# Communication avoiding algorithms for LU and QR factorizations

Laura Grigori

Alpines

INRIA Paris - LJLL, UPMC

February 2017

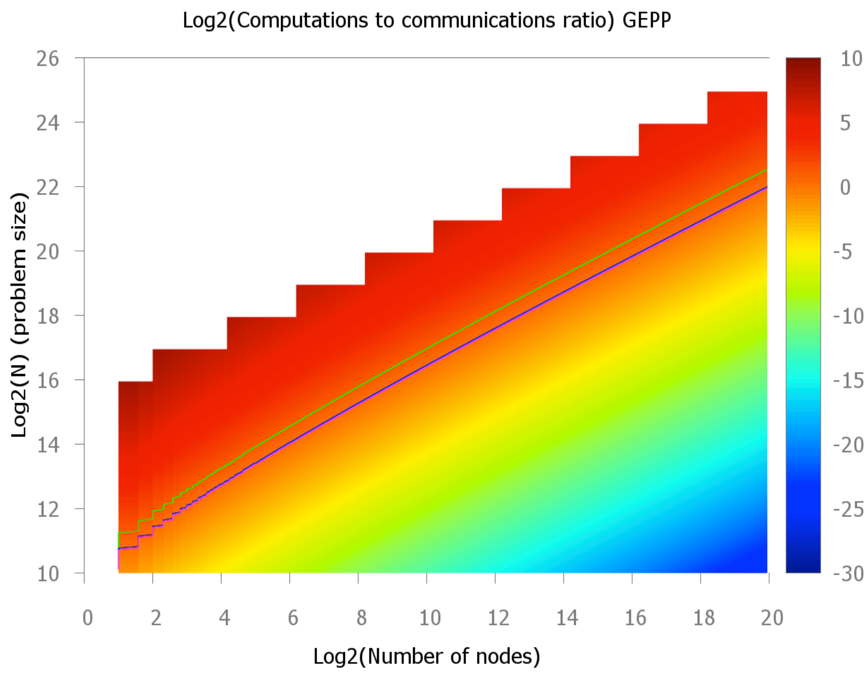
# Plan

- Motivation
- Communication complexity of linear algebra operations
- Communication avoiding for dense linear algebra
  - LU, QR, Rank Revealing QR factorizations
  - Progressively implemented in ScaLAPACK, LAPACK
  - Algorithms for multicore processors
- Conclusions

# Approaches for reducing communication

- Tuning
  - Overlap communication and computation, at most a factor of 2 speedup

- Same numerical algorithm, different schedule of the computation
  - Block algorithms for NLA
    - Barron and Swinnerton-Dyer, 1960
    - ScaLAPACK, Blackford et al 97
  - Cache oblivious algorithms for NLA
    - Gustavson 97, Toledo 97, Frens and Wise 03, Ahmed and Pingali 00

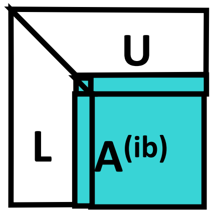



- Same algebraic framework, different numerical algorithm
  - The approach used in CA algorithms
  - More opportunities for reducing communication, may affect stability

# Evolution of numerical libraries

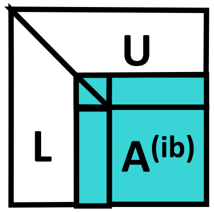
## LINPACK (70's)

- vector operations, uses BLAS1/2
- HPL benchmark based on Linpack LU factorization



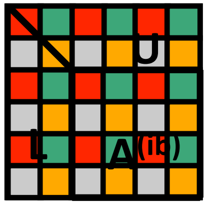

## LAPACK (80's)

- Block versions of the algorithms used in LINPACK
- Uses BLAS3



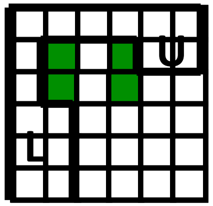

## ScaLAPACK (90's)

- Targets distributed memories
- 2D block cyclic distribution of data
- PBLAS based on message passing




## PLASMA (2008): new algorithms

- Targets many-core
- Block data layout
- Low granularity, high asynchronicity

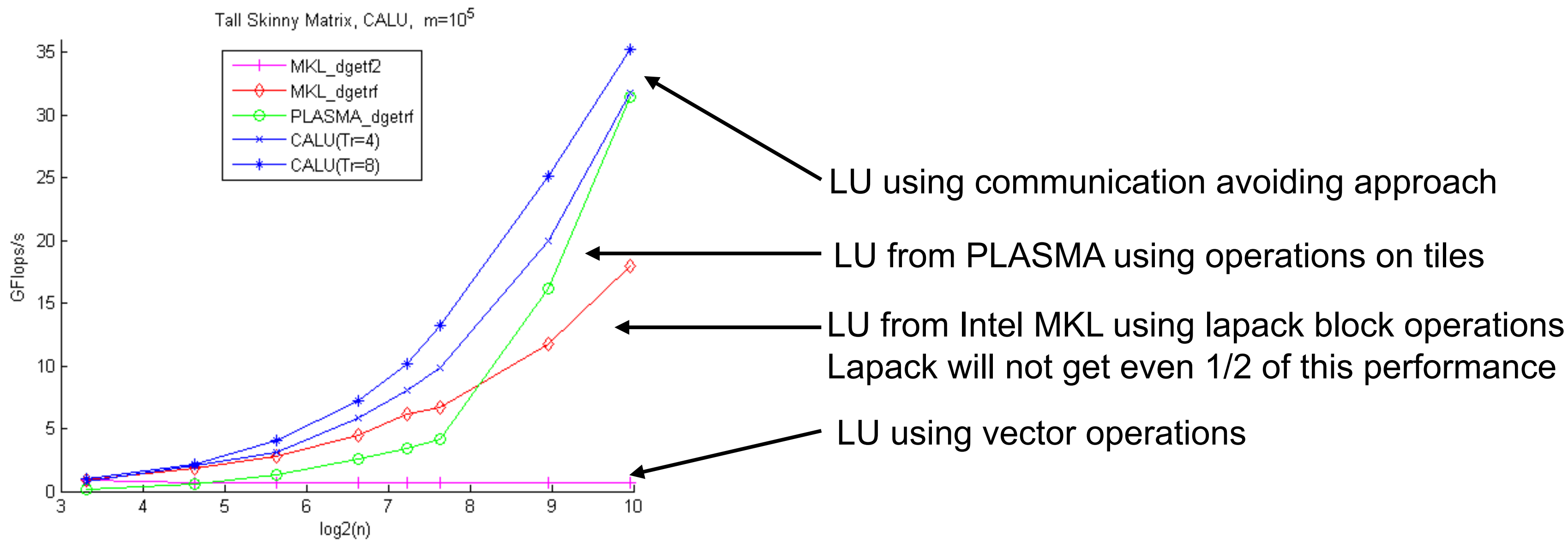



Project developed by U Tennessee Knoxville, UC Berkeley, other collaborators.

Source: inspired from J. Dongarra, UTK, J. Langou, CU Denver

# Evolution of numerical libraries

- Did we need new algorithms?
  - Results on two-socket, quad-core Intel Xeon EMT64 machine, 2.4 GHz per core, peak performance 76.5 Gflops/s
  - LU factorization of an m-by-n matrix, m=$10^5$ and n varies from 10 to 1000



# Communication Complexity of Dense Linear Algebra

- Matrix multiply, using $2n^3$ flops (sequential or parallel)
  - Hong-Kung (1981), Irony/Tishkin/Toledo (2004)
  - Lower bound on Bandwidth = $\Omega$ (#flops / $M^{1/2}$ )
  - Lower bound on Latency = $\Omega$ (#flops / $M^{3/2}$ )

- Same lower bounds apply to LU using reduction
  - Demmel, LG, Hoemmen, Langou 2008

$$\begin{pmatrix} I & & -B \\ A & I & \\ & & I \end{pmatrix} = \begin{pmatrix} I & & \\ A & I & \\ & & I \end{pmatrix} \cdot \begin{pmatrix} I & & -B \\ & I & AB \\ & & I \end{pmatrix}$$

- And to almost all direct linear algebra [Ballard, Demmel, Holtz, Schwartz, 09]

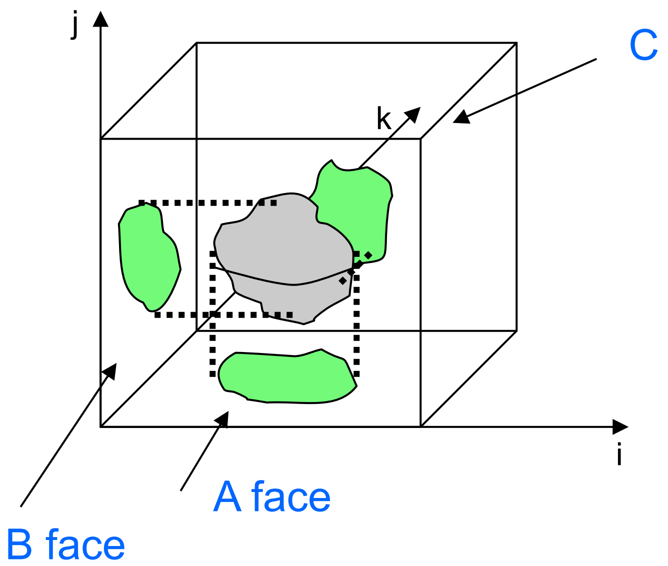
# Lower bounds for linear algebra

- Computation modelled as an n-by-n-by-n set of lattice points
  (i,j,k) represents the operation $c(i,j) \mathrel{+}= f_{ij}(\, g_{ijk}\, (\, a(i,k)*b(k,j))\, )\, )$
- The computation is divided in S phases
- Each phase contains exactly M (the fast memory size) load and store instructions
- Determine how many flops the algorithm can compute in each phase, by applying discrete Loomis-Whitney inequality:

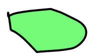
$$w^2 \leq N_A N_B N_C$$

Algorithms in direct linear algebra:

$$\begin{aligned} &for\ i,j,k = 1:n \\ &\quad c(i,j) = f_{ij}(g_{ijk}(a(i,k),b(k,j))) \\ &endfor \end{aligned}$$




 - set of points in $R^3$, represent w arithmetics

 - orthogonal projections of the points onto coordinate planes $N_A, N_B, N_C$ represent values of A, B, C

# Lower bounds for matrix multiplication (contd)

- Discrete Loomis-Whitney inequality:

$$w^2 \leq N_A N_B N_C$$

- Since there are at most 2M elements of A, B, C in a phase, the bound is:

$$w \leq 2\sqrt{2} M^{3/2}$$

- The number of phases S is #flops/w, and hence the lower bound on communication is:

$$\#\,messages(S) \geq \frac{\#\,flops}{w} = \Omega\left(\frac{\#\,flops}{M^{3/2}}\right)$$

$$\#\,loads/stores \geq \Omega\left(\frac{\#\,flops}{M^{1/2}}\right)$$

# Sequential algorithms and communication bounds

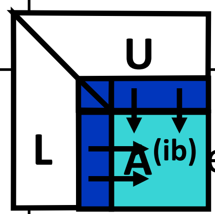
| Algorithm | Minimizing #words (not #messages) | Minimizing #words and #messages |
|---|---|---|
| Cholesky | LAPACK | [Gustavson, 97] [Ahmed, Pingali, 00] |
| LU | LAPACK (few cases) [Toledo,97], [Gustavson, 97] both use partial pivoting | [LG, Demmel, Xiang, 08] [Khabou, Demmel, LG, Gu, 12] uses tournament pivoting |
| QR | LAPACK (few cases) [Elmroth,Gustavson,98] | [Frens, Wise, 03], 3x flops [Demmel, LG, Hoemmen, Langou, 08] [Ballard et al, 14] |
| RRQR | | [Demmel, LG, Gu, Xiang 11] uses tournament pivoting, 3x flops |

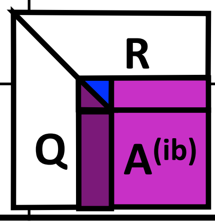
- Only several references shown for block algorithms (LAPACK), cache-oblivious algorithms and communication avoiding algorithms
- CA algorithms exist also for SVD and eigenvalue computation

# 2D Parallel algorithms and communication bounds

- If memory per processor = $n^2 / P$, the lower bounds become
  #words_moved ≥ $\Omega ( n^2 / P^{1/2} )$,  #messages ≥ $\Omega ( P^{1/2} )$


| Algorithm | Minimizing #words (not #messages) | Minimizing #words and #messages |
|---|---|---|
| Cholesky | ScaLAPACK | ScaLAPACK |
| LU | ScaLAPACK<br>es partial pivoting | [LG, Demmel, Xiang, 08]<br>[Khabou, Demmel, LG, Gu, 12]<br>uses tournament pivoting |
| QR | ScaLAPACK | [Demmel, LG, Hoemmen, Langou, 08]<br>[Ballard et al, 14] |
| RRQR | ScaLAPACK | [Demmel, LG, Gu, Xiang 13]<br>uses tournament pivoting, 3x flops |




- Only several references shown, block algorithms (ScaLAPACK) and communication avoiding algorithms
- CA algorithms exist also for SVD and eigenvalue computation

