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

\[
\text{communication} = \begin{cases}
\# \text{ flops} \times \text{time\_per\_flop} \\
\# \text{ words moved} / \text{bandwidth} \\
\# \text{ messages} \times \text{latency}
\end{cases}
\]
Why avoid communication? (2/3)

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  – # flops * time_per_flop
  – # words moved / bandwidth
  – # messages * latency

\[ \text{communication} \]

• Time_per_flop \ll 1/ \text{bandwidth} \ll \text{latency}
Why avoid communication? (2/3)

- Running time of an algorithm is sum of 3 terms:
  - # flops * time_per_flop
  - # words moved / bandwidth
  - # messages * latency

- Time_per_flop << 1/ bandwidth << latency

- Gaps growing exponentially with time [FOSC]

<table>
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- Running time of an algorithm is sum of 3 terms:
  - \( \# \text{flops} \times \text{time\_per\_flop} \)
  - \( \# \text{words moved} / \text{bandwidth} \)
  - \( \# \text{messages} \times \text{latency} \)

- Time\_per\_flop \( \ll \) 1/ bandwidth \( \ll \) latency
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- Avoid communication to save time
Why Minimize Communication? (3/3)

Source: John Shalf, LBL
Why Minimize Communication? (3/3)

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Why Minimize Communication? (3/3)

Minimize communication to save energy

Source: John Shalf, LBL
Alternative Cost Model for Algorithms?
Alternative Cost Model for Algorithms?

Total distance moved by beads on an abacus
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
Sample Speedups

- Up to $12x$ faster for 2.5D matmul on 64K core IBM BG/P
- Up to $3x$ faster for tensor contractions on 2K core Cray XE/6
- Up to $6.2x$ faster for All-Pairs-Shortest-Path on 24K core Cray CE6
- Up to $2.1x$ faster for 2.5D LU on 64K core IBM BG/P
- Up to $11.8x$ faster for direct N-body on 32K core IBM BG/P
- Up to $13x$ faster for Tall Skinny QR on Tesla C2050 Fermi NVIDIA GPU
- Up to $6.7x$ faster for symeig(band A) on 10 core Intel Westmere
- Up to $2x$ faster for 2.5D Strassen on 38K core Cray XT4
- Up to $4.2x$ faster for MiniGMG benchmark bottom solver, using CA-BiCGStab ($2.5x$ for overall solve)
  - $2.5x / 1.5x$ for combustion simulation code
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.”

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CA-GMRES (Hoemmen, Mohiyuddin, Yelick, JD)
“Tall-Skinny” QR (Grigori, Hoemmen, Langou, JD)
Outline

• Survey state of the art of CA (Comm-Avoiding) algorithms
  – Review previous Matmul algorithms
  – CA $O(n^3)$ 2.5D Matmul
  – TSQR: Tall-Skinny QR
  – CA Strassen Matmul
• Beyond linear algebra
  – Lower bound proof for linear algebra
  – Extending lower bounds to “any algorithm with arrays”
  – Progress toward optimal algorithms
• CA-Krylov methods
• Conclusions
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Summary of CA Linear Algebra

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  • Mostly not attained by algorithms in standard libraries

• Being added to libraries: Sca/LAPACK, PLASMA, MAGMA

• Large speed-ups possible

• Autotuning to find optimal implementation

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• Ditto for “Iterative” Linear Algebra
Lower bound for all “n³-like” linear algebra

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

\[ \#\text{words\_moved (per processor)} = \Omega\left(\frac{\#\text{flops (per processor)}}{M^{1/2}}\right) \]
Lower bound for all “$n^3$-like” linear algebra

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• Parallel case: assume either load or memory balanced
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  – Matmul
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$$\text{#words}_\text{moved} (\text{per processor}) = \Omega(\text{#flops (per processor) } / M^{1/2})$$

• 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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\[ \#\text{words\_moved (per processor)} = \Omega(\#\text{flops (per processor)} / M^{1/2}) \]

\[ \#\text{messages\_sent} \geq \#\text{words\_moved} / \text{largest\_message\_size} \]

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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, APSP
  – New algorithms, with new numerical properties, new ways to encode answers, new data structures
  – Not just loop transformations (need those too!)

• Only a few sparse algorithms so far
  – Ex: Matmul of “random” sparse matrices
  – Ex: Sparse Cholesky of matrices with “large” separators

• Lots of work in progress
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• Beyond linear algebra
  – Lower bound proof for linear algebra
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  – Progress toward optimal algorithms

• CA-Krylov methods

• Conclusions
Naïve Matrix Multiply

\{\text{implies } C = C + A*B\}

for \(i = 1\) to \(n\)

\hspace{1cm}

for \(j = 1\) to \(n\)

\hspace{1cm}

for \(k = 1\) to \(n\)

\[ C(i,j) = C(i,j) + A(i,k) \times B(k,j) \]
Naïve Matrix Multiply

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

\{\text{implements } C = C + A \times B\}

\text{for } i = 1 \text{ to } n

\{\text{read row } i \text{ of } A \text{ into fast memory}\} \quad \ldots \quad n^2 \text{ reads altogether}

\text{for } j = 1 \text{ to } n

\{\text{read } C(i,j) \text{ into fast memory}\} \quad \ldots \quad n^2 \text{ reads altogether}

\{\text{read column } j \text{ of } B \text{ into fast memory}\} \quad \ldots \quad n^3 \text{ reads altogether}

\text{for } k = 1 \text{ to } n

C(i,j) = C(i,j) + A(i,k) \times B(k,j)

\{\text{write } C(i,j) \text{ back to slow memory}\} \quad \ldots \quad n^2 \text{ writes altogether}

n^3 + 3n^2 \text{ reads/writes altogether} - \text{dominates } 2n^3 \text{ arithmetic}
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}
    $C[i,j] = C[i,j] + A[i,k] \times B[k,j]$ \{do a matrix multiply on $b$-by-$b$ blocks\}
    {write block $C[i,j]$ back to slow memory}
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\} \quad ... $b^2 \times (n/b)^2 = n^2$ reads
  For $k = 1$ to $n/b$
    \{read block $A[i,k]$ into fast memory\} \quad ... $b^2 \times (n/b)^3 = n^3/b$ reads
    \{read block $B[k,j]$ into fast memory\} \quad ... $b^2 \times (n/b)^3 = n^3/b$ reads
    $C[i,j] = C[i,j] + A[i,k] \times B[k,j]$ \{do a matrix multiply on $b$-by-$b$ blocks\}
    \{write block $C[i,j]$ back to slow memory\} \quad ... $b^2 \times (n/b)^2 = n^2$ writes

\[2n^3/b + 2n^2 \text{ reads/writes} \ll 2n^3 \text{ arithmetic - Faster!}\]
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: $3b^2 \leq M$, so #reads/writes $\geq 3^{1/2}n^3/M^{1/2} + 2n^2$

• Attains lower bound $= \Omega (\#\text{flops} / M^{1/2})$
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: \(3b^2 \leq M\), so \#reads/writes \(\geq 3^{1/2}n^3/M^{1/2} + 2n^2\)
• Attains lower bound \(= \Omega (\text{#flops} / M^{1/2})\)

