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:
  - \( \# \text{flops} \times \text{time}_{\text{per fop}} \)
  - \( \# \text{words moved} / \text{bandwidth} \)
  - \( \# \text{messages} \times \text{latency} \)

- \( \text{time}_{\text{per fop}} \ll 1 / \text{bandwidth} \ll \text{latency} \)

- Gaps growing exponentially with time [FOSC]

<table>
<thead>
<tr>
<th></th>
<th>Annual improvements</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time_per_flop</td>
<td>Bandwidth</td>
</tr>
<tr>
<td><strong>Network</strong> 59%</td>
<td>26%</td>
</tr>
<tr>
<td><strong>DRAM</strong> 23%</td>
<td>23%</td>
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- Avoid communication to save time
Why Minimize Communication? (3/3)

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

Minimize communication to save energy

Source: John Shalf, LBL
Goals

• Redesign algorithms to *avoid* communication
  • Between all memory hierarchy levels
    • L1 ↔ L2 ↔ DRAM ↔ network, etc

• Attain lower bounds if possible
  • Current algorithms often far from lower bounds
  • Large speedups and energy savings possible
President Obama cites Communication-Avoiding Algorithms in the FY 2012 Department of Energy Budget Request to Congress:

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


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 $O(n^3)$ 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
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Summary of CA Linear Algebra

• “Direct” Linear Algebra
  • Lower bounds on communication for linear algebra problems like Ax=b, least squares, Ax = λx, SVD, etc
  • Mostly not attained by algorithms in standard libraries
  • New algorithms that attain these lower bounds
    • Being added to libraries: Sca/LAPACK, PLASMA, MAGMA
      • Large speed-ups possible
  • Autotuning to find optimal implementation

• Ditto for “Iterative” Linear Algebra
Lower bound for all “$n^3$-like” linear algebra

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

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

• Parallel case: assume either load or memory balanced

• Holds for
  – Matmul
Lower bound for all “n³-like” linear algebra

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

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

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

• 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 Aᵏ)
  – Dense and sparse matrices (where #flops \(<<\) n³)
  – Sequential and parallel algorithms
  – Some graph-theoretic algorithms (eg Floyd-Warshall)
Lower bound for all “$n^3$-like” linear algebra

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

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

$$\# \text{messages\_sent (per processor)} = \Omega(\# \text{flops (per processor)} / M^{3/2})$$

- 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 $A^k$)

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SIAM SIAG/Linear Algebra Prize, 2012
Ballard, D., Holtz, Schwartz
Can we attain these lower bounds?

• Do conventional dense algorithms as implemented in LAPACK and ScaLAPACK attain these bounds?
  – Often not

• If not, are there other algorithms that do?
  – Yes, for much of dense linear algebra
  – New algorithms, with new numerical properties, new ways to encode answers, new data structures
  – Not just loop transformations (need those too!)

• Only a few sparse algorithms so far

• Lots of work in progress
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• CA-Krylov methods
Naïve Matrix Multiply

\[
\{\text{implements } C = C + A*B\}
\]

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

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

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

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

{implements $C = C + A \times B$}
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 $n$
    $C(i,j) = C(i,j) + A(i,k) \times B(k,j)$
    {write $C(i,j)$ back to slow memory}  ...  $n^2$ writes altogether

$n^3 + 3n^2$ reads/writes altogether – dominates $2n^3$ arithmetic
Consider \( A, B, C \) to be \( \frac{n}{b} \)-by-\( \frac{n}{b} \) 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 \( \frac{n}{b} \)
  for \( j = 1 \) to \( \frac{n}{b} \)
    \{read block \( C(i, j) \) into fast memory\}
  for \( k = 1 \) to \( \frac{n}{b} \)
    \{read block \( A(i, k) \) into fast memory\}
    \{read block \( B(k, j) \) into fast memory\}
    \( C(i, j) = C(i, j) + A(i, k) \cdot B(k, j) \) \{do a matrix multiply on 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 \textit{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\} \hspace{1cm} \ldots \hspace{0.5cm} b^2 \times (n/b)^2 = n^2 \text{ reads}
  For \( k = 1 \) to \( n/b \)
    \{read block \( A(i,k) \) into fast memory\} \hspace{1cm} \ldots \hspace{0.5cm} b^2 \times (n/b)^3 = n^3/b \text{ reads}
    \{read block \( B(k,j) \) into fast memory\} \hspace{1cm} \ldots \hspace{0.5cm} b^2 \times (n/b)^3 = n^3/b \text{ 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\} \hspace{1cm} \ldots \hspace{0.5cm} b^2 \times (n/b)^2 = n^2 \text{ writes}

\[
2n^3/b + 2n^2 \text{ reads/writes} \ll 2n^3 \text{ arithmetic} \quad \text{- Faster!}
\]
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 \(= \Omega \left( \#\text{flops} / M^{1/2} \right) \)

• But what if we don’t know \(M\)?

