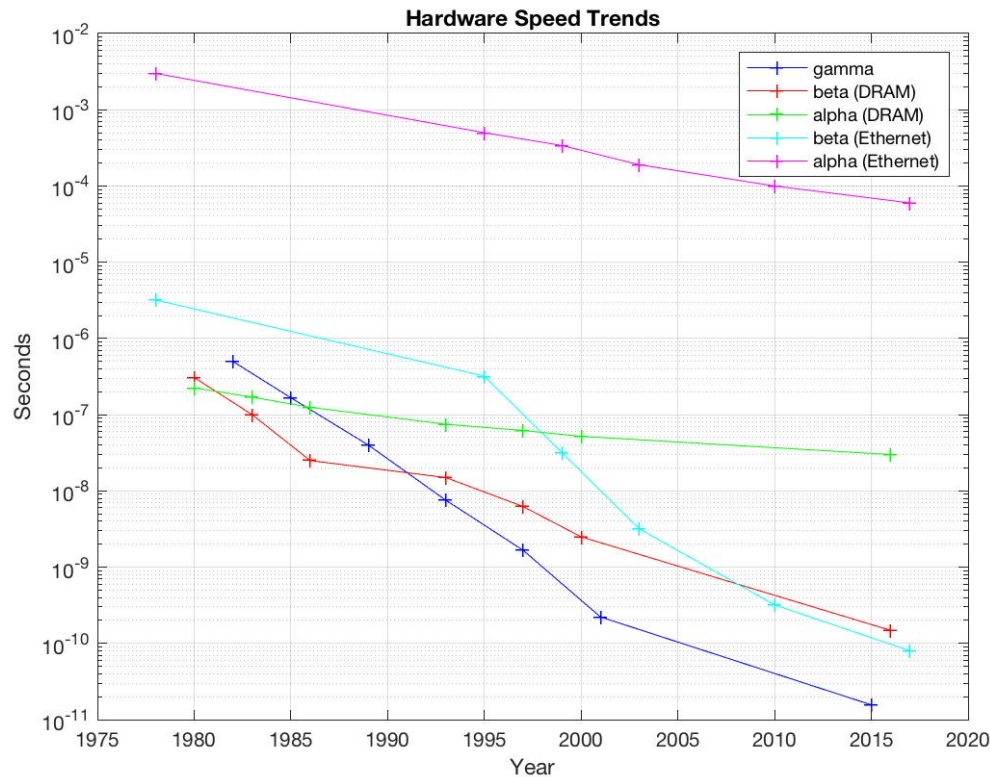
Algorithms have two costs (measured in time or energy):

1. Arithmetic (FLOPS)
2. Communication: moving data between
 - levels of a memory hierarchy (sequential case)
 - processors over a network (parallel case).



Why avoid communication? (2/3)

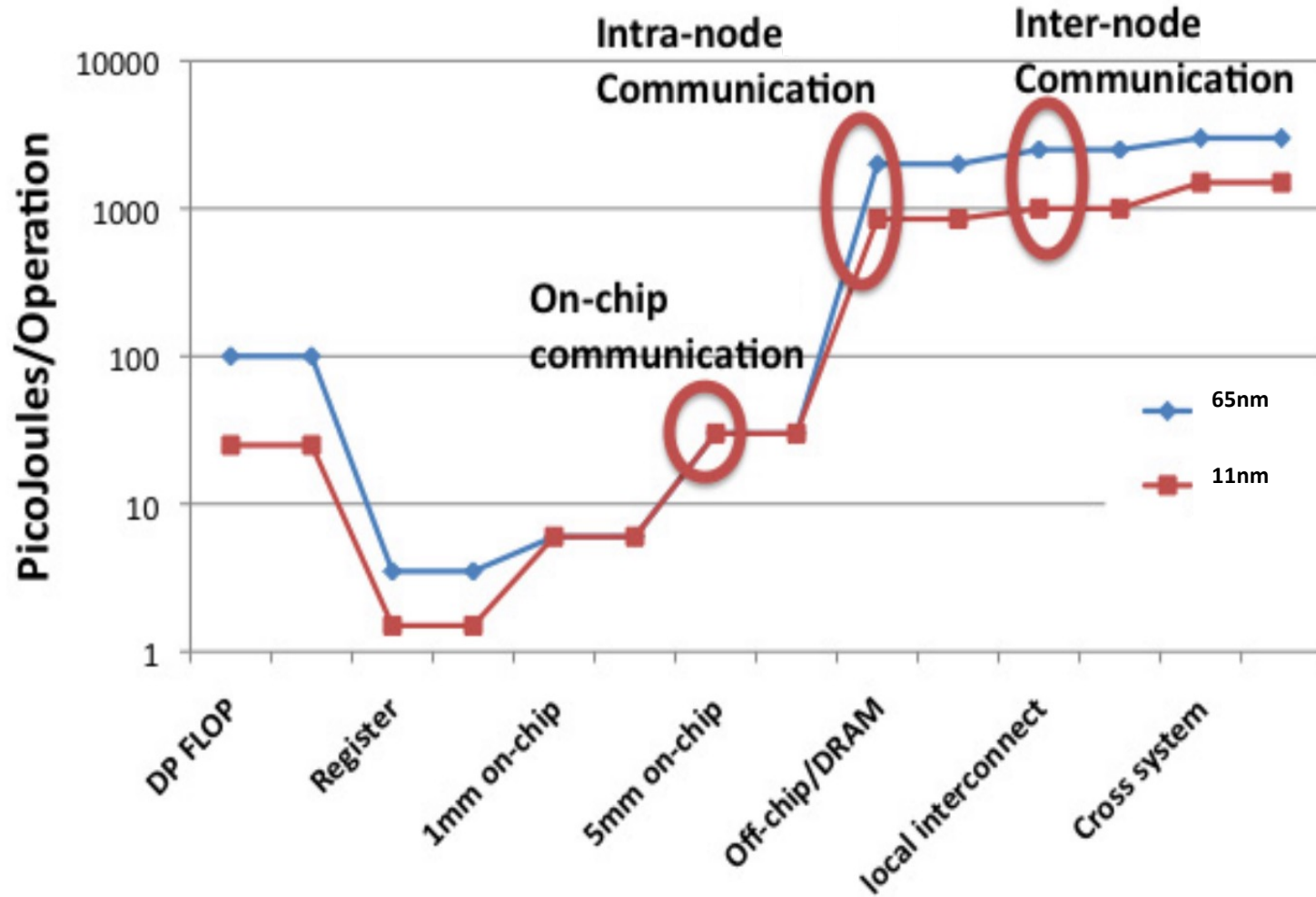
- Running time of an algorithm is sum of 3 terms:
 - # flops * time_per_flop
 - # words moved / bandwidth
 - # messages * latency } communication
- Time_per_flop (γ) \ll 1/ bandwidth (β) \ll latency (α)



Data from
Patterson &
Hennessey, 2019

Why avoid communication? (3/3)

Same story for saving energy



Goals

- Redesign algorithms to *avoid* communication
 - Between all memory hierarchy levels
 - $L1 \leftrightarrow L2 \leftrightarrow \text{DRAM} \leftrightarrow \text{network, etc}$
- Attain lower bounds if possible
 - Classical algorithms often far from lower bounds
 - Large speedups and energy savings possible
- Automate implementation of communication-avoiding (CA) algorithms

Sample Speedups

- Doing same operations, just in a different order
 - Up to **12x** faster for 2.5D dense matmul on 64K core IBM BG/P
 - Up to **100x** faster for 1.5D sparse-dense matmul on 1536 core Cray XC30
 - Up to **6.2x** faster for 2.5D All-Pairs-Shortest-Path on 24K core Cray XE6
 - Up to **11.8x** faster for direct N-body on 32K core IBM BG/P
- Mathematically identical answer, but different algorithm
 - Up to **13x** faster for Tall Skinny QR on Tesla C2050 Fermi NVIDIA GPU
 - Up to **6.7x** faster for syeig(band A) on 10 core Intel Westmere
 - Up to **4.2x** faster for BiCGStab (MiniGMG bottom solver) on 24K core Cray XE6
 - Up to **5.1x** faster for coordinate descent LASSO on 3K core Cray XC30
- Different algorithm, different approximate answer
 - Up to **16x** faster for SVM on a 1536 core Cray XC30
 - Up to **135x** faster for ImageNet training on 2K Intel KNL nodes

Sample Speedups

- Doing same operations, just in a different order

**Ideas adopted by Nervana, “deep learning” startup,
acquired by Intel in August 2016**

Kwasniewski, Hoefler, et al (Best Student Paper, SC’19)

- Mathematically identical answer, but different algorithm

SIAG on Supercomputing Best Paper Prize, 2016

(D., Grigori, Hoemmen, Langou)

Released in LAPACK 3.7, 2016

LAPACK 3.10: Householder Reconstruction, 2021

- Different algorithm, different approximate answer

IPDPS 2015 Best Paper Prize (You, D. Czechowski, Song, Vuduc)

ICPP 2018 Best Paper Prize (You, Zhang, Hsieh, D., Keutzer)

2019: Idea (LARS) adopted by industry standard benchmark MLPerf

Outline

- Linear Algebra
 - Communication Lower Bounds for classical direct linear algebra
 - CA 2.5D Matmul
 - TSQR - Tall-Skinny QR
 - Iterative Methods for linear algebra
- Machine Learning
 - Training Neural Nets – “ImageNet training in minutes”
 - Convolutional Neural Nets
- And Beyond
 - Extending communication lower bounds and optimal algorithms to general loop nests

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Summary of CA Linear Algebra

- “Direct” Linear Algebra
 - Lower bounds on communication for linear algebra problems like $Ax=b$, least squares, $Ax = \lambda x$, SVD, etc
 - Only some attained by algorithms in standard libraries
 - LAPACK, ScaLAPACK, ...
 - New algorithms needed to attain these lower bounds
 - New numerical properties, ways to encode answers, data structures, not just loop transformations
 - Autotuning to find optimal implementation (eg GPTune)
 - Sparse matrices: depends on sparsity structure
- Ditto for “Iterative” Linear Algebra

Lower bound for all “n³-like” linear algebra

- Let M = “fast” memory size (per processor)

$$\#words_moved \text{ (per processor)} = \Omega(\#flops \text{ (per processor)} / M^{1/2})$$

- Parallel case: assume either load or memory balanced
- Holds for
 - Matmul

Lower bound for all “n³-like” linear algebra

- Let M = “fast” memory size (per processor)

$$\#words_moved \text{ (per processor)} = \Omega(\#flops \text{ (per processor)} / M^{1/2})$$

$$\#messages_sent \geq \#words_moved / largest_message_size$$

- Parallel case: assume either load or memory balanced
- Holds for
 - Matmul, BLAS, LU, QR, eig, SVD, tensor contractions, ...
 - Some whole programs (sequences of these operations, no matter how individual ops are interleaved, eg A^k)
 - Dense and sparse matrices (where $\#flops \ll n^3$)
 - Sequential and parallel algorithms
 - Some graph-theoretic algorithms (eg Floyd-Warshall)

