Communication-Avoiding Algorithms for Linear Algebra and Beyond

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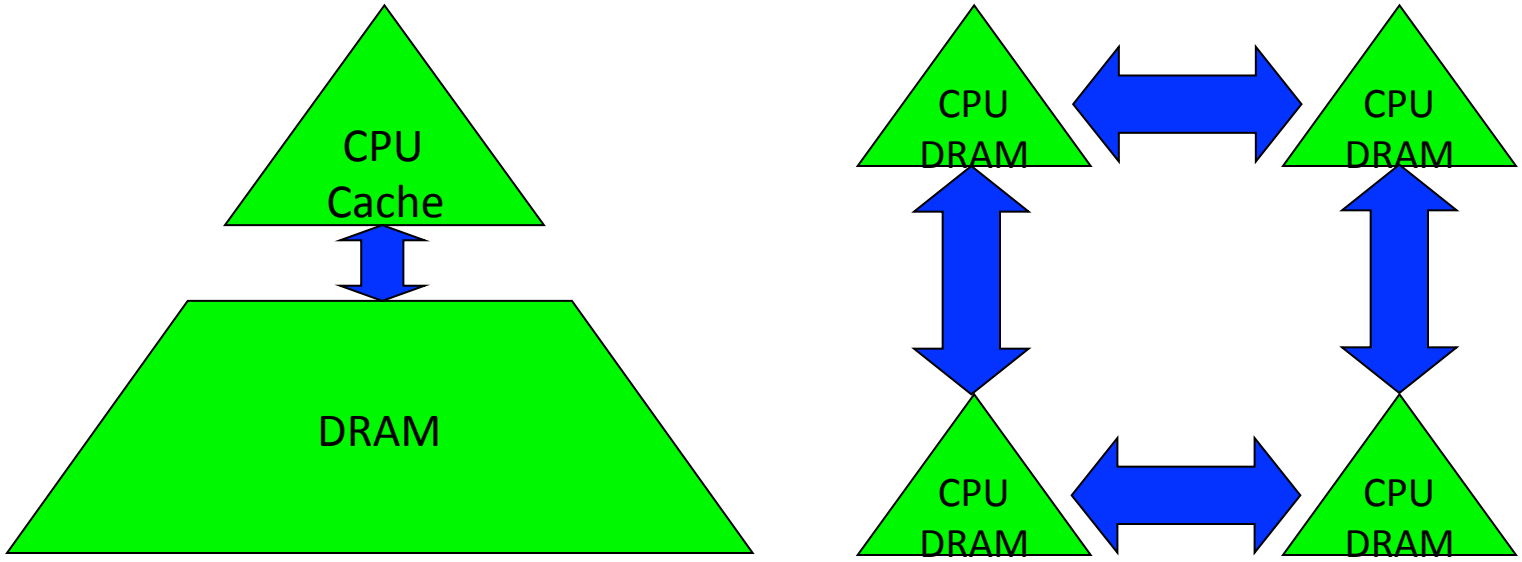
Why avoid communication? (1/3)