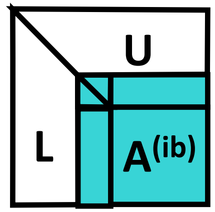
# LU factorization (as in ScaLAPACK pdgetrf)


LU factorization on a $P = P_r \times P_c$ grid of processors

For ib = 1 to n-1 step b

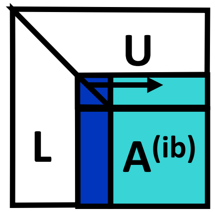
$A^{(ib)} = A(ib{:}n,\ ib{:}n)$

#messages



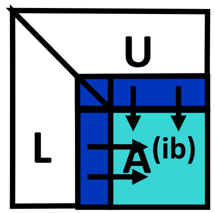

(1) Compute panel factorization — $O(n \log_2 P_r)$

- find pivot in each column, swap rows




(2) Apply all row permutations — $O(n/b(\log_2 P_c + \log_2 P_r))$

- broadcast pivot information along the rows
- swap rows at left and right

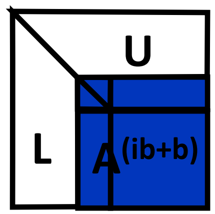



(3) Compute block row of U — $O(n/b \log_2 P_c)$

- broadcast right diagonal block of L of current panel

(4) Update trailing matrix — $O(n/b(\log_2 P_c + \log_2 P_r))$

- broadcast right block column of L
- broadcast down block row of U



# Block QR factorization

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = Q_1 \begin{pmatrix} R_{11} & R_{12} \\ & A_{22}^{\ 1} \end{pmatrix}$$

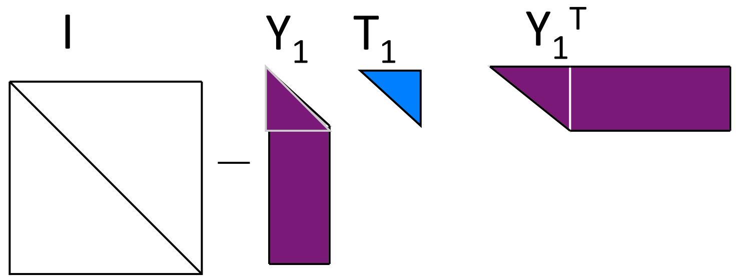
Block QR algebra:

1. Compute panel factorization:

$$\begin{pmatrix} \mathrm{A}_{11} \\ \mathrm{A}_{12} \end{pmatrix} = \mathrm{Q}_1 \begin{pmatrix} R_{11} \\ \\ \end{pmatrix}, \quad Q_1 = H_1 H_2 \ldots H_b$$

2. Compute the compact representation:

$$\mathrm{Q}_1 = I - Y_1 T_1 Y_1^T$$



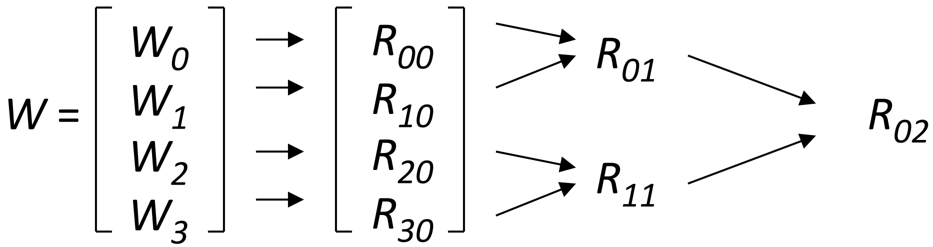

3. Update the trailing matrix:

$$\left(I - Y_1 T_1^T Y_1^T\right)\begin{pmatrix} A_{12} \\ A_{22} \end{pmatrix} = \begin{pmatrix} A_{12} \\ A_{22} \end{pmatrix} - Y_1\left(T_1^T\left(Y_1^T\begin{pmatrix} A_{12} \\ A_{22} \end{pmatrix}\right)\right) = \begin{pmatrix} R_{12} \\ A_{22}^1 \end{pmatrix}$$

4. The algorithm continues recursively on the trailing matrix.

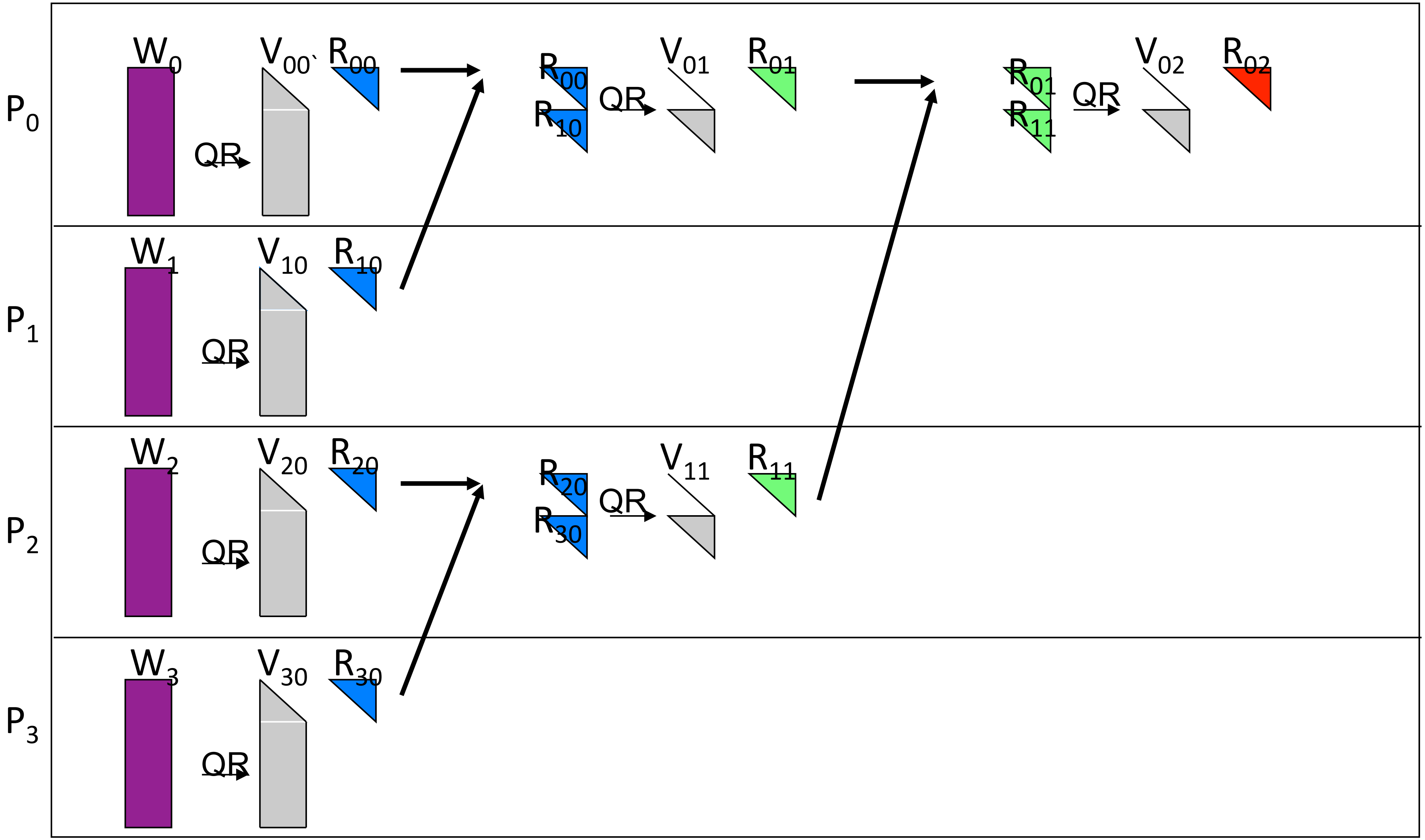
# TSQR: QR factorization of a tall skinny matrix using Householder transformations

- QR decomposition of m x b matrix W,  m >> b
  - P processors, block row layout
- Classic Parallel Algorithm
  - Compute Householder vector for each column
  - Number of messages ∝ b log P
- Communication Avoiding Algorithm
  - Reduction operation, with QR as operator
  - Number of messages ∝ log P




J. Demmel, LG, M. Hoemmen, J. Langou, 08

# Parallel TSQR




References: Golub, Plemmons, Sameh 88, Pothen, Raghavan, 89, Da Cunha, Becker, Patterson, 02

# Algebra of TSQR

Parallel:

$$
W = \begin{bmatrix} W_0 \\ W_1 \\ W_2 \\ W_3 \end{bmatrix}
\begin{tikzcd}[row sep=small]
{} \arrow[r] & R_{00} \arrow[dr] & & \\
{} \arrow[r] & R_{10} \arrow[r] & R_{01} \arrow[dr] & \\
& & & R_{02} \\
{} \arrow[r] & R_{20} \arrow[r] & R_{11} \arrow[ur] & \\
{} \arrow[r] & R_{30} \arrow[ur] & &
\end{tikzcd}
$$

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

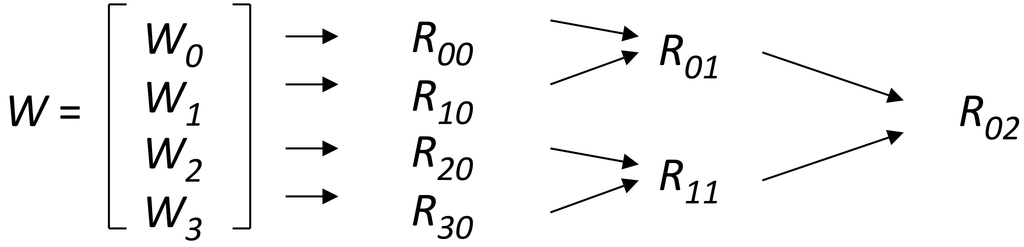
$$
\begin{pmatrix} R_{00} \\ R_{10} \\ \hline R_{20} \\ R_{30} \end{pmatrix} = \begin{pmatrix} Q_{01}R_{01} \\ \hline Q_{11}R_{11} \end{pmatrix} = \begin{pmatrix} Q_{01} & \\ \hline & Q_{11} \end{pmatrix} \cdot \begin{pmatrix} R_{01} \\ \hline R_{11} \end{pmatrix} \qquad \begin{pmatrix} R_{01} \\ \hline R_{11} \end{pmatrix} = Q_{02}R_{02}
$$

Q is represented implicitly as a product

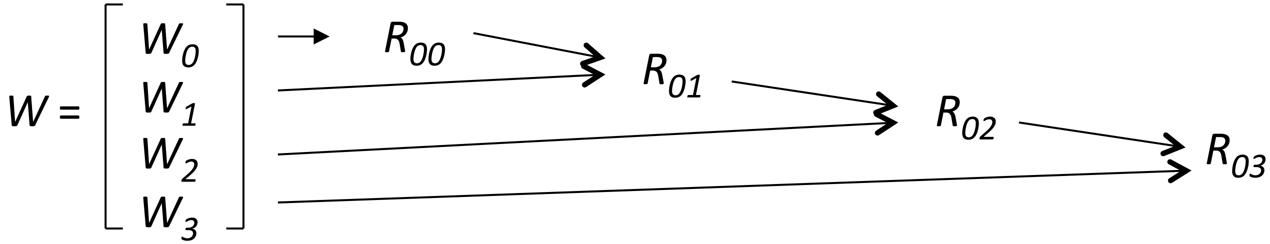
Output: $\{Q_{00}, Q_{10}, Q_{00}, Q_{20}, Q_{30}, Q_{01}, Q_{11}, Q_{02}, R_{02}\}$

# Flexibility of TSQR and CAQR algorithms

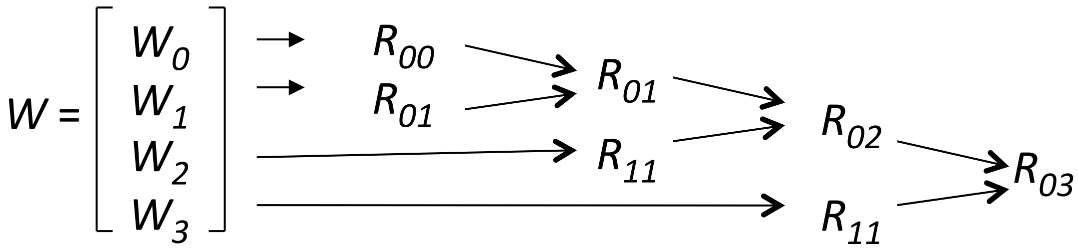
Parallel:




Sequential:




Dual Core:



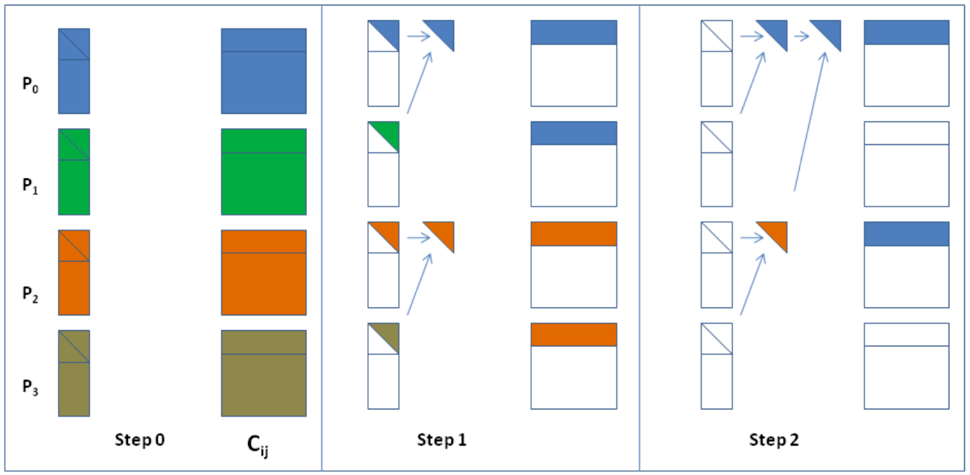

Reduction tree will depend on the underlying architecture, could be chosen dynamically

# Algebra of TSQR

Parallel:

$$W = \begin{bmatrix} W_0 \\ W_1 \\ W_2 \\ W_3 \end{bmatrix} \begin{array}{c} \rightarrow \\ \rightarrow \\ \rightarrow \\ \rightarrow \end{array} \begin{array}{c} R_{00} \\ R_{10} \\ R_{20} \\ R_{30} \end{array} \begin{array}{c} \searrow \\ \nearrow \\ \searrow \\ \nearrow \end{array} \begin{array}{c} R_{01} \\ \\ R_{11} \end{array} \begin{array}{c} \searrow \\ \nearrow \end{array} R_{02}$$

CAQR



# QR for General Matrices

- Cost of CAQR vs ScaLAPACK's PDGEQRF
  - n x n matrix on $P^{1/2}$ x $P^{1/2}$ processor grid, block size b
  - Flops: $(4/3)n^3/P + (3/4)n^2 b \log P/P^{1/2}$ vs $(4/3)n^3/P$
  - Bandwidth: $(3/4)n^2 \log P/P^{1/2}$ vs same
  - Latency: $2.5\ n \log P$ / **b** vs $1.5\ n \log\ P$

- Close to optimal (modulo log P factors)
  - Assume: $O(n^2/P)$ memory/processor, $O(n^3)$ algorithm,
  - Choose b near $n / P^{1/2}$ (its upper bound)
  - Bandwidth lower bound:

    $\Omega(n^2 /P^{1/2})$ – just log(P) smaller
  - Latency lower bound:

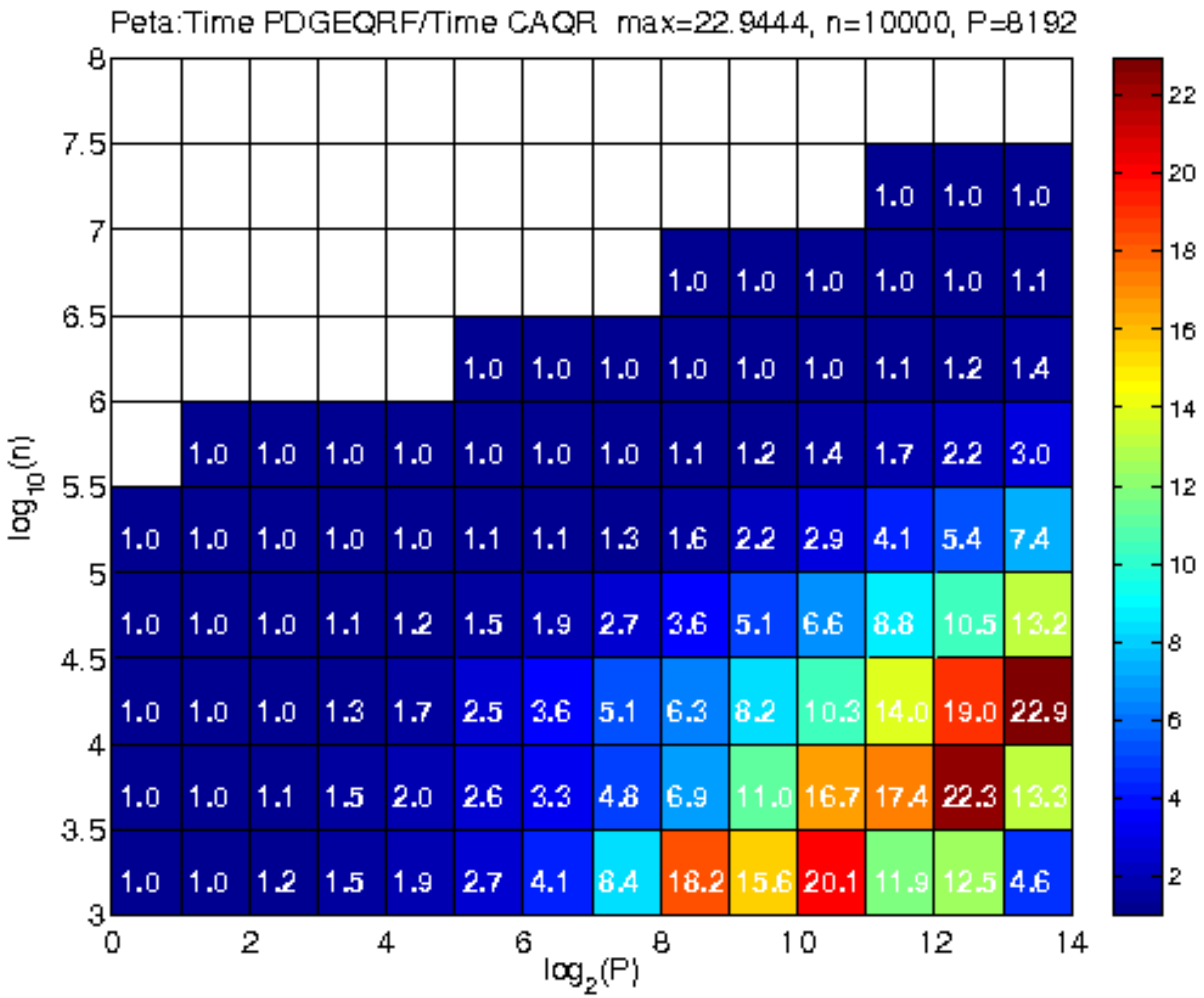
    $\Omega(P^{1/2})$ – just polylog(P) smaller

# Performance of TSQR vs Sca/LAPACK

- Parallel
  - Intel Xeon (two socket, quad core machine), 2010
    - Up to **5.3x speedup** (8 cores, $10^5$ x 200)
  - Pentium III cluster, Dolphin Interconnect, MPICH, 2008
    - Up to **6.7x speedup** (16 procs, 100K x 200)
  - BlueGene/L, 2008
    - Up to **4x speedup** (32 procs, 1M x 50)
  - Tesla C 2050 / Fermi (Anderson et al)
    - Up to **13x** (110,592 x 100)
  - Grid – **4x** on 4 cities vs 1 city (Dongarra, Langou et al)
  - QR computed locally using recursive algorithm (Elmroth-Gustavson) – enabled by TSQR

- Results from many papers, for some see [Demmel, LG, Hoemmen, Langou, SISC 12], [Donfack, LG, IPDPS 10].

# Modeled Speedups of CAQR vs ScaLAPACK




Petascale
up to 22.9x

IBM Power 5
up to 9.7x

“Grid”
up to 11x

Petascale machine with 8192 procs, each at 500 GFlops/s, a bandwidth of 4 GB/s.

$$\gamma = 2 \cdot 10^{-12} s, \alpha = 10^{-5} s, \beta = 2 \cdot 10^{-9} s / word.$$

# Impact

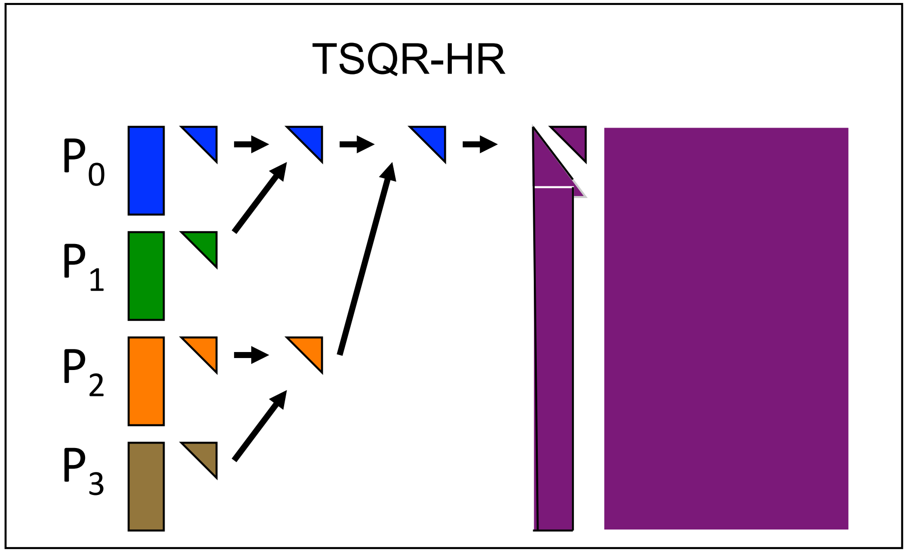
- TSQR/CAQR implemented in
  - Intel Data analytics library
  - GNU Scientific Library
  - ScaLAPACK
  - Spark for data mining

- CALU implemented in
  - Cray's libsci
  - To be implemented in lapack/scapalack

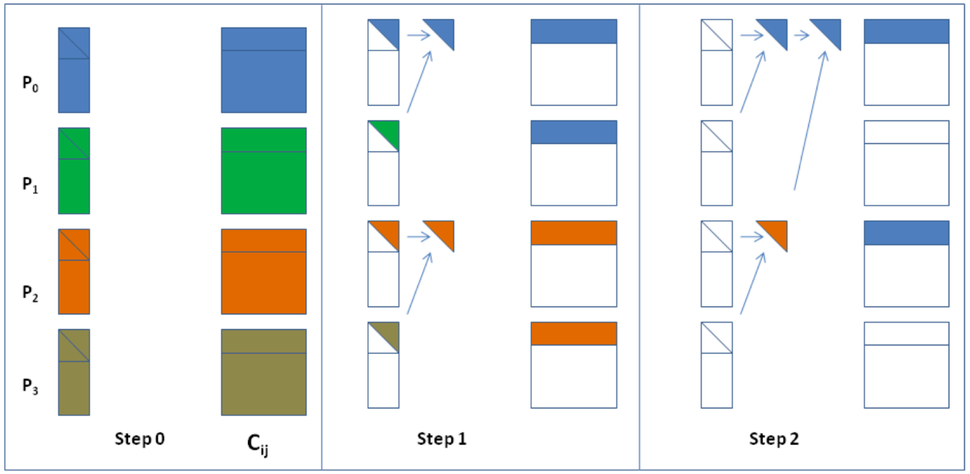
# Algebra of TSQR

Parallel:

$$W = \begin{bmatrix} W_0 \\ W_1 \\ W_2 \\ W_3 \end{bmatrix} \begin{array}{l} \rightarrow R_{00} \\ \rightarrow R_{10} \\ \rightarrow R_{20} \\ \rightarrow R_{30} \end{array} \begin{array}{l} \searrow \\ \nearrow \\ \searrow \\ \nearrow \end{array} \begin{array}{l} R_{01} \\ \\ R_{11} \end{array} \begin{array}{l} \searrow \\ \nearrow \end{array} R_{02}$$




CAQR



# Reconstruct Householder vectors from TSQR

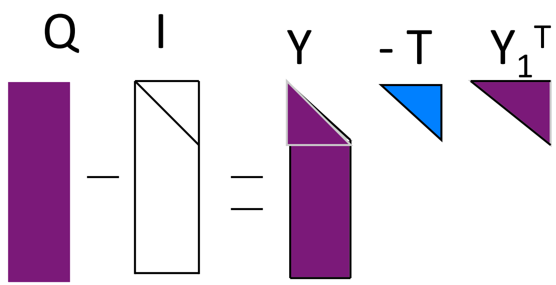
The QR factorization using Householder vectors

$$W = QR = (I - YTY_1^T)R$$

can be re-written as an LU factorization

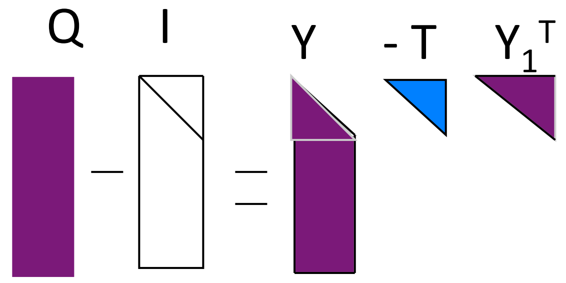
$$W - R = Y(-TY_1^T)R$$

$$Q - I = Y(-TY_1^T)$$



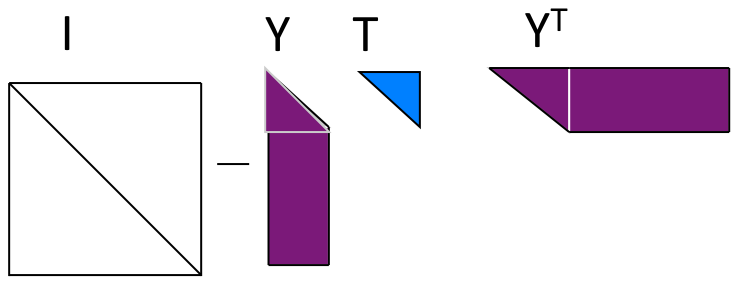
# Reconstruct Householder vectors TSQR-HR