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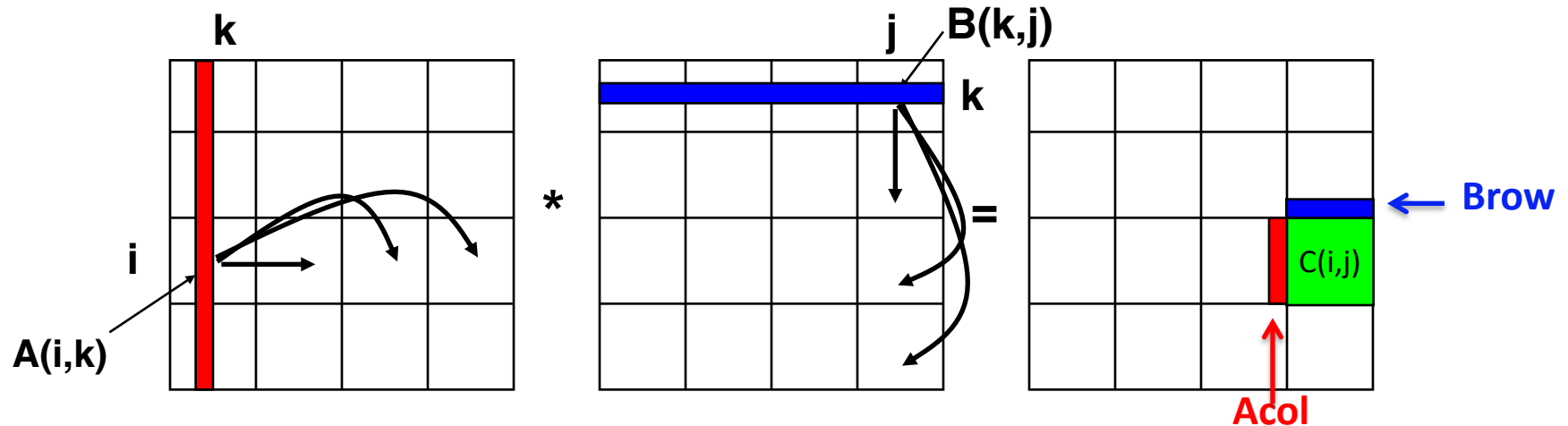
SIAM SIAG/Linear Algebra Prize, 2012

(Ballard, D., Holtz, Schwartz)

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SUMMA– $n \times n$ matmul on $P^{1/2} \times P^{1/2}$ grid (nearly) optimal using minimum memory $M=O(n^2/P)$



For $k=0$ to $n/b-1$... $b = \text{block size} = \text{\#cols in } A(i,k) = \text{\#rows in } B(k,j)$
 for all $i = 1$ to $P^{1/2}$
 owner of $A(i,k)$ broadcasts it to whole processor row (using binary tree)
 for all $j = 1$ to $P^{1/2}$
 owner of $B(k,j)$ broadcasts it to whole processor column (using bin. tree)
 Receive $A(i,k)$ into $Acol$
 Receive $B(k,j)$ into $Brow$
 $C_{\text{myproc}} = C_{\text{myproc}} + Acol * Brow$

Summary of dense parallel algorithms attaining communication lower bounds

- Assume $n \times n$ matrices on P processors
- Minimum Memory per processor = $M = O(n^2 / P)$
- Recall lower bounds:
#words_moved = $\Omega((n^3 / P) / M^{1/2}) = \Omega(n^2 / P^{1/2})$
#messages = $\Omega((n^3 / P) / M^{3/2}) = \Omega(P^{1/2})$
- SUMMA attains this lower bound
- Does ScaLAPACK attain these bounds?
 - For #words_moved: mostly, except nonsym. Eigenproblem
 - For #messages: asymptotically worse, except Cholesky
- New algorithms attain all bounds, up to polylog(P) factors
 - Cholesky, LU, QR, Sym. and Nonsym eigenproblems, SVD

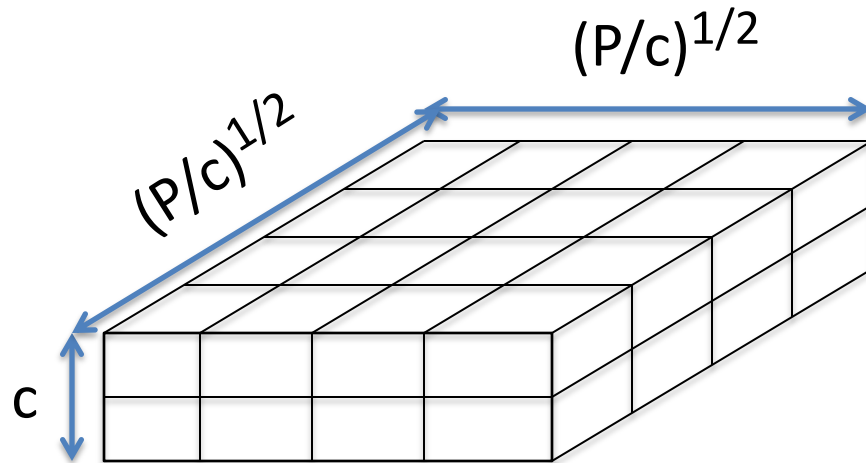
Can we do Better?

Can we do better?

- Aren't we already optimal?
- Why assume $M = O(n^2/p)$, i.e. minimal?
 - Lower bound still true if more memory
 - Can we attain it?
- Special case: “3D Matmul”
 - Uses $M = O(n^2/p^{2/3})$
 - Dekel, Nassimi, Sahni [81], Bernstein [89], Agarwal, Chandra, Snir [90], Johnson [93], Agarwal, Balle, Gustavson, Joshi, Palkar [95]
- Not always $p^{1/3}$ times as much memory available...

2.5D Matrix Multiplication

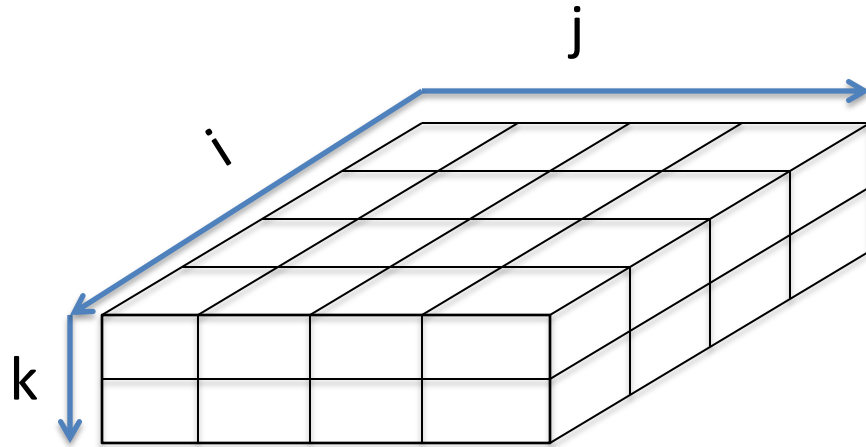
- Assume can fit cn^2/P data per processor, $c > 1$
- Processors form $(P/c)^{1/2} \times (P/c)^{1/2} \times c$ grid



Example: $P = 32, c = 2$

2.5D Matrix Multiplication

- Assume can fit cn^2/P data per processor, $c > 1$
- Processors form $(P/c)^{1/2} \times (P/c)^{1/2} \times c$ grid



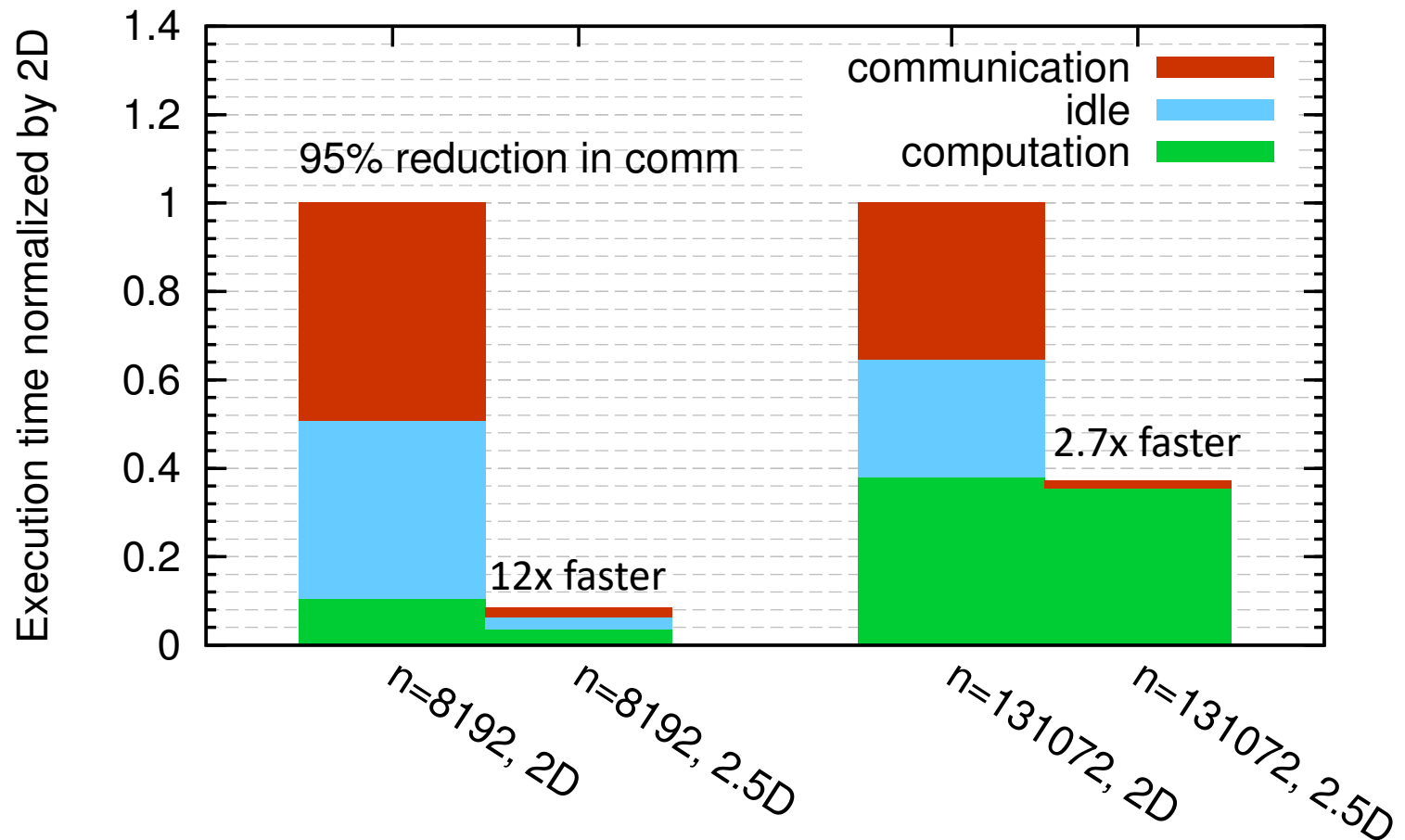
Initially $P(i,j,0)$ owns $A(i,j)$ and $B(i,j)$
each of size $n(c/P)^{1/2} \times n(c/P)^{1/2}$

- (1) $P(i,j,0)$ broadcasts $A(i,j)$ and $B(i,j)$ to $P(i,j,k)$
- (2) Processors at level k perform $1/c$ -th of SUMMA, i.e. $1/c$ -th of $\sum_m A(i,m)*B(m,j)$
- (3) Sum-reduce partial sums $\sum_m A(i,m)*B(m,j)$ along k -axis so $P(i,j,0)$ owns $C(i,j)$

2.5D Matmul on BG/P, 16K nodes / 64K cores

c = 16 copies

Matrix multiplication on 16,384 nodes of BG/P



Distinguished Paper Award, EuroPar'11 (Solomonik, D.)

