Practicality of Large Scale Fast Matrix Multiplication

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Introduction

- Classical matrix multiplication is nearly ubiquitous, even though asymptotically faster algorithms have been know since 1969
- Concerns about fast matrix multiplication:
  - Practical speed
  - Stability
- This talk addresses both concerns

Outline

- Strassen's algorithm
- New parallel algorithm
  - Communication optimal
  - Faster in practice
- Stability of Strassen
  - Normwise error bound
  - Diagonal scaling, improved error bounds
  - Stability experiments

Recall: Strassen's fast matrix multiplication

Strassen's original algorithm uses 7 multiplies and 18 adds for $n = 2$.
It is applied recursively (blockwise).

$$
\begin{aligned}
M_1 &= (A_{11} + A_{22}) \cdot (B_{11} + B_{22}) \\
M_2 &= (A_{21} + A_{22}) \cdot B_{11} \\
M_3 &= A_{11} \cdot (B_{12} - B_{22}) \\
M_4 &= A_{22} \cdot (B_{21} - B_{11}) \\
M_5 &= (A_{11} + A_{12}) \cdot B_{22} \\
M_6 &= (A_{21} - A_{11}) \cdot (B_{11} + B_{12}) \\
M_7 &= (A_{12} - A_{22}) \cdot (B_{21} + B_{22})
\end{aligned}
$$

$$
\begin{aligned}
C_{11} &= M_1 + M_4 - M_5 + M_7 \\
C_{12} &= M_3 + M_5 \\
C_{21} &= M_2 + M_4 \\
C_{22} &= M_1 - M_2 + M_3 + M_6
\end{aligned}
$$

$$
\begin{array}{r} n/2\,\{ \\ n/2\,\{ \end{array}
\begin{array}{|c|c|}\hline C_{11} & C_{12} \\ \hline C_{21} & C_{22} \\ \hline \end{array}
=
\begin{array}{|c|c|}\hline A_{11} & A_{12} \\ \hline A_{21} & A_{22} \\ \hline \end{array}
\bullet
\begin{array}{|c|c|}\hline B_{11} & B_{12} \\ \hline B_{21} & B_{22} \\ \hline \end{array}
$$

$$T(n) = 7 \cdot T(n/2) + O(n^2)$$

$$T(n) = \Theta\left(n^{\log_2 7}\right)$$

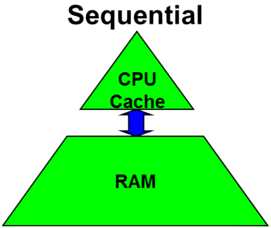
Improved by Winograd to 15 additions

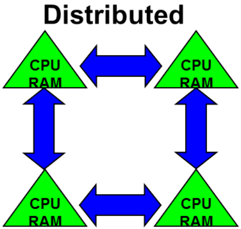
Communication costs

Two kinds of costs:

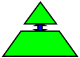
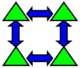
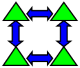
- Arithmetic (FLOPs)
- Communication: moving data between
  - levels of a memory hierarchy (sequential case)
  - over a network connecting processors (parallel case)

Communication is becoming more expensive relative to computation

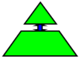
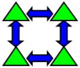
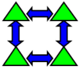




Communication lower bounds for matrix multiplication

	Strassen:	Classic (cubic):
 Sequential	$\Omega\left(\left(\frac{n}{\sqrt{M}}\right)^{\log_2 7} M\right)$	$\Omega\left(\left(\frac{n}{\sqrt{M}}\right)^{\log_2 8} M\right)$
 Distributed	$\Omega\left(\left(\frac{n}{\sqrt{M}}\right)^{\log_2 7} \frac{M}{P}\right)$	$\Omega\left(\left(\frac{n}{\sqrt{M}}\right)^{\log_2 8} \frac{M}{P}\right)$
 Distributed	$\Omega\left(\frac{n^2}{P^{2/\log_2 7}}\right)$	$\Omega\left(\frac{n^2}{P^{2/\log_2 8}}\right)$

Algorithms attaining these bounds?