1. Perform TSQR
2. Form Q explicitly (tall-skinny orthonormal factor)
3. Perform LU decomposition: *Q - I = LU*

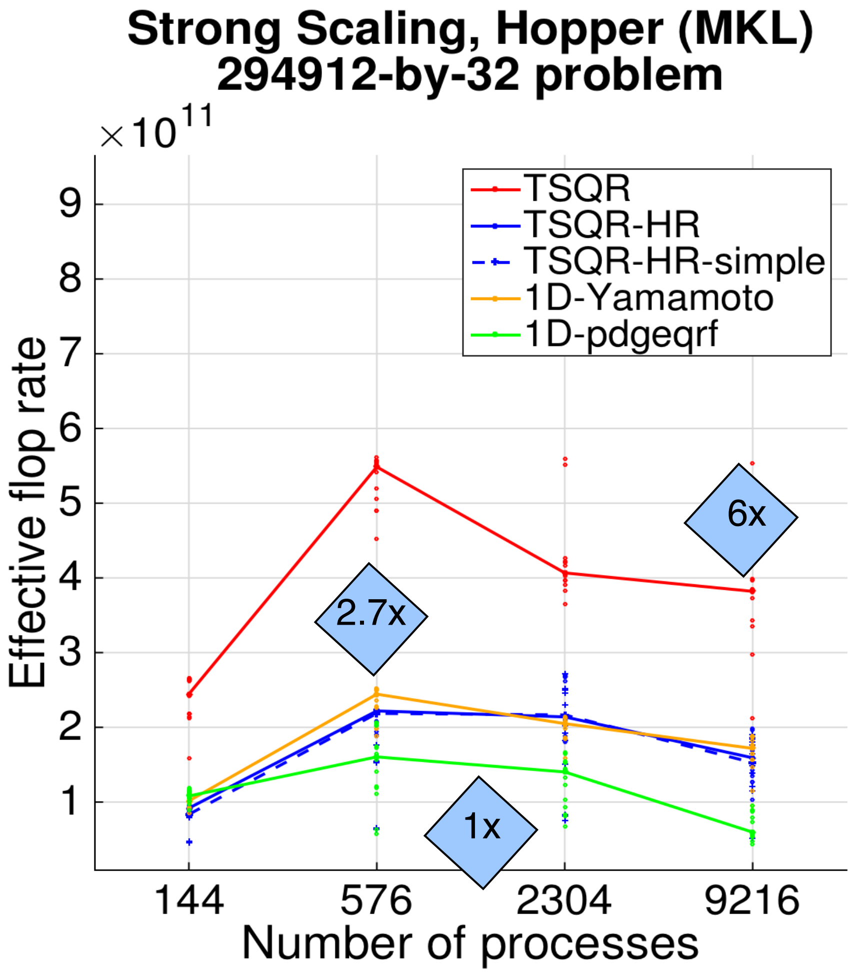


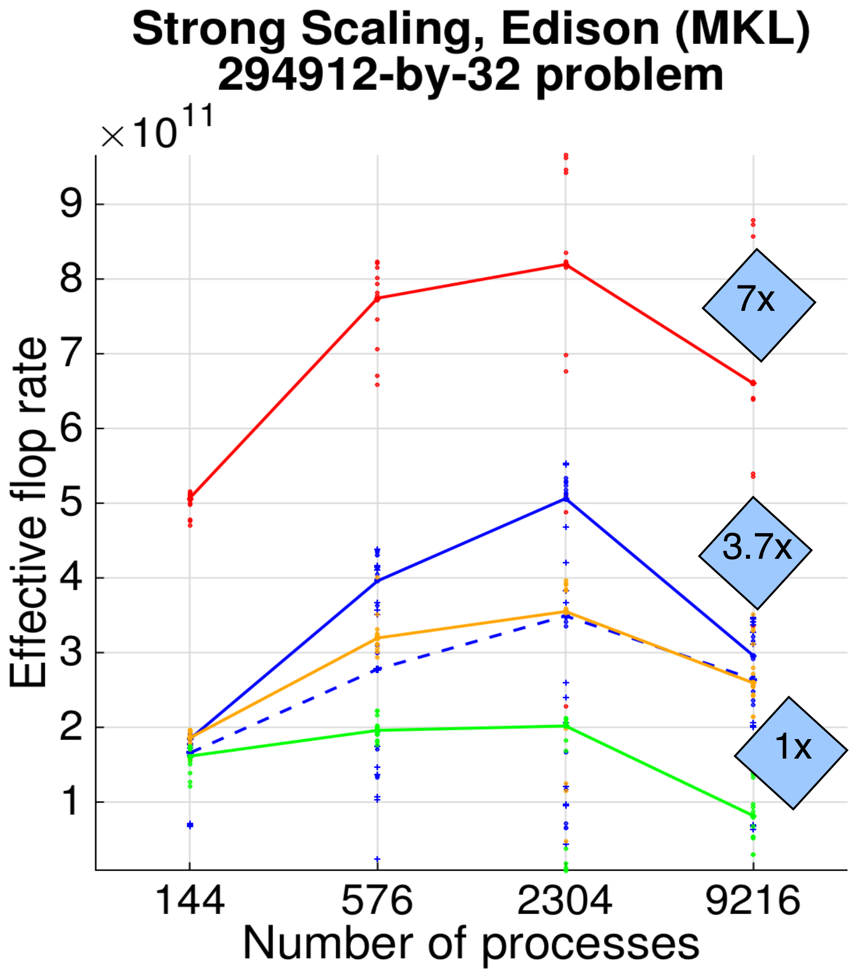

4. Set $Y = L$
5. Set $T = -U\,Y_1^{-T}$

$$I - YTY^T = I - \begin{bmatrix} Y_1 \\ Y_2 \end{bmatrix} T \begin{bmatrix} Y_1^T & Y_2^T \end{bmatrix}$$



# Strong scaling




- Hopper: Cray XE6 (NERSC) – 2 x 12-core AMD Magny-Cours (2.1 GHz)
- Edison: Cray CX30 (NERSC) – 2 x 12-core Intel Ivy Bridge (2.4 GHz)
- Effective flop rate, computed by dividing $2mn^2 - 2n^3/3$ by measured runtime

Ballard, Demmel, LG, Jacquelin, Knight, Nguyen, and Solomonik, 2015.

# The LU factorization of a tall skinny matrix

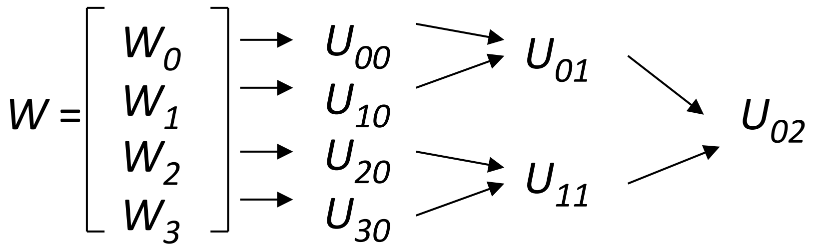
First try the obvious generalization of TSQR.

$$W = \begin{pmatrix} W_0 \\ W_1 \\ W_2 \\ W_3 \end{pmatrix} = \underbrace{\begin{pmatrix} \Pi_{00} & & & \\ & \Pi_{10} & & \\ & & \Pi_{20} & \\ & & & \Pi_{30} \end{pmatrix}}_{\Pi_0} \cdot \begin{pmatrix} L_{00} & & & \\ & L_{10} & & \\ & & L_{20} & \\ & & & L_{30} \end{pmatrix} \cdot \begin{pmatrix} U_{00} \\ U_{10} \\ U_{20} \\ U_{30} \end{pmatrix}$$

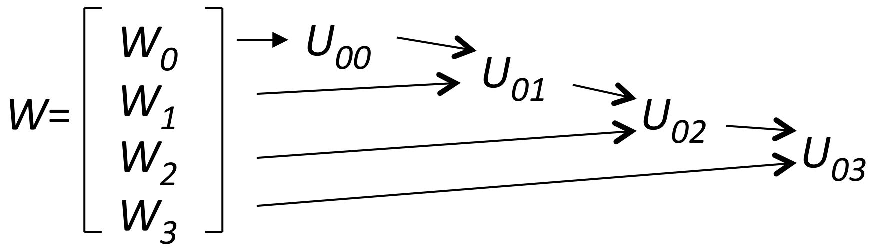
$$\begin{pmatrix} U_{00} \\ U_{10} \\ U_{20} \\ U_{30} \end{pmatrix} = \underbrace{\begin{pmatrix} \Pi_{01} & \\ & \Pi_{11} \end{pmatrix}}_{\Pi_1} \cdot \begin{pmatrix} L_{01} & \\ & L_{11} \end{pmatrix} \cdot \begin{pmatrix} U_{01} \\ U_{11} \end{pmatrix} \qquad \begin{pmatrix} U_{01} \\ U_{11} \end{pmatrix} = \underbrace{\Pi_{02}}_{\Pi_2} L_{02} U_{02}$$

# Obvious generalization of TSQR to LU

- Block parallel pivoting:
  - uses a binary tree and is optimal in the parallel case




- Block pairwise pivoting:
  - uses a flat tree and is optimal in the sequential case
  - introduced by Barron and Swinnerton-Dyer, 1960: block LU factorization used to solve a system with 100 equations on EDSAC 2 computer using an auxiliary magnetic-tape
  - used in PLASMA for multicore architectures and FLAME for out-of-core algorithms and for multicore architectures



# Stability of the LU factorization

- The backward stability of the LU factorization of a matrix A of size n-by-n

$$\left\| |\hat{L}| \cdot |\hat{U}| \right\|_\infty \le (1 + 2(n^2 - n) g_w) \|A\|_\infty$$

depends on the growth factor

$$g_W = \frac{\max_{i,j,k} |a_{ij}^k|}{\max_{i,j} |a_{ij}|}$$

where $a_{ij}^k$ are the values at the k-th step.

- $g_W \le 2^{n-1}$ , attained for Wilkinson matrix

but in practice it is on the order of $n^{2/3}$ -- $n^{1/2}$

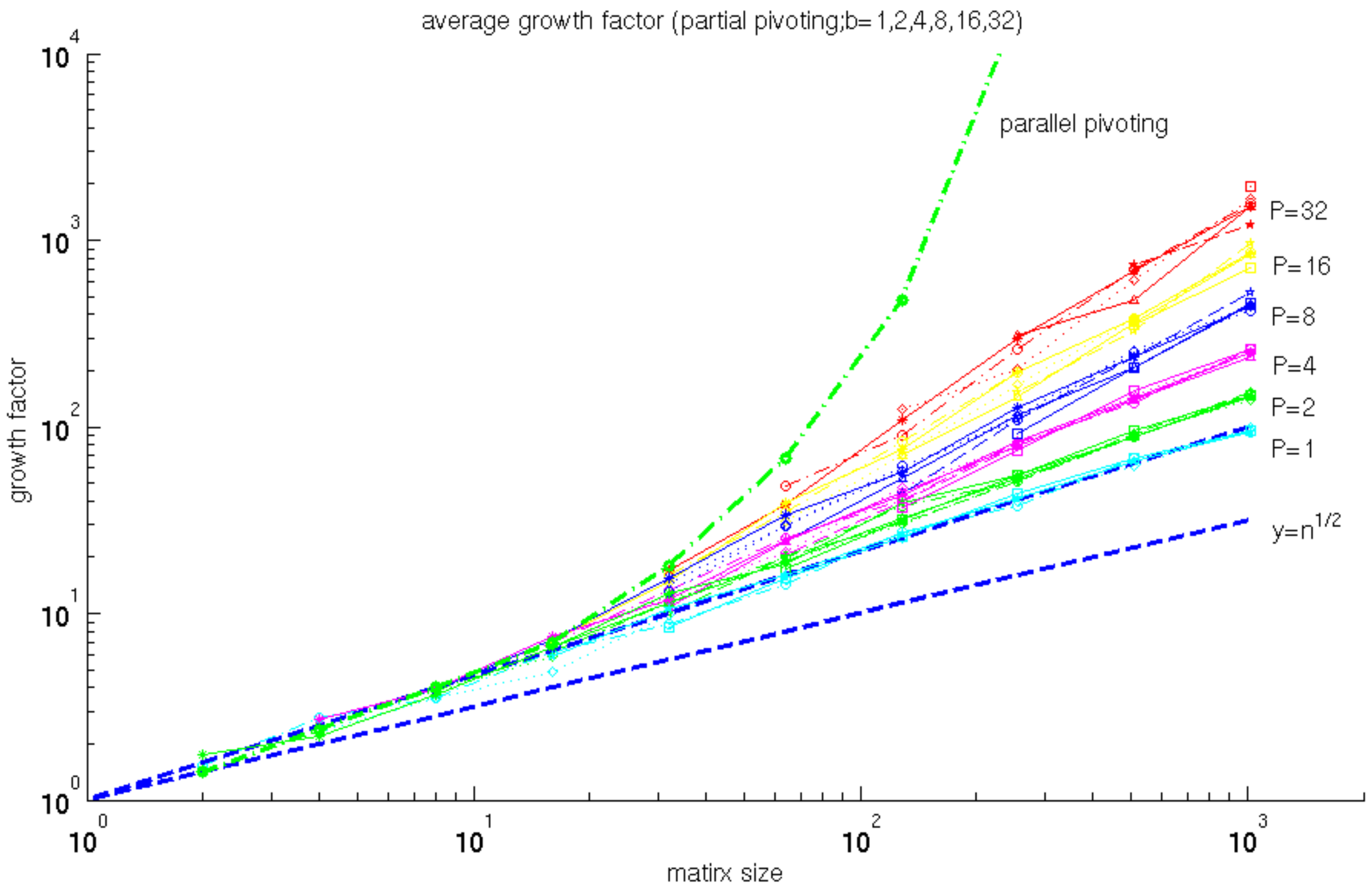
$$A = diag(\pm 1)\begin{pmatrix} 1 & 0 & 0 & \cdots & 0 & 1 \\ -1 & 1 & & \cdots & 0 & 1 \\ -1 & -1 & 1 & \ddots & 0 & 1 \\ \vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\ -1 & -1 & \cdots & -1 & 1 & 1 \\ -1 & -1 & \cdots & -1 & -1 & 1 \end{pmatrix}$$

- Two reasons considered to be important for the average case stability [Trefethen and Schreiber, 90] :

- the multipliers in L are small,

- the correction introduced at each elimination step is of rank 1.