• Or if there are multiple levels of fast memory?

• How do we write the algorithm?
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
```
Recursive Matrix Multiplication (RMM) (2/2)

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 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 \cdot 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
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 $n/b-1$  
... $b = \text{block size} = \#\text{cols in } A(i,k) = \#\text{rows in } B(k,j)$

for all $i = 1$ to $P^{1/2}$

owner of $A(i,k)$ broadcasts it to whole processor row (using binary tree)

for all $j = 1$ to $P^{1/2}$

owner of $B(k,j)$ broadcasts it to whole processor column (using bin. tree)

Receive $A(i,k)$ into $Acol$

Receive $B(k,j)$ into $Brow$

$C_{\text{myproc}} = C_{\text{myproc}} + Acol \times Brow$
Summary of dense parallel algorithms attaining communication lower bounds

- Assume nxn matrices on P processors
- Minimum Memory per processor = \( M = O\left(\frac{n^2}{P}\right) \)
- 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 = \( \Omega\left(\frac{n^3}{P} / M^{3/2}\right) = \Omega\left(\frac{P^{1/2}}{P}\right) \)
- 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 $p^{1/3} \times p^{1/3} \times p^{1/3}$ 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…
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• CA-Krylov methods
2.5D Matrix Multiplication

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

Example: \( P = 32, \ c = 2 \)
2.5D Matrix Multiplication

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

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

1. $P(i,j,0)$ broadcasts $A(i,j)$ and $B(i,j)$ to $P(i,j,k)$
2. Processors at level $k$ perform $1/c$-th of SUMMA, i.e. $1/c$-th of $\Sigma_m A(i,m)*B(m,j)$
3. Sum-reduce partial sums $\Sigma_m A(i,m)*B(m,j)$ along k-axis so $P(i,j,0)$ owns $C(i,j)$
2.5D Matmul on BG/P, 16K nodes / 64K cores

Matrix multiplication on 16,384 nodes of BG/P

- 2.5D MM
- 2D MM

Using $c=16$ matrix copies

- 12X faster
- 2.7X faster
2.5D Matmul on BG/P, 16K nodes / 64K cores

c = 16 copies

Matrix multiplication on 16,384 nodes of BG/P

95% reduction in comm

12x faster

2.7x faster

Distinguished Paper Award, EuroPar’11 (Solomonik, D.)
SC’11 paper by Solomonik, Bhavele, 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 = 3n²
• Increase P by a factor of c → total memory increases by a factor of c
• Notation for timing model:
  – γₜ, βₜ, αₜ = secs per flop, per wordMoved, per message of size m
• \( T(cP) = n^3/(cP) \left[ \gammaₜ + \betaₜ/M^{1/2} + \alphaₜ/(mM^{1/2}) \right] \)
  = \( T(P)/c \)
• Notation for energy model:
  – γₑ, βₑ, αₑ = joules for same operations
  – δₑ = joules per word of memory used per sec
  – εₑ = joules per sec for leakage, etc.
• \( E(cP) = cP \left\{ n^3/(cP) \left[ \gammaₑ + \betaₑ/M^{1/2} + \alphaₑ/(mM^{1/2}) \right] + \deltaₑMT(cP) + \varepsilonₑT(cP) \right\} \)
  = \( E(P) \)
Perfect Strong Scaling – in Time and Energy (2/2)

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

- 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?
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TSQR: QR of a Tall, Skinny matrix

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

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

\[ \begin{pmatrix} R_{01} \\ R_{11} \end{pmatrix} = \begin{pmatrix} Q_{02} & R_{02} \end{pmatrix} \]
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} \}
TSQR: An Architecture-Dependent Algorithm

Parallel:
\[ W = \begin{bmatrix} W_0 \\ W_1 \\ W_2 \\ W_3 \end{bmatrix} \rightarrow \begin{bmatrix} R_{00} \\ R_{10} \\ R_{20} \\ R_{30} \end{bmatrix} \rightarrow \begin{bmatrix} R_{01} \\ R_{11} \end{bmatrix} \rightarrow R_{02} \]

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

Dual Core:
\[ W = \begin{bmatrix} W_0 \\ W_1 \\ W_2 \\ W_3 \end{bmatrix} \rightarrow \begin{bmatrix} R_{00} \\ R_{01} \\ R_{11} \end{bmatrix} \rightarrow \begin{bmatrix} R_{02} \\ R_{03} \end{bmatrix} \]

Multicore / Multisocket / Multirack / Multisite / Out-of-core: ?
Can choose reduction tree dynamically
TSQR Performance Results

• Parallel
  – Intel Clovertown
    – Up to \textbf{8x} speedup (8 core, dual socket, 10M x 10)
  – Pentium III cluster, Dolphin Interconnect, MPICH
    • Up to \textbf{6.7x} speedup (16 procs, 100K x 200)
  – BlueGene/L
    • Up to \textbf{4x} speedup (32 procs, 1M x 50)
  – Tesla C 2050 / Fermi
    • Up to \textbf{13x} (110,592 x 100)
  – Grid – \textbf{4x} on 4 cities vs 1 city (Dongarra, Langou et al)
  – Cloud – \textbf{1.6x slower than accessing data twice} (Gleich and Benson)
• Sequential
  – “\textit{Infinite speedup}” for out-of-core on PowerPC laptop
    • As little as 2x slowdown vs (predicted) infinite DRAM
    • LAPACK with virtual memory never finished
• SVD costs about the same
• Joint work with Grigori, Hoemmen, Langou, Anderson, Ballard, Keutzer, others
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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 \( W_4' \)

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

Choose b pivot rows, call them \( W_{12}' \)
Choose b pivot rows, call them \( W_{34}' \)

\[ W_{12}', W_{34}' = P_{1234} \cdot L_{1234} \cdot U_{1234} \]

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
2.5D vs 2D LU
With and Without Pivoting

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

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

• Integration into applications (on IBM BG/Q)
  – CTF (with ANL): symmetric tensor contractions
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
**Communication Lower Bounds for Strassen-like matmul algorithms**

<table>
<thead>
<tr>
<th>Classical $O(n^3)$ matmul:</th>
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<tbody>
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<td>$#\text{words}_\text{moved} = \Omega \left( M(n/M^{1/2})^3 / P \right)$</td>
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<th>Strassen’s $O(n^{\lg 7})$ matmul:</th>
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<th>Strassen-like $O(n^\omega)$ matmul:</th>
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<td>$#\text{words}_\text{moved} = \Omega \left( M(n/M^{1/2})^\omega / P \right)$</td>
</tr>
</tbody>
</table>

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

BFS

A·B

T₀·S₀ T₁·S₁ T₂·S₂ T₃·S₃ T₄·S₄ T₅·S₅ T₆·S₆

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

DFS

A·B

T₀·S₀ T₁·S₁ T₂·S₂ T₃·S₃ T₄·S₄ T₅·S₅ T₆·S₆

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

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

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

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

- “ Blocked” code
  for i1 = 1:b:n, for j1 = 1:b:n, for k1 = 1:b:n
  for i2 = 0:b-1, for j2 = 0:b-1, for k2 = 0:b-1
  i=i1+i2, j = j1+j2, k = k1+k2
  C(i,j)+=A(i,k)*B(k,j)

- Thm: Picking $b = M^{1/2}$ attains lower bound:
  $\#\text{words\_moved} = \Omega(n^3/M^{1/2})$
- 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

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

- 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 = \(\Omega(n^3/M_{SHBL}^{1})\) = \(\Omega(n^3/M^{1/2})\)
  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 $\Delta$
  $\Delta = \begin{pmatrix}
  1 & 0 & F \\
  1 & 0 & P(i) \\
  0 & 1 & P(j)
\end{pmatrix}$
- Solve LP for $x = [x_i, x_j]^T$: $\max 1^T x \text{ s.t. } \Delta x \leq 1$
  - Result: $x = [1,1], 1^T x = 2 = s_{HBL}$
- Thm: $\# \text{words}_\text{moved} = \Omega(n^2/M_{S_{HBL}-1}) = \Omega(n^2/M^1)$
  Attained by block sizes $M^{x_i}, M^{x_j} = M^1, M^1$
N-Body Speedups on IBM-BG/P (Intrepid)