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

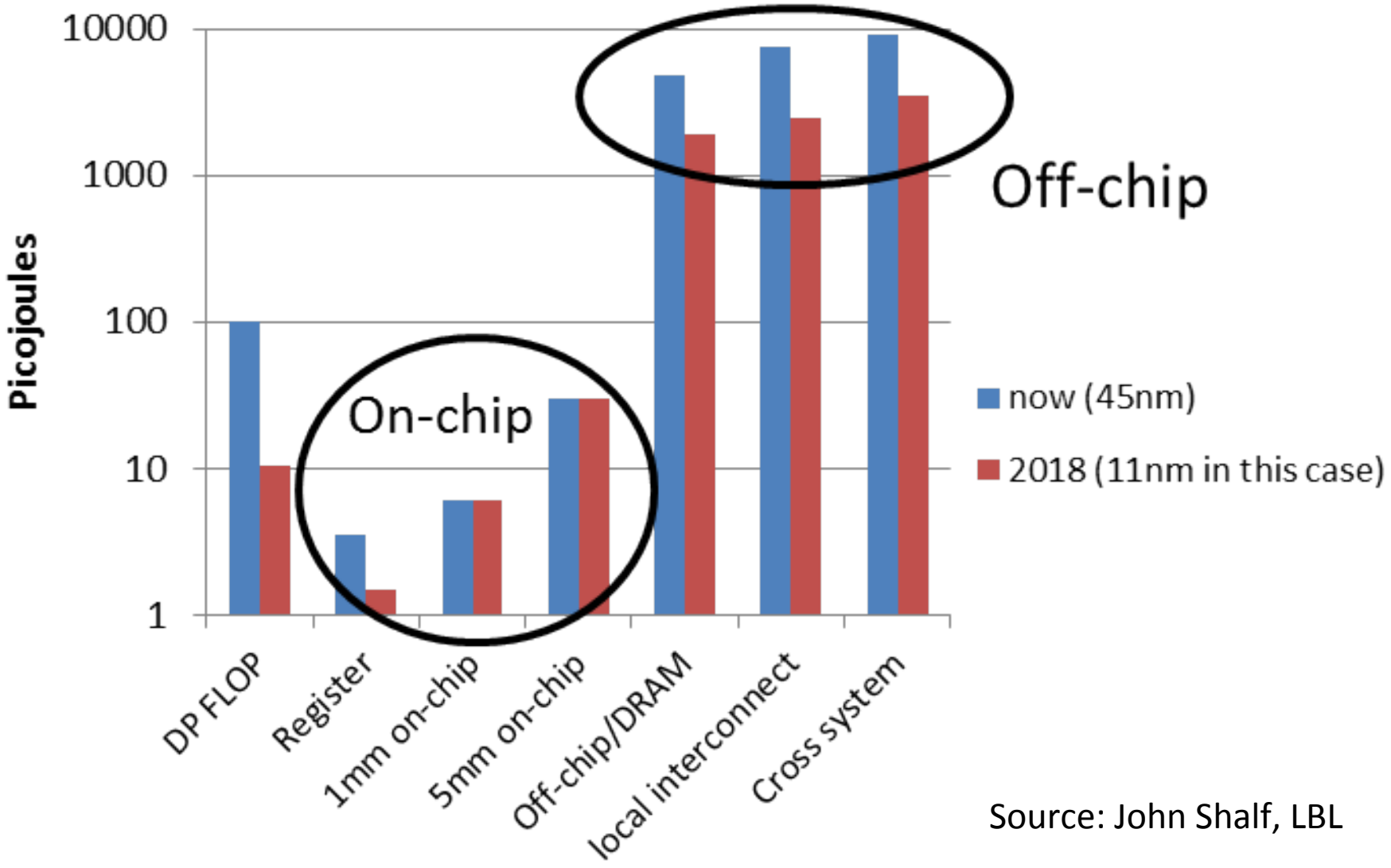
- Time_per_flop << 1/ bandwidth << latency
  - Gaps growing exponentially with time [FOSC]

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

- Avoid communication to save time

Why Minimize Communication? (3/3)

Minimize communication to save energy



Source: John Shalf, LBL

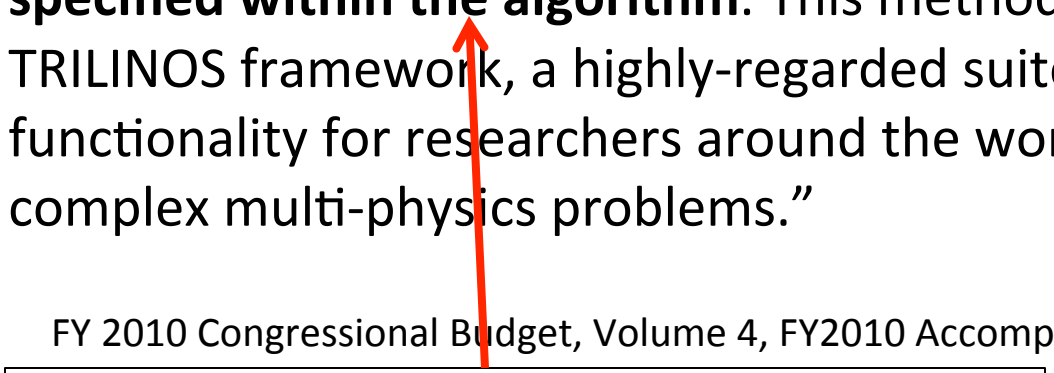
Goals

- Redesign algorithms to *avoid* communication
  - Between all memory hierarchy levels
    - L1 ↔ L2 ↔ DRAM ↔ network, etc
- Attain lower bounds if possible
  - Current algorithms often far from lower bounds
  - Large speedups and energy savings possible

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.