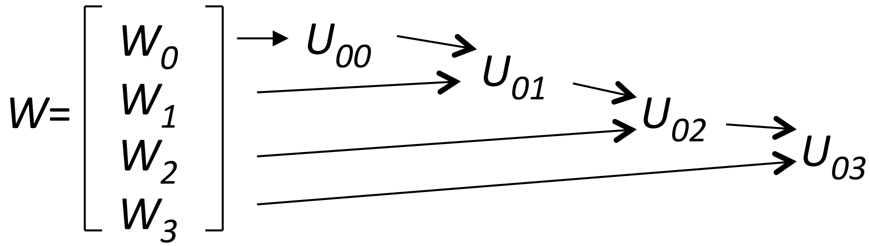
# Block parallel pivoting

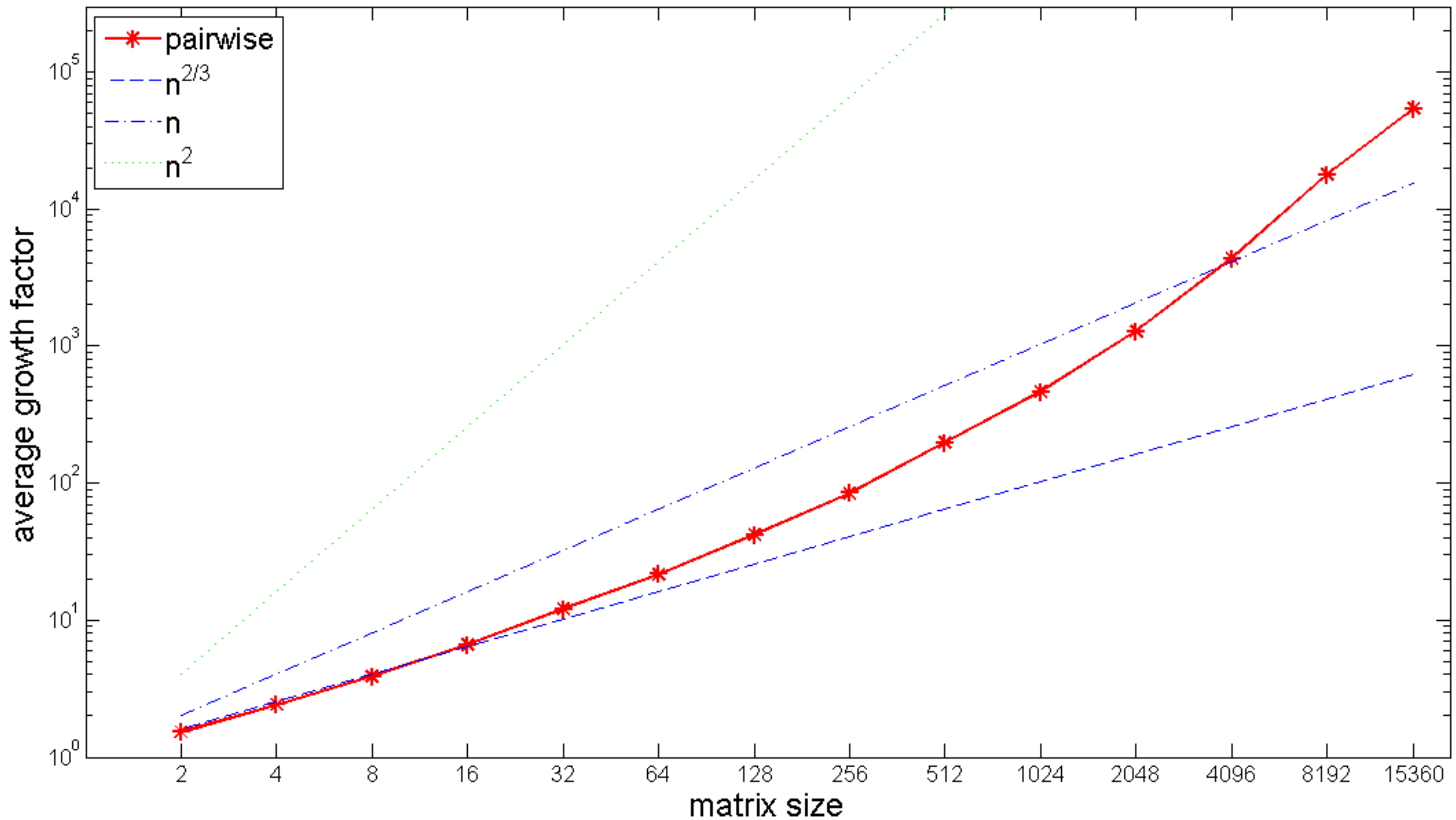



- Unstable for large number of processors P
- When P=number rows, it corresponds to parallel pivoting, known to be unstable (Trefethen and Schreiber, 90)

# Block pairwise pivoting

- Results shown for random matrices
- Will become unstable for large matrices



# Tournament pivoting - the overall idea

- At each iteration of a block algorithm

$$A = \begin{array}{c} \begin{array}{cc} b & n-b \end{array} \\ \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \end{array} \begin{array}{l} \\ \left.\right\}\, b \\ \left.\right\}\, n-b \end{array} \text{, where } \quad W = \begin{pmatrix} A_{11} \\ A_{21} \end{pmatrix}$$

  - Preprocess W to find at low communication cost good pivots for the LU factorization of W, return a permutation matrix P.
  - Permute the pivots to top, ie compute PA.
  - Compute LU with no pivoting of W, update trailing matrix.

$$PA = \begin{pmatrix} L_{11} & \\ L_{21} & I_{n-b} \end{pmatrix} \begin{pmatrix} U_{11} & U_{12} \\ & A_{22} - L_{21}U_{12} \end{pmatrix}$$

# Tournament pivoting for a tall skinny matrix

1) Compute GEPP factorization of each $W_{i.}$, find permutation $\Pi_0$

$$W = \begin{pmatrix} W_0 \\ \hline W_1 \\ \hline W_2 \\ \hline W_3 \end{pmatrix} = \begin{pmatrix} \Pi_{00} L_{00} U_{00} \\ \hline \Pi_{10} L_{10} U_{10} \\ \hline \Pi_{20} L_{20} U_{20} \\ \hline \Pi_{30} L_{30} U_{30} \end{pmatrix},$$

Pick b pivot rows, form $A_{00}$

Same for $A_{10}$

Same for $A_{20}$

Same for $A_{30}$

2) Perform $\log_2(P)$ times GEPP factorizations of 2b-by-b rows, find permutations $\Pi_1, \Pi_2$

$$\begin{pmatrix} A_{00} \\ A_{10} \\ \hline A_{20} \\ A_{30} \end{pmatrix} = \begin{pmatrix} \Pi_{01} L_{01} U_{01} \\ \hline \Pi_{11} L_{11} U_{11} \end{pmatrix}$$

Pick b pivot rows, form $A_{01}$

Same for $A_{11}$

$$\begin{pmatrix} A_{01} \\ A_{11} \end{pmatrix} = \underbrace{\Pi_{02}}_{\Pi_2} L_{02} U_{02}$$

3) Compute LU factorization with no pivoting of the permuted matrix:

$$\Pi_2^T \Pi_1^T \Pi_0^T W = LU$$

# Tournament pivoting

P$_0$

$$W_0 = \begin{pmatrix} 2 & 4 \\ 0 & 1 \\ 2 & 0 \\ 1 & 2 \end{pmatrix} = \Pi_0 L_0 U_0 \qquad \Pi_0^T W_0 = \begin{pmatrix} 2 & 4 \\ 2 & 0 \end{pmatrix}$$

P$_1$

$$W_1 = \begin{pmatrix} 2 & 0 \\ 0 & 0 \\ 4 & 1 \\ 1 & 0 \end{pmatrix} = \Pi_1 L_1 U_1 \qquad \Pi_1^T W_1 = \begin{pmatrix} 4 & 1 \\ 2 & 0 \end{pmatrix}$$

P$_2$

$$W_2 = \begin{pmatrix} 0 & 1 \\ 1 & 4 \\ 0 & 0 \\ 0 & 2 \end{pmatrix} = \Pi_2 L_2 U_2 \qquad \Pi_2^T W_2 = \begin{pmatrix} 1 & 4 \\ 0 & 2 \end{pmatrix}$$

P$_3$

$$W_3 = \begin{pmatrix} 2 & 1 \\ 0 & 2 \\ 1 & 0 \\ 4 & 2 \end{pmatrix} = \Pi_3 L_3 U_3 \qquad \Pi_3^T W_3 = \begin{pmatrix} 4 & 2 \\ 0 & 2 \end{pmatrix}$$

$$\overline{W}_0 = \begin{pmatrix} 2 & 4 \\ 2 & 0 \\ 4 & 1 \\ 2 & 0 \end{pmatrix} = \overline{\Pi}_0 \overline{L}_0 \overline{U}_0 \qquad \overline{\Pi}_0^T \overline{W}_0 = \begin{pmatrix} 4 & 1 \\ 2 & 4 \end{pmatrix}$$

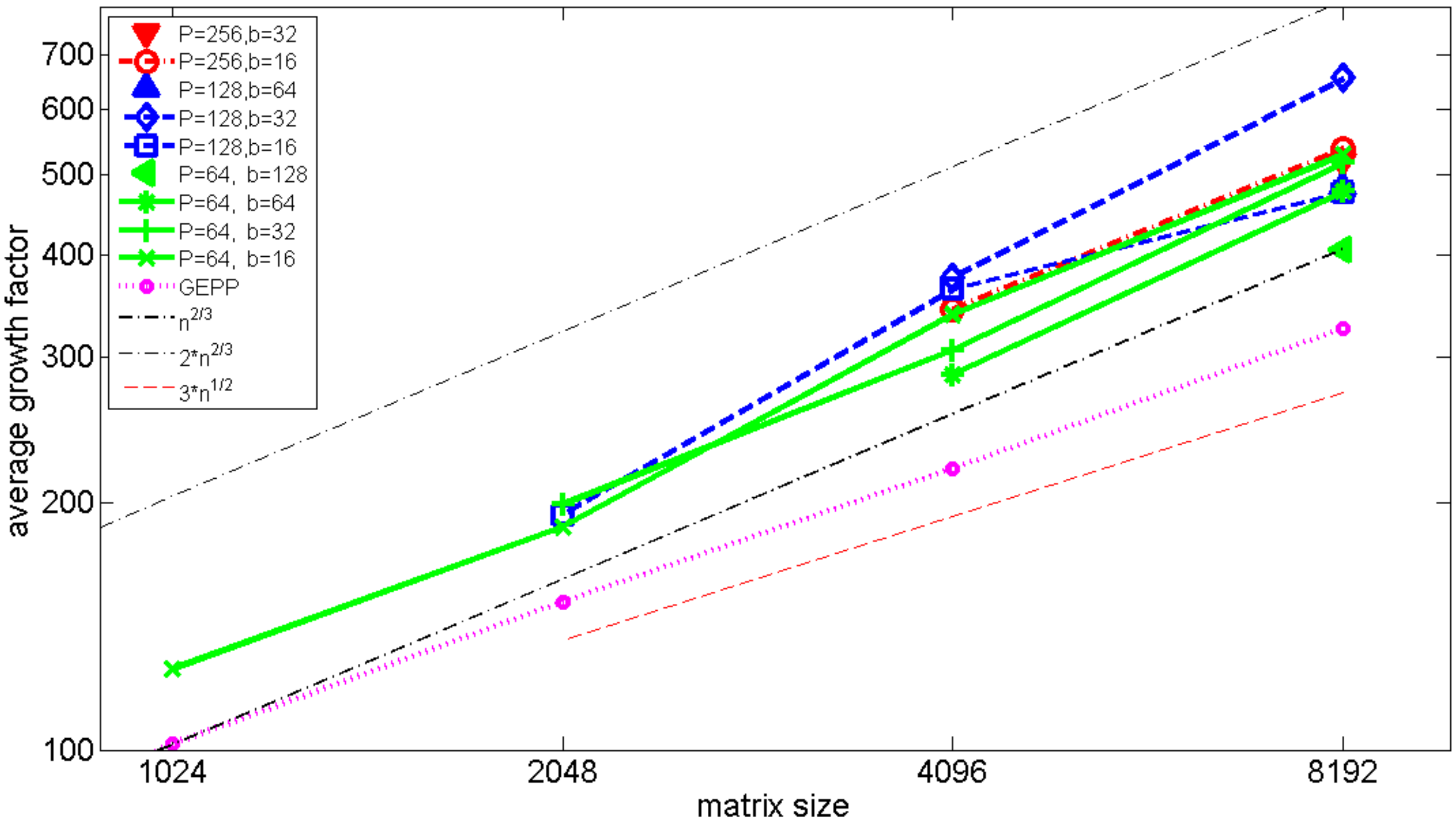
$$\overline{W}_2 = \begin{pmatrix} 1 & 4 \\ 0 & 2 \\ 4 & 2 \\ 0 & 2 \end{pmatrix} = \overline{\Pi}_2 \overline{L}_2 \overline{U}_2 \qquad \overline{\Pi}_2^T \overline{W}_2 = \begin{pmatrix} 4 & 2 \\ 1 & 4 \end{pmatrix}$$

$$\underline{W}_0 = \begin{pmatrix} 4 & 1 \\ 2 & 4 \\ 4 & 2 \\ 1 & 4 \end{pmatrix} = \underline{\Pi}_0 \underline{L}_0 \underline{U}_0 \qquad \underline{\Pi}_0^T \underline{W}_0 = \begin{pmatrix} 4 & 1 \\ 1 & 4 \end{pmatrix}$$