• But what if we don’t know M?
• Or if there are multiple levels of fast memory?
• Can use “Cache Oblivious” algorithm (divide and conquer)
SUMMA—n x n matmul on P^{1/2} x P^{1/2} grid (nearly) optimal using minimum memory M=O(n^2/P)

For k=0 to n/b-1  … b = block size = #cols in A(i,k) = #rows in B(k,j)
   for all i = 1 to P^{1/2}
      owner of A(i,k) broadcasts it to processor row i
   for all j = 1 to P^{1/2}
      owner of B(k,j) broadcasts it to processor column k
Receive A(i,k) into Acol
Receive B(k,j) into Brow
C_myproc = C_myproc + Acol * Brow
Summary of dense \textit{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\left(\frac{n^3}{P} / M^{1/2}\right) = \Omega\left(\frac{n^2}{P^{1/2}}\right)
  \#messages = \Omega\left(\frac{n^3}{P} / M^{3/2}\right) = \Omega\left(P^{1/2}\right)
Summary of dense *parallel* algorithms attaining communication lower bounds

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  - $\#\text{words}_\text{moved} = \Omega(\frac{n^3}{P} / M^{1/2}) = \Omega(\frac{n^2}{P^{1/2}})$
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- Does ScALAPACK attain these bounds?
  - For $\#\text{words}_\text{moved}$: mostly, except nonsym. Eigenproblem
  - For $\#\text{messages}$: asymptotically worse, except Cholesky
- New algorithms attain all bounds, up to polylog(P) factors
  - Cholesky, LU, QR, Sym. and Nonsym eigenproblems, SVD
    - Needed to replace partial pivoting in LU
    - Need randomization for Nonsym eigenproblem (so far)
Summary of dense \textit{parallel} algorithms attain communication lower bounds

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  \#\text{messages} & = \Omega\left( \frac{n^3}{P} / M^{3/2} \right) = \Omega\left( P^{1/2} \right)
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\textbf{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?
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]
• Not always $p^{1/3}$ times as much memory available...
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2.5D Matrix Multiplication

- Assume can fit $cn^2/P$ data per processor, $c > 1$
- Processors form $(P/c)^{1/2} \times (P/c)^{1/2} \times c$ 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 $n(c/P)^{1/2} \times n(c/P)^{1/2}$
2.5D Matrix Multiplication

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

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 $\sum_m A(i,m) \times B(m,j)$
3. Sum-reduce partial sums $\Sigma_m A(i,m) \times B(m,j)$ along $k$-axis so $P(i,j,0)$ owns $C(i,j)$
2.5D Matmul on BG/P, 16K nodes / 64K cores

Matrix multiplication on 16,384 nodes of BG/P

- 2.5D MM
- 2D MM

Using c=16 matrix copies

- 12X faster
- 2.7X faster

Percentage of machine peak: 0 to 100
2.5D Matmul on BG/P, 16K nodes / 64K cores

c = 16 copies

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95% reduction in comm

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

SC’11 paper by Solomonik, Bhatatele, 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.

• Note for timing model:
  - \( \gamma_T \), \( \beta_T \), \( \alpha_T \) = seconds per flop, per word moved, per message of size m.

  \[ T(cP) = \frac{n^3}{cP} \left[ \gamma_T + \frac{\beta_T}{M^{1/2}} + \frac{\alpha_T}{(mM^{1/2})} \right] = T(P)/c \]

• Note for energy model:
  - \( \gamma_E \), \( \beta_E \), \( \alpha_E \) = joules for same operations.
  - \( \delta_E \) = joules per word of memory used per sec.
  - \( \epsilon_E \) = joules per sec for leakage, etc.

  \[ E(cP) = cP \{ \frac{n^3}{cP} \left[ \gamma_T + \frac{\beta_T}{M^{1/2}} + \frac{\alpha_T}{(mM^{1/2})} \right] + \delta_E MT(cP) + \epsilon_E T(cP) \} = E(P) \]

• Extends to N-body, Strassen, …

• Can prove lower bounds on needed network (eg 3D torus for matmul).
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 = 3n²
• Increase P by a factor of c \( \Rightarrow \) total memory increases by a factor of c
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) = \frac{n^3}{cP} \left[ \gamma_T + \frac{\beta_T}{\sqrt{M}} + \frac{\alpha_T}{(mM)^{1/2}} \right]
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• Extends to N-body, Strassen, …
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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 $c$ $\Rightarrow$ total memory increases by a factor of $c$
• Notation for timing model:
  $\quad \gamma_T, \beta_T, \alpha_T = \text{secs per flop, per word\_moved, per message of size } m$
• $T(cP) = n^3/(cP) \left[ \gamma_T + \beta_T/M^{1/2} + \alpha_T/(mM^{1/2}) \right]$
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 $c$ $\Rightarrow$ total memory increases by a factor of $c$
• Notation for timing model:
  $\gamma_T, \beta_T, \alpha_T =$ secs per flop, per word\_moved, per message of size $m$
• $T(cP) = \frac{n^3}{(cP)} \left[ \gamma_T + \frac{\beta_T}{M^{1/2}} + \frac{\alpha_T}{(mM^{1/2})} \right]$
  $= \frac{T(P)}{c}$
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 wordMoved, per message of size m
• T(cP) = n^3/(cP) [ γ_T + β_T/M^{1/2} + α_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.
Perfect Strong Scaling – in Time and Energy

- Every time you add a processor, you should use its memory M too
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  - \(\gamma_T, \beta_T, \alpha_T\) = secs per flop, per word\_moved, per message of size m
- \(T(cP) = \frac{n^3}{cP} \left[ \gamma_T + \beta_T/M^{1/2} + \alpha_T/(mM^{1/2}) \right] = T(P)/c\)
- Notation for energy model:
  - \(\gamma_E, \beta_E, \alpha_E\) = joules for same operations
  - \(\delta_E\) = joules per word of memory used per sec
  - \(\varepsilon_E\) = joules per sec for leakage, etc.
- \(E(cP) = cP \left\{ \frac{n^3}{cP} \left[ \gamma_E + \beta_E/M^{1/2} + \alpha_E/(mM^{1/2}) \right] + \delta_E MT(cP) + \varepsilon_E T(cP) \right\}\)
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 $c \Rightarrow$ total memory increases by a factor of $c$
- Notation for timing model:
  - $\gamma_T, \beta_T, \alpha_T = \text{secs per flop, per word moved, per message of size } m$
  - $T(cP) = n^3/(cP) [ \gamma_T + \beta_T/M^{1/2} + \alpha_T/(mM^{1/2}) ]$
  - $= T(P)/c$
- Notation for energy model:
  - $\gamma_E, \beta_E, \alpha_E = \text{joules for same operations}$
  - $\delta_E = \text{joules per word of memory used per sec}$
  - $\epsilon_E = \text{joules per sec for leakage, etc.}$
- $E(cP) = cP \{ n^3/(cP) [ \gamma_E + \beta_E/M^{1/2} + \alpha_E/(mM^{1/2}) ] + \delta_E MT(cP) + \epsilon_E T(cP) \}$
  - $= E(P)$
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 = 3n²
- Increase P by a factor of c ➔ total memory increases by a factor of c
- Notation for timing model:
  - $\gamma_T$, $\beta_T$, $\alpha_T = \text{secs per flop, per word}_\text{moved, per message of size } m$
  - $T(cP) = n^3/(cP) \left[ \gamma_T + \beta_T/M^{1/2} + \alpha_T/(mM^{1/2}) \right] = T(P)/c$
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- Extends to N-body, Strassen, ...
- Can prove lower bounds on needed network (eg 3D torus for matmul)
Outline

