Communication-Avoiding Algorithms for Linear Algebra and Beyond

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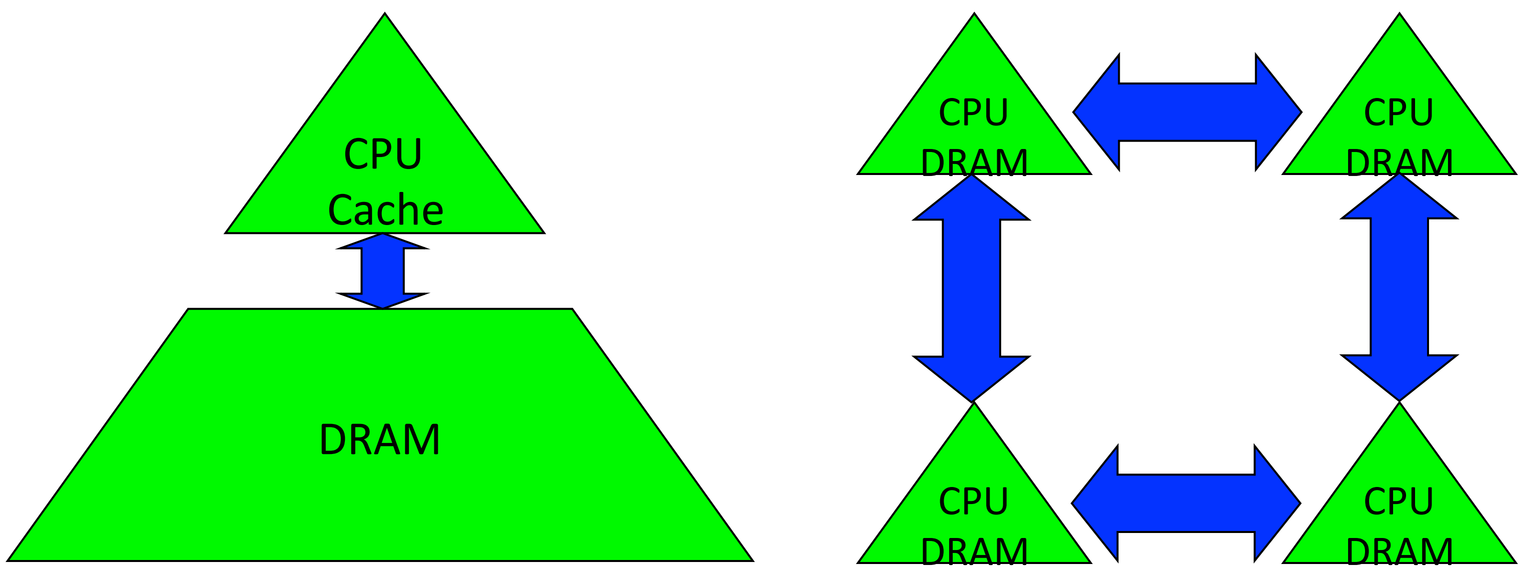
Why avoid communication? (1/3)

