Introduction to Communication-Avoiding Algorithms

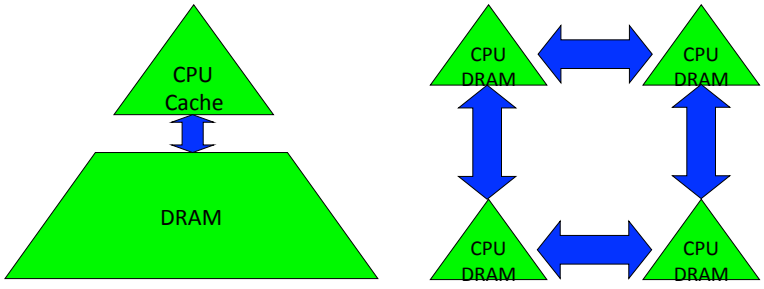
www.cs.berkeley.edu/~demmel/SC14_tutorial

Jim Demmel
EECS & Math Departments
UC Berkeley

Why avoid communication? (1/2)

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).



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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

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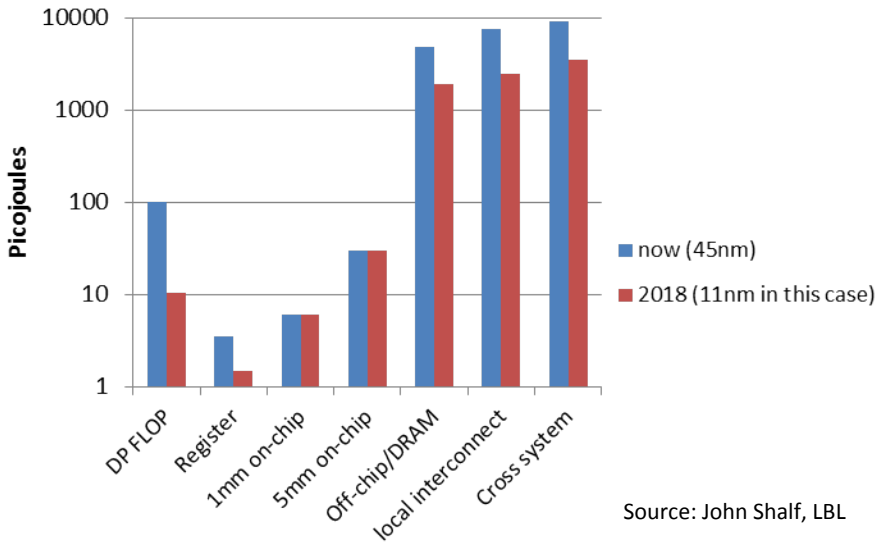
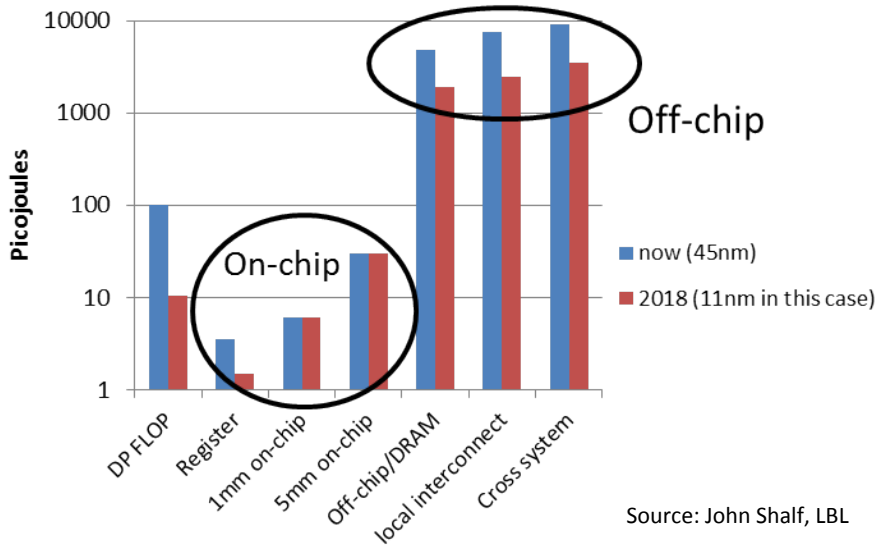
Why Minimize Communication? (2/2)



Source: John Shalf, LBL

Why Minimize Communication? (2/2)

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

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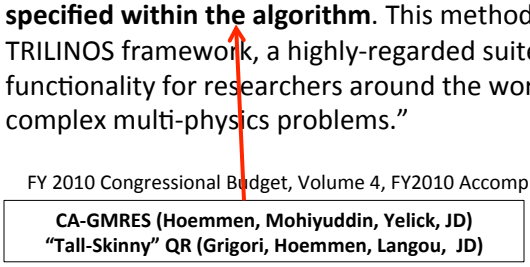
President Obama cites Communication-Avoiding Algorithms in the FY 2012 Department of Energy Budget Request to Congress:

"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.



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
- Austin Benson, Maryam Dehnavi, Mark Hoemmen, Shoaib Kamil, Marghoob Mohiyuddin
- Abhinav Bhatele, Aydin Buluc, Michael Christ, Ioana Dumitriu, Armando Fox, David Gleich, Ming Gu, Jeff Hammond, **Mike Heroux**, Olga Holtz, Kurt Keutzer, Julien Langou, Devin Matthews, Tom Scanlon, Michelle Strout, Sam Williams, Hua Xiang
- **Jack Dongarra, Jakub Kurzak**, Dulceneia Becker, Ichitaro Yamazaki, …
- Sivan Toledo, Alex Druinsky, Inon Peled
- Laura Grigori, Sebastien Cayrols, Simplice Donfack, Mathias Jacquelin, Amal Khabou, Sophie Moufawad, Mikolaj Szydlarski
- Members of ParLab, ASPIRE, BEBOP, CACHE, EASI, FASTMath, MAGMA, PLASMA
- Thanks to DOE, NSF, UC Discovery, INRIA, Intel, Microsoft, Mathworks, National Instruments, NEC, Nokia, NVIDIA, Samsung, Oracle
- bebop.cs.berkeley.edu

Summary of CA Algorithms

- "Direct" Linear Algebra
  - Lower bounds on communication for linear algebra problems like Ax=b, least squares, Ax = λx, SVD, etc
  - 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 programs accessing arrays (eg n-body)
- Ditto for "Iterative" Linear Algebra

Outline

- "Direct" Linear Algebra
  - Lower bounds on communication
  - New algorithms that attain these lower bounds
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Lower bound for all "direct" 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

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Lower bound for all "direct" 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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Lower bound for all "direct" linear algebra

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

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

#messages_sent (per processor) = Ω(#flops (per processor) / $M^{3/2}$)

- Parallel case: assume either load or memory balanced
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SIAM SIAG/Linear Algebra Prize, 2012
Ballard, D., Holtz, Schwartz

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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
- Only a few sparse algorithms so far
- Lots of work in progress
- Case study: Matrix Multiply

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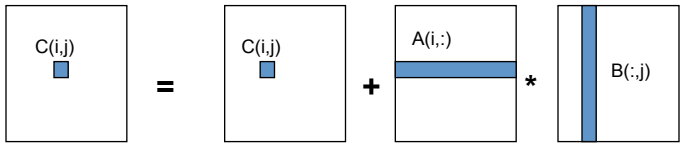
Naïve Matrix Multiply

```
{implements C = C + A*B}
for i = 1 to n

  for j = 1 to n


    for k = 1 to n
      C(i,j) = C(i,j) + A(i,k) * B(k,j)
```



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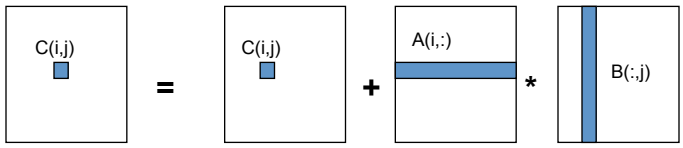
Naïve Matrix Multiply

```
{implements C = C + A*B}
for i = 1 to n
 {read row i of A into fast memory}
  for j = 1 to n
    {read C(i,j) into fast memory}
    {read column j of B into fast memory}
    for k = 1 to n
       C(i,j) = C(i,j) + A(i,k) * B(k,j)
    {write C(i,j) back to slow memory}
```



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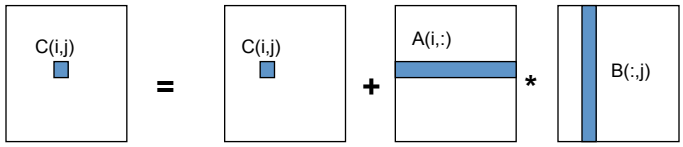
Naïve Matrix Multiply

```
{implements C = C + A*B}
for i = 1 to n
 {read row i of A into fast memory}          … n^2 reads altogether
  for j = 1 to n
    {read C(i,j) into fast memory}           … n^2 reads altogether
    {read column j of B into fast memory}    … n^3 reads altogether
    for k = 1 to n
       C(i,j) = C(i,j) + A(i,k) * B(k,j)
    {write C(i,j) back to slow memory}       … n^2 writes altogether
```



$n^3 + 3n^2$ reads/writes altogether – dominates $2n^3$ arithmetic

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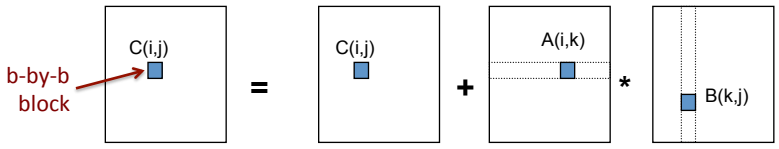
Blocked (Tiled) Matrix Multiply

Consider A,B,C to be n/b-by-n/b matrices of b-by-b subblocks where
b is called the block size; assume 3 b-by-b blocks fit in fast memory

```
for i = 1 to n/b
  for j = 1 to n/b
    {read block C(i,j) into fast memory}
    for k = 1 to n/b
        {read block A(i,k) into fast memory}
        {read block B(k,j) into fast memory}
        C(i,j) = C(i,j) + A(i,k) * B(k,j) {do a matrix multiply on blocks}
    {write block C(i,j) back to slow memory}
```



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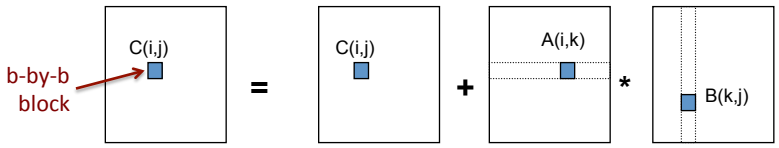
Blocked (Tiled) Matrix Multiply

Consider A,B,C to be n/b-by-n/b matrices of b-by-b subblocks where
b is called the block size; assume 3 b-by-b blocks fit in fast memory

```
for i = 1 to n/b
  for j = 1 to n/b
    {read block C(i,j) into fast memory}          ... b² × (n/b)² = n² reads
    for k = 1 to n/b
        {read block A(i,k) into fast memory}      ... b² × (n/b)³ = n³/b reads
        {read block B(k,j) into fast memory}      ... b² × (n/b)³ = n³/b reads
        C(i,j) = C(i,j) + A(i,k) * B(k,j) {do a matrix multiply on blocks}
    {write block C(i,j) back to slow memory}      ... b² × (n/b)² = n² writes
```



$2n^3/b + 2n^2$ reads/writes << $2n^3$ arithmetic - Faster!