• Survey state of the art of CA (Comm-Avoiding) algorithms
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• Conclusions
TSQR: QR of a Tall, Skinny matrix

\[ W = \begin{pmatrix} W_0 \\ W_1 \\ W_2 \\ W_3 \end{pmatrix} \]
TSQR: QR of a Tall, Skinny matrix

\[
W = \begin{pmatrix} W_0 \\ W_1 \\ W_2 \\ W_3 \end{pmatrix} = \begin{pmatrix} Q_{00} & R_{00} \\ Q_{10} & R_{10} \\ Q_{20} & R_{20} \\ Q_{30} & R_{30} \end{pmatrix}
\]
TSQR: QR of a Tall, Skinny matrix

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W = \begin{pmatrix}
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\]

\[
\begin{pmatrix}
R_{00} \\
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R_{20} \\
R_{30}
\end{pmatrix} = \begin{pmatrix}
Q_{01} & R_{01} \\
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\]

Output = \{ Q_{00}, Q_{10}, Q_{20}, Q_{30}, Q_{01}, Q_{11}, Q_{02}, R_{02} \}
TSQR: An Architecture-Dependent Algorithm

Parallel: $W = \begin{bmatrix} W_0 \\ W_1 \\ W_2 \\ W_3 \end{bmatrix} \rightarrow R_{00} \rightarrow R_{10} \rightarrow R_{01} \rightarrow R_{02} \rightarrow R_{11} \rightarrow R_{30} \rightarrow R_{30} \rightarrow R_{02}$
TSQR: An Architecture-Dependent Algorithm

Parallel: \[ \begin{bmatrix} W_0 \\ W_1 \\ W_2 \\ W_3 \end{bmatrix} \rightarrow R_{00} \rightarrow R_{10} \rightarrow R_{01} \rightarrow R_{02} \]

Sequential: \[ \begin{bmatrix} W_0 \\ W_1 \\ W_2 \\ W_3 \end{bmatrix} \rightarrow R_{00} \rightarrow R_{01} \rightarrow R_{02} \rightarrow R_{03} \]

Dual Core: Can choose reduction tree dynamically

Multi-core / Multi-socket / Multi-rack / Multi-site / Out-of-core: ?
TSQR: An Architecture-Dependent Algorithm

Parallel: \( W = \begin{bmatrix} W_0 \\ W_1 \\ W_2 \\ W_3 \end{bmatrix} \rightarrow R_{00} \rightarrow R_{10} \rightarrow R_{01} \rightarrow R_{02} \)

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

Can choose reduction tree dynamically
TSQR Performance Results

- **Parallel Speedups**
  - Up to $8x$ on 8 core Intel Clovertown
  - Up to $6.7x$ on 16 processor Pentium cluster
  - Up to $4x$ on 32 processor IBM Blue Gene
  - Up to $13x$ on NVidia GPU
  - Up to $4x$ on 4 cities vs 1 city (Dongarra, Langou et al)
  - **Only 1.6x slower** on Cloud than just accessing data twice (Gleich and Benson)

- **Sequential Speedup**
  - “**Infinite**” for out-of-core on PowerPC laptop

- **SVD costs about the same**
  - Joint work with Grigori, Hoemmen, Langou, Anderson, Ballard, Keutzer, others

Data from Grey Ballard, Mark Hoemmen, Laura Grigori, Julien Langou, Jack Dongarra, Michael Anderson
Outline

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Communication Lower Bounds for Strassen-like matmul algorithms

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 achievable?

Classical $O(n^3)$ matmul:
$\#\text{words moved} = \Omega(M(n/M^{1/2})^3/P)$

Strassen's $O(n \lg^7)$ matmul:
$\#\text{words moved} = \Omega(M(n/M^{1/2}) \lg^7/P)$

Strassen-like $O(n^\omega)$ matmul:
$\#\text{words moved} = \Omega(M(n/M^{1/2})^\omega/P)$
Communication Lower Bounds for Strassen-like matmul algorithms

Classical
$O(n^3)$ matmul:

$\#\text{words}\_\text{moved} = \Omega \left( M(n/M^{1/2})^3 / P \right)$
Communication Lower Bounds for Strassen-like matmul algorithms

Classical $O(n^3)$ matmul:
$$\#\text{words}_\text{moved} = \Omega\left(\frac{M(n/M^{1/2})^3}{P}\right)$$

Strassen’s $O(n^{\lg 7})$ matmul:
$$\#\text{words}_\text{moved} = \Omega\left(\frac{M(n/M^{1/2})^{|\lg 7|}}{P}\right)$$
Communication Lower Bounds for Strassen-like matmul algorithms

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- **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)
Performance Benchmarking, Strong Scaling Plot
Franklin (Cray XT4) n = 94080

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Invited to appear as Research Highlight in CACM
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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)
Recall optimal sequential Matmul

• Naïve code
  for i=1:n, for j=1:n, for k=1:n,
  \[ C(i,j) += A(i,k) \times B(k,j) \]

• “Blocked” code
  for i = 1:n/b, for j = 1:n/b, for k = 1:n/b
  \[ C[i,j] += A[i,k] \times B[k,j] \quad \ldots \quad \text{b x b matmul} \]
Recall optimal sequential Matmul

• Naïve code
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• Thm: Picking \( b = M^{1/2} \) attains lower bound:
  \[ \# \text{words}_\text{moved} = \Omega(n^3/M^{1/2}) \]
• Where does 1/2 come from?
Where do lower and matching upper bounds on communication come from? (1/3)

• Originally for $C = A \times B$ by Irony/Tiskin/Toledo (2004)

• Proof idea
  – Suppose we can upper bound $\#\text{operations}$ doable with data in fast memory of size $M$, by $\#\text{operations} \leq G$
  – So to do $F = \#\text{total\_operations}$, need to fill fast memory at least $F/G$ times, and so $\#\text{words\_moved} \geq MF/G$

• Hard part: finding $G$
Where do lower and matching upper bounds on communication come from? (1/3)

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• Harder part: Attaining lower bound
  – Need to “block” all operations to perform $\sim G$ operations on every chunk of $M$ words of data
Proof of communication lower bound (2/3)
Proof of communication lower bound (2/3)

Cube representing $C(1,1) = A(1,3) \cdot B(3,1)$

"C face"

"A face"

"B face"
Proof of communication lower bound (2/3)

If we have at most $M$ “A squares”, $M$ “B squares”, and $M$ “C squares”, how many cubes $G$ can we have?
Proof of communication lower bound (3/3)

\[ G = \# \text{ cubes in black box with} \]
\[ \text{side lengths } x, y \text{ and } z \]
\[ = \text{Volume of black box} \]
\[ = x \cdot y \cdot z \]
\[ = (xz \cdot zy \cdot yx)^{1/2} \]
\[ = (\#A\square s \cdot \#B\square s \cdot \#C\square s)^{1/2} \]
\[ \leq M^{3/2} \]
Proof of communication lower bound (3/3)