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

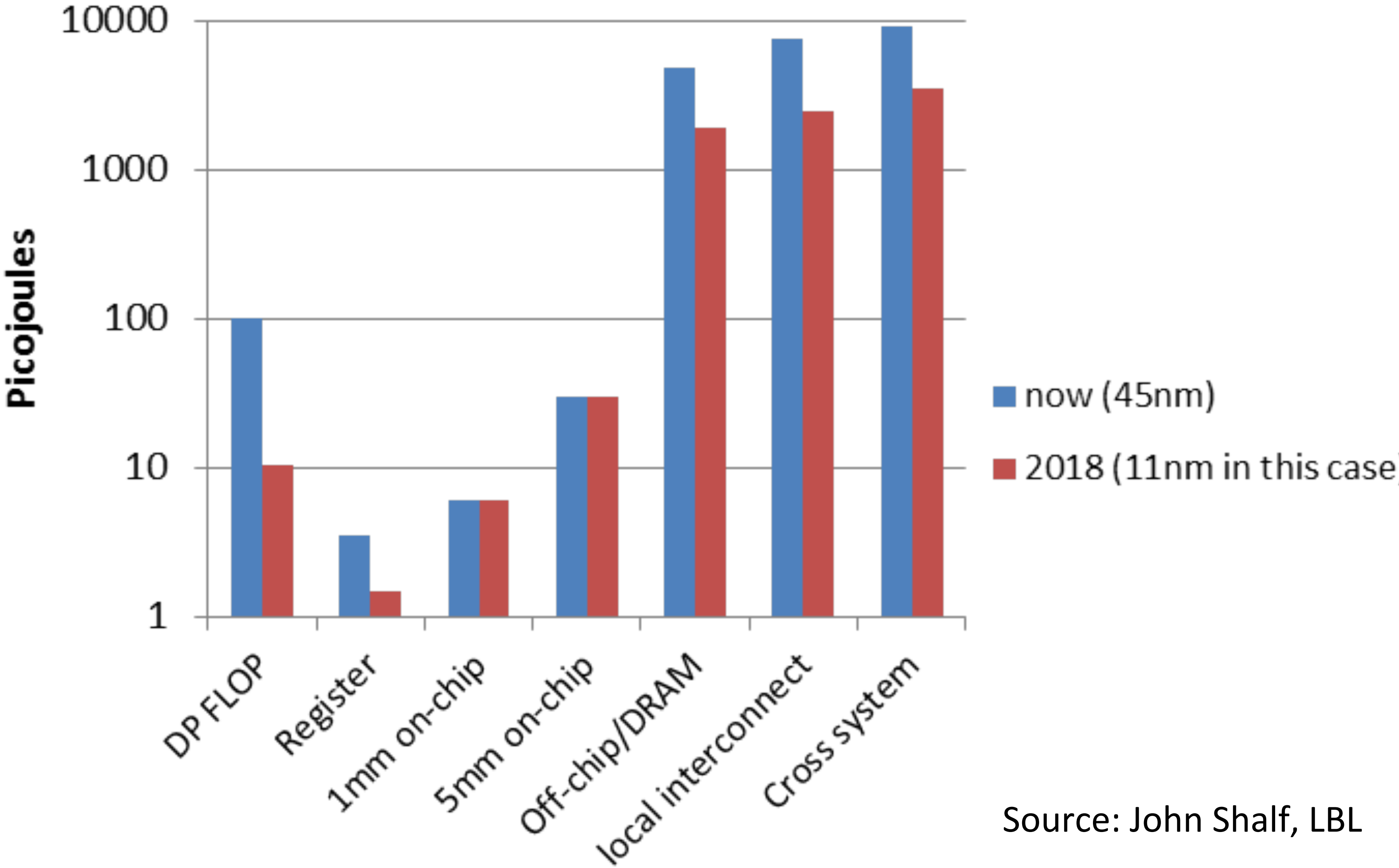
communication

- Time_per_flop << 1/ bandwidth << latency
  - Gaps growing exponentially with time [FOSC]

Annual improvements			
Time_per_flop		Bandwidth	Latency
59%	Network	26%	15%
	DRAM	23%	5%

- Avoid communication to save time

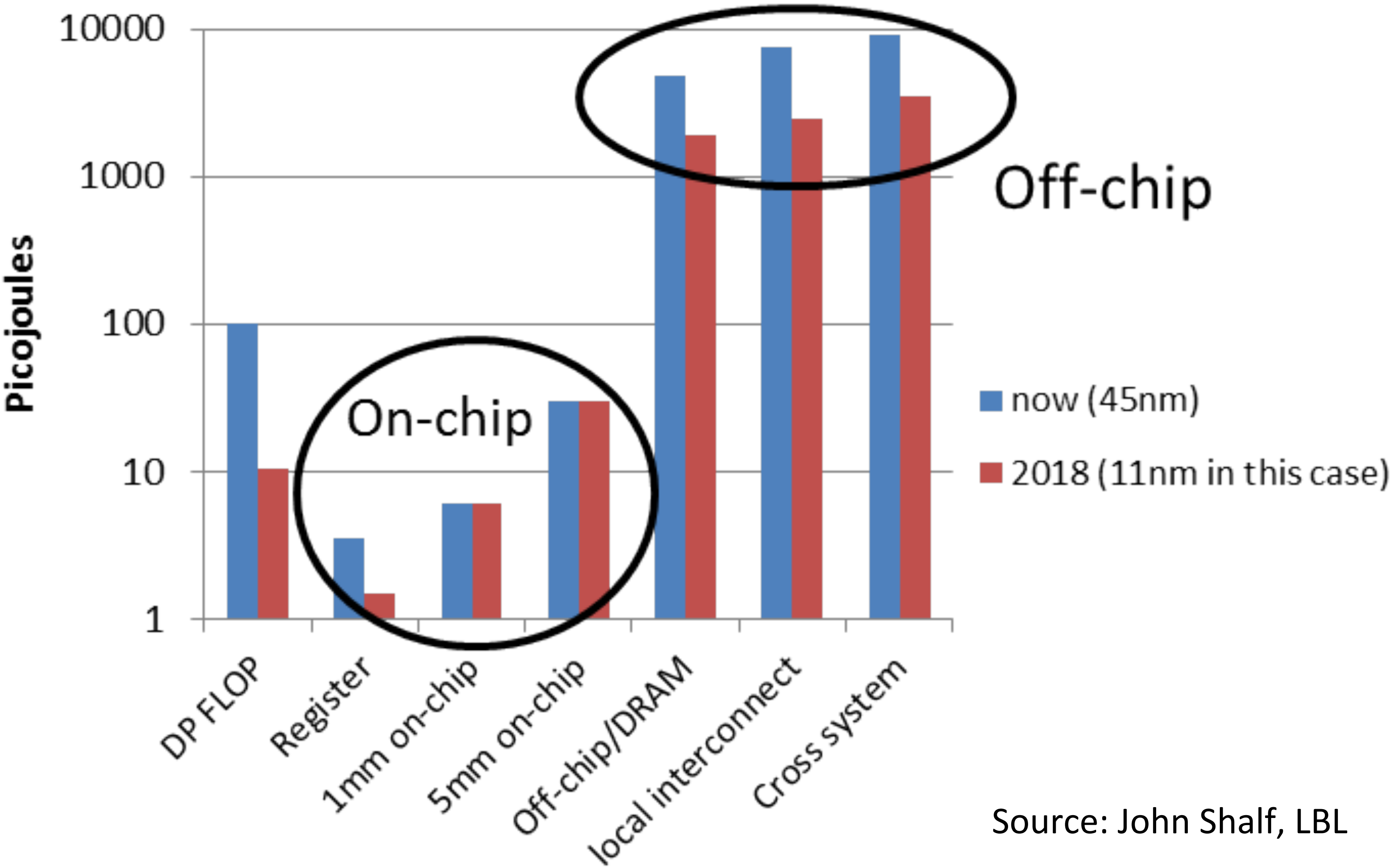
Why Minimize Communication? (3/3)