	Strassen:	Classic (cubic):
 Sequential	$\Omega\left(\left(\frac{n}{\sqrt{M}}\right)^{\log_2 7} M\right)$	$\Omega\left(\left(\frac{n}{\sqrt{M}}\right)^{\log_2 8} M\right)$
 Distributed	$\Omega\left(\left(\frac{n}{\sqrt{M}}\right)^{\log_2 7} \frac{M}{P}\right)$	$\Omega\left(\left(\frac{n}{\sqrt{M}}\right)^{\log_2 8} \frac{M}{P}\right)$
 Distributed	$\Omega\left(\frac{n^2}{P^{2/\log_2 7}}\right)$	$\Omega\left(\frac{n^2}{P^{2/\log_2 8}}\right)$

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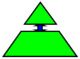
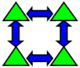
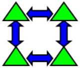
 Sequential	$\Omega\left(\left(\frac{n}{\sqrt{M}}\right)^{\log_2 7} M\right)$	$\Omega\left(\left(\frac{n}{\sqrt{M}}\right)^{\log_2 8} M\right)$
 Distributed	$\Omega\left(\left(\frac{n}{\sqrt{M}}\right)^{\log_2 7} \frac{M}{P}\right)$	$\Omega\left(\left(\frac{n}{\sqrt{M}}\right)^{\log_2 8} \frac{M}{P}\right)$
 Distributed	$\Omega\left(\frac{n^2}{P^{2/\log_2 7}}\right)$	$\Omega\left(\frac{n^2}{P^{2/\log_2 8}}\right)$

Our new algorithm

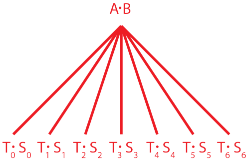
Lessons from lower bounds

- Don't use a classical algorithm for the communication
  - Strassen can communicate less than classical
- Make local multiplies as large as possible
- Use all available memory, up to $O(n^2/P^{2/\log_2 7})$
  - Communication bound decreases with increased memory
- Send memory size messages to minimize latency

Main Idea of CAPS algorithm

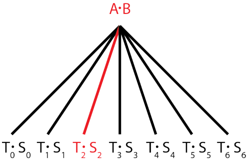
At each level of recursion tree, choose either breadth-first or depth-first traversal of the recursion tree

Breadth-First-Search (BFS)



- Runs all 7 multiplies in parallel
  - each uses $P/7$ processors
- Requires $7/4$ as much extra memory
- Requires communication, but
- All BFS minimizes communication if possible

Depth-First-Search (DFS)

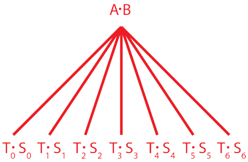


- Runs all 7 multiplies sequentially
  - each uses all P processors
- Requires $1/4$ as much extra memory
- No immediate communication
- Increases bandwidth by factor of $7/4$
- Increases latency by factor of 7

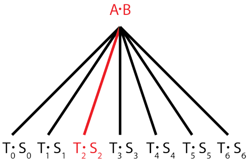
Main Idea of CAPS algorithm

At each level of recursion tree, choose either breadth-first or depth-first traversal of the recursion tree

Breadth-First-Search (BFS)



Depth-First-Search (DFS)