G = # cubes in black box with side lengths x, y and z
= Volume of black box
= x·y·z
= (xz · zy · yx)\(^{1/2}\)
= (\(#A\bigcirc\)s · \(#B\bigcirc\)s · \(#C\bigcirc\)s \(^{1/2}\)
\leq M^{3/2}

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

Thm (Loomis & Whitney, 1949)

G = # cubes in 3D set = Volume of 3D set
\leq (\text{area}(A\ projection) \cdot \text{area}(B\ projection) \cdot \text{area}(C\ projection))^{1/2}
\leq M^{3/2}
New theorem, applied to Matmul
(Christ, D., Knight, Scanlon, Yelick)

• 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

\[
\begin{bmatrix}
i & j & k \\
1 & 0 & 1 \\
0 & 1 & 1 \\
1 & 1 & 0 \\
\end{bmatrix}
\]

Δ = 

\[
\begin{bmatrix}
A \\
B \\
C \\
\end{bmatrix}
\]

• Thm: #words_moved = Ω(n^3/M_{SHBL}^{-1}) = Ω(n^{3/2})
New theorem, applied to Matmul
(Christ, D., Knight, Scanlon, Yelick)

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Δ

\[
\begin{pmatrix}
A \\
B \\
C \\
\end{pmatrix}
\]

• Solve LP for \(x = [x_i, x_j, x_k]^T\): \(\max 1^T x \quad \text{s.t.} \quad \Delta x \leq 1\)
  
  — Result: \(x = [1/2, 1/2, 1/2]^T, 1^T x = 3/2 = s_{HBL}\)
New theorem, applied to Matmul
(Christ, D., Knight, Scanlon, Yelick)

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

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• Solve LP for \( x = [x_i, x_j, x_k]^T \): \( \max 1^T x \) s.t. \( \Delta x \leq 1 \)
  
  — Result: \( x = [1/2, 1/2, 1/2]^T \), \( 1^T x = 3/2 = s_{HBL} \)

• Thm: \#words\_moved = \( \Omega(n^3/M_{SHBL-1}^{1/2}) = \Omega(n^3/M^{1/2}) \)
  
  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 $j=1:n$, $F(i) + = \text{force}(P(i), P(j))$

• Record array indices in matrix $\Delta$

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

$$
\begin{pmatrix}
 i & j \\
 1 & 0 \\
 1 & 0 \\
 0 & 1 \\
\end{pmatrix}
$$

- Solve LP for $x = [x_i,x_j]^T$: max $1^T x$ s.t. $\Delta x \leq 1$
  - Result: $x = [1,1], 1^T x = 2 = s_{HBL}$
- Thm: $\#\text{words\_moved} = \Omega(n^2/M_{SHBL}^{-1}) = \Omega(n^2/M^1)$
  Attained by block sizes $M_i^{x_i}, M_j^{x_j} = M^1, M^1$
N-Body Speedups on IBM-BG/P (Intrepid) 8K cores, 32K particles

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

• Gravity, Turbulence, Molecular Dynamics, Plasma Simulation, …
Some Applications

- Gravity, Turbulence, Molecular Dynamics, Plasma Simulation, …
- Electron-Beam Lithography Device Simulation

– www.fxguide.com/featured/brave-new-hair/
– graphics.pixar.com/library/CurlyHairA/paper.pdf
Some Applications

• Gravity, Turbulence, Molecular Dynamics, Plasma Simulation, …
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• Hair …
  – www.fxguide.com/featured/brave-new-hair/
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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 $\Delta$

$$
\Delta = \begin{pmatrix}
i1 & i2 & i3 & i4 & i5 & i6 \\
1 & 0 & 1 & 0 & 0 & 1 \\
1 & 1 & 0 & 1 & 0 & 0 \\
0 & 1 & 1 & 0 & 1 & 0 \\
0 & 0 & 1 & 1 & 0 & 1 \\
0 & 1 & 0 & 0 & 0 & 1 \\
1 & 0 & 0 & 1 & 1 & 0 \\
\end{pmatrix}
$$
New Thm applied to Random Code

• for i1=1:n, for i2=1:n, ... , for i6=1:n
  
  \[ A1(i1,i3,i6) += \text{func1}(A2(i1,i2,i4),A3(i2,i3,i5),A4(i3,i4,i6)) \]
  \[ A5(i2,i6) += \text{func2}(A6(i1,i4,i5),A3(i3,i4,i6)) \]

• Record array indices in matrix \( \Delta \)

\[
\Delta = \begin{pmatrix}
1 & 0 & 1 & 0 & 0 & 1 \\
1 & 1 & 0 & 1 & 0 & 0 \\
0 & 1 & 1 & 0 & 1 & 0 \\
0 & 0 & 1 & 1 & 0 & 1 \\
0 & 1 & 0 & 0 & 0 & 1 \\
1 & 0 & 0 & 1 & 1 & 0
\end{pmatrix}
\]

• Solve LP for \( x = [x_1,...,x_6]^T \): max \( 1^T x \) s.t. \( \Delta x \leq 1 \)
  
  – Result: \( x = [2/7,3/7,1/7,2/7,3/7,4/7] \), \( 1^T x = 15/7 = s_{\text{HBL}} \)

• Thm: \#words\_moved = \( \Omega(n^6/M_{\text{HBL}}^{-1}) = \Omega(n^6/M^{8/7}) \)
  
  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
Approach to generalizing lower bounds

• Matmul
  
  for i=1:n, for j=1:n, for k=1:n,
  
  \[ C(i,j) += A(i,k) \times B(k,j) \]

• General case for i1=1:n, i2=1:m, …, ik=i3:i4
  
  \[ C(i1+2i3-i7) = \text{func}(A(i2+3i4,i1,i2,i1+i2,…), B(pnt(3i4)),…) \]

  \[ D(\text{something else}) = \text{func}(\text{something else}), … \]

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

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

• Goal: Communication lower bounds, optimal algorithms for any program that looks like this
Approach to generalizing lower bounds

- Matmul
  
  for i=1:n, for j=1:n, for k=1:n,
  
  \[ C(i,j) += A(i,k) \times B(k,j) \]
  
  => 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
  
  \[ C(i1+2*i3-i7) = \text{func}(A(i2+3*i4,i1,i2,i1+i2,…),B(pnt(3*i4)),…) \]
  
  D(something else) = \text{func}(something else), …
  
  => for (i1,i2,…,ik) in S = subset of \( Z^k \)
  
  Access locations indexed by group homomorphisms, e.g.
  
  \[ \phi(C(i1,i2,…,ik)) = (i1+2*i3-i7) \]
  
  \[ \phi(A(i1,i2,…,ik)) = (i2+3*i4,i1,i2,i1+i2,…), \]
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 $S = \text{subset of } \mathbb{Z}^3$
  
  Access locations indexed by (i,j), (i,k), (k,j)