Kwasniewski, Hoefler, et al (Best Student Paper, SC'19)

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TSQR: QR of a Tall, Skinny matrix

$$W = \begin{pmatrix} W_0 \\ W_1 \\ W_2 \\ W_3 \end{pmatrix}$$

$$\begin{pmatrix} R_{00} \\ R_{10} \\ R_{20} \\ R_{30} \end{pmatrix} = \begin{pmatrix} Q_{01} & R_{01} \\ Q_{11} & R_{11} \end{pmatrix}$$

$$\begin{pmatrix} R_{01} \\ R_{11} \end{pmatrix} = \begin{pmatrix} Q_{02} & R_{02} \end{pmatrix}$$

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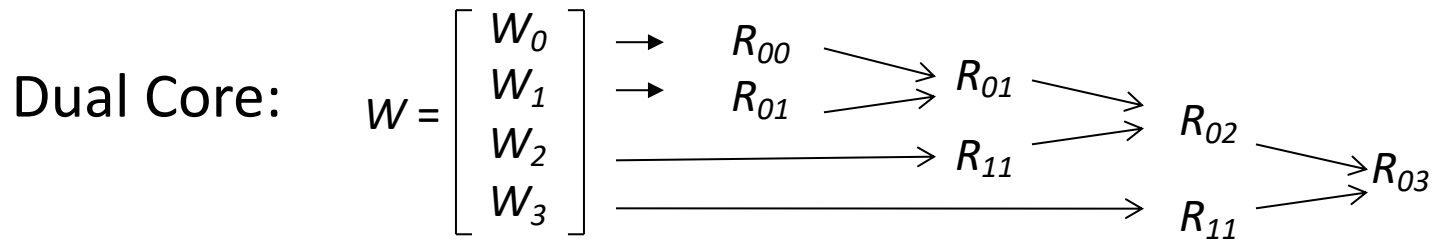
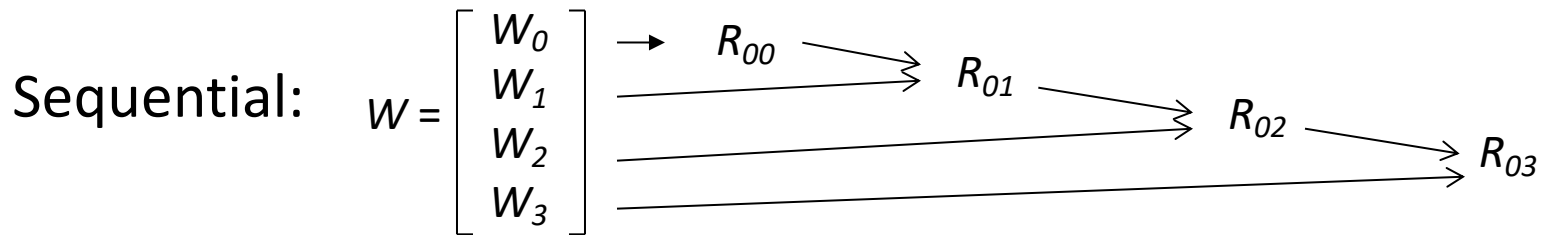
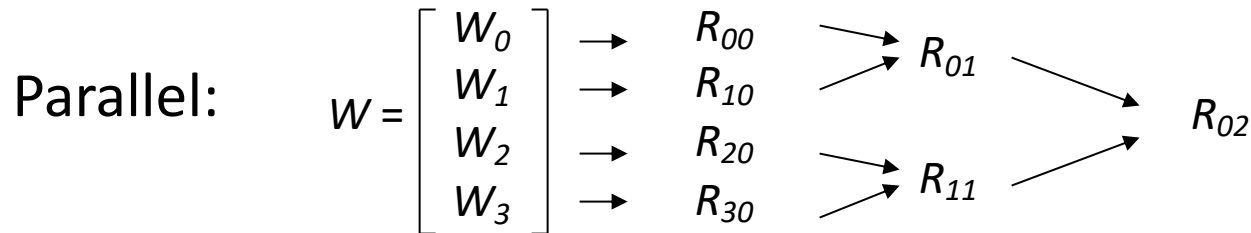
$$W = \begin{pmatrix} W_0 \\ W_1 \\ W_2 \\ W_3 \end{pmatrix} = \begin{pmatrix} Q_{00} R_{00} \\ Q_{10} R_{10} \\ Q_{20} R_{20} \\ Q_{30} R_{30} \end{pmatrix} = \begin{pmatrix} Q_{00} \\ Q_{10} \\ Q_{20} \\ Q_{30} \end{pmatrix} \cdot \begin{pmatrix} R_{00} \\ R_{10} \\ R_{20} \\ R_{30} \end{pmatrix}$$

$$\begin{pmatrix} R_{00} \\ R_{10} \\ R_{20} \\ R_{30} \end{pmatrix} = \begin{pmatrix} Q_{01} R_{01} \\ Q_{11} R_{11} \end{pmatrix} = \begin{pmatrix} Q_{01} \\ Q_{11} \end{pmatrix} \cdot \begin{pmatrix} R_{01} \\ R_{11} \end{pmatrix}$$

$$\begin{pmatrix} R_{01} \\ R_{11} \end{pmatrix} = \begin{pmatrix} Q_{02} R_{02} \end{pmatrix}$$

Output = $\{ Q_{00}, Q_{10}, Q_{20}, Q_{30}, Q_{01}, Q_{11}, Q_{02}, R_{02} \}$

TSQR: An Architecture-Dependent Algorithm



Multicore / Multisocket / Multirack / Multisite / Out-of-core: ?

Can choose reduction tree dynamically

TSQR Performance Results

- Parallel
 - Intel Clovertown
 - Up to **8x** speedup (8 core, dual socket, 10M x 10)
 - Pentium III cluster, Dolphin Interconnect, MPICH
 - Up to **6.7x** speedup (16 procs, 100K x 200)
 - BlueGene/L
 - Up to **4x** speedup (32 procs, 1M x 50)
 - Tesla C 2050 / Fermi
 - Up to **13x** (110,592 x 100)
 - Grid – **4x** on 4 cities vs 1 city (Dongarra, Langou et al)
 - Cloud – **1.6x slower than just accessing data twice** (Gleich and Benson)
- Sequential
 - “**Infinite speedup**” for out-of-core on PowerPC laptop
 - As little as 2x slowdown vs (predicted) infinite DRAM
 - LAPACK with virtual memory never finished
- SVD costs about the same
- Joint work with Grigori, Hoemmen, Langou, Anderson, Ballard, Keutzer, others

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Avoiding Communication in Iterative Linear Algebra

- k-steps of iterative solver for sparse $Ax=b$ or $Ax=\lambda x$
 - Does k SpMV's with A and starting vector
 - Many such “Krylov Subspace Methods”
 - Conjugate Gradients (CG), GMRES, Lanczos, Arnoldi, ...
- Goal: minimize communication
 - Assume matrix “well-partitioned”
 - Serial implementation
 - Conventional: $O(k)$ moves of data from slow to fast memory
 - **New: $O(1)$ moves of data – optimal**
 - Parallel implementation on p processors
 - Conventional: $O(k \log p)$ messages (k SpMV calls, dot prods)
 - **New: $O(\log p)$ messages - optimal**
- Lots of speed up possible (modeled and measured)
 - Price: some redundant computation
 - Challenges: Poor partitioning, Preconditioning, Num. Stability

Minimizing Communication of GMRES to solve $Ax=b$

- GMRES: find x in $\text{span}\{b, Ab, \dots, A^k b\}$ minimizing $\|Ax - b\|_2$

Standard GMRES

for $i=1$ to k

$w = A \cdot v(i-1) \dots SpMV$

$MGS(w, v(0), \dots, v(i-1))$

update $v(i), H$

endfor

solve LSQ problem with H

Communication-avoiding GMRES

$W = [v, Av, A^2v, \dots, A^k v]$

$[Q, R] = \text{TSQR}(W)$

\dots “Tall Skinny QR”

build H from R

solve LSQ problem with H

Sequential case: #words moved decreases by a factor of k

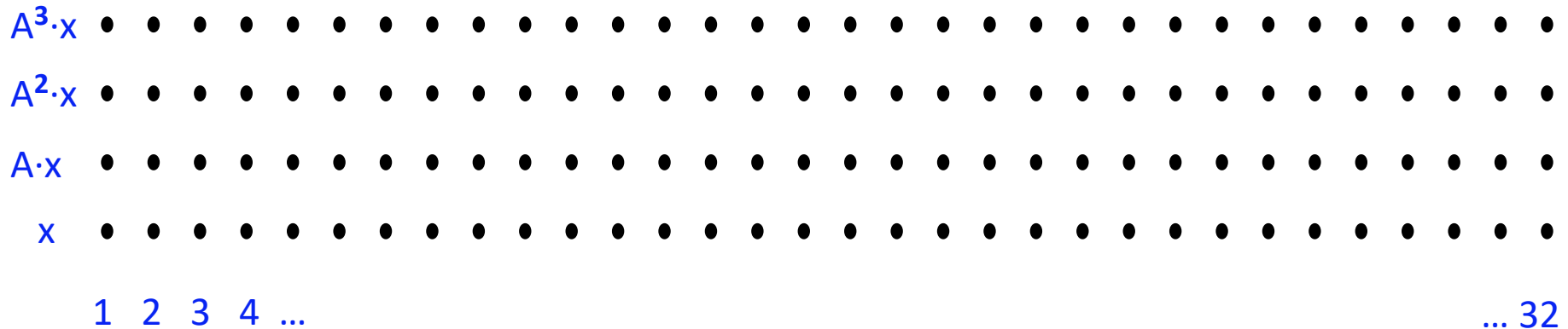
Parallel case: #messages decreases by a factor of k

- **Oops** – W from power method, precision lost!
- **Fix:** replace W by $[v, p_1(A)v, p_2(A)v, \dots, p_k(A)v]$
- Up to **2.3x** speedup for GMRES on 8 core Intel Clovertown (Hoemmen)
- Up to **4.2x** speedup for BiCGStab on 24K core Cray XE6 (Carson)

Communication Avoiding Kernels:

The Matrix Powers Kernel : $[Ax, A^2x, \dots, A^kx]$

- Replace k iterations of $y = A \cdot x$ with $[Ax, A^2x, \dots, A^kx]$

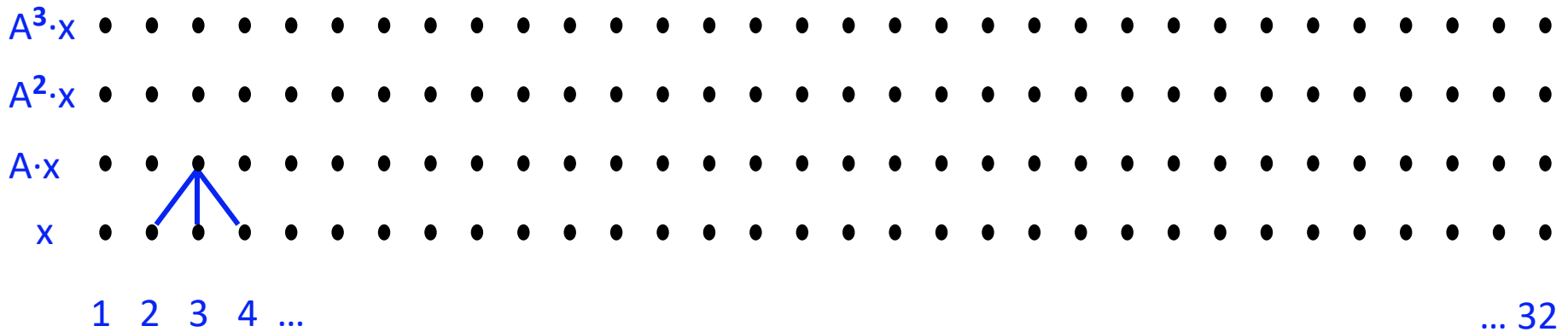


- Example: A tridiagonal, $n=32$, $k=3$
- Works for any “well-partitioned” A

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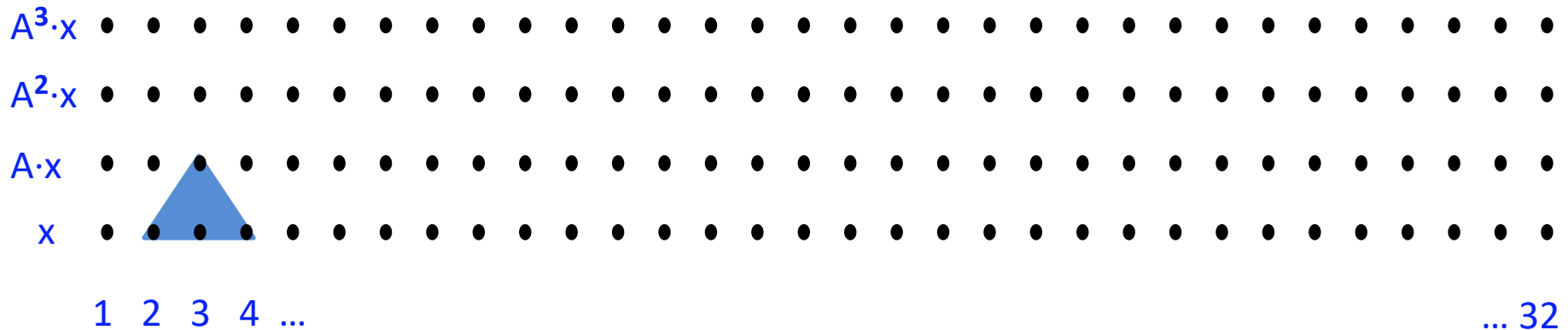