Outline

- Survey state of the art of CA (Comm-Avoiding) algorithms
  - CA O(n^3) 2.5D Matmul
  - CA Strassen Matmul
- Beyond linear algebra
  - Extending lower bounds to any algorithm with arrays
  - Communication-optimal N-body algorithm

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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 = λx, SVD, etc
  - Mostly not attained by algorithms in standard libraries
  - New algorithms that attain these lower bounds
    - Being added to libraries: Sca/LAPACK, PLASMA, MAGMA
    - Large speed-ups possible
  - Autotuning to find optimal implementation
- Ditto for "Iterative" Linear Algebra

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

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

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

#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

Summary of *dense* algorithms attaining communication lower bounds

- Do LAPACK and ScaLAPACK attain these bounds? Often not
- 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 = $\Omega((n^3/ P) / M^{3/2}) = \Omega(P^{1/2})$
- When 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
  - New numerical properties, new ways to encode answers, new data structures, not just loop transformations

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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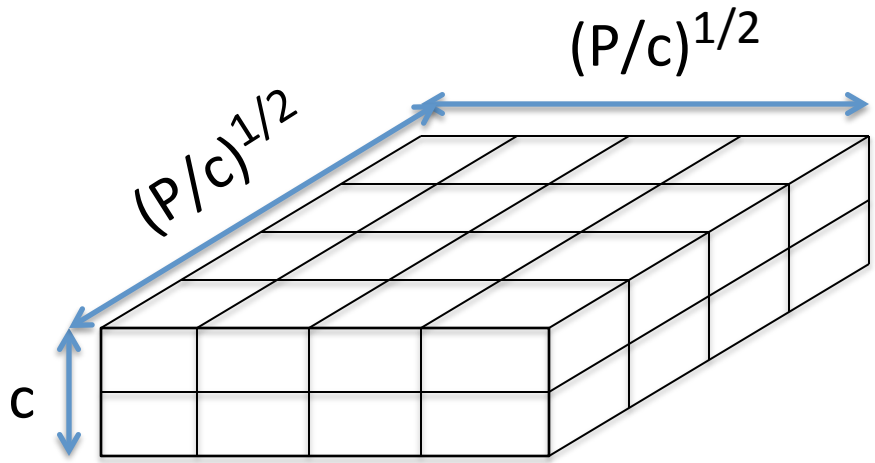
2.5D Matrix Multiplication