Source: John Shalf, LBL

Why Minimize Communication? (3/3)

Minimize communication to save energy



Source: John Shalf, LBL

Goals

- Redesign algorithms to *avoid* communication
  - Between all memory hierarchy levels
    - L1 $\leftrightarrow$ L2 $\leftrightarrow$ DRAM $\leftrightarrow$ network, etc
- Attain lower bounds if possible
  - Current algorithms often far from lower bounds
  - Large speedups and energy savings possible
- New lower bounds, optimal algorithms, for
  - Direct linear algebra (matmul, LU, QR, SVD, etc.)
  - Iterative linear algebra (conjugate grad., etc.)
  - Other algorithms that access arrays (n-body, etc.)

President Obama cites Communication-Avoiding Algorithms in the FY 2012 Department of Energy Budget Request to Congress:

"New Algorithm Improves Performance and Accuracy on Extreme-Scale Computing Systems. **On modern computer architectures, communication between processors takes longer than the performance of a floating point arithmetic operation by a given processor.** ASCR researchers have developed a new method, derived from commonly used linear algebra methods, to **minimize communications between processors and the memory hierarchy, by reformulating the communication patterns specified within the algorithm**. This method has been implemented in the TRILINOS framework, a highly-regarded suite of software, which provides functionality for researchers around the world to solve large scale, complex multi-physics problems."

FY 2010 Congressional Budget, Volume 4, FY2010 Accomplishments, Advanced Scientific Computing Research (ASCR), pages 65-67.

CA-GMRES (Hoemmen, Mohiyuddin, Yelick, JD)
"Tall-Skinny" QR (Grigori, Hoemmen, Langou, JD)

Outline

- Survey state of the art of CA (Comm-Avoiding) algorithms
  - CA $O(n^3)$ 2.5D Matmul
  - *APSP: All-Pairs-Shortest-Pahts (Buluc, Monday)*
  - *TSQR: Tall-Skinny QR (Gleich, Tuesday)*
  - *CA Strassen Matmul (Ballard, Tuesday)*
- Beyond linear algebra
  - Extending lower bounds to any algorithm with arrays
  - Communication-optimal N-body algorithm, join (?)
- CA-Krylov methods

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Lower bound for all "n^3-like" linear algebra

- Let M = "fast" memory size (per processor)

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

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

Lower bound for all "n^3-like" linear algebra

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

#messages_sent ≥ #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 << 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

Can we attain these lower bounds?

- Do conventional dense algorithms as implemented in LAPACK and ScaLAPACK attain these bounds?
  - Often not
- If not, are there other algorithms that do?
  - Yes, for much of dense linear algebra
  - New algorithms, with new numerical properties, new ways to encode answers, new data structures
  - Not just loop transformations (need those too!)
  - Being added to Sca/LAPACK, PLASMA, MAGMA, …
- Only a few sparse algorithms so far
- Lots of work in progress
- Ditto for iterative linear algebra

Summary of dense *parallel* algorithms attaining communication lower bounds

- Assume nxn 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 = $\Omega((n^3/ P) / M^{3/2}) = \Omega(P^{1/2})$
- 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?