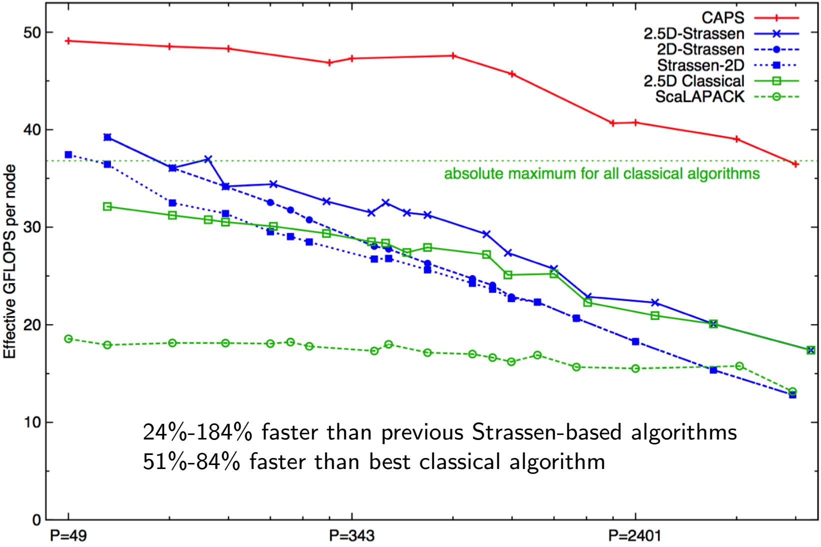
CAPS
    if enough memory **and** $P \geq 7$
        then BFS step
        else DFS step
    end if

Asymptotic costs analysis

		Flops	Bandwidth
Strassen	Lower Bound	$\frac{n^{\omega_0}}{P}$	$\max\left\{\frac{n^{\omega_0}}{PM^{\omega_0/2-1}}, \frac{n^2}{P^{2/\omega_0}}\right\}$
	2D-Strassen	$\frac{n^{\omega_0}}{P^{(\omega_0-1)/2}}$	$\frac{n^2}{P^{1/2}}$
	Strassen-2D	$\left(\frac{7}{8}\right)^{\ell}\frac{n^3}{P}$	$\left(\frac{7}{4}\right)^{\ell}\frac{n^2}{P^{1/2}}$
	CAPS	$\frac{n^{\omega_0}}{P}$	$\max\left\{\frac{n^{\omega_0}}{PM^{\omega_0/2-1}}, \frac{n^2}{P^{2/\omega_0}}\right\}$
Classical	Lower Bound	$\frac{n^3}{P}$	$\max\left\{\frac{n^3}{PM^{1/2}}, \frac{n^2}{P^{2/3}}\right\}$
	2D	$\frac{n^3}{P}$	$\frac{n^2}{P^{1/2}}$
	2.5D	$\frac{n^3}{P}$	$\max\left\{\frac{n^3}{PM^{1/2}}, \frac{n^2}{P^{2/3}}\right\}$

Performance of CAPS

Strong-scaling on Franklin (Cray XT4), $n = 94080$.



CAPS Summary

The CAPS matrix multiplication algorithm

- is communication optimal
  - matches the communication lower bounds
  - moves asymptotically less data than all existing algorithms
- is faster: asymptotically and in practice
  - faster than any parallel classical algorithm can be
  - faster than any parallel Strassen-based algorithm we are aware of
- applies to other fast matrix multiplication algorithms
  - but there might not be any other practical ones

Stability

- CAPS has the same stability properties as any other Strassen (Strassen-Winograd) algorithm.
- Weaker stability guarantee than classical, but still norm-wise stable.
- This can be improved through diagonal scaling.
  - Two best scaling schemes give incomparable bounds
  - Can check which bound is better in $O(n^2)$ time
- The improved error bounds match those of matrix factorization such as classical LU and QR.

Diagonal Scaling

Outside scaling: $D^A C D^B = (D^A A)(B D^B)$

- Scale so each row of A and each column of B has unit norm.
- Explicitly:
  - Let $D^A_{ii} = (\|A(i,:)\|)^{-1}$, and $D^B_{jj} = (\|B(:,j)\|)^{-1}$.
  - Scale $A' = D^A A$, and $B' = B D^B$.
  - Use Strassen for the product $C' = A'B'$.
  - Unscale $C = \left(D^A\right)^{-1} C' \left(D^B\right)^{-1}$.

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  - Unscale $C = \left(D^A\right)^{-1} C' \left(D^B\right)^{-1}$.

Inside scaling: $C = (AD)(D^{-1}B)$

- Scale so each column of A has the same norm as the corresponding row of B.
- Explicitly:
  - Let $D_{ii} = (\|A(:,i)\|/\|B(i,:)\|)^{-1/2}$.
  - Scale $A' = AD$, and $B' = D^{-1}B$.
  - Use Strassen for the product $C = A'B'$.