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Does blocked matmul attain lower bound?

- Recall: if 3 b-by-b blocks fit in fast memory of size M, then #reads/writes = $2n^3/b + 2n^2$
- Make b as large as possible: $3b^2 \le M$, so #reads/writes $\ge 2n^3/(M/3)^{1/2} + 2n^2$
- Attains lower bound $= \Omega$ (#flops / $M^{1/2}$)

- But what if we don't know M?
- Or if there are multiple levels of fast memory?
- How do we write the algorithm?

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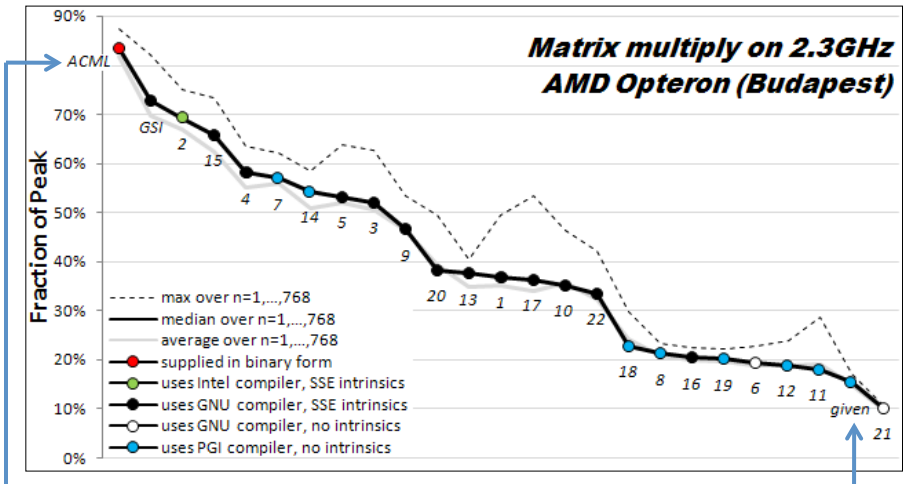
How hard is hand-tuning matmul, anyway?



- **Results of 22 student teams trying to tune matrix-multiply, in CS267 Spr09**
- **Students given "blocked" code to start with (7x faster than naïve)**
  - **Still hard to get close to vendor tuned performance (ACML) (another 6x)**
- **For more discussion, see www.cs.berkeley.edu/~volkov/cs267.sp09/hw1/results/**

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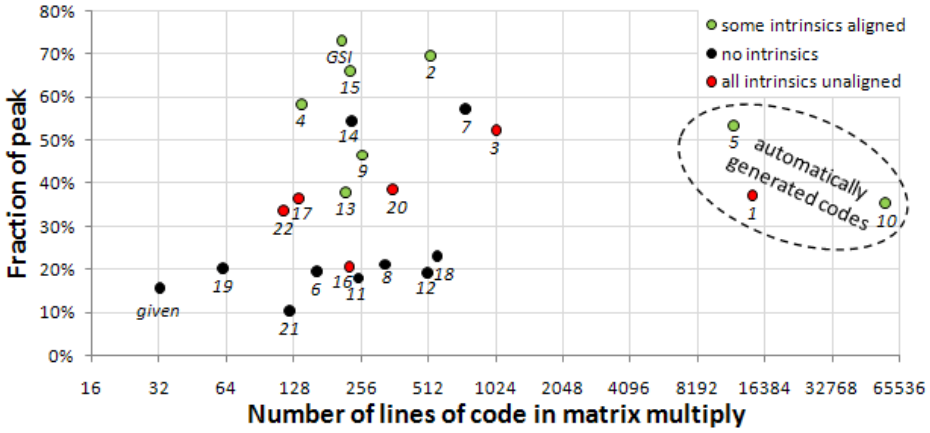
How hard is hand-tuning matmul, anyway?



Recursive Matrix Multiplication (RMM) (1/2)

- For simplicity: square matrices with $n = 2^m$
- $C = \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix} = A \cdot B = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \cdot \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}$

  $= \begin{pmatrix} A_{11}\cdot B_{11} + A_{12}\cdot B_{21} & A_{11}\cdot B_{12} + A_{12}\cdot B_{22} \\ A_{21}\cdot B_{11} + A_{22}\cdot B_{21} & A_{21}\cdot B_{12} + A_{22}\cdot B_{22} \end{pmatrix}$

- True when each A_{ij} etc 1x1 or n/2 x n/2

```
func C = RMM (A, B, n)
  if n = 1, C = A * B, else
    { C11 = RMM (A11 , B11 , n/2) + RMM (A12 , B21 , n/2)
      C12 = RMM (A11 , B12 , n/2) + RMM (A12 , B22 , n/2)
      C21 = RMM (A21 , B11 , n/2) + RMM (A22 , B21 , n/2)
      C22 = RMM (A21 , B12 , n/2) + RMM (A22 , B22 , n/2) }
  return
```

Recursive Matrix Multiplication (RMM) (2/2)

```
func C = RMM (A, B, n)
   if n=1, C = A * B, else
     { C11 = RMM (A11 , B11 , n/2) + RMM (A12 , B21 , n/2)
       C12 = RMM (A11 , B12 , n/2) + RMM (A12 , B22 , n/2)
       C21 = RMM (A21 , B11 , n/2) + RMM (A22 , B21 , n/2)
       C22 = RMM (A21 , B12 , n/2) + RMM (A22 , B22 , n/2)  }
   return
```

A(n) = # arithmetic operations in RMM(. , . , n)
= 8 · A(n/2) + 4(n/2)^2 if n > 1, else 1
= 2n^3 … same operations as usual, in different order

W(n) = # words moved between fast, slow memory by RMM(. , . , n)
= 8 · W(n/2) + 12(n/2)^2 if 3n^2 > M , else 3n^2
= O(n^3 / M$^{1/2}$ + n^2) … same as blocked matmul

"Cache oblivious", works for memory hierarchies, but not panacea

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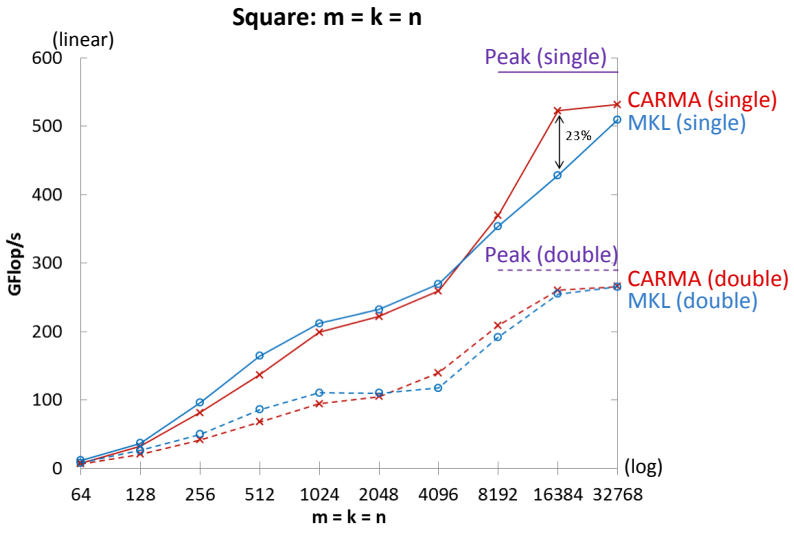
CARMA Performance: Shared Memory

Intel Emerald: 4 Intel Xeon X7560 x 8 cores, 4 x NUMA



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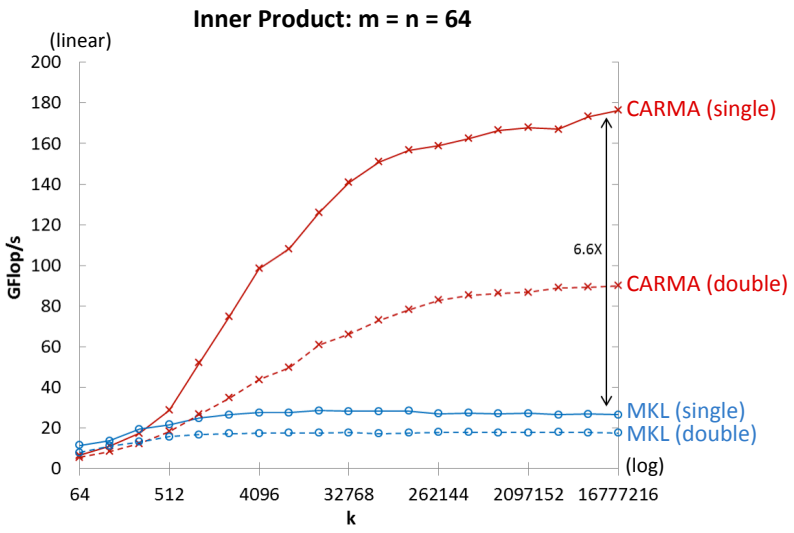
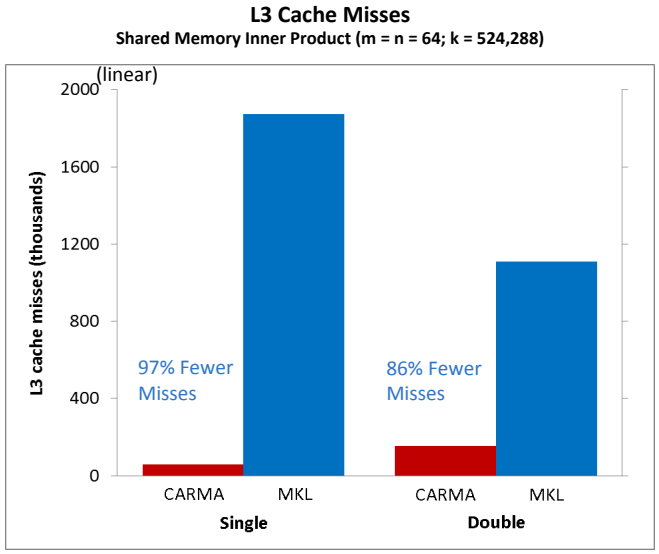


Why is CARMA Faster?