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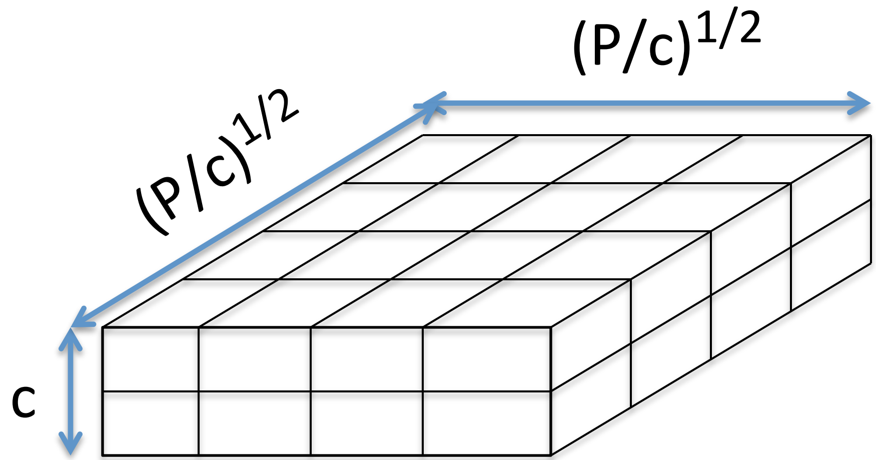
2.5D Matrix Multiplication

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



Example: P = 32, c = 2

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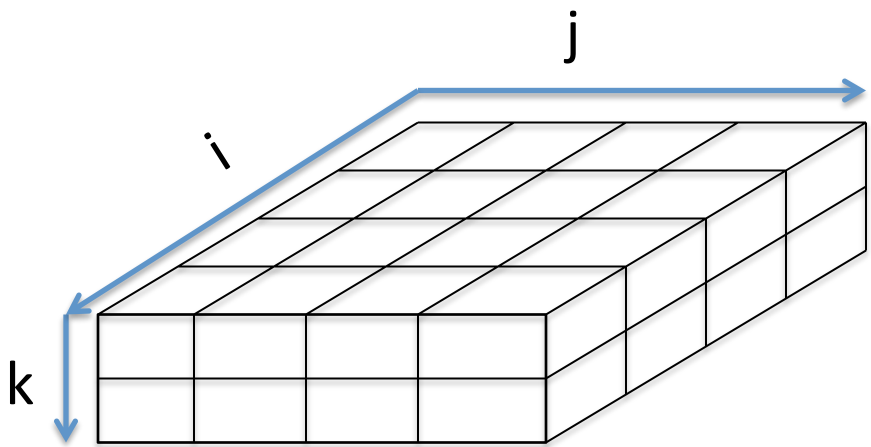
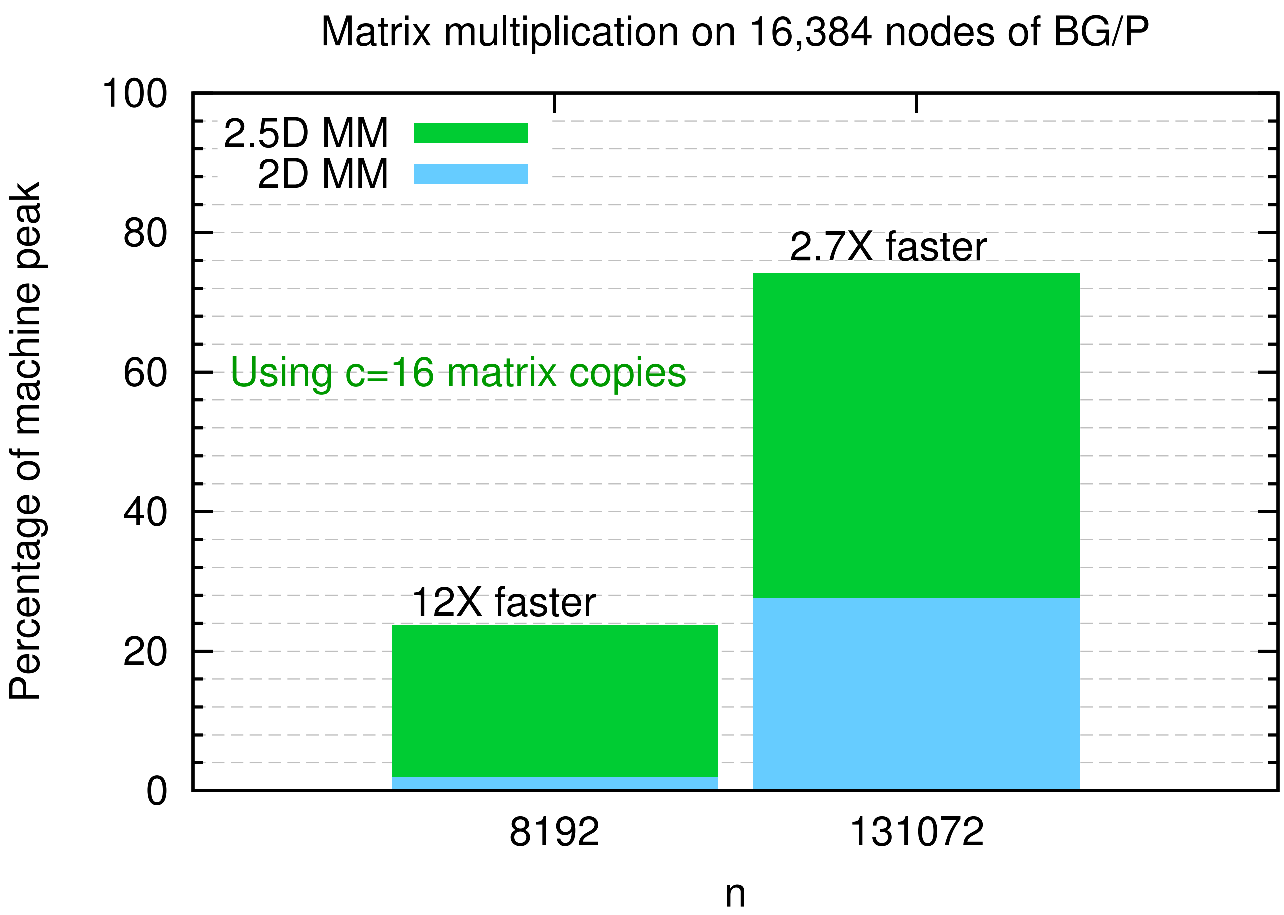