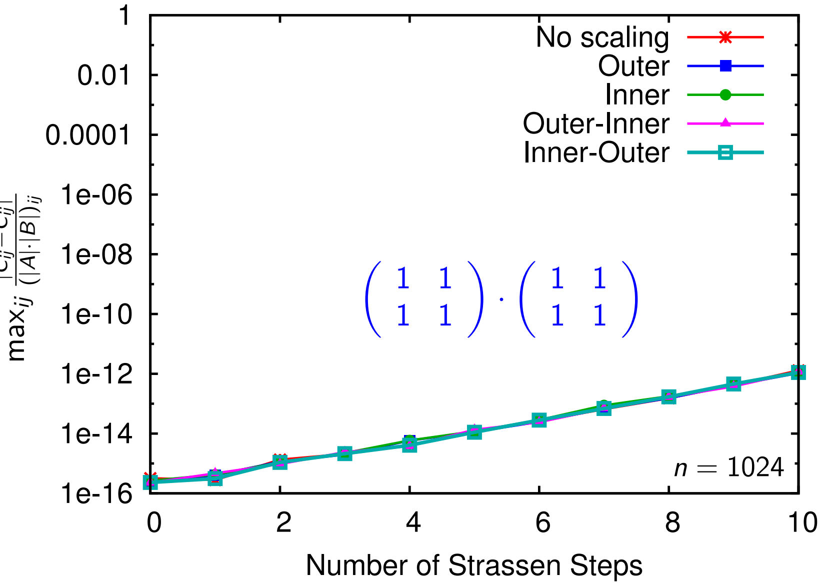
Error bounds

$$|C_{ij} - \hat{C}_{ij}| \leq O(\epsilon) f(n) \cdot \ldots$$

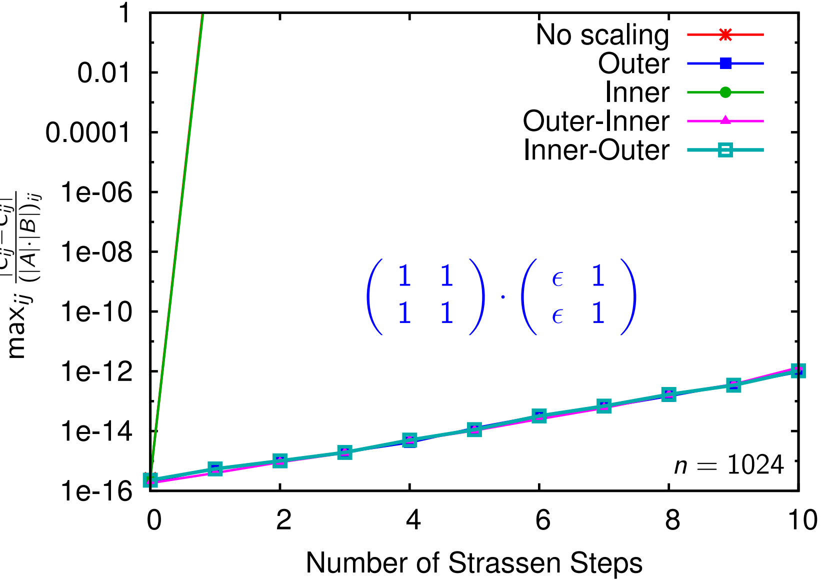
$$\begin{tikzcd}
 & \begin{array}{c}\text{Classical:}\\ (|A|\cdot|B|)_{ij}\end{array} \arrow[dl] \arrow[dr] & \\
\begin{array}{c}\text{Outside-Inside:}\\ \|A(i,:)\|\|B(:,j)\|\||D^A A|\cdot|BD^B|\|\end{array} \arrow[d] & & \begin{array}{c}\text{Inside-Outside:}\\ \|(AD)(i,:)\|\|(D^{-1}B)(:,j)\|\end{array} \arrow[d] \\
\begin{array}{c}\text{Outside:}\\ \|A(i,:)\|\|B(:,j)\|\end{array} \arrow[dr] & & \begin{array}{c}\text{Inside:}\\ \||A|\cdot|B|\|\end{array} \arrow[dl] \\
 & \begin{array}{c}\text{No Scaling:}\\ \|A\|\|B\|\end{array} &
\end{tikzcd}$$

$X \to Y$ means that bound X is stronger than bound Y.