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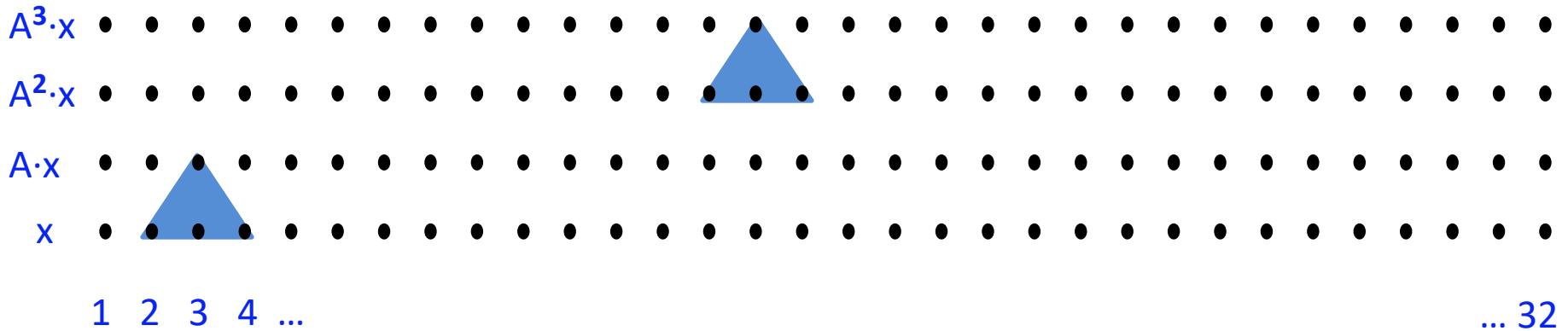


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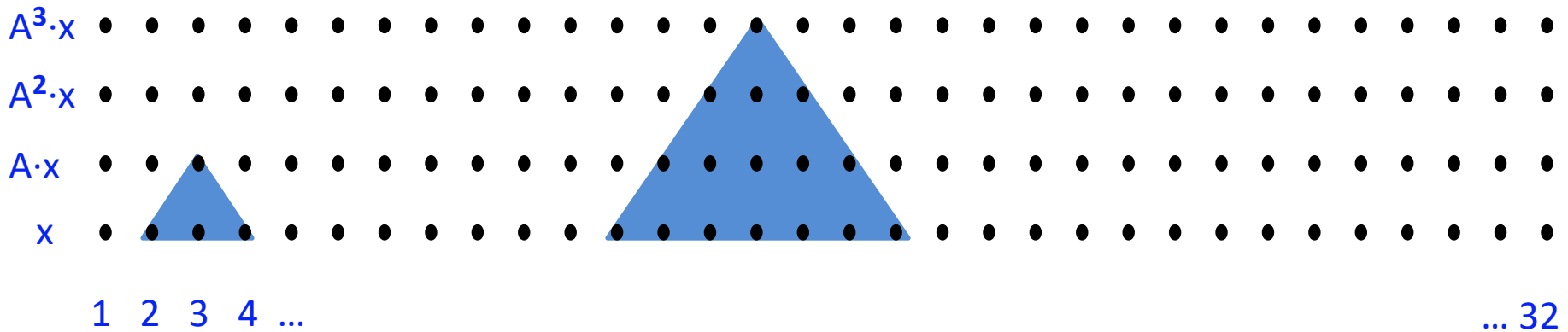


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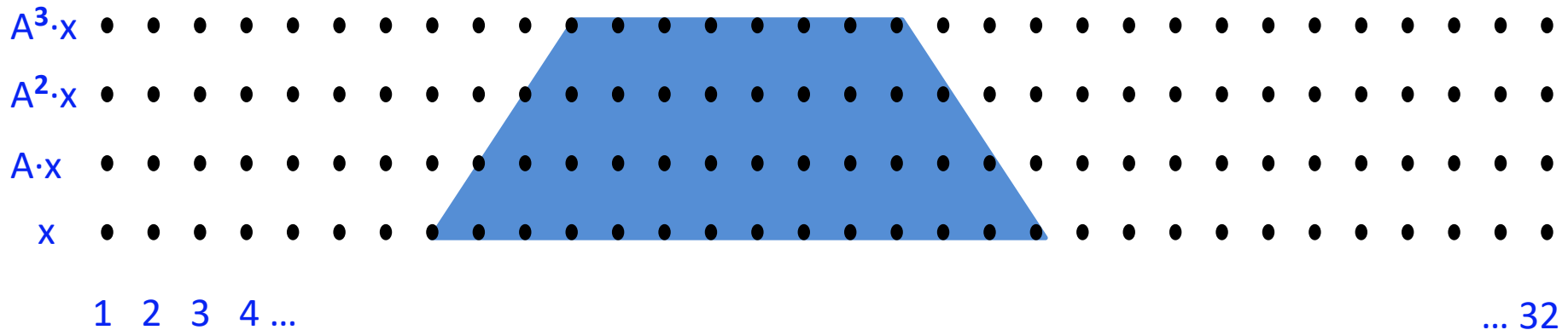


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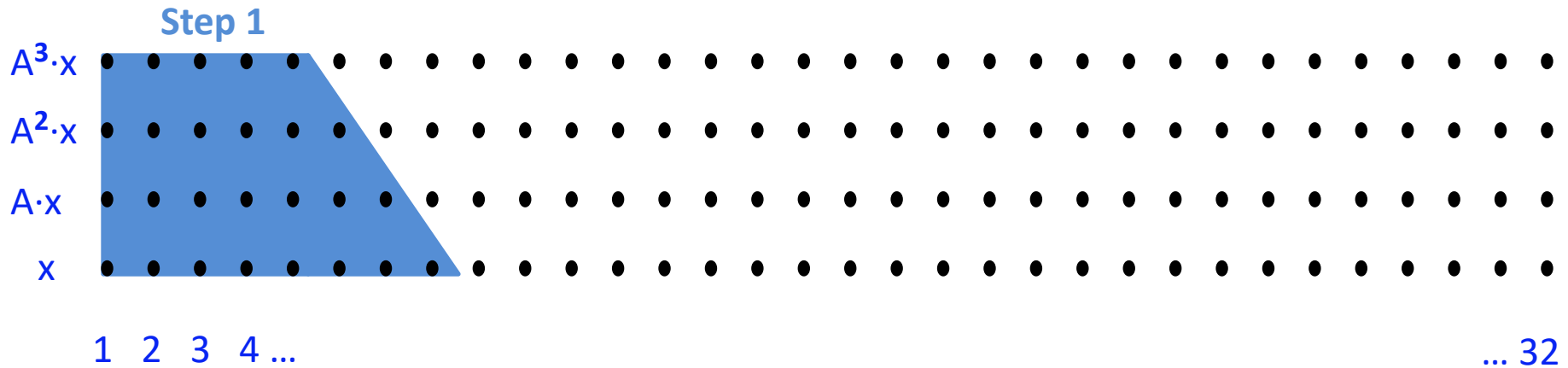


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- Sequential Algorithm

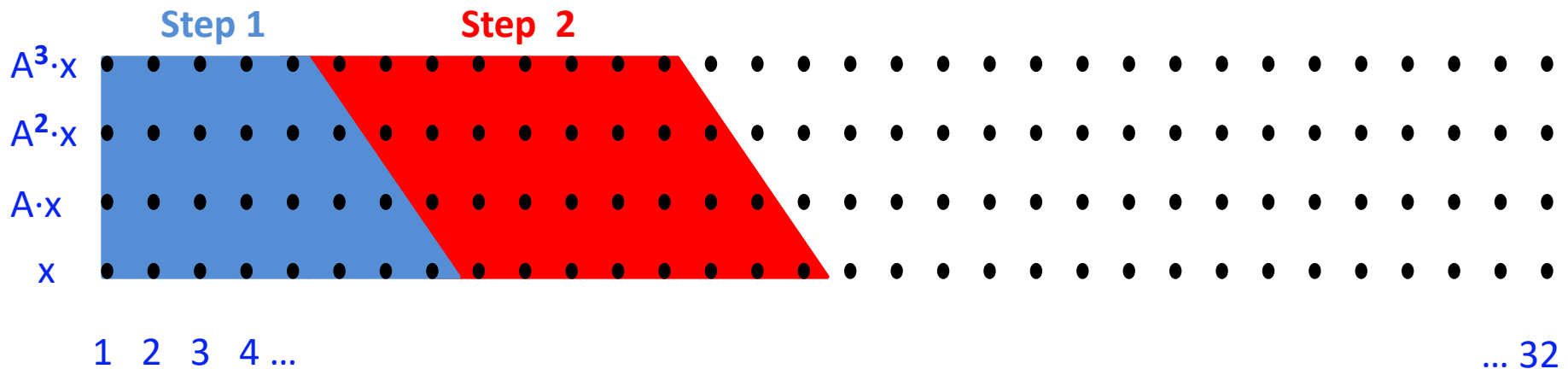


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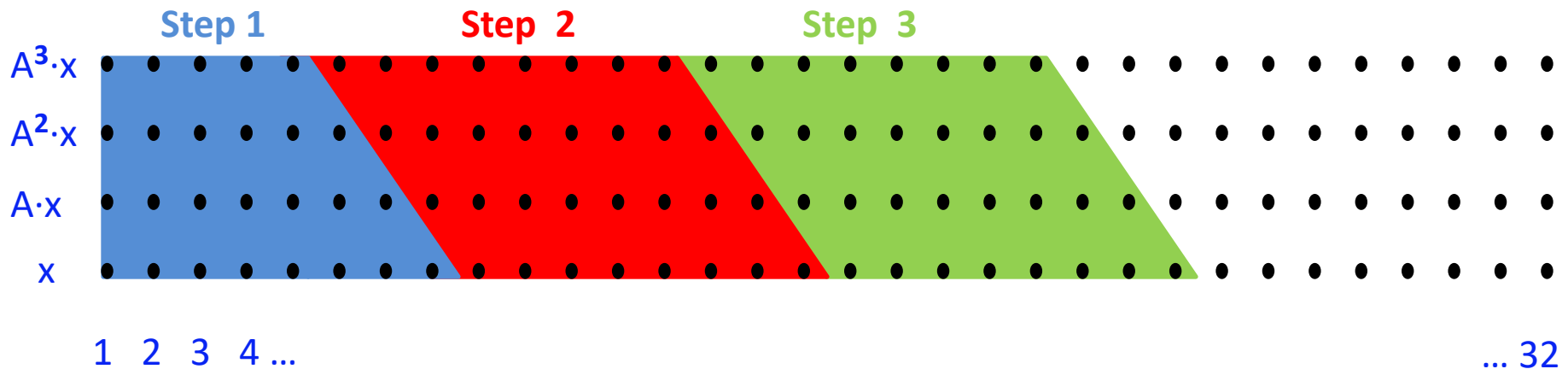