Initially P(i,j,0) owns A(i,j) and B(i,j) each of size $n(c/P)^{1/2} \times n(c/P)^{1/2}$

(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 Σ_m A(i,m)*B(m,j)
(3) Sum-reduce partial sums Σ_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



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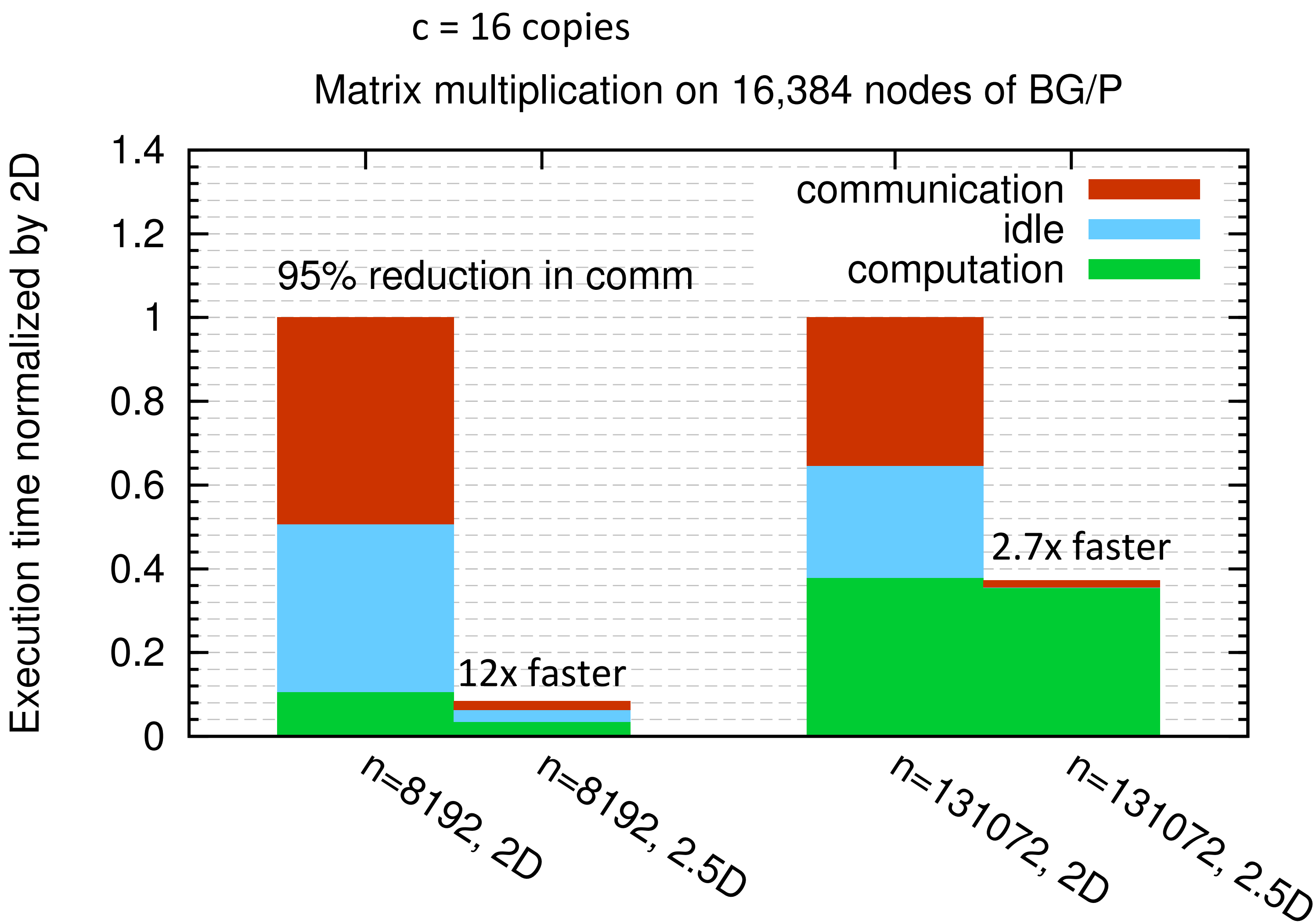