8K cores, 32K particles

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

Execution Time vs. Replication Factor

11.8x speedup
New Thm applied to Random Code

• for \(i_1=1:n\), for \(i_2=1:n\), ... , for \(i_6=1:n\)
  
  \[
  A_1(i_1,i_3,i_6) +\text{func1}(A_2(i_1,i_2,i_4),A_3(i_2,i_3,i_5),A_4(i_3,i_4,i_6))
  
  A_5(i_2,i_6) +\text{func2}(A_6(i_1,i_4,i_5),A_3(i_3,i_4,i_6))
  \]

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

\[
\begin{bmatrix}
1 & 0 & 1 & 0 & 0 & 1 \\
1 & 1 & 0 & 1 & 0 & 0 \\
0 & 1 & 1 & 0 & 1 & 0 \\
0 & 0 & 1 & 1 & 0 & 1 \\
0 & 0 & 1 & 1 & 0 & 1 \\
1 & 0 & 0 & 1 & 1 & 0 \\
\end{bmatrix}
\]

• Solve LP for \(x = [x_1,...,x_7]^T\): max \(1^T x\) s.t. \(\Delta x \leq 1\)
  
  \[\text{Result: } x = [2/7,3/7,1/7,2/7,3/7,4/7], \ 1^T x = 15/7 = s_{HBL} \]

• Thm: \#words_moved = \(\Omega(n^6/M^{S_{HBL} - 1}) = \Omega(n^6/M^{8/7})\)
  
  Attained by block sizes \(M^{2/7}, M^{3/7}, M^{1/7}, M^{2/7}, M^{3/7}, M^{4/7}\)
Where do lower and matching upper bounds on communication come from? (1/3)

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

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

• Hard part: finding $G$

• 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)

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

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

Thm (Loomis & Whitney, 1949)
G = # cubes in 3D set = Volume of 3D set
≤ (area(A shadow) · area(B shadow) · area(C shadow))^{1/2}
≤ M^{3/2}
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 \( \mathbb{Z}^3 \)
  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 $H < \mathbb{Z}^k$, $\text{rank}(H) \leq \Sigma_j s_j \ast \text{rank}(\phi_j(H))$

- 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 $s_{\text{HBL}} = \Sigma_j s_j$ subject to HBL-LP. Then
  
  $\#\text{words}_\text{moved} = \Omega (\#\text{iterations}/M^{s_{\text{HBL}}^{-1}})$
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, so far)
• Thm: (better news) Easy to write down LP explicitly in many cases of interest (eg all $\phi_j = \{\text{subset of indices}\}$)
• Thm: (good news) Easy to approximate, i.e. get upper or lower bounds on $s_{\text{HBL}}$
Is this bound attainable (2/2)?

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

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

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

Then for sequential algorithm, tile $i_j$ by $M^{x_j}$

• Ex: Matmul: $s = [1/2, 1/2, 1/2]^T = x$
• Extends to unimodular transforms of indices
Ongoing Work

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

- **k-steps of iterative solver for sparse Ax=b or Ax=λx**
  - Does k SpMVs with A and starting vector
  - Many such “Krylov Subspace Methods”
    - Conjugate Gradients (CG), GMRES, Lanczos, Arnoldi, ...

- **Goal: minimize communication**
  - Assume matrix “well-partitioned”
  - Serial implementation
    - Conventional: $O(k)$ moves of data from slow to fast memory
    - **New: $O(1)$ moves of data – optimal**
  - Parallel implementation on $p$ processors
    - Conventional: $O(k \log p)$ messages (k SpMV calls, dot prods)
    - **New: $O(\log p)$ messages - optimal**

- **Lots of speed up possible (modeled and measured)**
  - Price: some redundant computation
  - Challenges: Poor partitioning, Preconditioning, Num. Stability
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:
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- Replace $k$ iterations of $y = A \cdot x$ with $[Ax, A^2x, ..., A^kx]$
- Sequential Algorithm

- Example: A tridiagonal, $n=32$, $k=3$
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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 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

![Diagram showing parallel algorithm with processors 1 to 4]

- Example: A tridiagonal, \(n=32\), \(k=3\)