Good pivots for factorizing W

time

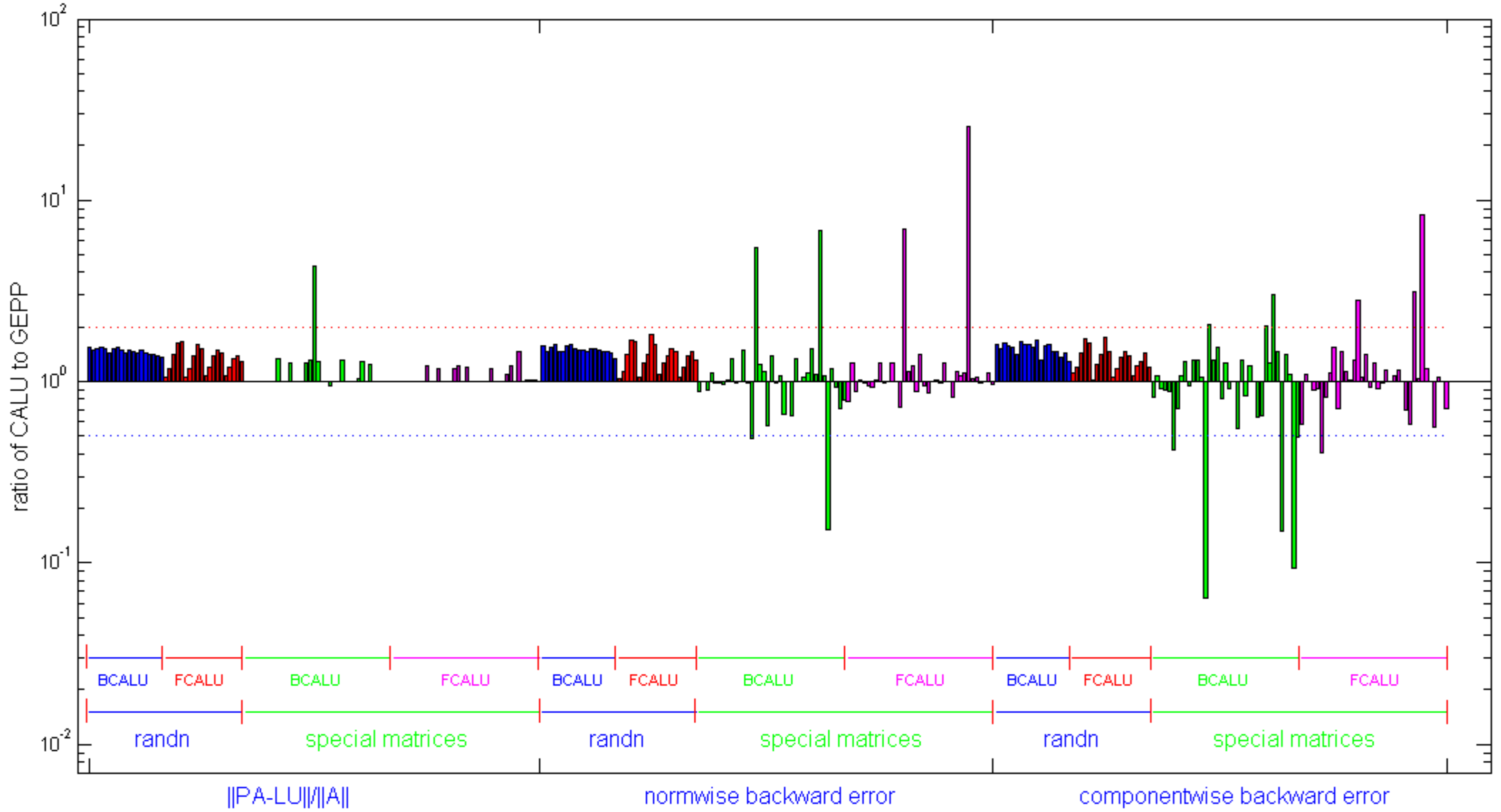
# Growth factor for binary tree based CALU




- Random matrices from a normal distribution
- Same behaviour for all matrices in our test, and |L| <= 4.2

# Stability of CALU (experimental results)

- Results show ||PA-LU||/||A||, normwise and componentwise backward errors, for random matrices and special ones
  - See [LG, Demmel, Xiang, SIMAX 2011] for details
  - BCALU denotes binary tree based CALU and FCALU denotes flat tree based CALU



# Our “proof of stability” for CALU

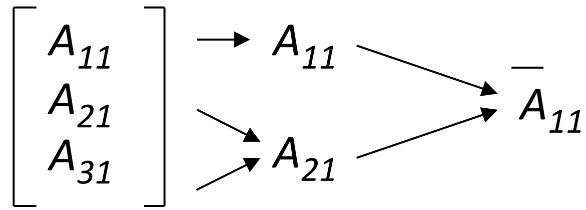
- CALU as stable as GEPP in following sense:

  In exact arithmetic, CALU process on a matrix A is equivalent to GEPP process on a larger matrix G whose entries are blocks of A and zeros.

- Example of one step of tournament pivoting:

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \\ A_{31} & A_{32} \end{pmatrix}$$

tournament pivoting:




$$G = \begin{pmatrix} \overline{A}_{11} & & \overline{A}_{12} \\ A_{21} & A_{21} & \\ & -A_{31} & A_{32} \end{pmatrix}$$

- Proof possible by using original rows of A during tournament pivoting (not the computed rows of U).

# Outline of the proof of stability for CALU

- Consider $A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \\ A_{31} & A_{32} \end{pmatrix}$, and the result of TSLU as $\begin{bmatrix} A_{11} \\ A_{21} \\ A_{31} \end{bmatrix}$

$$\begin{tikzcd}[row sep=small] & A_{11} \arrow[dr] & \\ \begin{bmatrix} A_{11} \\ A_{21} \\ A_{31} \end{bmatrix} \arrow[ur] \arrow[dr] & & \overline{A}_{11} \\ & A_{21} \arrow[ur] & \end{tikzcd}$$

- After the factorization of first panel by CALU, $A^s_{32}$ (the Schur complement of $A_{32}$) is not bounded as in GEPP,

$$\begin{pmatrix} \Pi_{11} & \Pi_{12} & \\ \Pi_{21} & \Pi_{22} & \\ & & I \end{pmatrix} \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \\ A_{31} & A_{32} \end{pmatrix} = \begin{pmatrix} \overline{A}_{11} & \overline{A}_{12} \\ \overline{A}_{21} & \overline{A}_{22} \\ A_{31} & A_{32} \end{pmatrix} = \begin{pmatrix} \overline{L}_{11} & & \\ \overline{L}_{21} & I & \\ \overline{L}_{31} & & I \end{pmatrix} \begin{pmatrix} \overline{U}_{11} & \overline{U}_{12} \\ & A^s_{22} \\ & A^s_{32} \end{pmatrix}$$

- but $A^s_{32}$ can be obtained by GEPP on larger matrix G formed from blocks of A

$$G = \begin{pmatrix} \overline{A}_{11} & & \overline{A}_{12} \\ A_{21} & A_{21} & \\ & -A_{31} & A_{32} \end{pmatrix} = \begin{pmatrix} \overline{L}_{11} & & \\ A_{21}\overline{U}_{11}^{-1} & L_{21} & \\ & -L_{31} & I \end{pmatrix} \begin{pmatrix} \overline{U}_{11} & & \overline{U}_{12} \\ & U_{21} & -L_{21}^{-1}A_{21}\overline{U}_{11}^{-1}\overline{U}_{12} \\ & & A^s_{32} \end{pmatrix}$$

- GEPP on G does not permute and

$$L_{31}L_{21}^{-1}A_{21}\overline{U}_{11}^{-1}\overline{U}_{12} + A^s_{32} = L_{31}U_{21}\overline{U}_{11}^{-1}\overline{U}_{12} + A^s_{32} = A_{31}\overline{U}_{11}^{-1}\overline{U}_{12} + A^s_{32} = \overline{L}_{31}\overline{U}_{12} + A^s_{32} = A_{32}$$

# LU factorization and low rank matrices

- For low rank matrices, the factorization of $A_1$ computed as following might not be stable

  Compute PA=LU by using GEPP — L(k+1:end,k) = A(k+1:end,k)/A(k,k)

  Permute the matrix $A_1$=PA

  Compute LU with no pivoting $A_1=L_1U_1$ — L(k+1:end,k) = L(k+1:end,k)* (1/A(k,k))

- Example A = randn(6,3)*randn(3,5), max(abs(L)) = 1, max(abs($L_1$)) = $10^{15}$

After 4 steps of factorization of PA we obtain:

$$PA^4 = \begin{pmatrix} 1.0000 & & & & \\ 0.1729 & 1.0000 & & & \\ 0.6061 & 0.8608 & 1.0000 & & \\ 0.5776 & 0.0543 & 0.3264 & 1.0000 & \\ 0.4789 & -0.2877 & -0.1545 & 2.3333 & \boxed{2.3e-16} \\ -0.3264 & -0.7514 & -0.4597 & 1.7778 & \boxed{8.3e-17} \end{pmatrix} \cdot \begin{pmatrix} 4.4766 & 3.0163 & -4.7390 & 4.2180 & -0.8164 \\ & -1.5439 & -0.4703 & 1.9267 & 1.0925 \\ & & 1.6149 & 2.3623 & 0.3167 \\ & & & 9.9e-16 & 1.6e-16 \\ & & & & 1 \end{pmatrix}$$

Schur complement after 4 elimination steps

After 4 steps of factorization of $A_1$ we obtain:

$$A_1^4 = \begin{pmatrix} 1.0000 & & & & \\ 0.1729 & 1.0000 & & & \\ 0.6061 & 0.8608 & 1.0000 & & \\ 0.5776 & 0.0543 & 0.3264 & 1.0000 & \\ 0.4789 & -0.2877 & -0.1545 & 2.3333 & \boxed{4.9e-32} \\ -0.3264 & -0.7514 & -0.4597 & 1.7778 & \boxed{-7.4e-17} \end{pmatrix} \cdot \begin{pmatrix} 4.4766 & 3.0163 & -4.7390 & 4.2180 & -0.8164 \\ & -1.5439 & -0.4703 & 1.9267 & 1.0925 \\ & & 1.6149 & 2.3623 & 0.3167 \\ & & & 9.9e-16 & 1.6e-16 \\ & & & & 1 \end{pmatrix}$$

# LU_PRRP: LU with panel rank revealing pivoting

- Pivots are selected by using strong rank revealing QR on each panel
- The factorization after one panel elimination is written as

$$PA = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} I_b & \\ A_{21}A_{11}^{-1} & I_{n-b} \end{pmatrix} \begin{pmatrix} A_{11} & A_{12} \\ & A_{22} - A_{21}A_{11}^{-1}A_{12} \end{pmatrix}$$

$A_{21} A_{11}^{-1}$ is computed through strong rank revealing QR
and $\max(|A_{21} A_{11}^{-1}|)_{ij} \le f$

- LU_PRRP and CALU_PRRP stable for pathological cases (Wilkinson matrix) and matrices from two real applications (Voltera integral equation - Foster, a boundary value problem - Wright) on which GEPP fails.