- **General case**
  
  for i1=1:n, for i2 = i1:m, ... for ik = i3:i4
  
  $C(i1+2*i3-i7) = \text{func}(A(i2+3*i4,i1,i2,i1+i2,...),B(\text{pnt}(3*i4)),...)$
  
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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
  \[ C(i1+2*i3-i7) = \text{func}(A(i2+3*i4,i1,i2,i1+i2,...),B(\text{pnt}(3*i4)),...) \]
  D(something else) = \text{func}(something else), ... 
=> for (i1,i2,...,ik) in S = subset of Z^k
  Access locations indexed by group homomorphisms, eg
  \[ \phi_C (i1,i2,...,ik) = (i1+2*i3-i7) \]
  \[ \phi_A (i1,i2,...,ik) = (i2+3*i4,i1,i2,i1+i2,...), ... \]
Approach to generalizing lower bounds

• Matmul
  
  for i=1:n, for j=1:n, for k=1:n,
  
  \[ C(i,j) += A(i,k) \times B(k,j) \]

  => for (i,j,k) in S = subset of Z³
  
  Access locations indexed by (i,j), (i,k), (k,j)

• General case
  
  for i1=1:n, for i2 = i1:m, ... for ik = i3:i4
  
  \[ C(i1+2*i3-i7) = \text{func}(A(i2+3*i4,i1,i2,i1+i2,...),B(pnt(3*i4)),...) \]
  
  \[ D(\text{something else}) = \text{func}(\text{something else}), ... \]

  => for (i1,i2,...,ik) in S = subset of Z^k
  
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  \[ \phi_C(i1,i2,...,ik) = (i1+2*i3-i7) \]
  
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• Goal: Communication lower bounds, optimal algorithms for any program that looks like this
General Communication Bound

• Given subset of loop iterations, how much data do we need?
General Communication Bound

- Given subset of loop iterations, how much data do we need?
  - Given subset $S$ of $\mathbb{Z}^k$, group homomorphisms $\phi_1, \phi_2, \ldots, \phi_m$ bound $|S|$ in terms of $|\phi_1(S)|, |\phi_2(S)|, \ldots, |\phi_m(S)|$
General Communication Bound

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  – Given subset \( S \) of \( \mathbb{Z}^k \), group homomorphisms \( \phi_1, \phi_2, \ldots, \phi_m \)
    bound \( |S| \) in terms of \( |\phi_1(S)|, |\phi_2(S)|, \ldots, |\phi_m(S)| \)
• Def: Hölder-Brascamp-Lieb LP (HBL-LP) for \( s_1, \ldots, s_m \):
    for all subgroups \( H < \mathbb{Z}^k \), \( \text{rank}(H) \leq \sum_j s_j \text{rank}(\phi_j(H)) \)
General Communication Bound

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• Thm (extension of Christ/Tao/Carbery/Bennett): Given $s_1,\ldots,s_m$
  $|S| \leq \prod_j |\phi_j(S)|^{S_j}$
General Communication Bound

• Given subset of loop iterations, how much data do we need?
  – Given subset $S$ of $\mathbb{Z}^k$, group homomorphisms $\phi_1, \phi_2, \ldots, \phi_m$ bound $|S|$ in terms of $|\phi_1(S)|, |\phi_2(S)|, \ldots, |\phi_m(S)|$

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• Thm (extension of Christ/Tao/Carbery/Bennett): Given $s_1, \ldots, s_m$
  $|S| \leq \prod_j |\phi_j(S)|^{s_j}$

• Thm: Given a program with array refs given by $\phi_j$, choose $s_j$ to minimize $s_{HBL} = \sum_j s_j$ subject to HBL-LP. Then
  $\#\text{words\_moved} = \Omega(\#\text{iterations}/M^{s_{HBL}^{-1}})$
Is this bound attainable (1/2)?
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• But first: Can we write it down?
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- Thm: (bad news) HBL-LP reduces to Hilbert’s 10th problem over Q
  - conjectured to be undecidable
- Thm: (good news) Another LP with same solution is decidable (but expensive):

Let \( L = (V_1, V_2, \ldots) \) be countable list of all subspaces of \( Q^n \)

\[
i = 0 \\
\text{repeat} \\
i = i + 1 \\
\text{until polytope determined by inequalities from } (V_1, \ldots, V_i) \text{ is right one}
\]
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- Thm: (better news) Enough to use \( L = \) lattice of kernels of \( \phi_1, \phi_2, \ldots, \phi_m \)
  - Similar to result of Valdimarsson in continuum case
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• Thm: (better news) Enough to use \( L = \) lattice of kernels of \( \phi_1, \phi_2, \ldots, \phi_m \)
  – Similar to result of Valdimarsson in continuum case
  – Corollary (Dedekind) If \( m=3 \), only need to consider 28 subspaces
Is this bound attainable (2/2)?

• Given bound, need to reorder loop iterations, or assign them to different processors, to maximize $|S| = \#\_\text{loop\_iterations}$ using data that fits in memory: $|\phi_1(S)| + |\phi_2(S)| + \ldots + |\phi_m(S)| \leq M$

• Assume best case: can execute iterations in any order
  – Ex: matmul, because just summing

• Thm: When all $\phi_k = \{\text{subset of indices}\}$, dual of HBL-LP gives optimal tile sizes:
  
  HBL-LP: minimize $1^T s$ s.t. $s^T \Delta \geq 1^T$, $\Delta(k,j) = \text{rank}(\phi_k(<i_j>))$
  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: $s = [1/2, 1/2, 1/2]^T = x$

• Ex: N-body, “random code”

• Extends to case where HBL-LP determined by independent groups
  – Tiling code means tessellating $Z^k$ with polytopes
Ongoing Work

• Implement/improve algorithms to generate for lower bounds, optimal algorithms

• Have yet to find a case where we cannot attain lower bound – can we prove this?

• Hardest, practical case: Loop-carried dependencies – Ex: $C(i,j) = \text{func}(C(i,j), A(i,k), B(k,j), C(i-1,j))$

• Only some reorderings/tessellations correct – How close can we get to “optimal”?

• Extend “perfect scaling” results for time and energy by using extra memory – “n.5D algorithms”

• Incorporate into compilers
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Outline

• Survey state of the art of CA (Comm-Avoiding) algorithms
  – Review previous Matmul algorithms
  – CA $O(n^3)$ 2.5D Matmul
  – TSQR: Tall-Skinny QR
  – CA Strassen Matmul

• Beyond linear algebra
  – Lower bound proof for linear algebra
  – Extending lower bounds to “any algorithm with arrays”
  – Progress toward optimal algorithms

• CA-Krylov methods

• Conclusions
Avoiding Communication in Iterative Linear Algebra

- k-steps of iterative solver for sparse $Ax=b$ or $Ax=\lambda x$
  - Does $k$ SpMVs with $A$ and starting vector
  - Many such “Krylov Subspace Methods”
    - Conjugate Gradients (CG), GMRES, Lanczos, Arnoldi, ...
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• Goal: minimize communication
  – Assume matrix “well-partitioned”
Avoiding Communication in Iterative Linear Algebra