Parallel MatMul with 2D Processor Layout

- P processors in $P^{1/2}$ x $P^{1/2}$ grid
  - Processors communicate along rows, columns
- Each processor owns $n/P^{1/2}$ x $n/P^{1/2}$ submatrices of A,B,C
- Example: P=16, processors numbered from P_{00} to P_{33}
  - Processor P_{ij} owns submatrices A_{ij}, B_{ij} and C_{ij}

C = A * B

P_{00}	P_{01}	P_{02}	P_{03}
P_{10}	P_{11}	P_{12}	P_{13}
P_{20}	P_{21}	P_{22}	P_{23}
P_{30}	P_{31}	P_{32}	P_{33}

P_{00}	P_{01}	P_{02}	P_{03}
P_{10}	P_{11}	P_{12}	P_{13}
P_{20}	P_{21}	P_{22}	P_{23}
P_{30}	P_{31}	P_{32}	P_{33}

P_{00}	P_{01}	P_{02}	P_{03}
P_{10}	P_{11}	P_{12}	P_{13}
P_{20}	P_{21}	P_{22}	P_{23}
P_{30}	P_{31}	P_{32}	P_{33}

SUMMA Algorithm

- SUMMA = Scalable Universal Matrix Multiply
  - Attains lower bounds:
    - Assume fast memory size $M = O(n^2/P)$ per processor – 1 copy of data
    - #words_moved = $\Omega(\text{\#flops} / M^{1/2}) = \Omega((n^3/P) / (n^2/P)^{1/2}) = \Omega(n^2 / P^{1/2})$
    - #messages = $\Omega(\text{\#flops} / M^{3/2}) = \Omega((n^3/P) / (n^2/P)^{3/2}) = \Omega(P^{1/2})$
  - Can accommodate any processor grid, matrix dimensions & layout
  - Used in practice in PBLAS = Parallel BLAS
    - www.netlib.org/lapack/lawns/lawn{96,100}.ps

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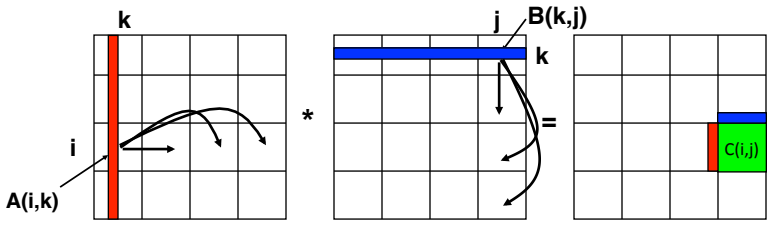
SUMMA – n x n matmul on $P^{1/2}$ x $P^{1/2}$ grid



- C(i, j) is $n/P^{1/2}$ x $n/P^{1/2}$ submatrix of C on processor P_{ij}
- A(i,k) is $n/P^{1/2}$ x b submatrix of A
- B(k,j) is b x $n/P^{1/2}$ submatrix of B
- C(i,j) = C(i,j) + Σ_k A(i,k)*B(k,j)
  - summation over submatrices
- Need not be square processor grid

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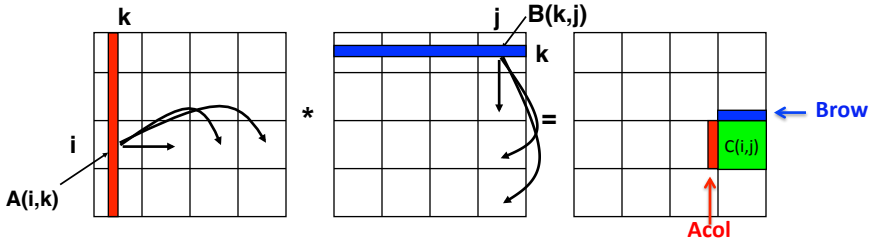
SUMMA– n x n matmul on $P^{1/2}$ x $P^{1/2}$ grid



For k=0 to n/b-1
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_myproc = C_myproc + Acol * Brow

- Attains bandwidth lower bound
- Attains latency lower bound if b near maximum $n/P^{1/2}$

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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

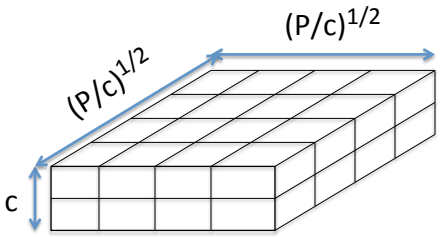
Can we do Better?

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?
  - Special case: "3D Matmul": uses M = $O(n^2/P^{2/3})$
    - Dekel, Nassimi, Sahni [81], Bernsten [89], Agarwal, Chandra, Snir [90], Johnson [93], Agarwal, Balle, Gustavson, Joshi, Palkar [95]
    - Processors arranged in $P^{1/3}$ x $P^{1/3}$ x $P^{1/3}$ grid
    - Processor (i,j,k) performs C(i,j) = C(i,j) + A(i,k)*B(k,j), where each submatrix is $n/P^{1/3}$ x $n/P^{1/3}$
  - M = $O(n^2/P^{2/3})$ is $P^{1/3}$ times the minimium
    - Not always that much memory available…

2.5D Matrix Multiplication

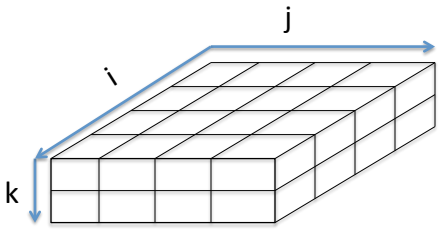
- Assume can fit cn^2/P data per processor, $c>1$
- Processors form $(P/c)^{1/2}$ x $(P/c)^{1/2}$ x c grid



Example: P = 32, c = 2

2.5D Matrix Multiplication

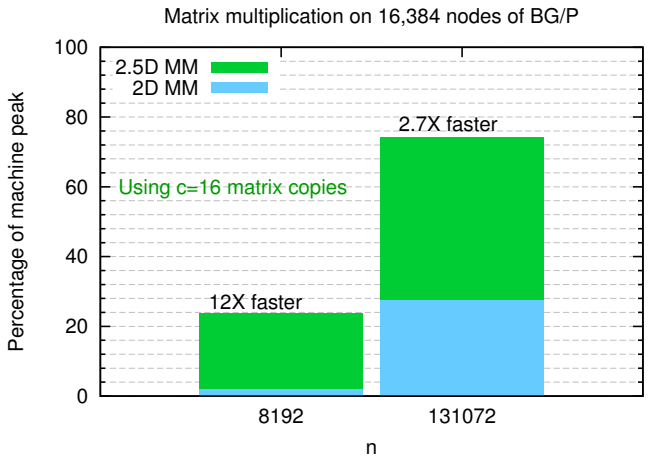
- Assume can fit cn^2/P data per processor, $c > 1$
- Processors form $(P/c)^{1/2}$ x $(P/c)^{1/2}$ x c grid



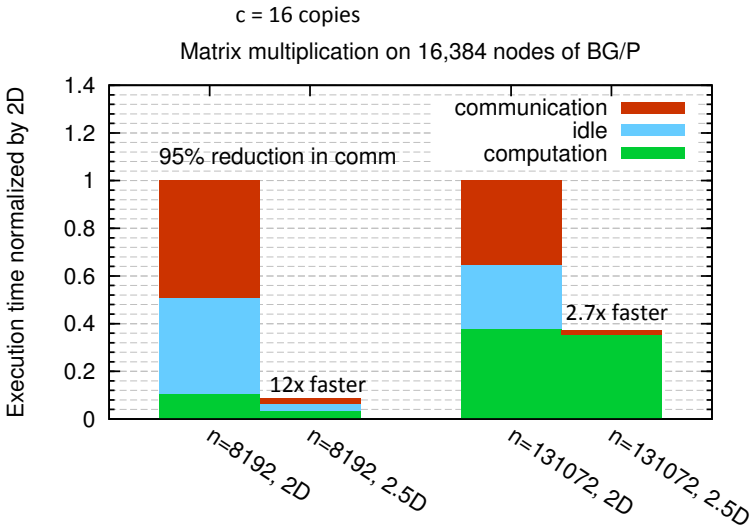
Initially P(i,j,0) owns A(i,j) and B(i,j) each of size $n(c/P)^{1/2}$ x $n(c/P)^{1/2}$

(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)

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



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



Distinguished Paper Award, EuroPar'11
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.
- $E(cP) = cP \{ n^3/(cP) [\gamma_E + \beta_E/M^{1/2} + \alpha_E/(mM^{1/2})] + \delta_E MT(cP) + \varepsilon_E T(cP) \}$
  $= E(P)$
- Limit: $c \leq P^{1/3}$ (3D algorithm), if starting with 1 copy of inputs

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

- 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?
- See Andrew Gearhart's PhD thesis