- 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

2.5D Matrix Multiplication

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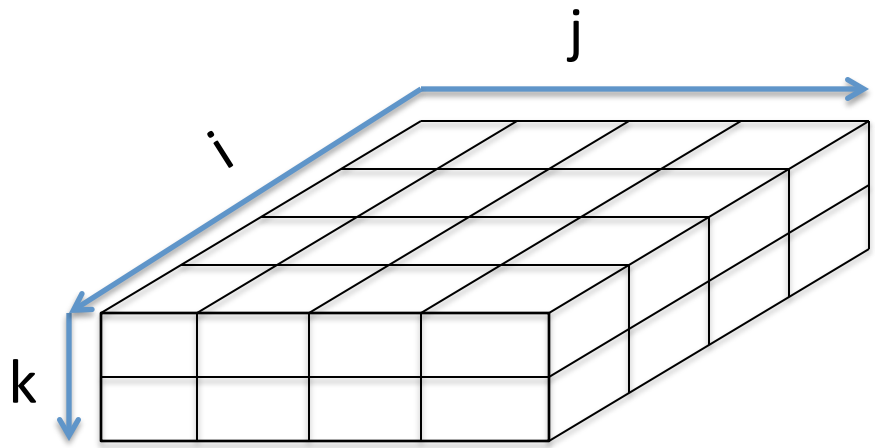
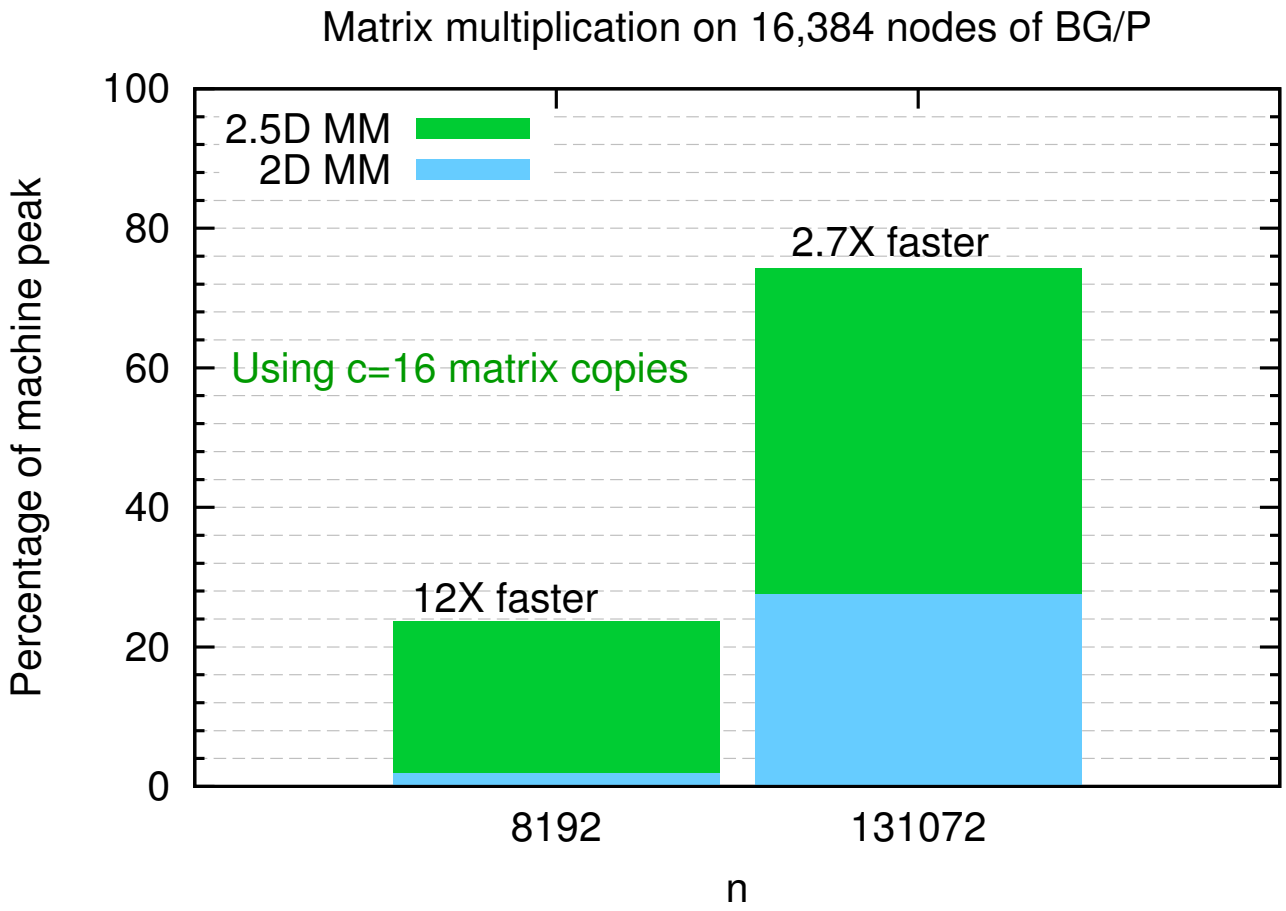


Initially P(i,j,0) owns A(i,j) and B(i,j)
each of size $n(c/P)^{1/2}$ x $n(c/P)^{1/2}$

(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)