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  - Assume matrix “well-partitioned”
  - Serial implementation
    - Conventional: $O(k)$ moves of data from slow to fast memory
    - **New: $O(1)$ moves of data – optimal**
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  - Parallel implementation on $p$ processors
    - Conventional: $O(k \log p)$ messages (k SpMV calls, dot prods)
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- Challenges:
  - Poor partitioning,
  - Preconditioning,
  - Num. Stability
Avoiding Communication in Iterative Linear Algebra

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• Lots of speed up possible (modeled and measured)
  – Price: some redundant computation
  – Challenges: Poor partitioning, Preconditioning, Num. Stability
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• Survey state of the art of CA (Comm-Avoiding) algorithms
  – Review previous Matmul algorithms
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  – CA Strassen Matmul

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• Conclusions
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 in Spring 2014/5
    • www.xsede.org
    • Free supercomputer accounts to do homework
    • Free autograding of homework
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- Jack Dongarra, 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 FASTMath, ParLab, ASPIRE, BEBOP, CACHE, EASI, MAGMA, PLASMA
- Thanks to DOE, NSF, UC Discovery, INRIA, Intel, Microsoft, Mathworks, National Instruments, NEC, Nokia, NVIDIA, Samsung, Oracle
- **bebop.cs.berkeley.edu**
Summary

Time to redesign all linear algebra, n-body, ... algorithms and software
(and compilers)
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Don’t Communic...
EXTRA SLIDES
Communication Avoiding Kernels:
The Matrix Powers Kernel : \([Ax, A^2x, ..., A^kx]\)

- Replace k iterations of \(y = A \cdot x\) with \([Ax, A^2x, ..., A^kx]\)

- Example: A tridiagonal, \(n=32, k=3\)
- Works for any “well-partitioned” \(A\)
Communication Avoiding Kernels: The Matrix Powers Kernel: \([Ax, A^2x, \ldots, A^kx]\)

- Replace \(k\) iterations of \(y = A \cdot x\) with \([Ax, A^2x, \ldots, A^kx]\)

Example: A tridiagonal, \(n=32\), \(k=3\)
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- Replace \(k\) iterations of \(y = A \cdot x\) with \([Ax, A^2x, ..., A^kx]\)
- 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 \(y = A \cdot x\) with \([Ax, A^2x, ..., A^kx]\)

- Parallel Algorithm

- Example: A tridiagonal, \(n=32\), \(k=3\)
- Each processor works on (overlapping) trapezoid
The Matrix Powers Kernel: \([Ax, A^2x, ..., A^kx]\) on a general matrix (nearest \(k\) neighbors on a graph)

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

Simple block-row partitioning \(\rightarrow\) (hyper)graph partitioning

Top-to-bottom processing \(\rightarrow\)
Traveling Salesman Problem
Minimizing Communication of GMRES to solve $Ax=b$

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

**Standard GMRES**
for $i=1$ to $k$

- $w = A \cdot v(i-1)$ ... $SpMV$
- $\text{MGS}(w, v(0), ..., v(i-1))$
- update $v(i)$, $H$
endfor

solve LSQ problem with $H$

**Communication-avoiding GMRES**

- $W = [v, Av, A^2v, ..., A^kv]$
- $[Q, R] = \text{TSQR}(W)$
  
  
  ... “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!
Matrix Powers Kernel + TSQR in GMRES

Relative norm of residual $\|Ax - b\|$

- Original GMRES
- CA-GMRES (Monomial basis)
- CA-GMRES (Newton basis)

Iteration count

$10^0$ $10^{-1}$ $10^{-2}$ $10^{-3}$ $10^{-4}$ $10^{-5}$
Speed ups of GMRES on 8-core Intel Clovertown

Requires Co-tuning Kernels

[MHDY09]
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

\[
P = [p_{sk}, A p_{sk}, \ldots, A^s p_{sk}],
\]

\[
Q = [q_{sk-1}, A q_{sk-1}, \ldots, A^s q_{sk-1}],
\]

\[
R = [r_{sk}, A r_{sk}, \ldots, A^s r_{sk}].
\]

//Compute the \( 1 \times (3s + 3) \) Gram vector.
\[
g = (r_0^*)^T [P, Q, R]
\]

//Compute the \((3s + 3) \times (3s + 3)\) Gram matrix
\[
G = \begin{bmatrix}
P^T \\
Q^T \\
R^T
\end{bmatrix}
\begin{bmatrix}
P & Q & R
\end{bmatrix}
\]

For \( \ell = 0 \) to \( s \),
\[
b^{\ell}_{sk} = \begin{bmatrix} B_1 (\cdot, \cdot)^T & 0_{s+1}^T & 0_{s+1}^T \end{bmatrix}^T
\]

\[
c^{\ell}_{sk-1} = \begin{bmatrix} 0_{s+1}^T & B_2 (\cdot, \cdot)^T & 0_{s+1}^T \end{bmatrix}^T
\]

\[
d^{\ell}_{sk} = \begin{bmatrix} 0_{s+1}^T & 0_{s+1} & B_3 (\cdot, \cdot)^T \end{bmatrix}^T
\]

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

For \( j = 0 \) to \( \lfloor \frac{s}{2} \rfloor - 1 \), Do
\[
\alpha_{sk+j} = \langle g \cdot d_{sk+j}^0, g \cdot b_{sk+j}^1 \rangle \\
\langle g \cdot d_{sk+j}^0, g \cdot b_{sk+j}^1 \rangle
\]

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

For \( \ell = 0 \) to \( s - 2j + 1 \), Do
\[
c_{sk+j}^\ell = d_{sk+j}^\ell - \alpha_{sk+j} b_{sk+j}^{\ell+1}
\]

//such that \([P, Q, R] c_{sk+j}^\ell = A^\ell q_{sk+j}\)
\[
\omega_{sk+j} = \langle c_{sk+j+1}^{\ell+1}, G c_{sk+j+1}^\ell \rangle \\
\langle c_{sk+j+1}^{\ell+1}, G c_{sk+j+1}^\ell \rangle
\]

\[
x_{sk+j+1} = x_{sk+j} + \alpha_{sk+j} P s_{sk+j} + \omega_{sk+j} q_{sk+j}
\]

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

For \( \ell = 0 \) to \( s - 2j \), Do
\[
d_{sk+j+1}^\ell = c_{sk+j+1}^\ell - \omega_{sk+j} c_{sk+j}^{\ell+1}
\]

//such that \([P, Q, R] d_{sk+j+1}^\ell = A^\ell r_{sk+j+1}\)
\[
\beta_{sk+j} = \langle g \cdot d_{sk+j}^\ell, g \cdot b_{sk+j}^{\ell+1} \rangle \\
\langle g \cdot d_{sk+j}^\ell, g \cdot b_{sk+j}^{\ell+1} \rangle \times \frac{\alpha_j}{\omega_j}
\]

\[
p_{sk+j+1} = r_{sk+j+1} + \beta_{sk+j} b_{sk+j}^{\ell+1}
\]