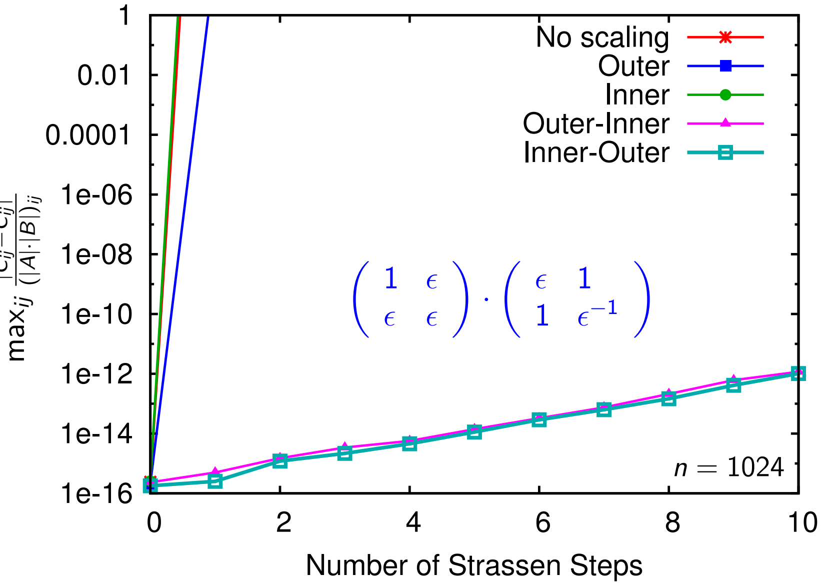
Scaling example: easy case



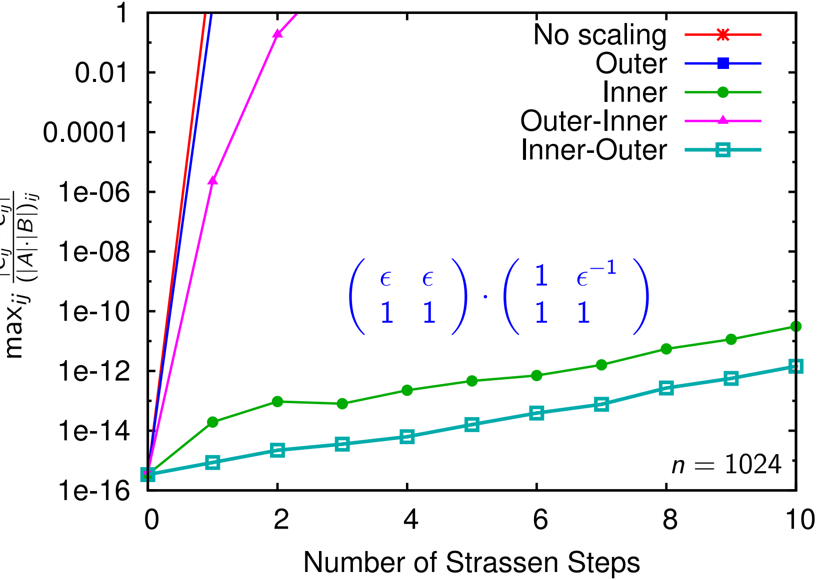
Scaling example: needs outer scaling



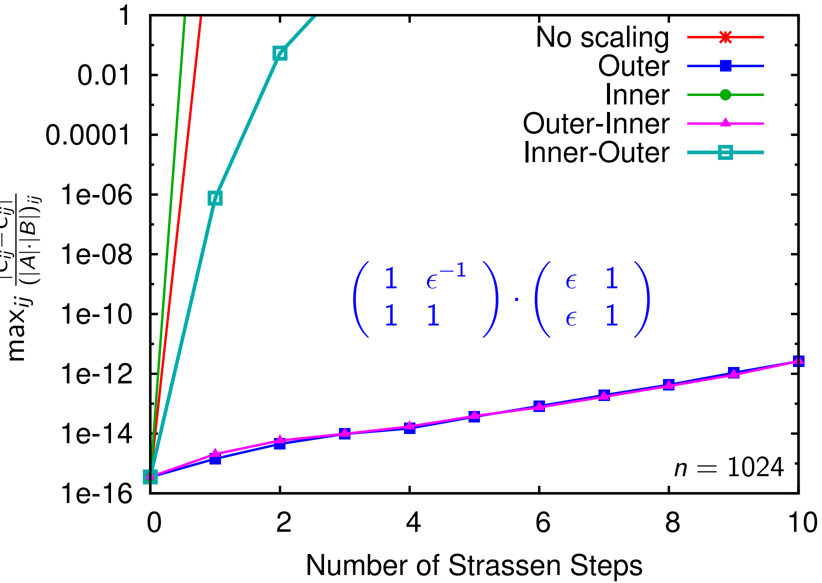
Scaling example: needs inner and outer



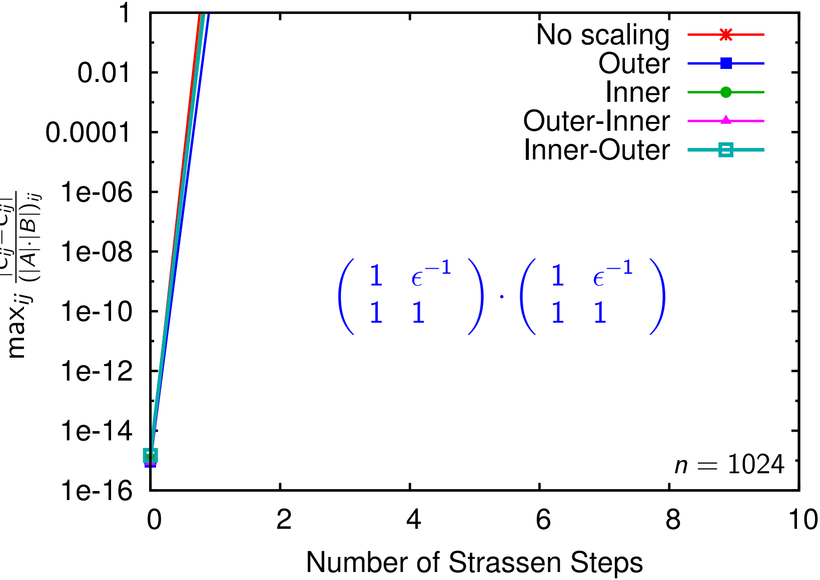
Scaling example: inner-outer better than outer-inner



Scaling example: outer-inner better than inner-outer



Scaling example: problems scaling can't fix



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$X \rightarrow Y$ means that bound X is stronger than bound Y.

Stability summary

- Scaling improves error bound of Strassen
  - To be comparable to many other algorithms
  - But still not a good as classical algorithm
- Applies to other fast matrix multiplication algorithms
- Inner-then-outer or outer-then-inner scaling are best
- Can choose between them by evaluating their bounds
- Open problem: simultaneously attain inner and outer scaling bounds?

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Thank You!

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Technical Report EECS-2012-90, UC Berkeley, May 2012.
Submitted to SC 2012.

Extra slides

1. Previous Parallel Strassen
2. Data Layout
3. Strassen-Winograd Algorithm
4. Hardware scaling
5. Time breakdown
6. Small problems

Previous parallel Strassen-based algorithms

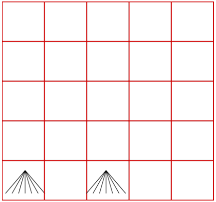
2D-Strassen: [Luo, Drake 95]

Run classical 2D inter-processors.