Handling Heterogeneity

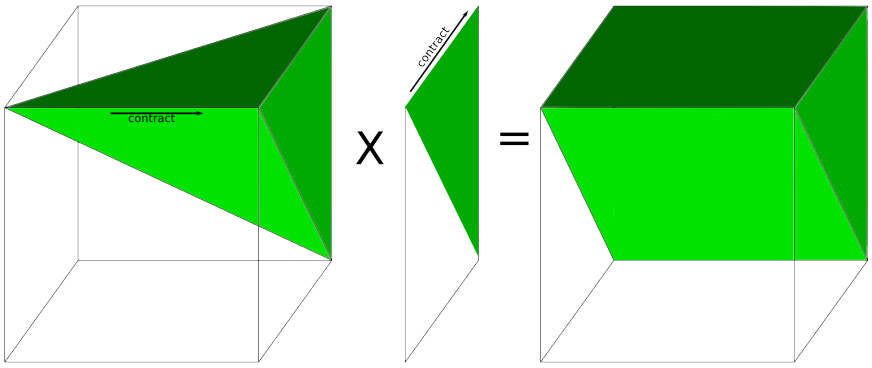
- Suppose each of P processors could differ
  - γ_i = sec/flop, β_i = sec/word, α_i = sec/message, M_i = memory
- What is optimal assignment of work F_i to minimize time?
  - $T_i = F_i \gamma_i + F_i \beta_i / M_i^{1/2} + F_i \alpha_i / M_i^{3/2} = F_i [\gamma_i + \beta_i / M_i^{1/2} + \alpha_i / M_i^{3/2}] = F_i \xi_i$
  - Choose F_i so $\Sigma_i F_i = n^3$ and minimizing $T = \max_i T_i$
  - Answer: $F_i = n^3(1/\xi_i)/\Sigma_j(1/\xi_j)$ and $T = n^3/\Sigma_j(1/\xi_j)$
- Optimal Algorithm for nxn matmul
  - Recursively divide into 8 half-sized subproblems
  - Assign subproblems to processor i to add up to F_i flops
- Works for Strassen, other algorithms...

Application to Tensor Contractions

- Ex: $C(i,j,k) = \Sigma_{mn} A(i,j,m,n)*B(m,n,k)$
  - Communication lower bounds apply
- Complex symmetries possible
  - Ex: B(m,n,k) = B(k,m,n) = …

  - Solomonik, Hammond, Matthews

$$C(i,j,k) = \Sigma_m A(i,j,m)*B(m,k)$$



A
3-fold symm

B
2-fold symm

C
2-fold symm

Application to Tensor Contractions

- Ex: $C(i,j,k) = \Sigma_{mn} A(i,j,m,n)*B(m,n,k)$
  - Communication lower bounds apply
- Complex symmetries possible
  - Ex: B(m,n,k) = B(k,m,n) = …
  - d-fold symmetry can save up to d!-fold flops/memory
- Heavily used in electronic structure calculations
  - Ex: NWChem, for coupled cluster (CC) approach to Schroedinger eqn.
- CTF: Cyclops Tensor Framework
  - Exploits 2.5D algorithms, symmetries
  - Up to **3x faster** running CC than NWChem on 3072 cores of Cray XE6
  - Solomonik, Hammond, Matthews

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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TSQR: QR of a Tall, Skinny matrix

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

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

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

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

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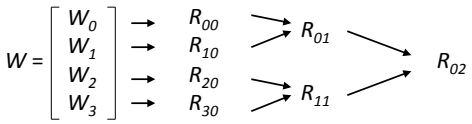
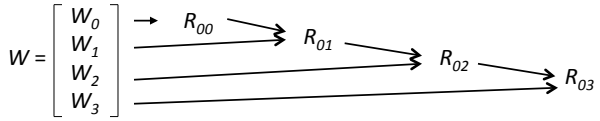
TSQR: An Architecture-Dependent Algorithm

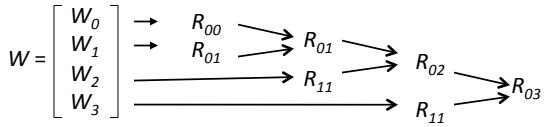
Parallel:



Sequential:



Dual Core:



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 (Dongarra et al)
  - Cloud – **~2 map-reduces** (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
- Building block for QR of a general matrix
- Joint work with Grigori, Hoemmen, Langou, Anderson, Ballard, Keutzer, others

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Using similar idea for TSLU as TSQR: Use reduction tree, to do "Tournament Pivoting"

$$W^{nxb} = \begin{pmatrix} W_1 \\ W_2 \\ W_3 \\ W_4 \end{pmatrix} = \begin{pmatrix} P_1 \cdot L_1 \cdot U_1 \\ P_2 \cdot L_2 \cdot U_2 \\ P_3 \cdot L_3 \cdot U_3 \\ P_4 \cdot L_4 \cdot U_4 \end{pmatrix}$$

Choose b pivot rows of W_1, call them W_1'
Choose b pivot rows of W_2, call them W_2'
Choose b pivot rows of W_3, call them W_3'
Choose b pivot rows of W_4, call them W_4'

$$\begin{pmatrix} W_1' \\ W_2' \\ W_3' \\ W_4' \end{pmatrix} = \begin{pmatrix} P_{12} \cdot L_{12} \cdot U_{12} \\ P_{34} \cdot L_{34} \cdot U_{34} \end{pmatrix}$$

Choose b pivot rows, call them W_{12}'

Choose b pivot rows, call them W_{34}'

$$\begin{pmatrix} W_{12}' \\ W_{34}' \end{pmatrix} = P_{1234} \cdot L_{1234} \cdot U_{1234}$$

Choose b pivot rows

- Go back to W and use these b pivot rows
  - Move them to top, do LU without pivoting
  - Extra work, but lower order term
- Thm: As numerically stable as Partial Pivoting on a larger matrix

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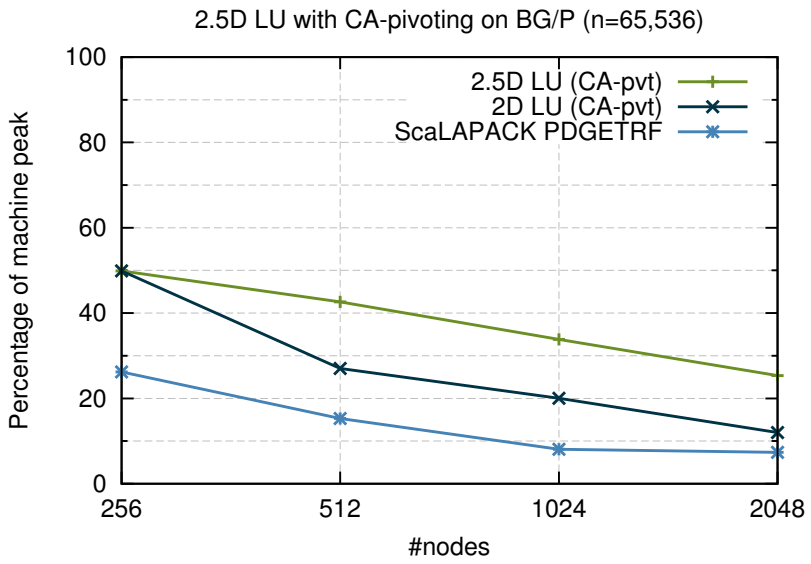
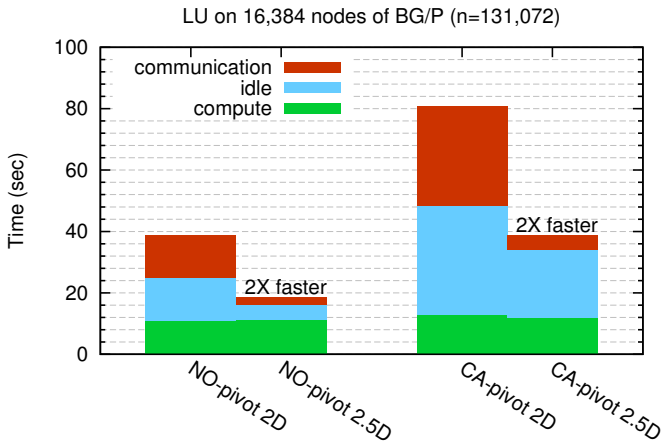
LU Speedups from Tournament Pivoting and 2.5D



2.5D vs 2D LU
With and Without Pivoting

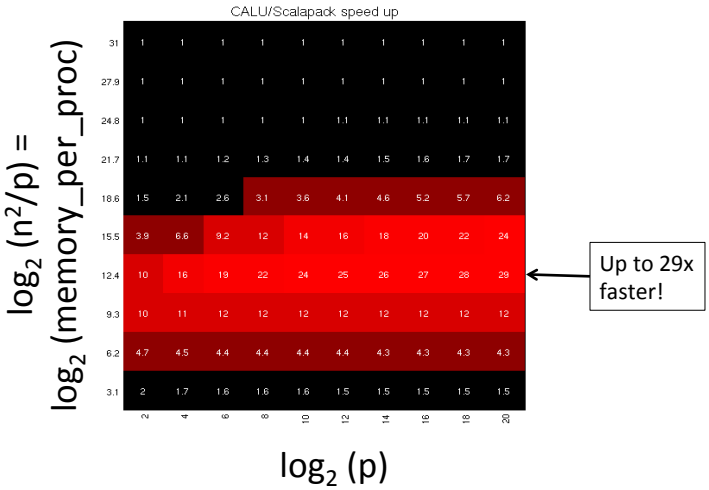


Thm: Perfect Strong Scaling impossible, because Latency*Bandwidth = $\Omega(n^2)$

Exascale Machine Parameters
Source: DOE Exascale Workshop

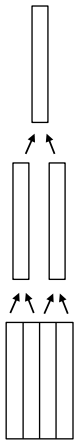
- 2^20 ≈ 1,000,000 nodes
- 1024 cores/node (a billion cores!)
- 100 GB/sec interconnect bandwidth
- 400 GB/sec DRAM bandwidth
- 1 microsec interconnect latency
- 50 nanosec memory latency
- 32 Petabytes of memory
- 1/2 GB total L1 on a node