Distinguished Paper Award, EuroPar'11 (Solomonik, D.)
SC'11 paper by Solomonik, Bhatele, D.

Perfect Strong Scaling – in Time and Energy

- Every time you add a processor, you should use its memory M too
- Start with minimal number of procs: $PM = 3n^2$
- Increase P by a factor of c ➔ total memory increases by a factor of c
- Notation for timing model:
  - γ_T, β_T, α_T = secs per flop, per word_moved, per message of size m
- $T(cP) = n^3/(cP)\ [\ \gamma_T + \beta_T/M^{1/2} + \alpha_T/(mM^{1/2})\ ]$

  $= T(P)/c$
- Notation for energy model:
  - γ_E, β_E, α_E = joules for same operations
  - δ_E = joules per word of memory used per sec
  - ε_E = joules per sec for leakage, etc.
- $E(cP) = cP\ \{\ n^3/(cP)\ [\ \gamma_E + \beta_E/M^{1/2} + \alpha_E/(mM^{1/2})\ ] + \delta_E M T(cP) + \varepsilon_E T(cP)\ \}$

  $= E(P)$
- Perfect scaling extends to N-body, Strassen, …

Ongoing Work

- Lots more work on
  - Algorithms:
    - BLAS, LU, LDL^T, QR, other pivoting schemes, eigenproblems, …
      - QR with column pivoting
    - Sparse matrices, All-pairs-shortest-path, …
    - Both 2D (c=1) and 2.5D (c>1)
    - But only bandwidth may decrease with c>1, not latency
  - Platforms:
    - Multicore, cluster, GPU, cloud, heterogeneous, low-energy, …
  - Software:
    - Integration into Sca/LAPACK, PLASMA, MAGMA,…
- Integration into applications (on IBM BG/Q)
  - CTF (with ANL): symmetric tensor contractions

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Recall optimal sequential Matmul

- Naïve code
  for i=1:n, for j=1:n, for k=1:n, C(i,j)+=A(i,k)*B(k,j)

- "Blocked" code:
  ... write A as n/b-by-n/b matrix of b-by-b blocks A[i,j]
  ... ditto for B, C
  for i = 1:n/b, for j = 1:n/b, for k = 1:n/b,
  C[i,j] += A[i,k] * B[k,j] ... b-by-b matrix multiply

- Thm: Picking b = $M^{1/2}$ attains lower bound:
  #words_moved = $\Omega(n^3/M^{1/2})$
- Where does **1/2** come from?

New Thm applied to Matmul

- for i=1:n, for j=1:n, for k=1:n, C(i,j) += A(i,k)*B(k,j)
- Record array indices in matrix Δ

$$\Delta = \begin{array}{c} \\ \\ \\ \end{array}\begin{array}{c} \begin{array}{ccc} i & j & k \end{array} \\ \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 0 \end{pmatrix} \end{array} \begin{array}{c} \\ A \\ B \\ C \end{array}$$

- Solve LP for $x = [xi,xj,xk]^T$: max $\mathbf{1}^T x$ s.t. $\Delta\, x \le \mathbf{1}$
  - Result: $x = [1/2, 1/2, 1/2]^T$, $\mathbf{1}^T x = 3/2 = s_{HBL}$
- Thm: #words_moved = $\Omega(n^3/M^{s_{HBL}-1}) = \Omega(n^3/M^{1/2})$

Attained by block sizes $M^{xi}, M^{xj}, M^{xk} = M^{1/2}, M^{1/2}, M^{1/2}$

New Thm applied to Direct N-Body

- for i=1:n, for j=1:n, F(i) += force(P(i) , P(j))
- Record array indices in matrix Δ