Thm: Works up to $c = P^{1/3}$, then stops

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



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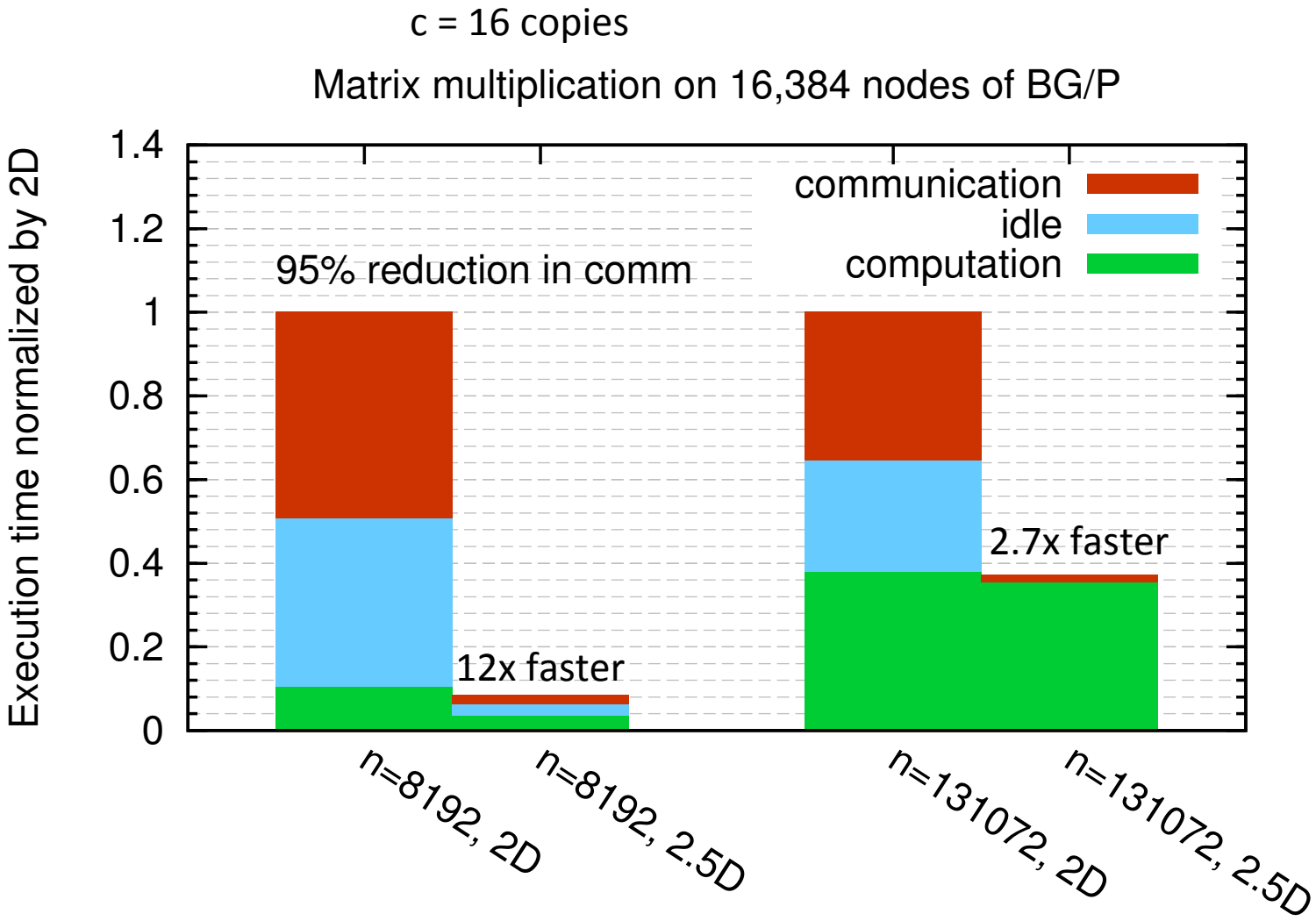

Distinguished Paper Award, EuroPar'11 (Solomonik, D.)

SC'11 paper by Solomonik, Bhatele, D.

Perfect Strong Scaling – in Time and Energy (1/2)

- 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.
- $E(cP) = cP \{ n^3/(cP) [\gamma_E + \beta_E/M^{1/2} + \alpha_E/(mM^{1/2})] + \delta_E MT(cP) + \varepsilon_E T(cP) \}$
  $= E(P)$

Perfect Strong Scaling – in Time and Energy (2/2)

- $T(cP) = n^3/(cP) \left[\gamma_T + \beta_T/M^{1/2} + \alpha_T/(mM^{1/2}) \right] = T(P)/c$
- $E(cP) = cP \{ n^3/(cP) \left[\gamma_E + \beta_E/M^{1/2} + \alpha_E/(mM^{1/2}) \right] + \delta_E MT(cP) + \varepsilon_E T(cP) \} = E(P)$

- Perfect scaling extends to N-body, Strassen, …
- We can use these models to answer many questions, including:

- What is the minimum energy required for a computation?
- Given a maximum allowed runtime **T** , what is the minimum energy **E** needed to achieve it?
- Given a maximum energy budget **E** , what is the minimum runtime **T** that we can attain?
- The ratio **P** = **E/T** gives us the average power required to run the algorithm. Can we minimize the average power consumed?
- Given an algorithm, problem size, number of processors and target energy efficiency (GFLOPS/W), can we determine a set of architectural parameters to describe a conforming computer architecture?