Exascale predicted speedups for Gaussian Elimination: 2D CA-LU vs ScaLAPACK-LU



Other CA algorithms

- Need for pivoting arises beyond LU, in QR
  - Choose permutation P so that leading columns of A*P = Q*R span column space of A – Rank Revealing QR (RRQR)
  - Usual approach like Partial Pivoting
    - Put longest column first, update rest of matrix, repeat
    - Hard to do using BLAS3 at all, let alone hit lower bound
  - Use Tournament Pivoting
    - Each round of tournament selects best b columns from two groups of b columns, either using usual approach or something better (Gu/Eisenstat)
    - Thm: This approach ``reveals the rank'' of A in the sense that the leading rxr submatrix of R has singular values "near" the largest r singular values of A; ditto for trailing submatrix
  - Idea extends to other pivoting schemes
    - Cholesky with diagonal pivoting
    - LU with complete pivoting
    - LDL^T with complete pivoting



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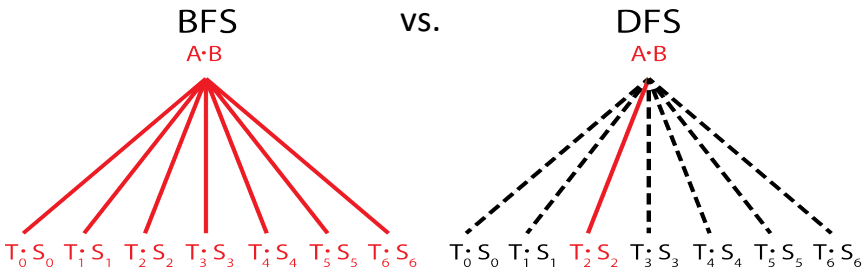
Communication Lower Bounds for Strassen-like matmul algorithms

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 appeared in JACM
- Is the lower bound attainable?

Communication Avoiding Parallel Strassen *(CAPS)*

BFS vs. DFS

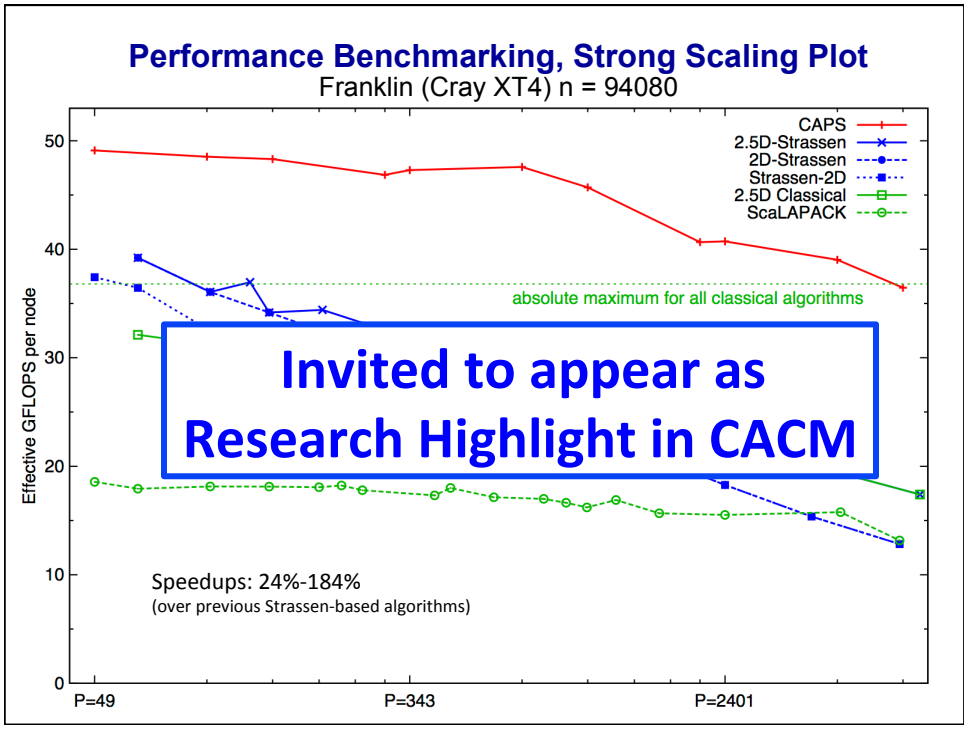


Runs all 7 multiplies in parallel
Each on P/7 processors
Needs 7/4 as much memory

Runs all 7 multiplies sequentially
Each on all P processors
Needs 1/4 as much memory

```
CAPS
  If EnoughMemory and P ≥ 7
    then BFS step
    else DFS step
  end if
```

In practice, how to best interleave BFS and DFS is a "tuning parameter"

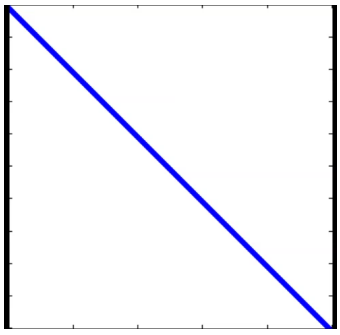


Symmetric Band Reduction

- Grey Ballard and Nick Knight
- $A \Rightarrow QAQ^T = T$, where
  - $A=A^T$ is banded
  - T tridiagonal
  - Similar idea for SVD of a band matrix
- Use alone, or as second phase when A is dense:
  - Dense ⇒ Banded ⇒ Tridiagonal
- Implemented in LAPACK's sytrd
- Algorithm does not satisfy communication lower bound theorem for applying orthogonal transformations
  - It can communicate even less!

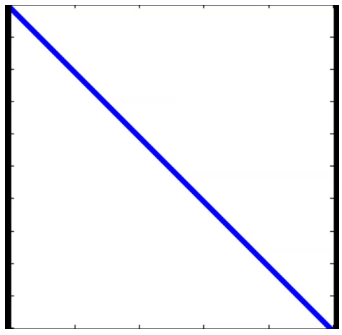
Conventional vs CA - SBR

Touch all data 4 times



Conventional

Touch all data once



Communication-Avoiding

Many tuning parameters
Right choices reduce #words_moved by factor M/bw, not just $M^{1/2}$

Speedups of Sym. Band Reduction vs LAPACK's DSBTRD

- Up to **17x** on Intel Gainestown, vs MKL 10.0
  - n=12000, b=500, 8 threads
- Up to **12x** on Intel Westmere, vs MKL 10.3
  - n=12000, b=200, 10 threads
- Up to **25x** on AMD Budapest, vs ACML 4.4
  - n=9000, b=500, 4 threads
- Up to **30x** on AMD Magny-Cours, vs ACML 4.4
  - n=12000, b=500, 6 threads

- Neither MKL nor ACML benefits from multithreading in DSBTRD
  - Best sequential speedup vs MKL: **1.9x**
  - Best sequential speedup vs ACML: **8.5x**

What about sparse matrices? (1/3)

- If matrix quickly becomes dense, use dense algorithm
- Ex: All Pairs Shortest Path using Floyd-Warshall
- Similar to matmul: Let D = A, then
  for k = 1:n, for i = 1:n, for j=1:n
  D(i,j) = min(D(i,j), D(i,k) + D(k,j))
- But can't reorder outer loop for 2.5D, need another idea
- Abbreviate D(i,j) = min(D(i,j),$\min_k$(A(i,k)+B(k,j)) by D = A⊙B
  - Dependencies ok, 2.5D works, just different semiring
- Kleene's Algorithm:

D = **DC-APSP**(A,n)
D = A, Partition D = [[D11,D12];[D21,D22]] into n/2 x n/2 blocks
D11 = **DC-APSP**(D11,n/2),
D12 = D11 ⊙ D12, D21 = D21 ⊙ D11, D22 = D21 ⊙ D12,
D22 = **DC-APSP**(D22,n/2),
D21 = D22 ⊙ D21, D12 = D12 ⊙ D22, D11 = D12 ⊙ D21,

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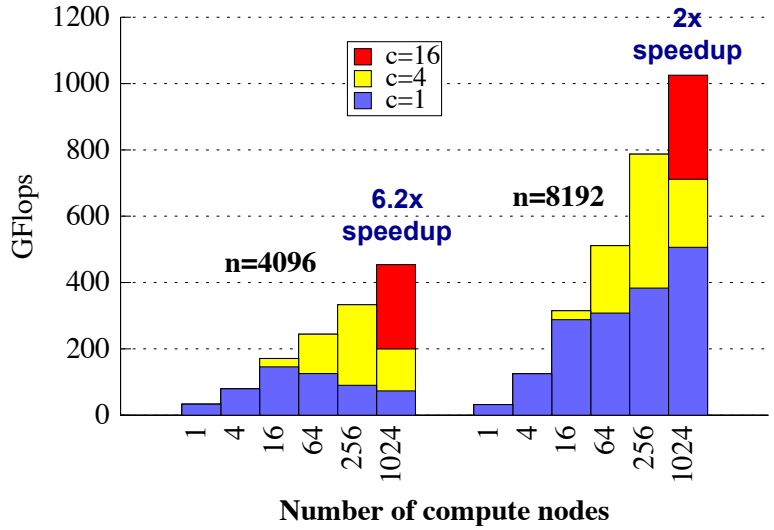
Performance of 2.5D APSP using Kleene

Strong Scaling on Hopper (Cray XE6 with 1024 nodes = 24576 cores)



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What about sparse matrices? (2/3)

- If parts of matrix becomes dense, optimize those
- Ex: Cholesky on matrix A with good separators
- Thm (Lipton,Rose,Tarjan,'79) If all balanced separators of G(A) have at least w vertices, then G(chol(A)) has clique of size w
  - Need to do dense Cholesky on w x w submatrix
- Thm: #Words_moved = $\Omega(w^3/M^{1/2})$ etc
- Thm (George,'73) Nested dissection gives optimal ordering for 2D grid, 3D grid, similar matrices
  - w = n for 2D n x n grid, w = n^2 for 3D n x n x n grid
- Sequential multifrontal Cholesky attains bounds
- PSPACES (Gupta, Karypis, Kumar) is a parallel sparse multifrontal Cholesky package
  - Attains 2D and 2.5D lower bounds (using optimal dense Cholesky on separators)

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What about sparse matrices? (3/3)