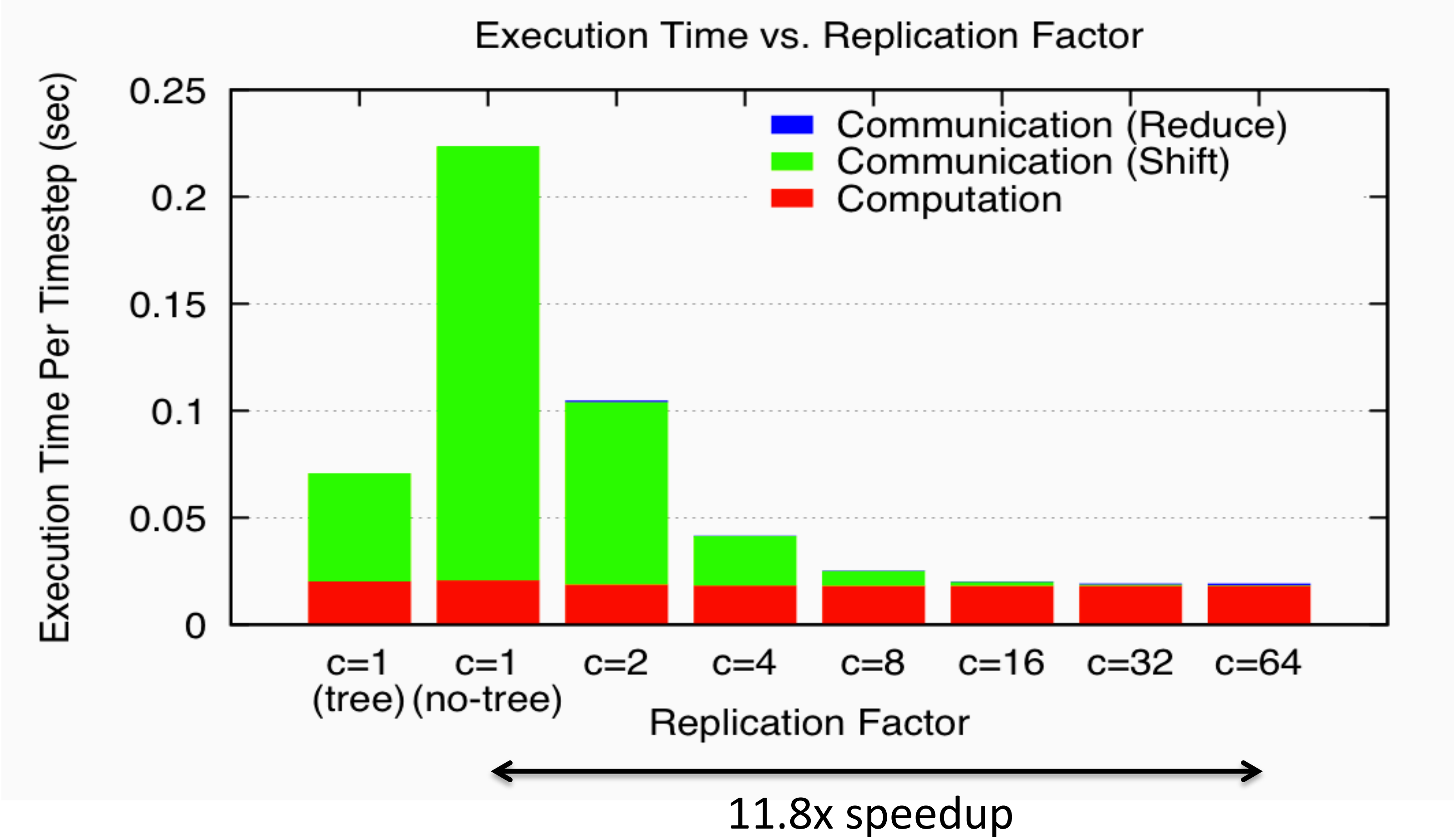
$$\Delta = \begin{array}{c} \\ \\ \\ \\ \end{array}\begin{array}{cc} i & j \\ \left(\begin{array}{c} 1 \\ 1 \\ 0 \end{array}\right. & \left.\begin{array}{c} 0 \\ 0 \\ 1 \end{array}\right) \end{array}\begin{array}{l} \\ F \\ P(i) \\ P(j) \end{array}$$

- Solve LP for $x = [xi,xj]^T$: max $\mathbf{1}^T x$ s.t. $\Delta\, x \le \mathbf{1}$
  - Result: $x = [1,1]$, $\mathbf{1}^T x = 2 = s_{HBL}$
- Thm: #words_moved $= \Omega(n^2/M^{s_{HBL}-1}) = \Omega(n^2/M^1)$