A. Khabou, J. Demmel, LG, M. Gu, 2012

# Growth factor in exact arithmetic

- Matrix of size m-by-n, reduction tree of height H=log(P).
- (CA)LU_PRRP select pivots using strong rank revealing QR (A. Khabou, J. Demmel, LG, M. Gu, SIMAX 2013)
- "In practice" means observed/expected/conjectured values.

| | CALU | GEPP | CALU_PRRP | LU_PRRP |
|---|---|---|---|---|
| Upper bound | $2^{n(\log(P)+1)-1}$ | $2^{n-1}$ | $(1+2b)^{(n/b)\log(P)}$ | $(1+2b)^{(n/b)}$ |
| In practice | $n^{2/3}$ -- $n^{1/2}$ | $n^{2/3}$ -- $n^{1/2}$ | $(n/b)^{2/3}$ -- $(n/b)^{1/2}$ | $(n/b)^{2/3}$ -- $(n/b)^{1/2}$ |

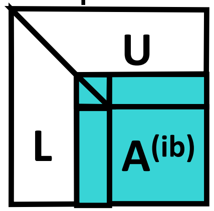
Better bounds →

- For a matrix of size $10^7$-by-$10^7$ (using petabytes of memory)

  $n^{1/2} = 10^{3.5}$

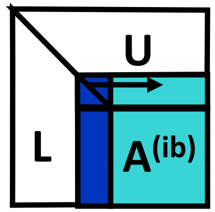
# CALU – a communication avoiding LU factorization

- Consider a 2D grid of P processors $P_r$-by-$P_c$ , using a 2D block cyclic layout with square blocks of size b.




For ib = 1 to n-1 step b
    $A^{(ib)} = A(ib{:}n, ib{:}n)$

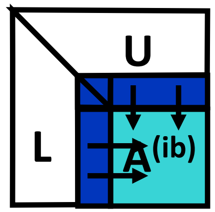
(1) Find permutation for current panel using TSLU $O(n/b \log_2 P_r)$




(2) Apply all row permutations (pdlaswp) $O(n/b(\log_2 P_c + \log_2 P_r))$

- broadcast pivot information along the rows of the grid

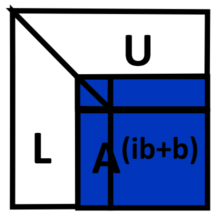
(3) Compute panel factorization (dtrsm)




$O(n/b \log_2 P_c)$

(4) Compute block row of U (pdtrsm)

- broadcast right diagonal part of L of current panel




(5) Update trailing matrix (pdgemm) $O(n/b(\log_2 P_c + \log_2 P_r))$

- broadcast right block column of L
- broadcast down block row of U

# LU for General Matrices

- Cost of CALU vs ScaLAPACK's PDGETRF
  - n x n matrix on $P^{1/2}$ x $P^{1/2}$ processor grid, block size b
  - Flops: $(2/3)n^3/P + (3/2)n^2b / P^{1/2}$ vs $(2/3)n^3/P + n^2b/P^{1/2}$
  - Bandwidth: $n^2 \log P/P^{1/2}$ vs same
  - Latency: $3 n \log P / \mathbf{b}$ vs $1.5 n \log P + 3.5n \log P / b$

- Close to optimal (modulo log P factors)
  - Assume: $O(n^2/P)$ memory/processor, $O(n^3)$ algorithm,
  - Choose b near $n / P^{1/2}$ (its upper bound)
  - Bandwidth lower bound:
    $\Omega(n^2 /P^{1/2})$ – just log(P) smaller
  - Latency lower bound:
    $\Omega(P^{1/2})$ – just polylog(P) smaller

# Performance vs ScaLAPACK

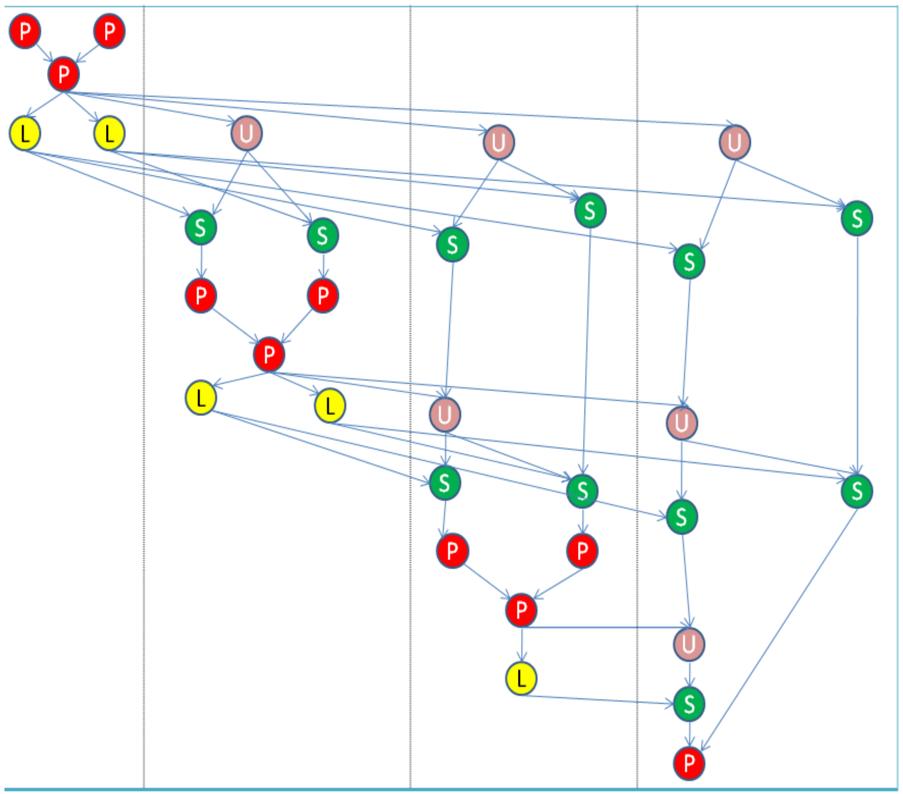
- Parallel TSLU (LU on tall-skinny matrix)
  - IBM Power 5
    - Up to **4.37x** faster (16 procs, 1M x 150)
  - Cray XT4
    - Up to **5.52x** faster (8 procs, 1M x 150)

- Parallel CALU (LU on general matrices)
  - Intel Xeon (two socket, quad core)
    - Up to **2.3x** faster (8 cores, 10^6 x 500)
  - IBM Power 5
    - Up to **2.29x** faster (64 procs, 1000 x 1000)
  - Cray XT4
    - Up to **1.81x** faster (64 procs, 1000 x 1000)

- Details in SC08 (LG, Demmel, Xiang), IPDPS'10 (S. Donfack, LG).

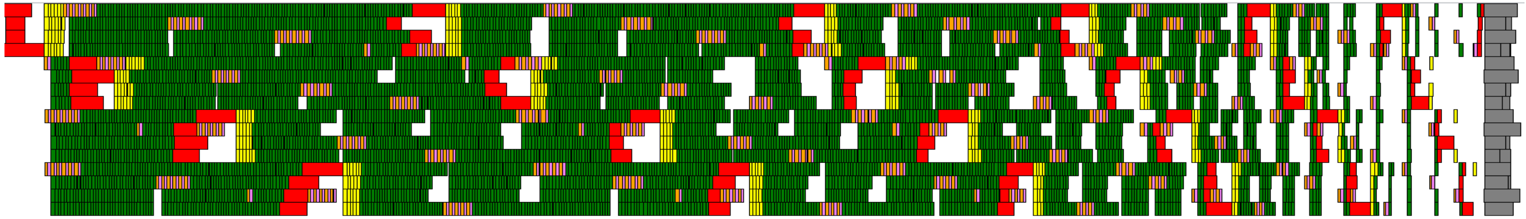
# CALU and its task dependency graph

- The matrix is partitioned into blocks of size T x b.
- The computation of each block is associated with a task.

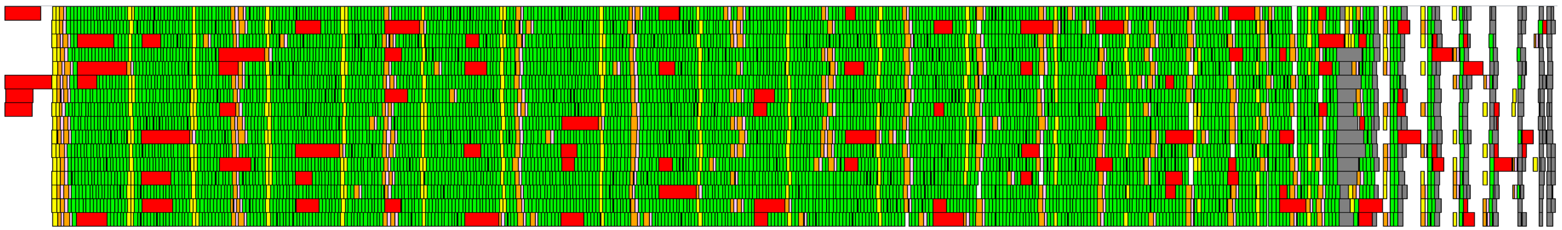



# Scheduling CALU's Task Dependency Graph

- Static scheduling
  - \+ Good locality of data
  - \- Ignores noise



- Dynamic scheduling
  - \+ Keeps cores busy
  - \- Poor usage of data locality
  - \- Can have large dequeue overhead



# Lightweight scheduling

- Emerging complexities of multi- and mani-core processors suggest a need for self-adaptive strategies
  - One example is work stealing
- Goal:
  - Design a tunable strategy that is able to provide a good trade-off between load balance, data locality, and dequeue overhead.
  - Provide performance consistency
- Approach: combine static and dynamic scheduling
  - Shown to be efficient for regular mesh computation [B. Gropp and V. Kale]

| | Design space | | |
|---|---|---|---|
| Data layout/scheduling | Static | Dynamic | Static/(%dynamic) |
| Column Major Layout (CM) | | √ | |
| Block Cyclic Layout (BCL) | √ | √ | √ |
| 2-level Block Layout (2l-BL) | √ | √ | √ |

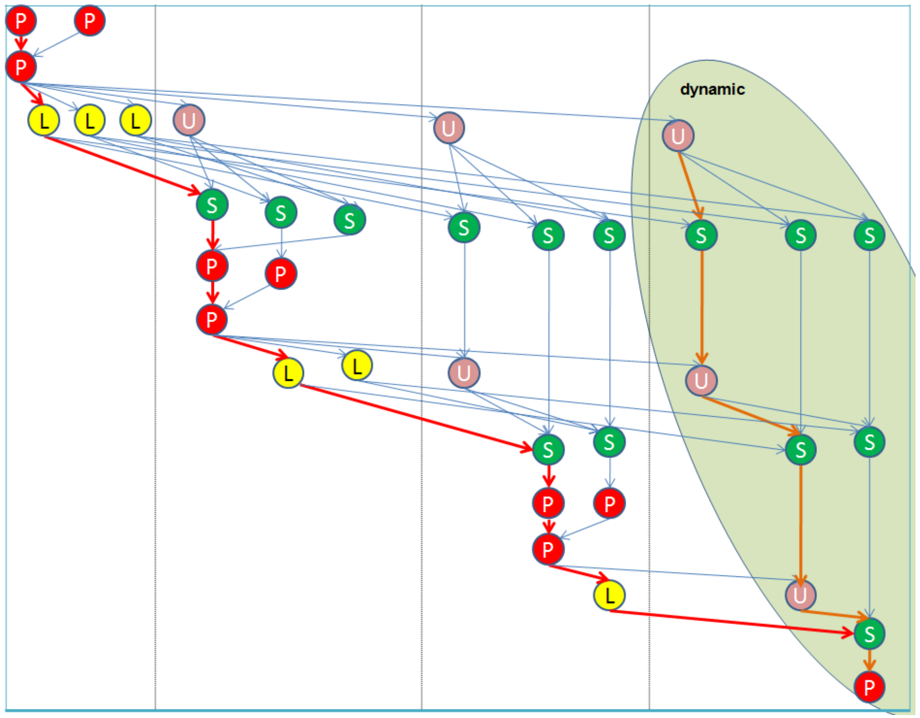
S. Donfack, LG, B. Gropp, V. Kale,IPDPS 2012

# Lightweight scheduling

- A self-adaptive strategy to provide
  - A good trade-off between load balance, data locality, and dequeue overhead.
  - Performance consistency
  - Shown to be efficient for regular mesh computation [B. Gropp and V. Kale]

Combined static/dynamic scheduling:

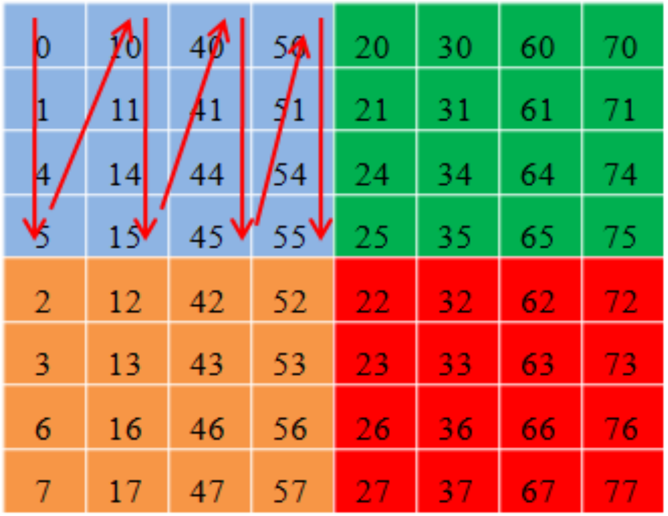
- A thread executes in priority its statically assigned tasks
- When no task ready, it picks a ready task from the dynamic part
- The size of the dynamic part is guided by a performance model