- If matrix stays very sparse, lower bound unattainable, new one?
- Ex: A*B, both diagonal: no communication in parallel case
- Ex: A*B, both are Erdos-Renyi: Prob(A(i,j)≠0) = d/n, d << $n^{1/2}$,iid
- Assumption: Algorithm is *sparsity-independent*: assignment of data and work to processors is sparsity-pattern-independent (but zero entries need not be communicated or operated on)
- Thm: A parallel algorithm that is sparsity-independent and load balanced for Erdos-Renyi matmul satisfies (in expectation)
  #Words_moved = $\Omega(\min(dn/P^{1/2}, d^2n/P))$
  - Proof exploits fact that reuse of entries of C = A*B unlikely
- Contrast general lower bound:
  #Words_moved = $\Omega(d^2n/(PM^{1/2}))$
- Attained by divide-and-conquer algorithm that splits matrices along dimensions most likely to minimize cost

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Summary of Direct Linear Algebra

- New lower bounds, optimal algorithms, big speedups in theory and practice
- Lots of ongoing work on
  - Algorithms:
    - 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
    - Sparse matrices
  - Platforms:
    - Multicore, cluster, GPU, cloud, heterogeneous, low-energy, …
  - Software:
    - Integration into Sca/LAPACK, PLASMA, MAGMA,…
- Integration of CTF into quantum chemistry/DFT applications
  - Aquarius, with ANL, UT Austin on IBM BG/Q, Cray XC30
  - Qbox, with LLNL, IBM, on IBM BG/Q
  - Q-Chem, work in progress
- Integration into big data analysis system based on Spark at AMPLab

Outline

- "Direct" Linear Algebra
  - Lower bounds on communication
  - New algorithms that attain these lower bounds
- Ditto for programs accessing arrays (eg n-body)
- Ditto for "Iterative" Linear Algebra

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

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

- Solve LP for x = $[x_i,x_j,x_k]^T$: max $\mathbf{1}^T x$ s.t. $\Delta x \le \mathbf{1}$
  - Result: x = $[1/2, 1/2, 1/2]^T$, $\mathbf{1}^T x = 3/2 = e$
- Thm: #words_moved = $\Omega(n^3/M^{e-1}) = \Omega(n^3/M^{1/2})$
  Attained by block sizes $M^{x_i}, M^{x_j}, M^{x_k} = M^{1/2}, M^{1/2}, M^{1/2}$

New Thm applied to Direct N-Body

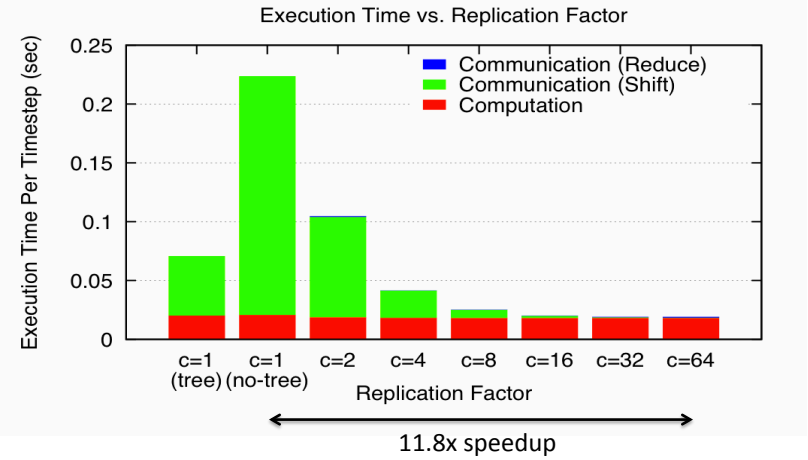
- for i=1:n, for j=1:n, F(i) += force(P(i) , P(j))
- Record array indices in matrix Δ

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

- 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 = e
- Thm: #words_moved = $\Omega(n^2/M^{e-1}) = \Omega(n^2/M^1)$
  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

Δ =

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,…,x6]^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 = e
- Thm: #words_moved = $\Omega(n^6/M^{e-1}) = \Omega(n^6/M^{8/7})$
  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 "projections", eg
  ϕ_C (i1,i2,…,ik) = (i1+2*i3-i7)
  ϕ_A (i1,i2,…,ik) = (i2+3*i4,i1,i2,i1+i2,…), …

General Communication Bound

- Thm: Given a program with array refs given by projections ϕ_j, then there is an $e \geq 1$ such that

  #words_moved = Ω (#iterations/M^{e-1})

  where e is the the value of a linear program:

  minimize $e = \Sigma_j e_j$ subject to

  $\text{rank}(H) \leq \Sigma_j e_j * \text{rank}(\phi_j(H))$ for all subgroups $H < Z^k$

- Proof depends on recent result in pure mathematics by Christ/Tao/Carbery/Bennett

Is this bound attainable (1/2)?

- But first: Can we write it down?
  - One inequality per subgroup $H < Z^d$, but still finitely many!
  - Thm (bad news): Writing down all inequalities in LP reduces to Hilbert's 10^{th} problem over Q
    - Could be undecidable: open question
  - Thm (good news): Another LP has same solution, is decidable (but expensive so far)
  - Thm: (better news) Easy to write LP down explicitly in many cases of interest (eg when subscript are subsets of indices)

Is this bound attainable (2/2)?

- Depends on loop dependencies
- Best case: none, or reductions (matmul)
- Thm: When all subscripts are subsets of indices, the solution x of the dual LP gives optimal tile sizes: M^{x1}, M^{x2}, …
- Ex: Linear algebra, n-body, "random code," join, …
- Conjecture: always attainable (modulo dependencies): work in progress

Ongoing Work

- Identify more decidable cases
  - Works for any 3 nested loops, or 3 different subscripts
- Automate generation of approximate LPs
- Extend "perfect scaling" results for time and energy by using extra memory
- Have yet to find a case where we cannot attain lower bound – can we prove this?
- Incorporate into compilers

Outline

- "Direct" Linear Algebra
  - Lower bounds on communication
  - New algorithms that attain these lower bounds
- Ditto for programs accessing arrays (eg n-body)
- Ditto for "Iterative" Linear Algebra

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"
- 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

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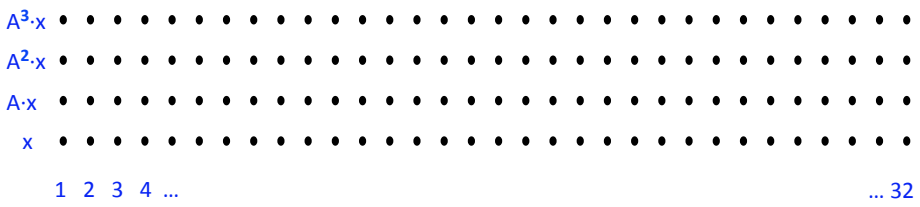
Communication Avoiding Kernels:
The Matrix Powers Kernel : [Ax, A^2x, …, A^kx]

- Replace k iterations of y = A·x with [Ax, A^2x, …, A^kx]



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

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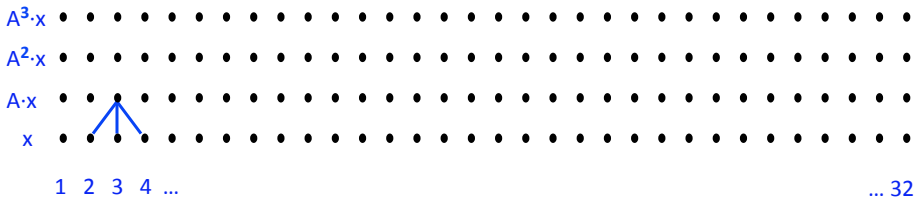

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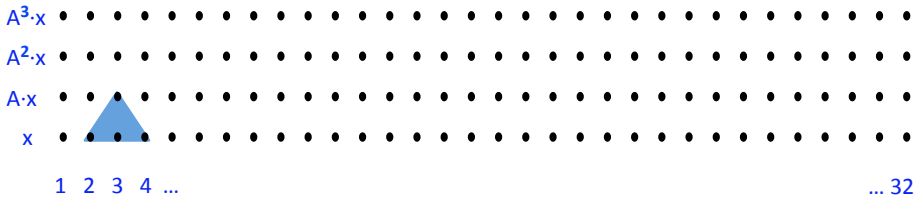

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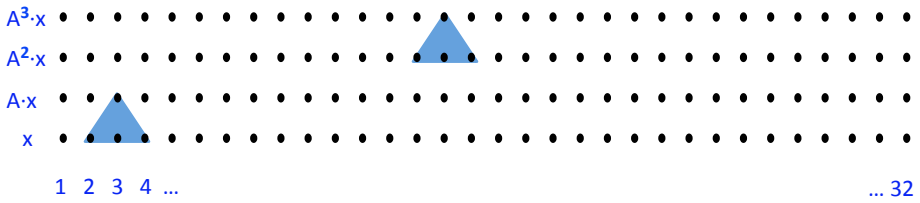

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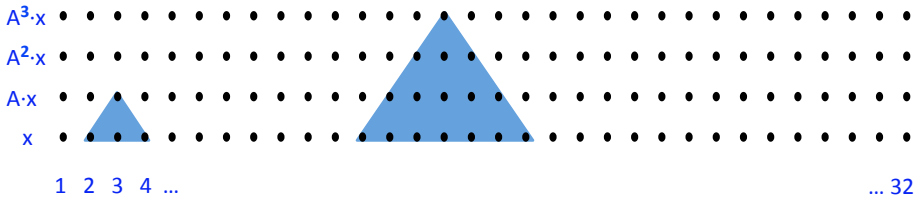

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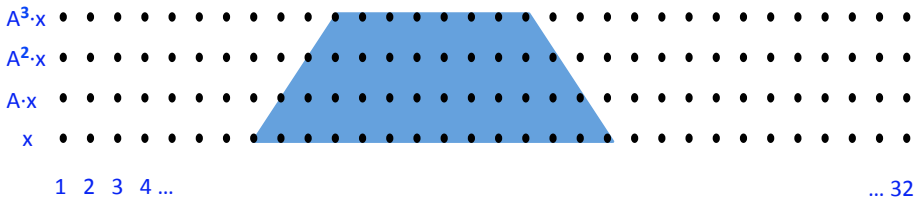