- Each processor works on (overlapping) trapezoid
Communication Avoiding Kernels:
The Matrix Powers Kernel: \([Ax, A^2x, \ldots, A^kx]\)

Same idea works for general sparse matrices

Simple block-row partitioning ⇒ (hyper)graph partitioning

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

- **GMRES**: find \( x \) in \( \text{span}\{b, Ab, \ldots, A^k b\} \) minimizing \( ||Ax-b||_2 \)

**Standard GMRES**

\[
\text{for } i=1 \text{ to } k \\
\quad w = A \cdot v(i-1) \quad \ldots \quad \text{SpMV} \\
\quad \text{MGS}(w, v(0), \ldots, v(i-1)) \\
\quad \text{update } v(i), H \\
\text{endfor} \\
\text{solve LSQ problem with } H
\]

**Communication-avoiding GMRES**

\[
W = [v, Av, A^2 v, \ldots, A^k v] \\
[Q,R] = \text{TSQR}(W) \\
\quad \ldots \quad \text{“Tall Skinny QR”} \\
\text{build } H \text{ from } R \\
\text{solve LSQ problem with } H
\]

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!
“Monomial” basis $[Ax, \ldots, A^kx]$ fails to converge

Different polynomial basis $[p_1(A)x, \ldots, p_k(A)x]$ does converge
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

\[
\begin{align*}
    P &= [p_{sk}, Ap_{sk}, \ldots, A^s p_{sk}], \\
    Q &= [q_{sk-1}, Aq_{sk-1}, \ldots, A^s q_{sk-1}], \\
    R &= [r_{sk}, Ar_{sk}, \ldots, A^s r_{sk}].
\end{align*}
\]

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

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

For \( \ell = 0 \) to \( s \),
\[
\begin{align*}
    b^\ell_{sk} &= \begin{bmatrix} B_1 (:, \ell)^T, 0_{s+1}^T, 0_{s+1}^T \end{bmatrix}^T \\
    c^\ell_{sk-1} &= \begin{bmatrix} 0_{s+1}^T, B_2 (:, \ell)^T, 0_{s+1}^T \end{bmatrix}^T \\
    d^\ell_{sk} &= \begin{bmatrix} 0_{s+1}^T, 0_{s+1}^T, B_3 (:, \ell)^T \end{bmatrix}^T
\end{align*}
\]

//such that \([P, Q, R] c^\ell_{sk+1} = A^\ell q_{sk+1} \]

For \( j = 0 \) to \( \left\lfloor \frac{s}{2} \right\rfloor - 1 \), Do
\[
\begin{align*}
    \alpha_{sk+j} &= \frac{\langle g, d^0_{sk+j} \rangle}{\langle g, b^0_{sk+j} \rangle} \\
    q_{sk+j} &= r_{sk+j} - \alpha_{sk+j} [P, Q, R] b^1_{sk+j} \\
    \omega_{sk+j} &= \frac{\langle c^1_{sk+j+1}, Gc^0_{sk+j+1} \rangle}{\langle c^1_{sk+j+1}, G c^1_{sk+j+1} \rangle} \\
    x_{sk+j+1} &= x_{sk+j} + \alpha_{sk+j} P s_{sk+j} + \omega_{sk+j} q_{sk+j} \\
    r_{sk+j+1} &= q_{sk+j} - \omega_{sk+j} [P, Q, R] c^1_{sk+j+1}
\end{align*}
\]

For \( \ell = 0 \) to \( s - 2j + 1 \), Do
\[
\begin{align*}
    \beta^\ell_{sk+j+1} &= \frac{\langle g, d^\ell_{sk+j+1} \rangle}{\langle g, b^\ell_{sk+j+1} \rangle} \times \frac{\alpha_{sk+j}}{\omega_{sk+j}} \\
    p_{sk+j+1} &= r_{sk+j+1} + \beta_{sk+j} p_{sk+j} - \beta_{sk+j} \omega_{sk+j} [P, Q, R] b^1_{sk+j}
\end{align*}
\]

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

EndDo

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

- Naive
- Monomial
- Newton
- Chebyshev
- Monomial+RR
- Newton+RR
- Chebyshev+RR
- Naive
- Naive+RR

<table>
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<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>
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”
For more details

• Bebop.cs.berkeley.edu

• CS267 – Berkeley’s Parallel Computing Course
  – Live broadcast in Spring 2013
    • [www.cs.berkeley.edu/~demmel](http://www.cs.berkeley.edu/~demmel)
    • All slides, video available
  – Prerecorded version broadcast in Spring 2013
    • [www.xsede.org](http://www.xsede.org)
    • Free supercomputer accounts to do homework
    • Free autograding of homework
Collaborators and Supporters

- Austin Benson, Maryam Dehnavi, Mark Hoemmen, Shoaib Kamil, Marghoob Mohiyuddin
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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 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

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

Don’t Communic...