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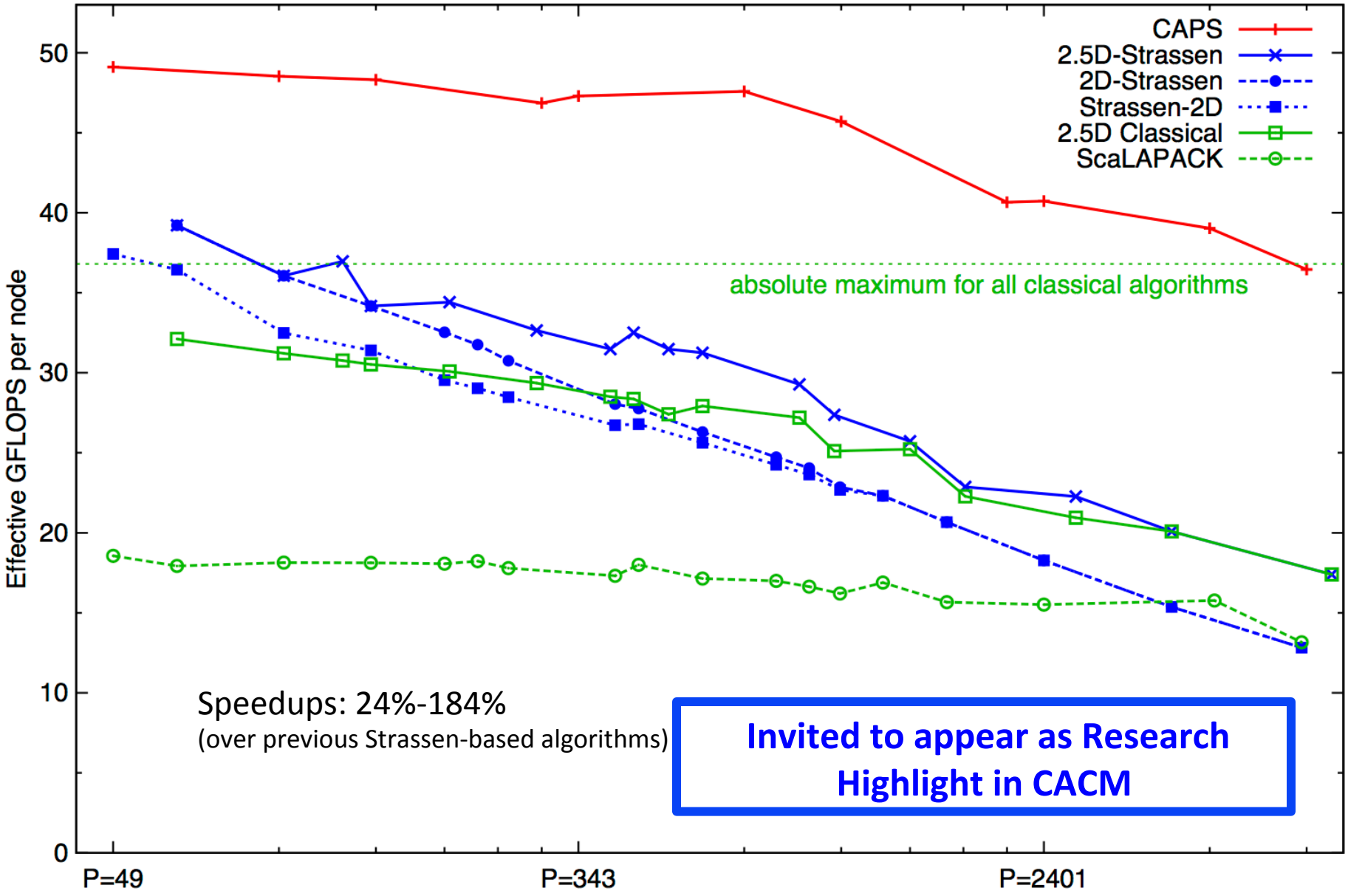
Communication Lower Bounds for Strassen-like matmul algorithms

Classical $O(n^3)$ matmul:	Strassen's $O(n^{lg7})$ matmul:	Strassen-like $O(n^{\omega})$ matmul:
#words_moved = $\Omega\,(M(n/M^{1/2})^3/P)$	#words_moved = $\Omega\,(M(n/M^{1/2})^{lg7}/P)$	#words_moved = $\Omega\,(M(n/M^{1/2})^{\omega}/P)$

- Proof: graph expansion (different from classical matmul)
  - Strassen-like: DAG must be "regular" and connected
- Extends up to $M = n^2 / p^{2/\omega}$
- Best Paper Prize (SPAA'11), Ballard, D., Holtz, Schwartz, also in JACM
- Is the lower bound attainable?