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

EndDo

EndDo
CA-BICGSTAB Convergence, $s=32$

With Residual Replacement (RR) a la Van der Vorst and Ye

<table>
<thead>
<tr>
<th>Replacement Its.</th>
<th>Naive</th>
<th>Monomial</th>
<th>Newton</th>
<th>Chebyshev</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>74 (1)</td>
<td>[7, 15, 24, 31, ..., 92, 97, 103] (17)</td>
<td>[67, 98] (2)</td>
<td>68 (1)</td>
</tr>
</tbody>
</table>
Speedups for GMG w/CA-KSM Bottom Solve

• Compared BICGSTAB vs. CA-BICGSTAB with s = 4 (monomial basis)
• Hopper at NERSC (Cray XE6), weak scaling: Up to 4096 MPI processes (1 per chip, 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
• Speedups for two BoxLib applications:
  – 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
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
    • Different kinds of “sparse matrices”
Outline

• Survey state of the art of CA (Comm-Avoiding) algorithms
  – Review previous Matmul algorithms
  – CA $O(n^3)$ 2.5D Matmul and LU
  – TSQR: Tall-Skinny QR
  – CA Strassen Matmul

• Beyond linear algebra
  – Extending lower bounds to any algorithm with arrays
  – Communication-optimal N-body algorithm

• CA-Krylov methods

• Related Topics
  – Write-Avoiding Algorithms
  – Reproducibility
Write-Avoiding Algorithms

• What if writes are more expensive than reads?
  – Nonvolatile Memory (Flash, PCM, ...)
  – Saving intermediates to disk in cloud (eg Spark)
  – Extra coherency traffic in shared memory

• Can we design “write-avoiding (WA)” algorithms?
  – Goal: find and attain better lower bound for writes
  – Thm: For classical matmul, possible to do asymptotically fewer writes than reads to given layer of memory hierarchy
  – Thm: Cache-oblivious algorithms cannot be write-avoiding
  – Thm: Strassen and FFT cannot be write-avoiding
Measured L3-DRAM traffic on Intel Nehalem Xeon-7560
Optimal \#DRAM reads = O(n^3/M^{1/2})
Optimal \#DRAM writes = n^2

Cache-Oblivious Matmul
\#DRAM reads close to optimal
\#DRAM writes much larger

Write-Avoiding Matmul
Total L3 misses close to optimal
Total DRAM writes much larger
Measured L3-DRAM traffic on Intel Nehalem Xeon-7560
Optimal #DRAM reads = \(O(n^3/M^{1/2})\)
Optimal #DRAM writes = \(n^2\)

Intel MKL Matmul
#DRAM reads >2x optimal
#DRAM writes much larger

Write-Avoiding Matmul
Total L3 misses close to optimal
Total DRAM writes much larger
Reproducibility

• Want bit-wise identical results from different runs of the same program on the same machine, possibly with different available resources
  – Needed for testing, debugging, correctness.
  – Requested by users (e.g. FEM, climate modeling, …)

• Hard just for summation, since floating point arithmetic is not associative because of roundoff
  – \((1e-16 + 1) - 1 \neq 1e-16 + (1 - 1)\)
Reproducible Floating Point Computation

• Get bit-wise identical answer when you type a.out again
• NA-Digest submission on 8 Sep 2010
  – From Kai Diethelm, at GNS-MBH
  – Sought reproducible parallel sparse linear equation solver, demanded by customers (construction engineers), otherwise they don’t believe results
  – Willing to sacrifice 40% - 50% of performance for it
• Email to ~110 Berkeley CSE faculty, asking about it
  – Most: “What?! How will I debug without reproducibility?”
  – Few: “I know better, and do careful error analysis”
  – S. Govindjee: needs it for fracture simulations
  – S. Russell: needs it for nuclear blast detection
Intel MKL non-reproducibility

Vector size: 1e6. Data aligned to 16-byte boundaries. For each input vector:
- Dot products are computed using 1, 2, 3 or 4 threads
- Absolute error = maximum – minimum
- Relative error = Absolute error / maximum absolute value

- Intel MKL 11.2 with CBWR: reproducible only for fixed number of threads and using the same instruction set (SSE2/AVX)
Goals/Approaches for Reproducible Sum

• Goals
  1. Same answer, independent of layout, #processors, order of summands
  2. Good performance (scales well)
  3. Portable (assume IEEE 754 only)
  4. User can choose accuracy

• Approaches
  – Guarantee fixed reduction tree (not 2. or 3.)
  – Use (very) high precision to get exact answer (not 2.)
  – Our approach (Nguyen, D.)
    • Oversimplified:
      1. Compute A = maximum absolute value (reproducible)
      2. Round all summands to one ulp in A
      3. Compute sum; rounding causes them to act like fixed point numbers
    • Possible with one reduction operation
Performance results on 1024 proc Cray XC30
1.2x to 3.2x slowdown vs fastest code, for n=1M
Reproducible Software and Hardware

• Software for Reproducible BLAS 1 available at bebop.cs.berkeley.edu/reproblas
  – BLAS2, 3 under development
• Used Chisel (hardware design language) to design one new instruction that would make reproducible summation as fast (and more accurate) than standard summation
• Industrial interest
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}
    $C(i,j) = C(i,j) + A(i,k) \times B(k,j)$  {do a matrix multiply on blocks}
    {write block $C(i,j)$ back to slow memory}

$$C(i,j) = C(i,j) + A(i,k) \times B(k,j)$$
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\} \( \ldots b^2 \times (n/b)^2 = n^2 \) reads

for \( k = 1 \) to \( n/b \)

\{read block \( A(i,k) \) into fast memory\} \( \ldots b^2 \times (n/b)^3 = n^3/b \) reads

\{read block \( B(k,j) \) into fast memory\} \( \ldots b^2 \times (n/b)^3 = n^3/b \) reads

\( C(i,j) = C(i,j) + A(i,k) \times B(k,j) \) \{do a matrix multiply on blocks\}

\{write block \( C(i,j) \) back to slow memory\} \( \ldots b^2 \times (n/b)^2 = n^2 \) writes

\[ 2n^3/b + 2n^2 \text{ reads/writes} \ll 2n^3 \text{ arithmetic} - \text{ Faster!} \]
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 \( n/2 \times n/2 \)

```python
func C = RMM (A, B, n)
    if n = 1, C = A * B, else
        {  C_{11} = RMM (A_{11} , B_{11} , n/2) + RMM (A_{12} , B_{21} , n/2)
           C_{12} = RMM (A_{11} , B_{12} , n/2) + RMM (A_{12} , B_{22} , n/2)
           C_{21} = RMM (A_{21} , B_{11} , n/2) + RMM (A_{22} , B_{21} , n/2)
           C_{22} = RMM (A_{21} , B_{12} , n/2) + RMM (A_{22} , B_{22} , n/2)  }
    return
```