  Attained by block sizes $M^{xi}, M^{xj} = M^1, M^1$

N-Body Speedups on IBM-BG/P (Intrepid) 8K cores, 32K particles

K. Yelick, E. Georganas, M. Driscoll, P. Koanantakool, E. Solomonik



New Thm applied to Random Code

- for i1=1:n, for i2=1:n, … , for i6=1:n
  A1(i1,i3,i6) += func1(A2(i1,i2,i4),A3(i2,i3,i5),A4(i3,i4,i6))
  A5(i2,i6) += func2(A6(i1,i4,i5),A3(i3,i4,i6))
- Record array indices
  in matrix Δ

$$\Delta = \begin{array}{cccccccc} & i1 & i2 & i3 & i4 & i5 & i6 & \\ & \left(\begin{array}{c} 1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 1 \end{array}\right. & \begin{array}{c} 0 \\ 1 \\ 1 \\ 0 \\ 0 \\ 0 \end{array} & \begin{array}{c} 1 \\ 0 \\ 1 \\ 1 \\ 1 \\ 0 \end{array} & \begin{array}{c} 0 \\ 1 \\ 0 \\ 1 \\ 1 \\ 1 \end{array} & \begin{array}{c} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 1 \end{array} & \left.\begin{array}{c} 1 \\ 0 \\ 0 \\ 1 \\ 1 \\ 0 \end{array}\right) & \begin{array}{c} A1 \\ A2 \\ A3 \\ A3,A4 \\ A5 \\ A6 \end{array} \end{array}$$

- Solve LP for $x = [x1,\ldots,x7]^T$: max $\mathbf{1}^T x$ s.t. $\Delta\, x \le \mathbf{1}$
  – Result: $x = [2/7,3/7,1/7,2/7,3/7,4/7]$, $\mathbf{1}^T x = 15/7 = s_{HBL}$
- Thm: #words_moved = $\Omega(n^6/M^{s_{HBL}-1}) = \Omega(n^6/M^{8/7})$
  Attained by block sizes $M^{2/7}, M^{3/7}, M^{1/7}, M^{2/7}, M^{3/7}, M^{4/7}$

Summary of Results Beyond LA (1/3)

- Extend communication lower bound proof from linear algebra to any program with
  - Inner loop iterations indexed by $(i_1,\ldots,i_d)$
  - Arrays in inner loop subscripted by linear functions of indices
  - Ex: $A(i_1,i_2-i_1,3i_1-4i_2+7i_4,\ldots)$, $B(ptr(i_5+6i_6))$, …
  - Can be dense or sparse, sequential or parallel, …
- Based on recent result of Bennett/Carbery/Christ/Tao
  - Generalizes **H**older, **B**rascamp-**L**ieb, Loomis-Whitney
  - Get linear program with one inequality per subgroup $H < Z^d$
  - Solution of linear program is s_{HBL}
  - Thm: #words_moved = $\Omega(\#loop\_iterations/M^{s_{HBL}-1})$

Summary of Results Beyond LA (2/3)

- Can we write down the lower bound?
  - One inequality per subgroup $H < Z^d$, but still finitely many
  - Thm (bad news): Writing down all the inequalities equivalent to solving Hilbert's 10^{th} Problem over Q
  - Thm (good news): Another LP has same solution, is decidable
  - Thm (better news): Easy to write down the LP explicitly in many cases of interest (eg when subscripts are just subsets of indices)
  - Also easy to get upper/lower bounds on s_{HBL}

Summary of Results Beyond LA (3/3)

- Can we attain the lower bound?
  - Depends on loop dependencies
  - Best case: none, or reductions (like matmul)
  - Thm: When subscripts are just subsets of indices, the solution x of the dual LP tells us the optimal tile sizes M^{x1}, M^{x2},…,M^{xd}
  - Ex: linear algebra, n-body, join, "random code", …
  - Conjecture: always attainable (modulo dependencies)

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Avoiding Communication in Iterative Linear Algebra

- k-steps of iterative solver for sparse Ax=b or Ax=λx
  - Does k SpMVs 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

For more details

- Bebop.cs.berkeley.edu
- CS267 – Berkeley's Parallel Computing Course
  - Live broadcast in Spring 2013
    - www.cs.berkeley.edu/~demmel
    - All slides, video available
  - Prerecorded version broadcast in Spring 2013
    - www.xsede.org
    - Free supercomputer accounts to do homework
    - Free autograding of homework

Collaborators and Supporters

- **James Demmel**, **Kathy Yelick**, Michael Anderson, Grey Ballard, Erin Carson, Aditya Devarakonda, Michael Driscoll, David Eliahu, Andrew Gearhart, Evangelos Georganas, Nicholas Knight, Penporn Koanantakool, Ben Lipshitz, Oded Schwartz, Edgar Solomonik, Omer Spillinger
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- bebop.cs.berkeley.edu

Summary

Time to redesign all linear algebra, n-body, …
algorithms and software
(and compilers)

Don't Communic…