Performance Benchmarking, Strong Scaling Plot

Franklin (Cray XT4) n = 94080



Speedups: 24%-184%
(over previous Strassen-based algorithms)

Invited to appear as Research Highlight in CACM

Ongoing Work

- Lots more work on
  - Algorithms:
    - BLAS, LDL^T, QR with pivoting, other pivoting schemes, eigenproblems, …
    - All-pairs-shortest-path, …
    - Both 2D (c=1) and 2.5D (c>1)
    - But only bandwidth may decrease with c>1, not latency
      - New lower bound on bandwidth*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
  for i1 = 1:b:n, for j1 = 1:b:n, for k1 = 1:b:n
    for i2 = 0:b-1, for j2 = 0:b-1, for k2 = 0:b-1
      i=i1+i2, j = j1+j2, k = k1+k2
      C(i,j)+=A(i,k)*B(k,j)

  } b x b matmul

- 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

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

- 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

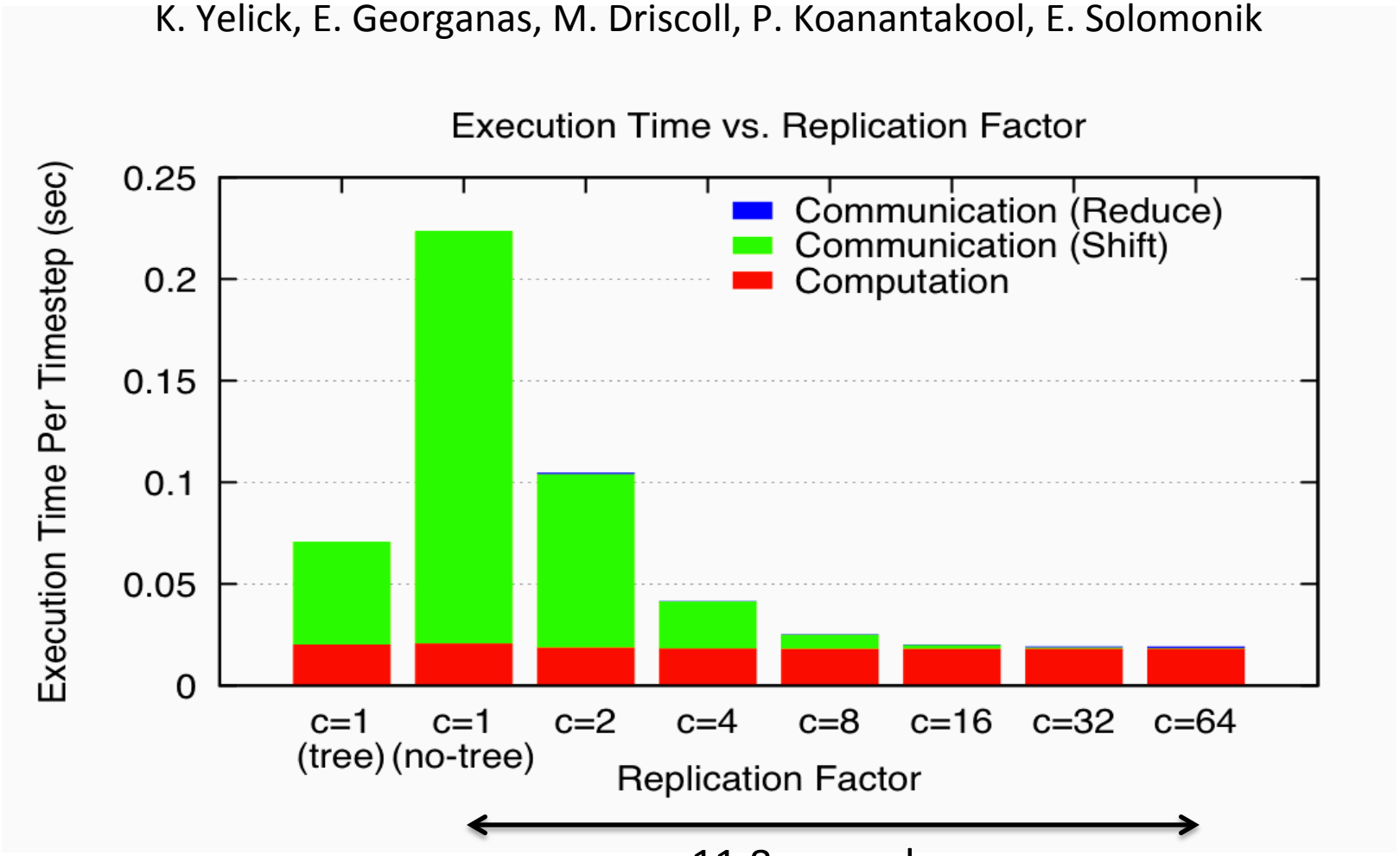
$$\Delta = \begin{array}{c} \begin{matrix} i & j \end{matrix} \\ \begin{pmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \end{pmatrix} \end{array} \begin{matrix} F \\ P(i) \\ P(j) \end{matrix}$$