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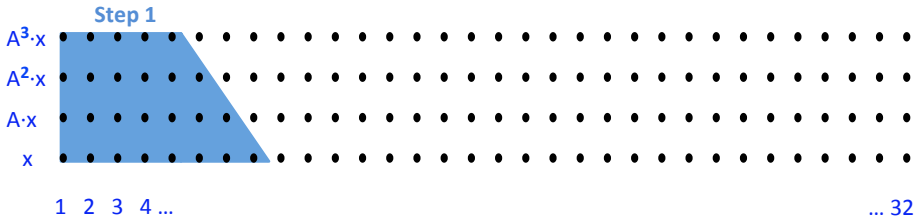
- Sequential Algorithm



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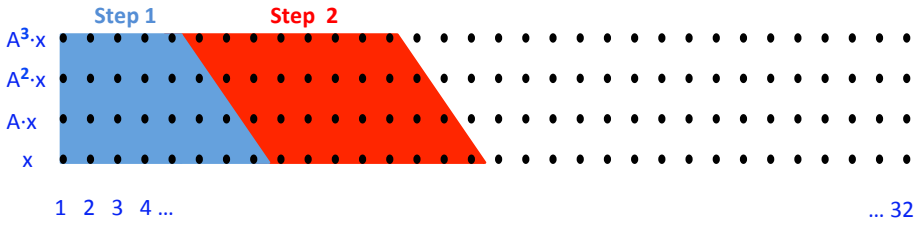

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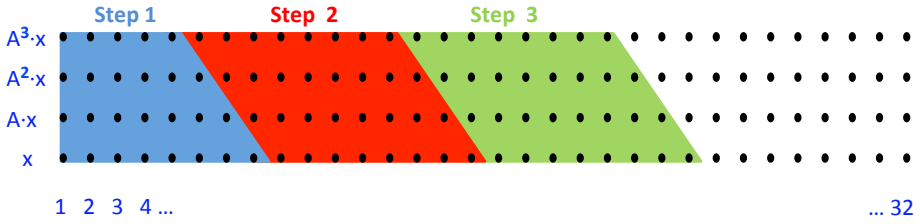

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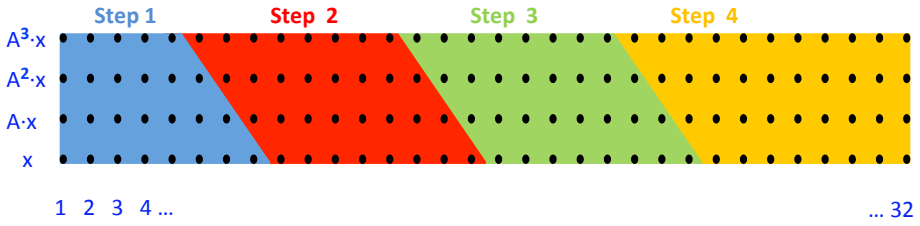

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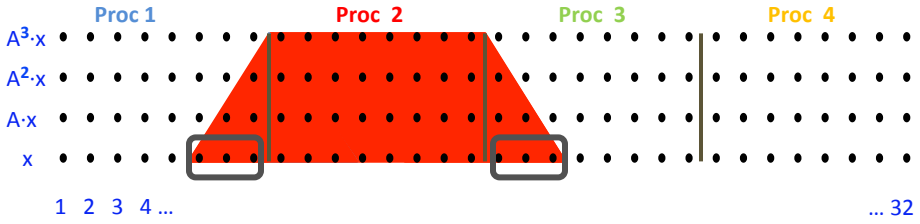
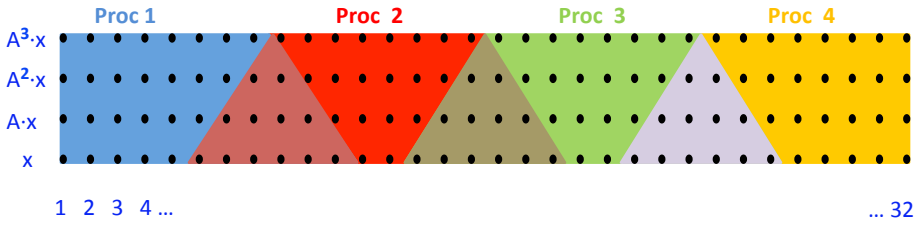
- Parallel Algorithm



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

Communication Avoiding Kernels:
The Matrix Powers Kernel : [Ax, A^2x, …, A^kx]

- Replace k iterations of y = A·x with [Ax, A^2x, …, A^kx]
- Parallel Algorithm



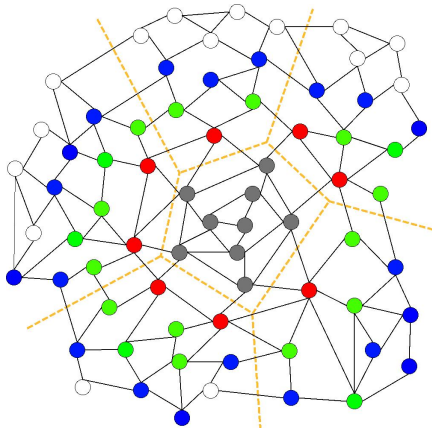
- Example: A tridiagonal, n=32, k=3
- Each processor works on (overlapping) trapezoid

Communication Avoiding Kernels:
The Matrix Powers Kernel : [Ax, A^2x, …, A^kx]

Same idea works for general sparse matrices

Simple block-row partitioning ➔
(hyper)graph partitioning

Left-to-right processing ➔
Traveling Salesman Problem



Minimizing Communication of GMRES to solve Ax=b

- GMRES: find x in span{b,Ab,…,A^kb} minimizing || Ax-b ||$_2$

Standard GMRES
for i=1 to k
  w = A · v(i-1) … *SpMV*
  MGS(w, v(0),…,v(i-1))
  update v(i), H
endfor
solve LSQ problem with H

Communication-avoiding GMRES
W = [v, Av, A^2v, … , A^kv]
[Q,R] = TSQR(W)
  … *"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!

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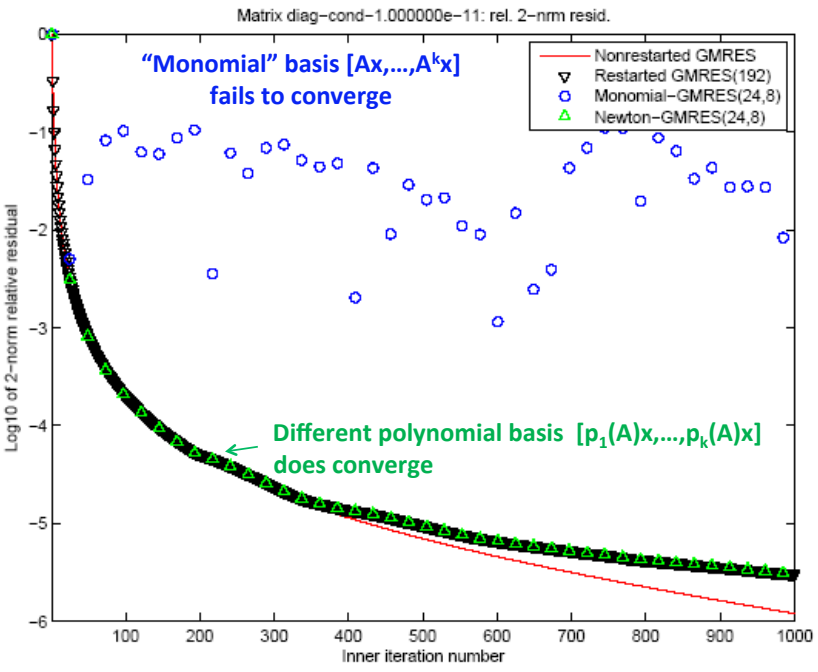

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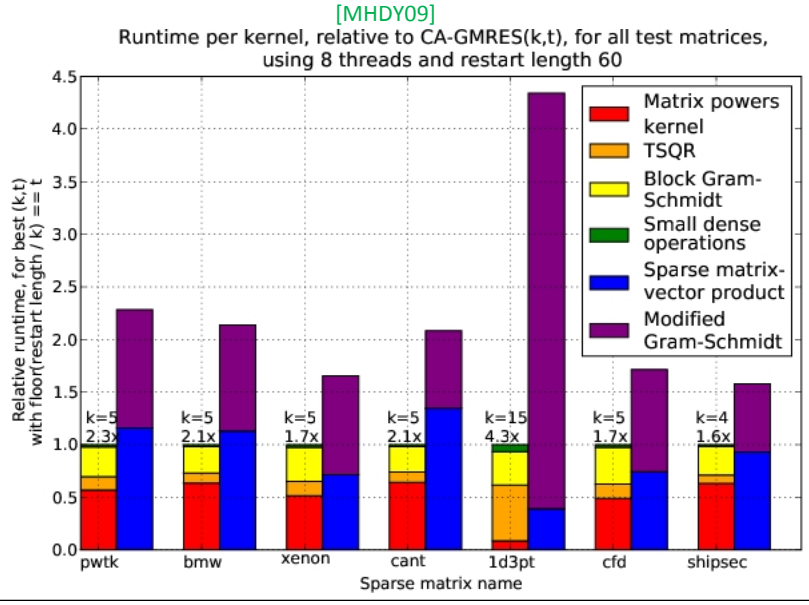
Speed ups of GMRES on 8-core Intel Clovertown

Requires Co-tuning Kernels

[MHDY09]



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CA-BiCGStab

Compute $r_0 = b - Ax_0$. Choose r_0^* arbitrary.
Set $p_0 = r_0$, $q_{-1} = 0_{N\times 1}$.
For $k = 0, 1, \ldots,$ until convergence, Do

$P = [p_{sk}, Ap_{sk}, \ldots, A^s p_{sk}]$
$Q = [q_{sk-1}, Aq_{sk-1}, \ldots, A^s q_{sk-1}]$
$R = [r_{sk}, Ar_{sk}, \ldots, A^s r_{sk}]$
//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,
$b^\ell_{sk} = \left[B_1(:,\ell)^T, 0^T_{s+1}, 0^T_{s+1}\right]^T$
$c^\ell_{sk-1} = \left[0^T_{s+1}, B_2(:,\ell)^T, 0^T_{s+1}\right]^T$
$d^\ell_{sk} = \left[0^T_{s+1}, 0^T_{s+1}, B_3(:,\ell)^T\right]^T$