- Same communication costs as classical 2D.

Run Strassen locally.

- Can't use Strassen on the full matrix size.



Extras

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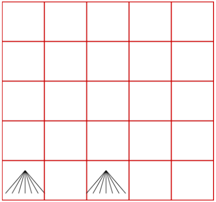


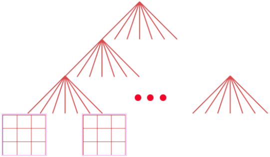
Strassen-2D: [Luo, Drake 95; Grayson, Shah, van de Geijn 95]

Run Strassen inter-processors

- This part can be done without communication.

Then run classical 2D.

- Communication costs grow exponentially with the number of Strassen steps.



▸ Extras

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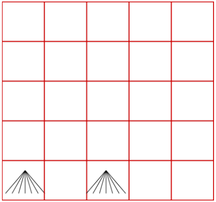

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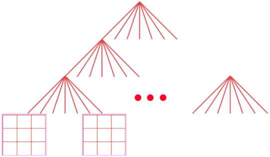
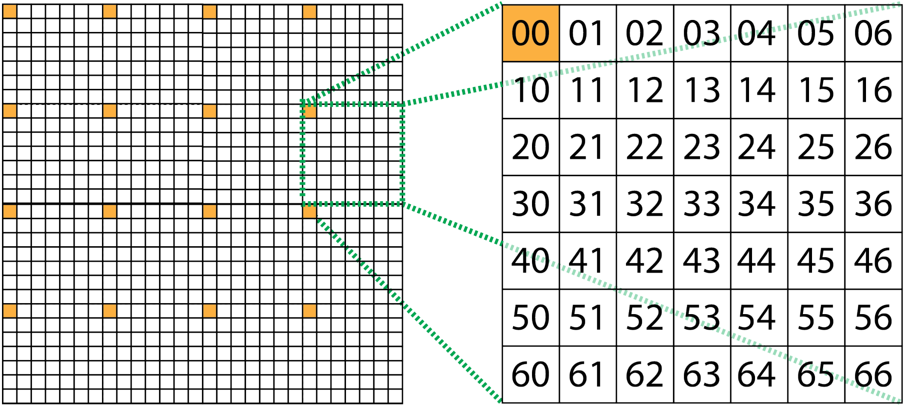


Neither is communication optimal

Extras

Data Layout



Extras

Strassen-Winograd Algorithm

$$\left(\begin{array}{c|c} C_{11} & C_{12} \\ \hline C_{21} & C_{22} \end{array}\right) = C = A \cdot B = \left(\begin{array}{c|c} A_{11} & A_{12} \\ \hline A_{21} & A_{22} \end{array}\right) \cdot \left(\begin{array}{c|c} A_{11} & A_{12} \\ \hline A_{21} & A_{22} \end{array}\right)$$

$$\begin{array}{lll} & & Q_i = S_i \cdot T_i \\ S_0 = A_{11} & T_0 = B_{11} & U_1 = Q_i + Q_4 \\ S_1 = A_{12} & T_1 = B_{21} & U_2 = U_1 + Q_5 \\ S_2 = A_{21} + A_{22} & T_2 = B_{12} + B_{11} & U_3 = U_1 + Q_5 \\ S_3 = S_2 - A_{12} & T_3 = B_{22} - T_2 & C_{11} = Q_1 + Q_2 \\ S_4 = A_{11} - A_{21} & T_4 = B_{22} - B_{12} & C_{12} = U_3 + Q_6 \\ S_5 = A_{12} + S_3 & T_5 = B_{22} & C_{21} = U_2 - Q_7 \\ S_6 = A_{22} & T_6 = T_3 - B_{21} & C_{22} = U_2 + Q_3 \end{array}$$