- 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

$\Delta =$

i1	i2	i3	i4	i5	i6	
1	0	1	0	0	1	A1
1	1	0	1	0	0	A2
0	1	1	0	1	0	A3
0	0	1	1	0	1	A3,A4
0	0	1	1	0	1	A5
1	0	0	1	1	0	A6

- 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 $M^{2/7},M^{3/7},M^{1/7},M^{2/7},M^{3/7},M^{4/7}$

Approach to generalizing lower bounds

- Matmul

  for i=1:n, for j=1:n, for k=1:n,

  C(i,j)+=A(i,k)*B(k,j)

  => for (i,j,k) in S = subset of Z^3

  Access locations indexed by (i,j), (i,k), (k,j)

- General case

  for i1=1:n, for i2 = i1:m, … for ik = i3:i4

  C(i1+2*i3-i7) = func(A(i2+3*i4,i1,i2,i1+i2,…),B(pnt(3*i4)),…)

  D(something else) = func(something else), …

  => for (i1,i2,…,ik) in S = subset of Z^k

  Access locations indexed by group homomorphisms, eg

  ϕ_C (i1,i2,…,ik) = (i1+2*i3-i7)

  ϕ_A (i1,i2,…,ik) = (i2+3*i4,i1,i2,i1+i2,…), …

- Can we bound #loop_iterations (= |S|)

  given bounds on #points in its images, i.e. bounds on $|\phi_C(S)|$, $|\phi_A(S)|$, … ?

General Communication Bound

- Given S subset of Z^k, group homomorphisms ϕ_1, ϕ_2, …, bound $|S|$ in terms of $|\phi_1(S)|$, $|\phi_2(S)|$, … , $|\phi_m(S)|$
- Def: Hölder-Brascamp-Lieb LP (HBL-LP) for $s_1,\ldots,s_m$:

  for all subgroups $H < Z^k$, $\quad \text{rank}(H) \le \Sigma_j\, s_j * \text{rank}(\phi_j(H))$
- Thm (Christ/Tao/Carbery/Bennett): Given $s_1,\ldots,s_m$

$$|S| \le \Pi_j\, |\phi_j(S)|^{s_j}$$

- Thm: Given a program with array refs given by ϕ_j, choose s_j to minimize $s_{HBL} = \Sigma_j\, s_j$ subject to HBL-LP. Then

$$\#\text{words\_moved} = \Omega\,(\#\text{iterations}/M^{s_{HBL}-1})$$

Is this bound attainable (1/2)?

- But first: Can we write it down?
- Thm: (bad news) HBL-LP reduces to Hilbert's 10^{th} problem over Q (conjectured to be undecidable)
- Thm: (good news) Another LP with same solution is decidable (but expensive, so far)
- Thm: (better news) Easy to write down LP explicitly in many cases of interest (eg all ϕ_j = {subset of indices})
- Thm: (good news) Easy to approximate, i.e. get upper or lower bounds on s_{HBL}

Is this bound attainable (2/2)?

- Depends on loop dependencies
- Best case: none, or reductions (matmul)
- Thm: When all ϕ_j = {subset of indices}, dual of HBL-LP gives optimal tile sizes:

  HBL-LP: minimize $1^T * s$ s.t. $s^T * \Delta \geq 1^T$

  Dual-HBL-LP: maximize $1^T * x$ s.t. $\Delta * x \leq 1$

  Then for sequential algorithm, tile i_j by M^{x_j}
- Ex: Matmul: $s = [\ 1/2\ ,\ 1/2\ ,\ 1/2\ ]^T = x$
- Extends to unimodular transforms of indices

Ongoing Work

- Accelerate decision procedure for lower bounds
  - Ex: At most 3 arrays, or 4 loop nests
- Have yet to find a case where we cannot attain lower bound – can we prove this?
- Extend "perfect scaling" results for time and energy by using extra memory
  - "n.5D algorithms"
- Incorporate into compilers

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
- Acta Numerica survey (in progress)

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…

With one exception:

Happy Birthday Michael!