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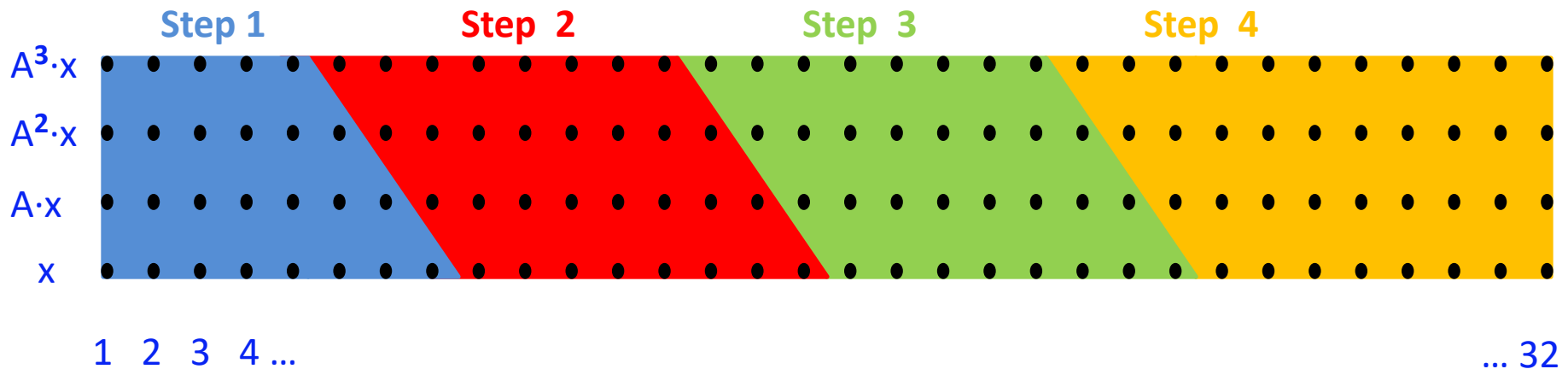


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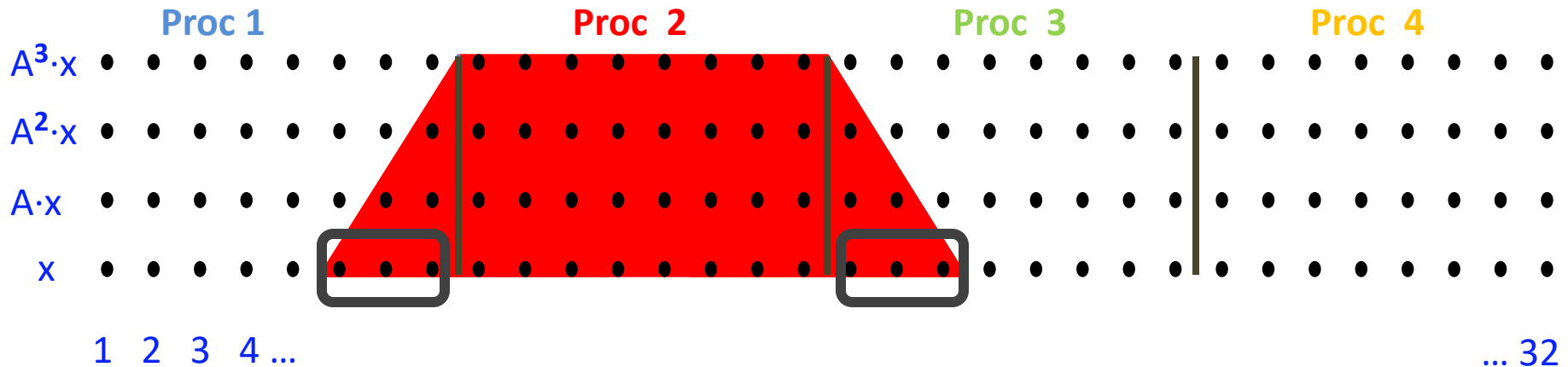


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- Parallel Algorithm

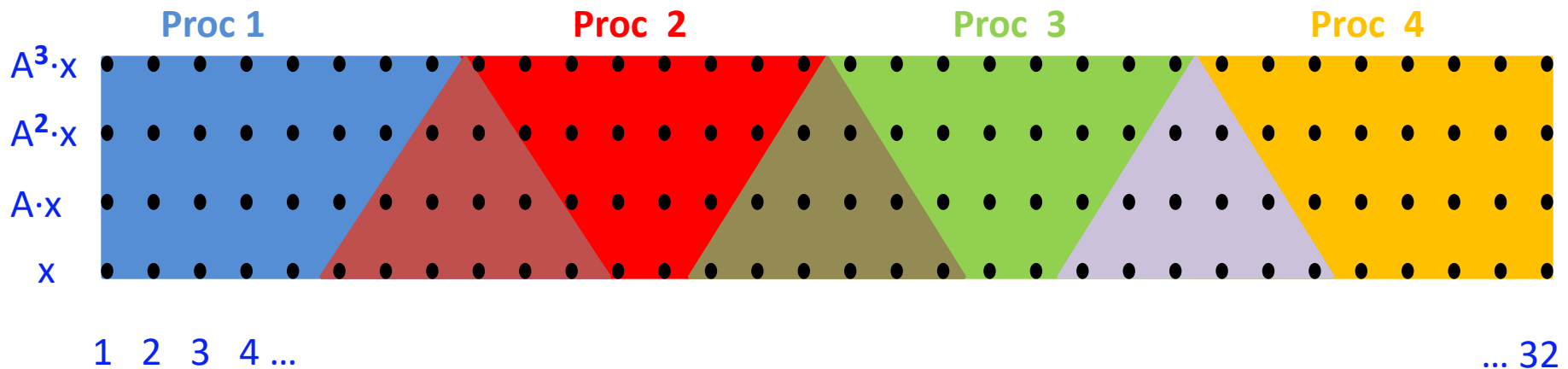


- Example: A tridiagonal, $n=32$, $k=3$
- Each processor communicates once with neighbors

Communication Avoiding Kernels:

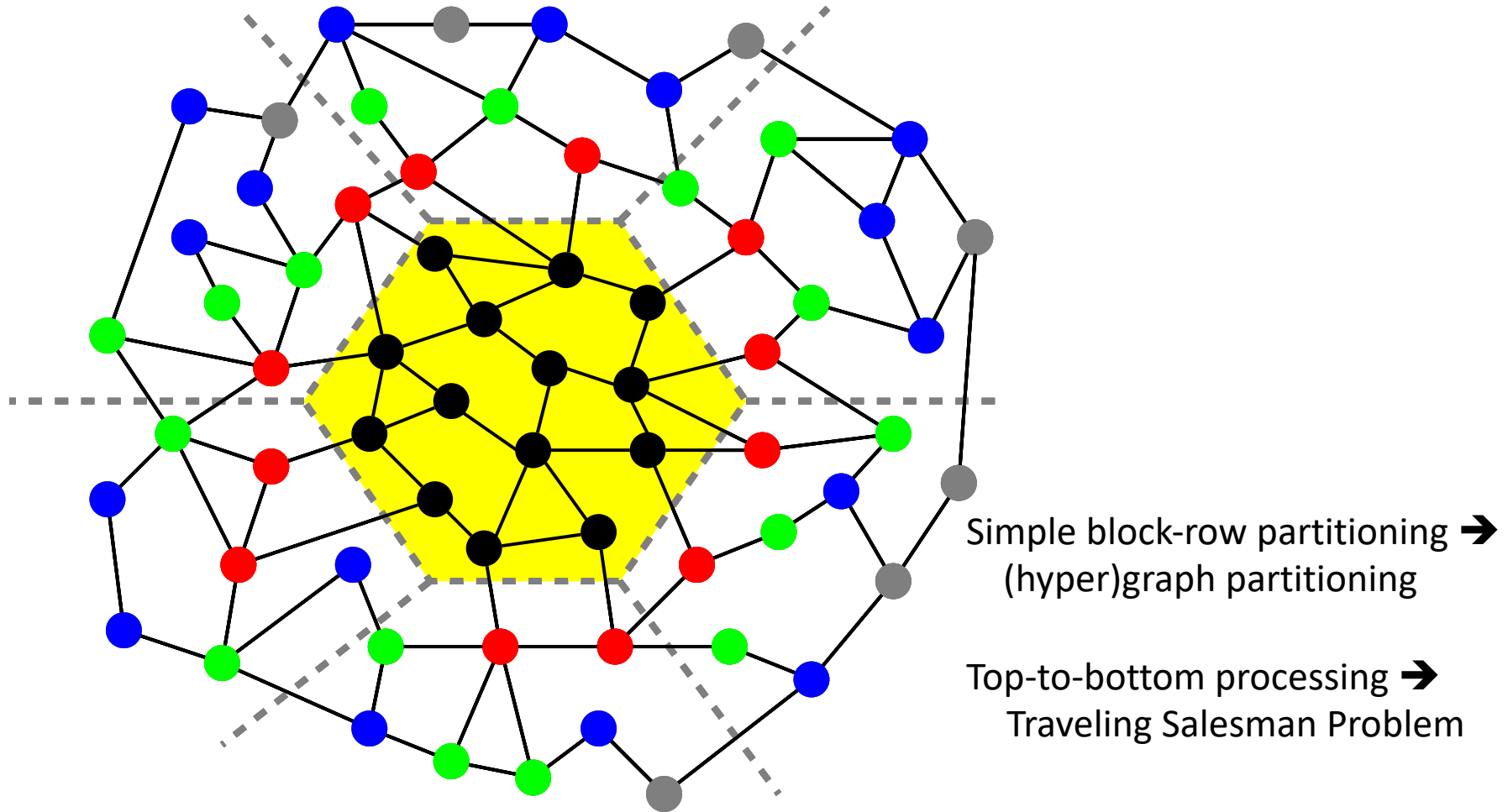
The Matrix Powers Kernel : $[Ax, A^2x, \dots, A^kx]$

- Replace k iterations of $y = A \cdot x$ with $[Ax, A^2x, \dots, A^kx]$
- Parallel Algorithm



- Example: A tridiagonal, $n=32$, $k=3$
- Each processor works on (overlapping) trapezoid

The Matrix Powers Kernel : $[Ax, A^2x, \dots, A^kx]$ on a general matrix (nearest k neighbors on a graph)



Same idea for general sparse matrices: k-wide neighboring region

Compute $r_0 = b - Ax_0$. Choose r_0^* arbitrary.

Set $p_0 = r_0$, $q_{-1} = 0_{N \times 1}$.