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Recursive Matrix Multiplication (RMM) (2/2)

```plaintext
func C = RMM (A, B, n)
    if n=1, C = A * B, else
        {  C_{11} = RMM (A_{11}, B_{11}, n/2) + RMM (A_{12}, B_{21}, n/2)
            C_{12} = RMM (A_{11}, B_{12}, n/2) + RMM (A_{12}, B_{22}, n/2)
            C_{21} = RMM (A_{21}, B_{11}, n/2) + RMM (A_{22}, B_{21}, n/2)
            C_{22} = RMM (A_{21}, B_{12}, n/2) + RMM (A_{22}, B_{22}, n/2)  }
    return

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

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

“Cache oblivious”, works for memory hierarchies, but not panacea
```
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/
How hard is hand-tuning matmul, anyway?
SUMMA—n x 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 $n/b-1$ … $b$ = block size = #cols in $A(i,k)$ = #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 $Brow$
$C_{_myproc} = C_{_myproc} + Acol \times Brow$
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 $p^{1/3} \times p^{1/3} \times p^{1/3}$ grid
  – Processor $(i,j,k)$ performs $C(i,j) = C(i,j) + A(i,k)B(k,j)$,
    where each submatrix is $n/p^{1/3} \times n/p^{1/3}$
• Not always that much memory available…
Perfect Strong Scaling – in Time and Energy (2/2)

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

- 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 \( P = \frac{E}{T} \) 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?
2.5D vs 2D LU
With and Without Pivoting

LU on 16,384 nodes of BG/P (n=131,072)

Thm: Perfect Strong Scaling impossible, because $\text{Latency} \times \text{Bandwidth} = \Omega(n^2)$
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
Outline

• Survey state of the art of CA (Comm-Avoiding) algorithms
  – Review previous Matmul algorithms
  – CA $O(n^3)$ 2.5D Matmul
  – TSQR: Tall-Skinny QR
  – CA $O(n^3)$ 2.5D LU
  – CA Strassen Matmul

• Beyond linear algebra
  – Extending lower bounds to any algorithm with arrays
  – Communication-optimal N-body algorithm

• CA-Krylov methods
Back to LU: 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
Exascale Machine Parameters

Source: DOE Exascale Workshop

- $2^{20} \approx 1,000,000$ 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

\[ \log_2 \left( \frac{n^2}{p} \right) = \frac{\log_2 \left( \text{memory\_per\_proc} \right)}{\log_2 (n^2/p)} = \log_2 (p) \]
Ongoing Work

• Lots more work on
  – Algorithms:
    • BLAS, LDL^T, QR with pivoting, other pivoting schemes, eigenproblems, ...
    • Sparse matrices, structured matrices
    • All-pairs-shortest-path, ...
    • Both 2D (c=1) and 2.5D (c>1)
    • But only bandwidth may decrease with c>1, not latency (eg LU)
  – Platforms:
    • Multicore, cluster, GPU, cloud, heterogeneous, low-energy, ...
  – Software:
    • Integration into Sca/LAPACK, PLASMA, MAGMA, ...

• Integration into applications
  – CTF (with ANL): symmetric tensor contractions
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)

• Thm: Picking b = M^{1/2} attains lower bound:
  #words_moved = Ω(n³/M^{1/2})

• Where does 1/2 come from?
Communication Avoiding Parallel Strassen (CAPS)

BFS vs. DFS

BFS

A·B

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

DFS

A·B

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

Best way to interleave BFS and DFS is a tuning parameter
Variable Loop Bounds are More Complicated

• Redundancy in n-body calculation $f(i,j)$, $f(j,i)$
• k-way n-body problems ("k-body") has even more

• Can achieve both communication and computation (symmetry exploiting) optimal
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 \( \mathbb{Z}^3 \)
  
  Access locations indexed by (i,j), (i,k), (k,j)

• General case
  
  for i1=1:n, for i2 = i1:m, ... for ik = i3:i4
  
  \[ C(i1+2*i3-i7) = \text{func}(A(i2+3*i4,i1,i2,i1+i2,...),B(pnt(3*i4)),...) \]
  
  \[ D(\text{something else}) = \text{func}(\text{something else}), ... \]

  => for (i1,i2,...,ik) in S = subset of \( \mathbb{Z}^k \)
  
  Access locations indexed by group homomorphisms, eg
  
  \[ \phi_C(i1,i2,...,ik) = (i1+2*i3-i7) \]
  
  \[ \phi_A(i1,i2,...,ik) = (i2+3*i4,i1,i2,i1+i2,...), ... \]

• 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 $\mathbb{Z}^k$, group homomorphisms $\phi_1, \phi_2, \ldots$, bound $|S|$ in terms of $|\phi_1(S)|, |\phi_2(S)|, \ldots, |\phi_m(S)|$

- Def: Hölder-Brascamp-Lieb LP (HBL-LP) for $s_1, \ldots, s_m$:
  for all subgroups $H < \mathbb{Z}^k$, $\text{rank}(H) \leq \sum_j s_j \ast \text{rank}(\phi_j(H))$

- Thm (Christ/Tao/Carbery/Bennett): Given $s_1, \ldots, s_m$
  $$|S| \leq \prod_j |\phi_j(S)|^{s_j}$$

- Thm: Given a program with array refs given by $\phi_j$, choose $s_j$ to minimize $s_{HBL} = \sum_j s_j$ subject to HBL-LP. Then
  $$\#\text{words}_\text{moved} = \Omega \left( \#\text{iterations}/M^{s_{HBL}^{-1}} \right)$$
Is this bound attainable?

• But first: Can we write it down?
• Thm: (bad news) HBL-LP reduces to Hilbert’s 10\textsuperscript{th} problem over Q (conjectured to be undecidable)
• Thm: (good news) Another LP with same solution is decidable
• Depends on loop dependencies
  – Best case: none, or reductions (like matmul)
• Thm: In many cases, solution $x$ of Dual HBL-LP gives optimal tiling
  – Ex: For Matmul, $x = [1/2, 1/2, 1/2]$ so optimal tiling is $M^{1/2} \times M^{1/2} \times M^{1/2}$
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 $\Delta$

\[
\begin{pmatrix}
  i & j \\
  1 & 0 & F \\
  1 & 0 & P(i) \\
  0 & 1 & P(j)
\end{pmatrix}
\]

• Solve LP for $x = [xi,xj]^T$: max $1^T x$ s.t. $\Delta x \leq 1$
  
  — Result: $x = [1,1]$, $1^T x = 2 = s_{HBL}$

• Thm: \#words\_moved = $\Omega(n^2/M^{SHBL-1}) = \Omega(n^2/M^1)$
  
  Attained by block sizes $M^{xi}, M^{xj} = M^1, M^1$
Is this bound attainable (1/2)?

- But first: Can we write it down?
- Thm: (bad news) HBL-LP reduces to Hilbert’s 10th problem over Q
  – conjectured to be undecidable
- Thm: (good news) Another LP with same solution is decidable (but expensive):

  Let \( L = (V_1, V_2, \ldots) \) be countable list of all subspaces of \( \mathbb{Q}^n \)
  
  \[
  i = 1 \\
  \text{repeat} \\
  \quad i = i + 1 \\
  \text{until polytope determined by inequalities from } (V_1, \ldots, V_i) \text{ is right one}
  \]

- Thm: (better news) Enough to search \( L = \) lattice of kernels of \( \phi_1, \phi_2, \ldots, \phi_m \)
  – Similar to result of Valdimarsson in continuum case
  – Corollary (Dedekind) If \( m=3 \), only need to consider 28 subspaces
- Thm: (even better news) Easy to write down LP explicitly in many simple cases of interest (eg all \( \phi_j = \{\text{subset of indices}\} \))
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