1. Compute $r_0 := b - Ax_0$; r_0^* arbitrary;
2. $p_0 := r_0$.
3. For $j = 0, 1, \ldots,$ 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. $\beta_j := \frac{(r_{j+1}, r_0^*)}{(r_j, r_0^*)} \frac{\alpha_j}{\omega_j}$
10. $p_{j+1} := r_{j+1} + \beta_j (p_j - \omega_j Ap_j)$
11. EndDo

For $j = 0$ to $\lfloor \frac{s}{2} \rfloor - 1$, Do
$\alpha_{sk+j} = \frac{<g, d^0_{sk+j}>}{<g, b^1_{sk+j}>}$
$q_{sk+j} = r_{sk+j} - \alpha_{sk+j}[P, Q, R] b^1_{sk+j}$
For $\ell = 0$ to $s - 2j + 1$, Do
$c^\ell_{sk+j} = d^\ell_{sk+j} - \alpha_{sk+j} b^{\ell+1}_{sk+j-1}$
//such that $[P, Q, R]\, c^\ell_{sk+j} = A^\ell q_{sk+j}$
$\omega_{sk+j} = \frac{<c^1_{sk+j+1}, Gc^0_{sk+j+1}>}{<c^1_{sk+j+1}, Gc^1_{sk+j+1}>}$
$x_{sk+j+1} = x_{sk+j} + \alpha_{sk+j} p_{sk+j} + \omega_{sk+j} q_{sk+j}$
$r_{sk+j+1} = q_{sk+j} - \omega_{sk+j}[P, Q, R] c^1_{sk+j+1}$
For $\ell = 0$ to $s - 2j$, Do
$d^\ell_{sk+j+1} = c^\ell_{sk+j+1} - \omega_{sk+j} c^{\ell+1}_{sk+j+1}$
//such that $[P, Q, R]\, d^\ell_{sk+j+1} = A^\ell r_{sk+j+1}$
$\beta_{sk+j} = \frac{<g, d^0_{sk+j+1}>}{<g, d^0_{sk+j}>} \times \frac{\alpha}{\omega}$
$p_{sk+j+1} = r_{sk+j+1} + \beta_{sk+j} p_{sk+j} - \beta_{sk+j}\omega_{sk+j}[P, Q, R] b^1_{sk+j}$
For $\ell = 0$ to $s - 2j$, Do
$b^\ell_{sk+j+1} = d^\ell_{sk+j+1} + \beta_{sk+j} b^\ell_{sk+j} - \beta_{sk+j}\omega_{sk+j} b^{\ell+1}_{sk+j}$
//such that $[P, Q, R]\, b^\ell_{sk+j+1} = A^\ell p_{sk+j+1}$.
EndDo
EndDo

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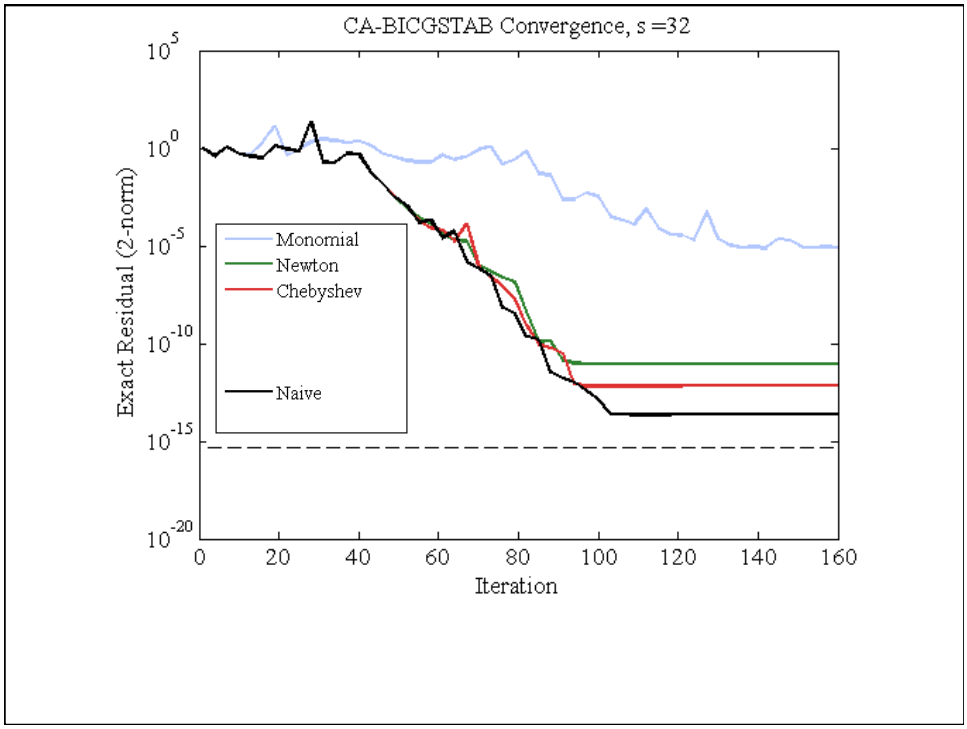
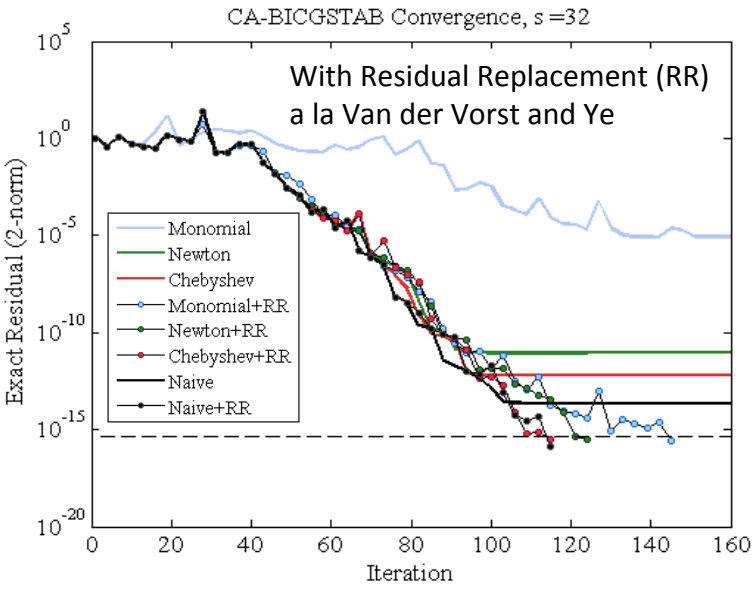
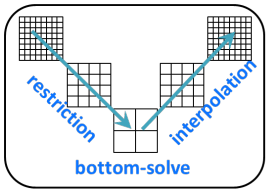




	Naive	Monomial	Newton	Chebyshev
Replacement Its.	74 **(1)**	[7, 15, 24, 31, …, 92, 97, 103] **(17)**	[67, 98] **(2)**	68 **(1)**

Sample Application Speedups

- Geometric Multigrid (GMG) w CA Bottom Solver
  - Compared **BICGSTAB** vs. **CA-BICGSTAB** with s = 4
  - Hopper at NERSC (Cray XE6), weak scaling: Up to 4096 MPI processes (24,576 cores total)



  - Speedups for miniGMG benchmark (HPGMG benchmark predecessor)
    - **4.2x** in bottom solve, **2.5x** overall GMG solve
  - Implemented as a solver option in BoxLib and CHOMBO AMR frameworks
    - 3D LMC (a low-mach number combustion code)
      - **2.5x** in bottom solve, **1.5x** overall GMG solve
    - 3D Nyx (an N-body and gas dynamics code)
      - **2x** in bottom solve, **1.15x** overall GMG solve
- Solve Horn-Schunck Optical Flow Equations
  - Compared **CG** vs. **CA-CG** with s = 3, **43%** faster on NVIDIA GT 640 GPU

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Tuning space for Krylov Methods

- Classifications of sparse operators for avoiding communication
  - Explicit indices or nonzero entries cause most communication, along with vectors
  - Ex: With stencils (all implicit) all communication for vectors

Nonzero entries \ Indices		Explicit (O(nnz))	Implicit (o(nnz))
	Explicit (O(nnz))	CSR and variations	Vision, climate, AMR, ...
	Implicit (o(nnz))	Graph Laplacian	Stencils

- Operations
  - [x, Ax, A^2x,…, A^kx] or [x, p_1(A)x, p_2(A)x, …, p_k(A)x]
  - Number of columns in x
  - [x, Ax, A^2x,…, A^kx] and [y, A^Ty, $(A^T)^2$y,…, $(A^T)^k$y], or [y, A^TAy, $(A^TA)^2$y,…, $(A^TA)^k$y],
  - return all vectors or just last one
- Cotuning and/or interleaving
  - W = [x, Ax, A^2x,…, A^kx] and {TSQR(W) or W^TW or … }
  - Ditto, but throw away W
- Preconditioned versions

Summary of Iterative Linear Algebra

- New Lower bounds, optimal algorithms, big speedups in theory and practice
- Lots of other progress, open problems
  - Many different algorithms reorganized
    - More underway, more to be done
  - Need to recognize stable variants more easily
  - Preconditioning
    - Hierarchically Semiseparable Matrices
  - Autotuning and synthesis
    - pOSKI for SpMV – available at bebop.cs.berkeley.edu
    - Different kinds of “sparse matrices”

For more details

- Bebop.cs.berkeley.edu
  - 155 page survey in Acta Numerica
- CS267 – Berkeley's Parallel Computing Course
  - Live broadcast in Spring 2015
    - www.cs.berkeley.edu/~demmel
    - All slides, video available
  - Prerecorded version broadcast since Spring 2013
    - www.xsede.org
    - Free supercomputer accounts to do homework
    - Free autograding of homework

Reproducible Floating Point Computation

- Do you get the same answer if you run the same program twice with the same input?
  - Not even on your multicore laptop!
- Floating point addition is nonassociative, summation order not reproducible
- First release of the ReproBLAS
  - Reproducible BLAS 1, independent of data order, number of processors, data layout, reduction tree, …
  - Sequential and distributed memory (MPI)
- bebop.cs.berkeley.edu/reproblas

Summary

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

Don’t Communic…

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