For $k = 0, 1, \dots$, until convergence, Do

$$P = [p_{sk}, Ap_{sk}, \dots, A^s p_{sk}]$$

$$Q = [q_{sk-1}, Aq_{sk-1}, \dots, A^s q_{sk-1}]$$

$$R = [r_{sk}, Ar_{sk}, \dots, A^s r_{sk}]$$

//Compute the $1 \times (3s+3)$ Gram vector.

$$g = (r_0^*)^T [P, Q, R]$$

//Compute the $(3s+3) \times (3s+3)$ Gram matrix

$$G = \begin{bmatrix} P^T \\ Q^T \\ R^T \end{bmatrix} [P \quad Q \quad R]$$

For $\ell = 0$ to s ,

$$b_{sk}^\ell = [B_1(:, \ell)^T, 0_{s+1}^T, 0_{s+1}^T]^T$$

$$c_{sk-1}^\ell = [0_{s+1}^T, B_2(:, \ell)^T, 0_{s+1}^T]^T$$

$$d_{sk}^\ell = [0_{s+1}^T, 0_{s+1}^T, B_3(:, \ell)^T]^T$$

1. Compute $r_0 := b - Ax_0$; r_0^* arbitrary;
2. $p_0 := r_0$.
3. For $j = 0, 1, \dots$, until convergence Do:
4. $\alpha_j := (r_j, r_0^*) / (Ap_j, r_0^*)$
5. $s_j := r_j - \alpha_j Ap_j$
6. $\omega_j := (As_j, s_j) / (As_j, As_j)$
7. $x_{j+1} := x_j + \alpha_j p_j + \omega_j s_j$
8. $r_{j+1} := s_j - \omega_j As_j$
9. $\beta_j := (r_{j+1}, r_0^*) / (r_j, r_0^*) \times \frac{\alpha_j}{\omega_j}$
10. $p_{j+1} := r_{j+1} + \beta_j (p_j - \omega_j Ap_j)$
11. EndDo

CA-BiCGStab

For $j = 0$ to $\lfloor \frac{s}{2} \rfloor - 1$, Do

$$\alpha_{sk+j} = \frac{\langle g, d_{sk+j}^0 \rangle}{\langle g, b_{sk+j}^1 \rangle}$$

$$q_{sk+j} = r_{sk+j} - \alpha_{sk+j} [P, Q, R] b_{sk+j}^1$$

For $\ell = 0$ to $s - 2j + 1$, Do

$$c_{sk+j}^\ell = d_{sk+j}^\ell - \alpha_{sk+j} b_{sk+j-1}^{\ell+1}$$

//such that $[P, Q, R] c_{sk+j}^\ell = A^\ell q_{sk+j}$

$$\omega_{sk+j} = \frac{\langle c_{sk+j+1}^1, Gc_{sk+j+1}^0 \rangle}{\langle c_{sk+j+1}^1, Gc_{sk+j+1}^1 \rangle}$$

$$x_{sk+j+1} = x_{sk+j} + \alpha_{sk+j} p_{sk+j} + \omega_{sk+j} q_{sk+j}$$

$$r_{sk+j+1} = q_{sk+j} - \omega_{sk+j} [P, Q, R] c_{sk+j+1}^1$$

For $\ell = 0$ to $s - 2j$, Do

$$d_{sk+j+1}^\ell = c_{sk+j+1}^\ell - \omega_{sk+j} c_{sk+j+1}^{\ell+1}$$

//such that $[P, Q, R] d_{sk+j+1}^\ell = A^\ell r_{sk+j+1}$

$$\beta_{sk+j} = \frac{\langle g, d_{sk+j+1}^0 \rangle}{\langle g, d_{sk+j}^0 \rangle} \times \frac{\alpha}{\omega}$$

$$p_{sk+j+1} = r_{sk+j+1} + \beta_{sk+j} p_{sk+j} - \beta_{sk+j} \omega_{sk+j} [P, Q, R] b_{sk+j}^1$$

For $\ell = 0$ to $s - 2j$, Do

$$b_{sk+j+1}^\ell = d_{sk+j+1}^\ell + \beta_{sk+j} b_{sk+j}^\ell - \beta_{sk+j} \omega_{sk+j} b_{sk+j}^{\ell+1}$$

//such that $[P, Q, R] b_{sk+j+1}^\ell = A^\ell p_{sk+j+1}$.

EndDo

EndDo

Outline

- Linear Algebra
 - Communication Lower Bounds for classical direct linear algebra
 - CA 2.5D Matmul
 - TSQR - Tall-Skinny QR
 - Iterative Methods for linear algebra
- **Machine Learning**
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 - Convolutional Neural Nets
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Training Neural Nets by Mini-Batch Stochastic Gradient Descent (SGD)

(You, Zhang, Hsieh, D., Keutzer, IPDPS 18)

- Iterate:
 - Pick a mini-batch of B data points
 - Update weights $W = W - \eta \cdot \nabla L(W)$
 - η = learning rate
 - $\nabla L(W)$ = gradient
- Data parallel version on P processors
 - Data partitioned, each processor gets B/P points
 - W_i replicated
 - Each processor computes $\nabla L(W)_i$ wrt its data
 - All-reduce: each processor computes
$$W_i = W_i - (\eta/P) \cdot \sum_{i=1}^P \nabla L(W)_i$$

$$\text{SGD: } W_i = W_i - (\eta/P) \cdot \sum_{i=1}^P \nabla L(W)_i$$

- Increase P to go faster: What are the bottlenecks?
- B/P decreases \Rightarrow less work per processor
 - Small matrix operations \Rightarrow locally communication bound
- Cost of each reduction $\sum_i \nabla L(W)_i$ grows
- Solution: increase B along with P
 - Maintain B/P \Rightarrow maintain processor efficiency
 - Try to converge in same #epochs (passes over data)
 - Same overall work, fewer reductions
- Oops: Convergence can be much worse
 - Convergence rate, test accuracy

Improving SGD convergence as B grows

- Facebook's strategy: adjust learning rate η
 - Increase B to kB \Rightarrow increase η to $k\eta$
 - Warmup rule: Start with smaller η , then increase
- Only worked up to B=1K for AlexNet (tried lots of tuning)
- Fix: Add Layer-wise Adaptive Rate Scaling (LARS)
 - $\|W\|/\|\nabla L(W)\|$ can vary by 233x between AlexNet layers
 - Let η be proportional to $\|W\|/\|\nabla L(W)\|$
 - (You, Gitman, Ginsburg, 2017)
 - Also need momentum, weight decay

ImageNet Training in Minutes

Speedup for AlexNet (for batchsize = 32K, changed LRN to BN)

Batch Size	Epochs	Top-1 Accuracy	Platform	Time
256	100	58.7%	8-core + K20 GPU	144 hrs
512	100	58.8%	DGX-1 station	6h 10m
4096	100	58.4%	DGX-1 station	2h 19m
32k	100	58.6%	512 KNLs	24m
32k	100	58.6%	1024 CPUs	11m

Speedup for ResNet50

Batch Size	Epochs	Top-1 Accuracy	Platform	Time
32	90	75.3%	CPU + M40 GPU	336h
256	90	75.3%	16 KNLs	45h
32K	90	75.4%	512 KNLs	60m
32K	90	75.4%	1600 CPUs	32m
32K	90	75.4%	2048 KNLs	20m

135x

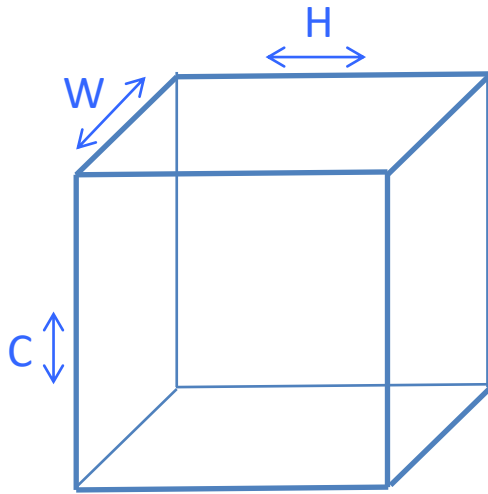
ImageNet Training in Minutes

- Best Paper Prize at ICPP 2018
- Open Source in Caffe, NVIDIA Caffe, Facebook Caffe 2 (PyTorch)
- Media coverage by CACM, EureKalert, Intel, NSF, Science Daily, Science NewsLine, etc.
- Subsequent work at Tencent reached 4 minutes
- LARS adopted by industry standard benchmark MLPerf in 2019

Outline

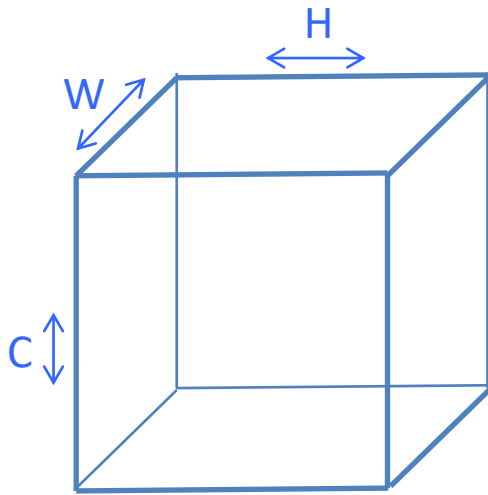
- Linear Algebra
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What CNNs compute