Extras

Implications for hardware scaling

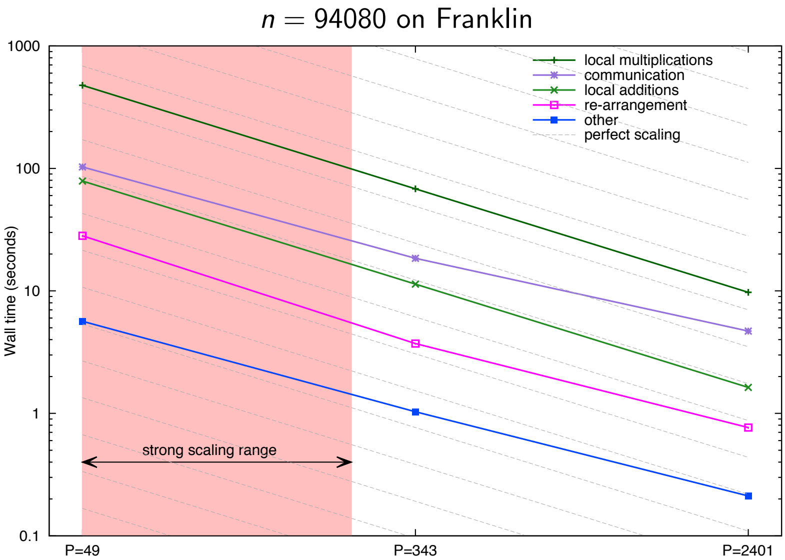
Requirements so that dense matrix multiplication is computation bound.

	Bandwidth Requirement	Latency Requirement
Classic	$\gamma M^{1/2} \gtrsim \beta$	$\gamma M^{3/2} \gtrsim \alpha$
Strassen	$\gamma M^{\omega_0/2-1} \gtrsim \beta$	$\gamma M^{\omega_0/2} \gtrsim \alpha$

Strassen performs fewer flops and less communication, but is more demanding on the hardware.

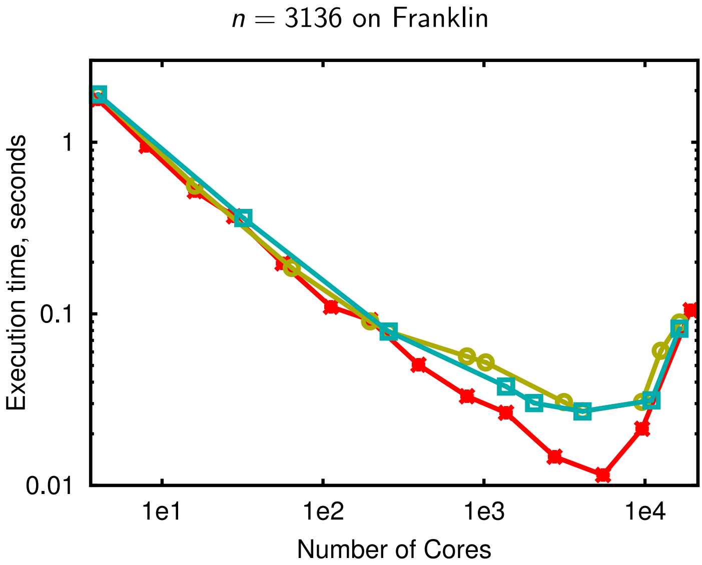
Extras

CAPS time breakdown



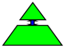
Extras

Performance on small problems



▸ Extras

Sequential recursive Strassen is communication optimal



Sequential

- Run Strassen algorithm recursively.
- When blocks are small enough, work in localy memory, so no further bandwidth cost

$$W(n,M) = \begin{cases} 7W(\frac{n}{2}, M) + O(n^2) & \text{if } 3n^2 > M \\ O(n^2) & \text{otherwise} \end{cases}$$

- Solution is

$$W(n,M) = O\left(\frac{n^{\omega_0}}{M^{\omega_0/2-1}}\right)$$

▸ Extras

Extra slides

1. Previous Parallel Strassen
2. Data Layout
3. Strassen-Winograd Algorithm
4. Hardware scaling
5. Time breakdown
6. Small problems