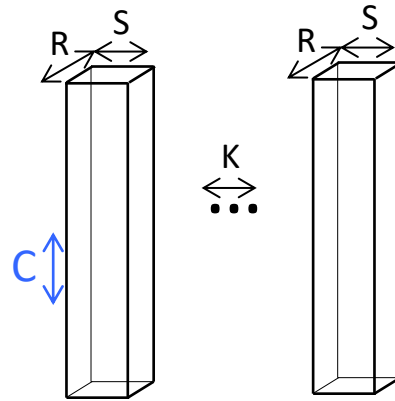


Image

What CNNs compute

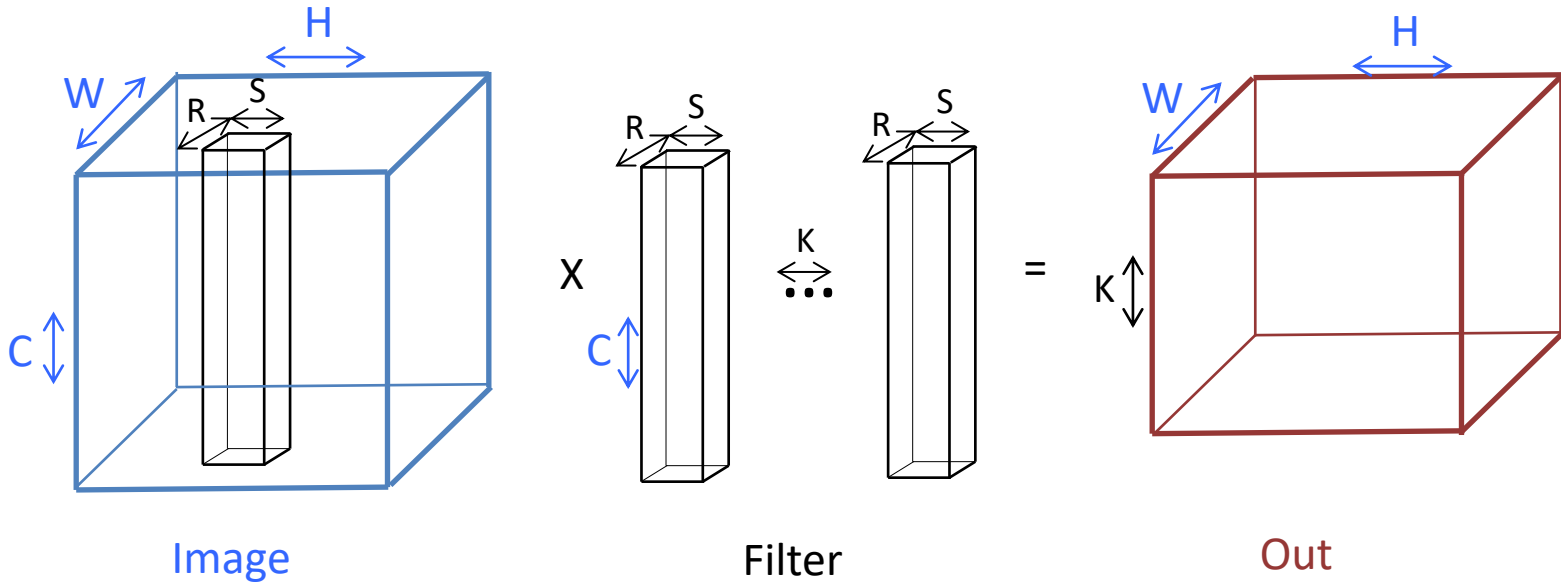


Image

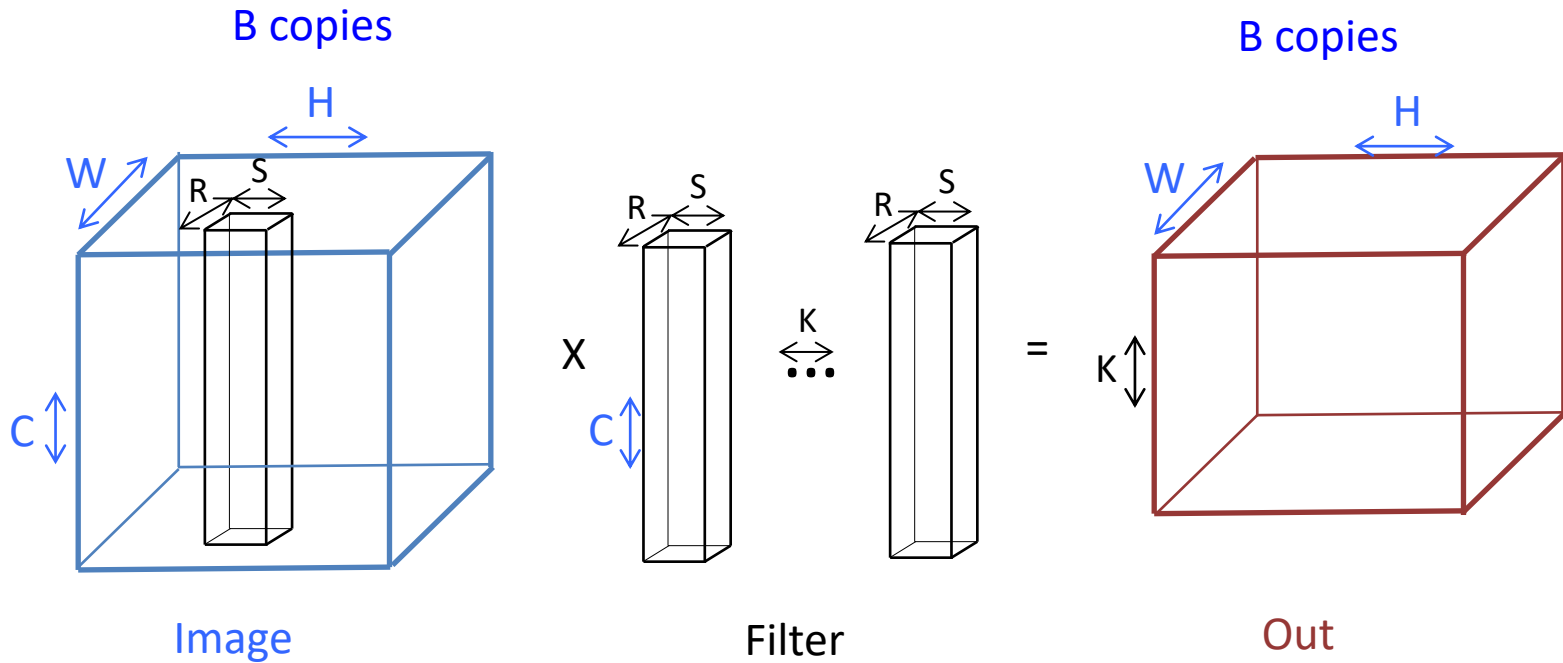


Filter

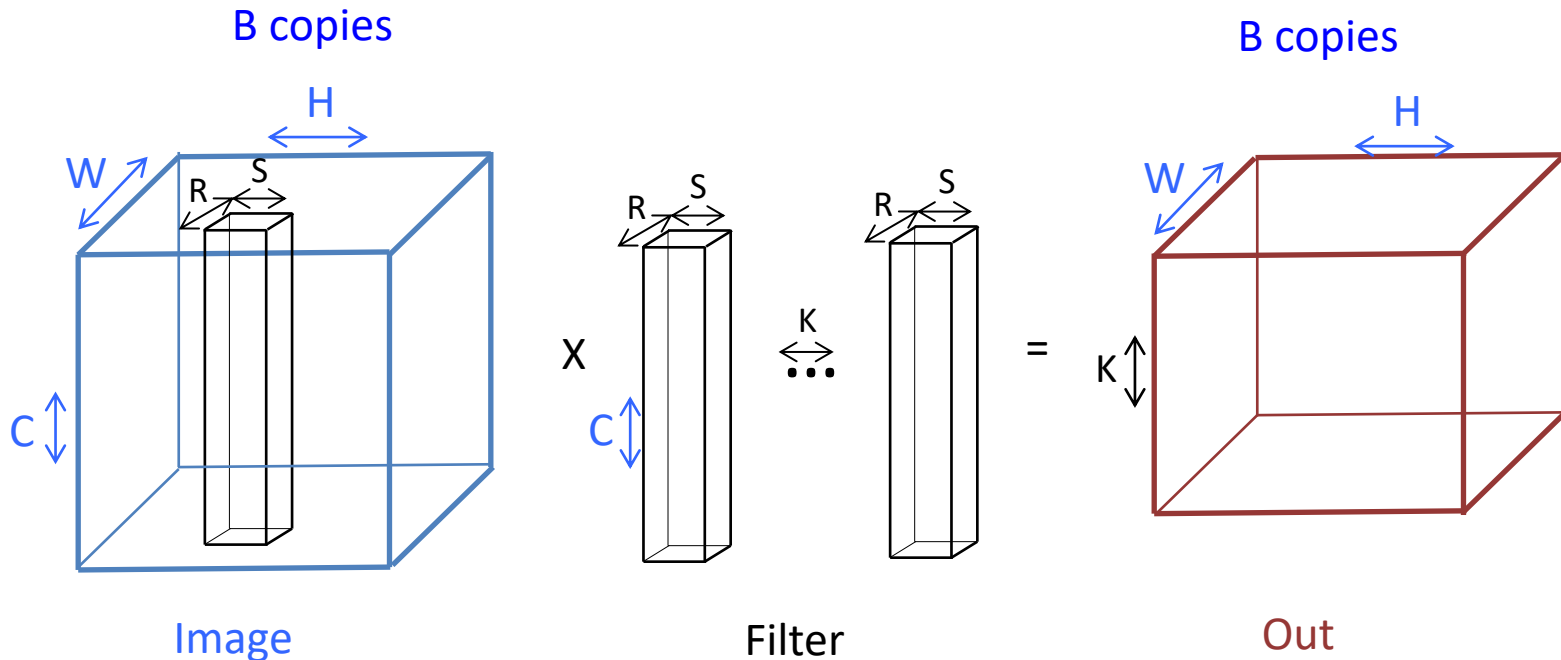
What CNNs compute



What CNNs compute



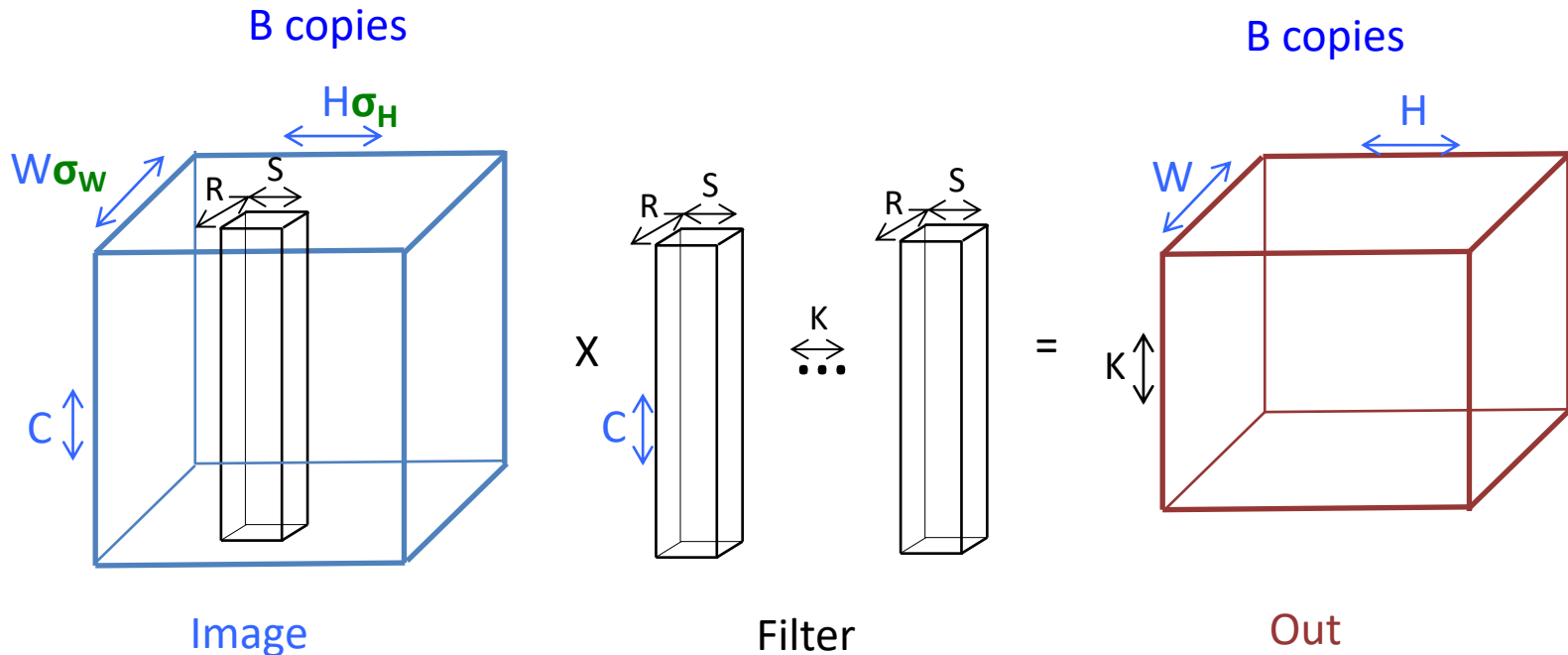
What CNNs compute



for $k=1:K$, for $h=1:H$, for $w=1:W$, for $r=1:R$,
for $s=1:S$, for $c=1:C$, for $b=1:B$

$$\text{Out}(k, h, w, b) += \text{Image}(r+w, s+h, c, b) * \text{Filter}(k, r, s, c)$$

What CNNs compute



for $k=1:K$, for $h=1:H$, for $w=1:W$, for $r=1:R$,
for $s=1:S$, for $c=1:C$, for $b=1:B$

$$\text{Out}(k, h, w, b) += \text{Image}(r + \sigma_W w, s + \sigma_H h, c, b) * \text{Filter}(k, r, s, c)$$

Communication Lower Bound for CNNs

- Let $N = \#iterations = KHWRSCB$, $M = \text{cache size}$
- $\#words\ moved = \Omega(\max(\dots 5\ \text{terms})$
 - BKHW, ... size of Out
 - $\sigma_H\sigma_W BCWH$, ... size of Image
 - CKRS, ... size of Filter
 - N/M , ... lower bound for large loop bounds
 - $N/(M^{1/2} (RS/(\sigma_H\sigma_W))^{1/2})$... lower bound for small filters)
- Any one of 5 terms may be largest
- Bottommost bound beats matmul by factor $(RS/(\sigma_H\sigma_W))^{1/2}$
 - Applies in common case when data does not fit in cache, but one $R \times S$ filter does
 - Tile needed to attain N/M too big to fit in loop bounds
- Thm: Always attainable! (computer generated proof)
 - Beats im2col in data movement for various practical sizes
- Improved constants in PASC'22
- Chen/Han/Wang (arxiv:1911.05662v3): HW accelerator

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Communication lower bounds and optimal algorithms for general loop nests

- for $i = 1:n$, for $j=1:n$, for $k = 1:n$
 $C(i,j) = C(i,j) + A(i,k)*B(k,j)$
- #Words moved between main memory and cache of size $M = \Omega(n^3 / M^{1/2})$, attainable
- For $(i_1, i_2, \dots, i_k) \in S \subseteq \mathbb{Z}^k$, do something with
 - $A(i_1), B(i_2, i_3+i_4), C(i_1-i_2, i_2+3*i_3- 5*i_4 +2, \dots), \dots$
- Thm: #Words moved = $\Omega(|S| / M^{e_{HBL}})$
(Christ, D., Knight, Scanlon, Yelick)
 - HBL = Hölder / Brascamp / Lieb
 - Uses results by Christ, Tao, others
- Thm: There exists an optimal tiling that attains this lower bound (D., Rusciano)

What's left?

- Dealing with small loop bounds
 - Ex: Matvec special case of Matmul, not optimizable
 - Special cases: CNNs
 - Thm: If all subscripts like $(i), (i,j)$, etc, and $S =$ parallelepiped, \exists tighter, attainable lower bound $(D., D_{inh})$
- Dealing with dependencies
 - Special cases: Linear algebra outside matmul, Floyd-Warshall, ...
- More realistic performance models than α, β, γ
 - Variable precision
 - Heterogeneous processors, accelerators, network topologies, differing costs of read and writes, ...
- Need to automate! (i.e. compilers)

Collaborators and Supporters

- **James Demmel, Kathy Yelick**, Vivek Bharadwaj, Grace Dinh, Tianyu Liang
- Peter Ahrens, Michael Anderson, Grey Ballard, Austin Benson, Erin Carson, Maryam Dehnavi, Aditya Devakonda, Michael Driscoll, David Eliahu, Andrew Gearhart, Evangelos Georganas, Mark Hoemmen, Shoaib Kamil, , Nicholas Knight, Penporn Koanantakool, Ben Lipshitz, Marghoob Mohiyuddin, Hong Diep Nguyen, Jason Riedy, Alex Rusciano, Oded Schwartz, Edgar Solomonik, Omer Spillinger, Yang You
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- bebop.cs.berkeley.edu

For more details

- Bebop.cs.berkeley.edu
 - 155 page linear algebra survey in Acta Numerica (2014)
 - Book in progress (with Ballard, Carson, Grigori)
- CS267 – Berkeley’s Parallel Computing Course
 - Slides available at <https://sites.google.com/lbl.gov/cs267-spr2023>
 - Recorded lectures also available at <https://sites.google.com/lbl.gov/cs267-spr2022>

Summary

Time to redesign all
linear algebra, machine learning, n-body, ...
algorithms and software, and compilers

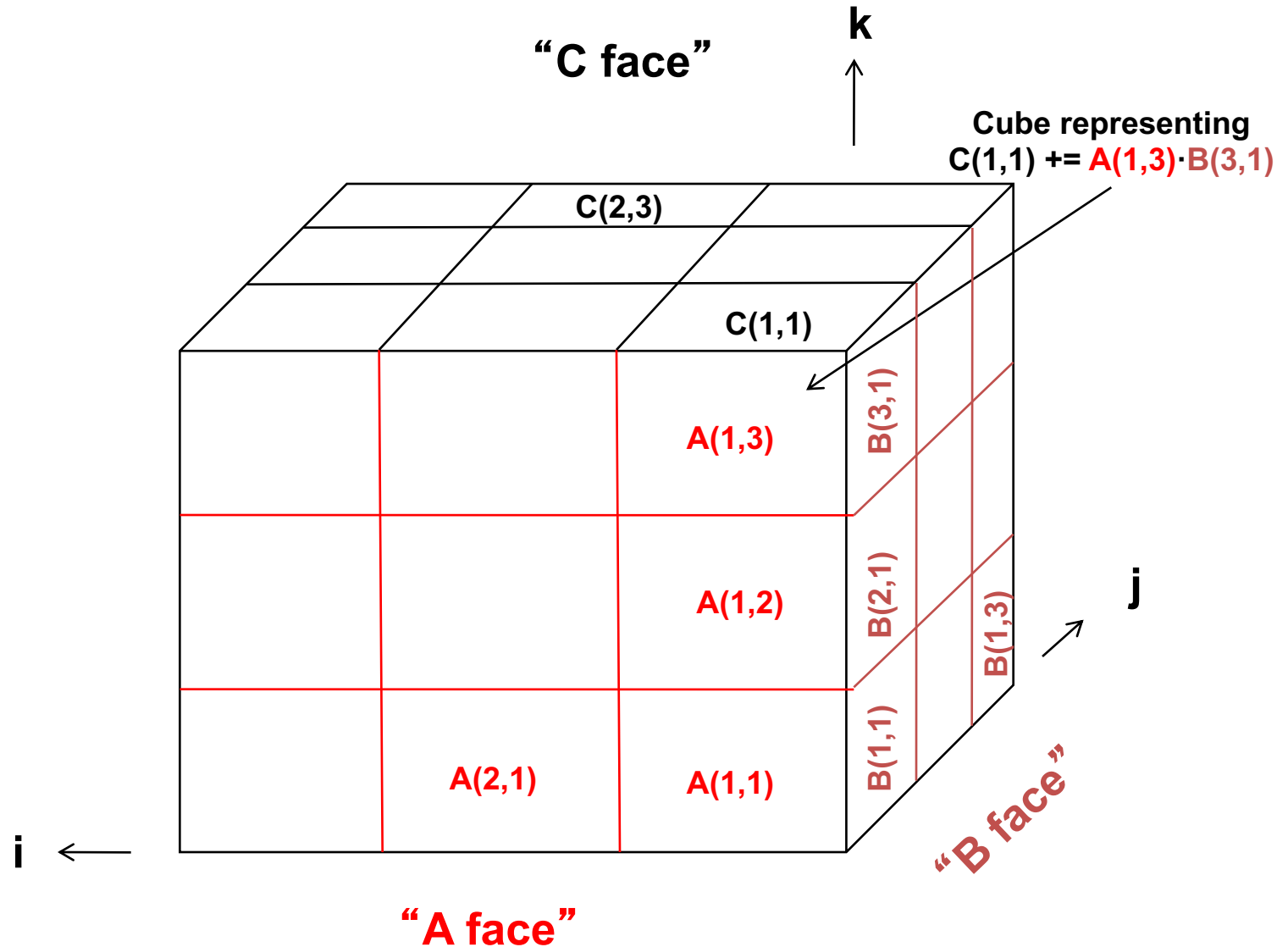
Don't Communic...

Backup slides

Proof of Communication Lower Bound on $C = A \cdot B$ (1/4)

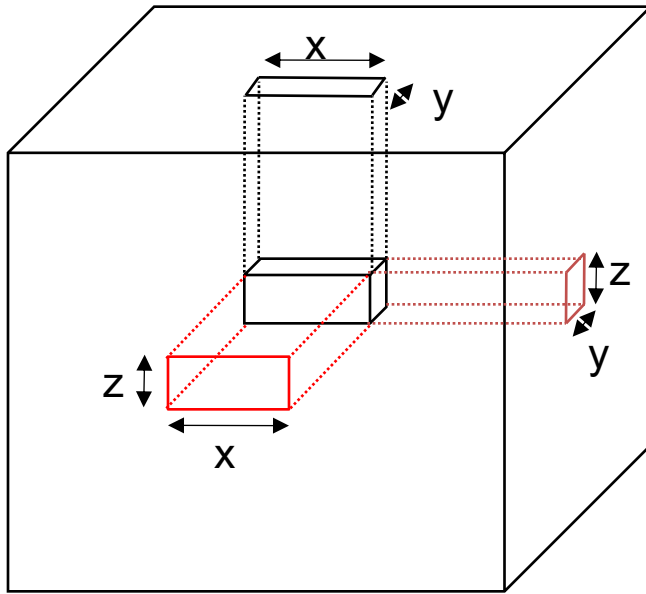
- Basic Counting Argument:
 - Only M entries of A , B and C are available in cache
 - Find an upper bound F on the number of different iterations $C(i,j) = C(i,j) + A(i,k) \cdot B(k,j)$ we can perform
 - Need to refill cache n^3/F times to complete algorithm
 - Need to read/write at least $M n^3/ F$ words to/from cache
- Represent iterations and data geometrically

Proof of Communication Lower Bound on $C = A \cdot B$ (2/4)

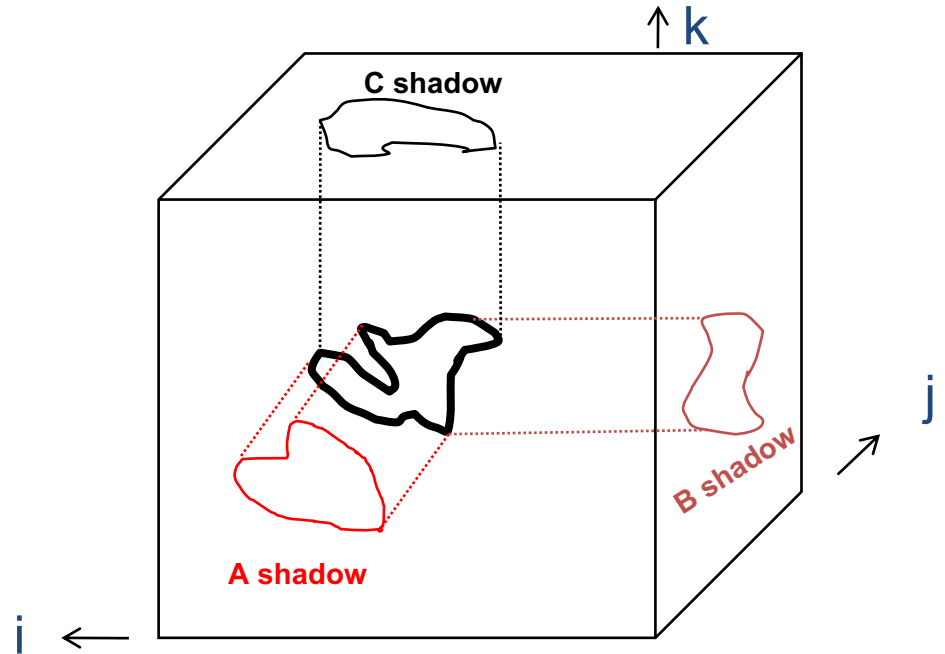


- If we have at most M “A squares”, “B squares”, and “C squares” on faces, how many cubes can we have?

Proof of Communication Lower Bound on $C = A \cdot B$ (3/4)



cubes in black box with
 side lengths x , y and z
 = Volume of black box
 = $x \cdot y \cdot z$
 = $(xz \cdot zy \cdot yx)^{1/2}$
 = $(\#A \square s \cdot \#B \square s \cdot \#C \square s)^{1/2}$



(i,k) is in **A shadow** if (i,j,k) in 3D set
 (j,k) is in **B shadow** if (i,j,k) in 3D set
 (i,j) is in **C shadow** if (i,j,k) in 3D set

Thm (Loomis & Whitney, 1949)

cubes in 3D set = Volume of 3D set
 $\leq (\text{area}(\mathbf{A shadow}) \cdot \text{area}(\mathbf{B shadow}) \cdot \text{area}(\mathbf{C shadow}))^{1/2}$

Proof of Communication Lower Bound on $C = A \cdot B$ (4/4)

- # loop iterations doable with M words of data = #cubes
 $\leq (\text{area}(A \text{ shadow}) \cdot \text{area}(B \text{ shadow}) \cdot \text{area}(C \text{ shadow}))^{1/2}$
 $\leq (M \cdot M \cdot M)^{1/2} = M^{3/2} = F$
- Need to read/write at least $M n^3 / F = \Omega(n^3 / M^{1/2}) = \Omega(\text{\#loop iterations} / M^{1/2})$ words to/from cache