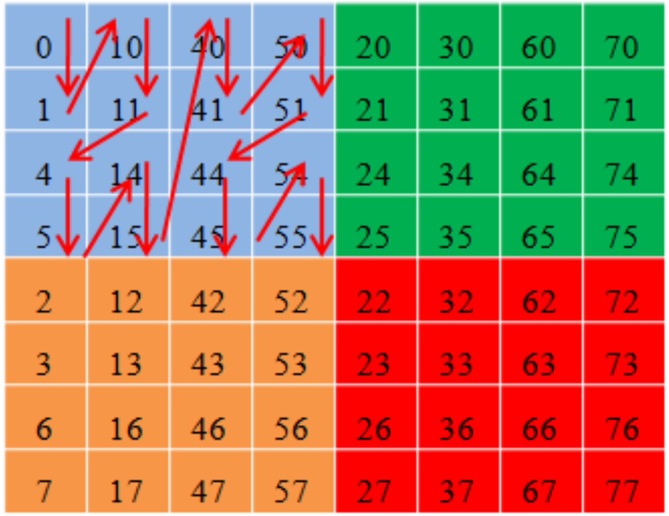

S. Donfack, LG, B. Gropp, V. Kale, 2012

# Data layout and other optimizations

- Three data distributions investigated
  - CM : Column major order for the entire matrix
  - BCL : Each thread stores contiguously (CM) the data on which it operates
  - 2l-BL : Each thread stores in blocks the data on which it operates



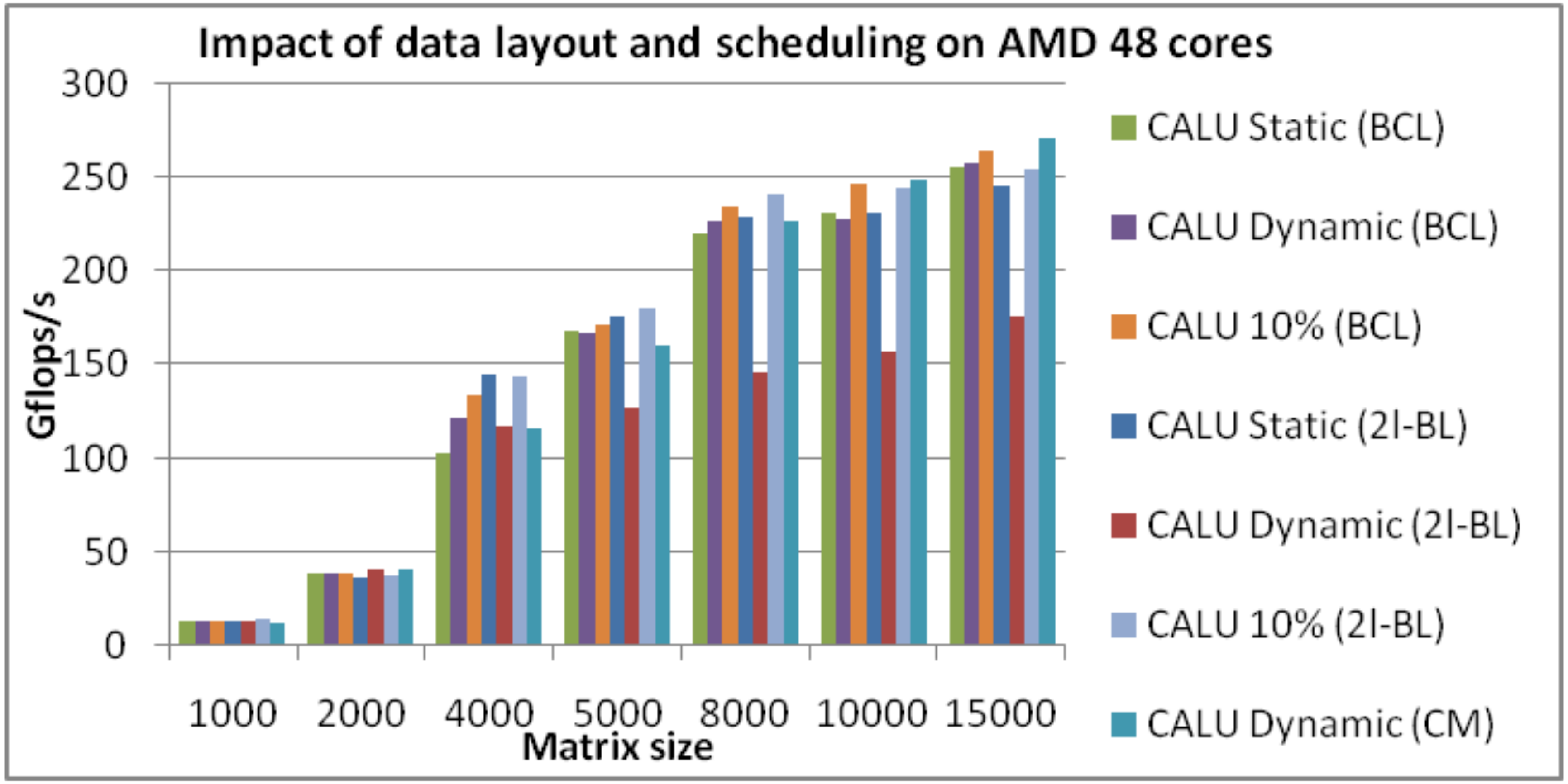

Block cyclic layout (BCL)




Two level block layout (2l-BL)

- And other optimizations
  - Updates (dgemm) performed on several blocks of columns (for BCL and CM layouts)

# Impact of data layout

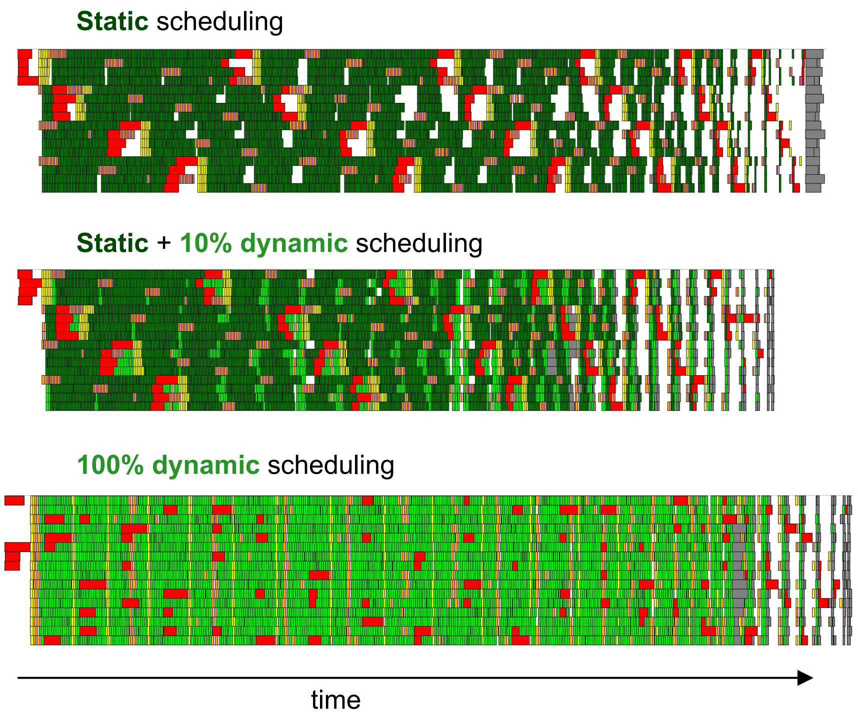


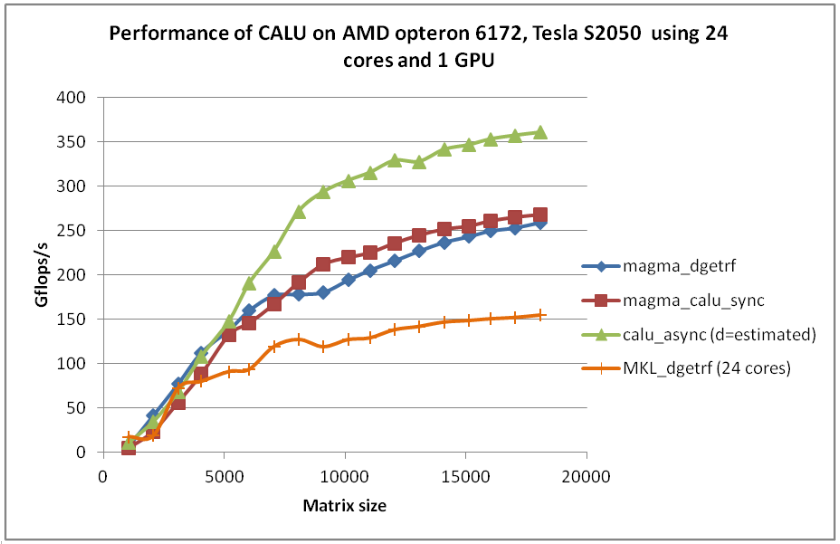

Eight socket, six core machine based on AMD Opteron processor (U. of Tennessee).

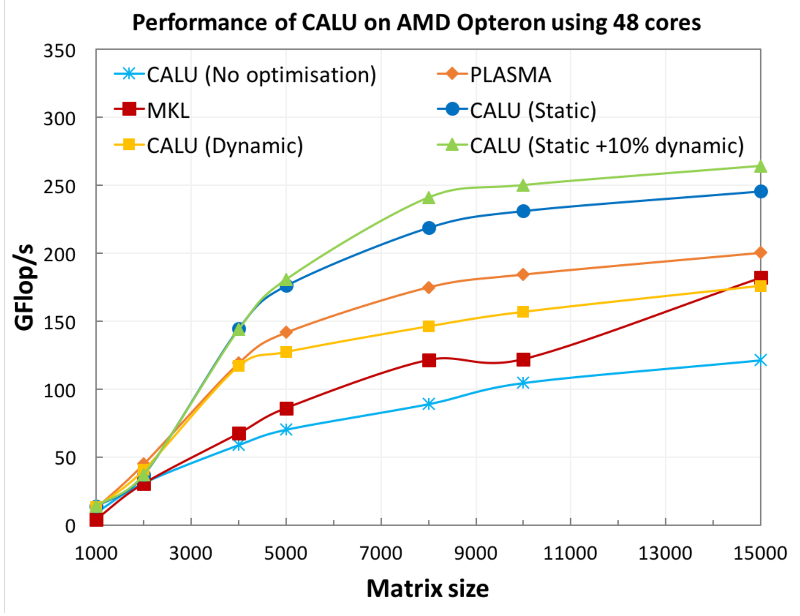
BCL : Each thread stores contiguously (CM) its data

2l-BL : Each thread stores in blocks its data

# Best performance of CALU on multicore architectures




- Reported performance for PLASMA uses LU with block pairwise pivoting.
- GPU data courtesy of S. Donfack

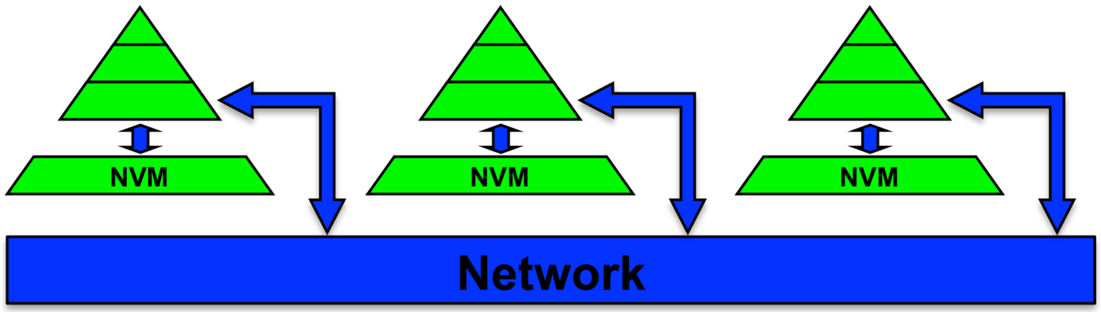
# Parallel write avoiding algorithms

Need to avoid writing suggested by emerging memory technologies, as NVMs:

- Writes more expensive (in time and energy) than reads
- Writes are less reliable than reads

Some examples:

- Phase Change Memory: Reads 25 us latency
  Writes: 15x slower than reads (latency and bandwidth)
  consume 10x more energy
- Conductive Bridging RAM - CBRAM
  Writes: use more energy (1pJ) than reads (50 fJ)
- Gap improving by new technologies such as XPoint and other FLASH alternatives, but not eliminated



# Parallel write-avoiding algorithms

- Matrix A does not fit in DRAM (of size M), need to use NVM (of size $n^2 / P$)

- Two lower bounds on volume of communication
  - Interprocessor communication: $\Omega(n^2 / P^{1/2})$
  - Writes to NVM: $n^2 / P$

- Result: any three-nested loop algorithm (matrix multiplication, LU,..), must asymptotically exceed at least one of these lower bounds
  - If $\Omega(n^2 / P^{1/2})$ words are transferred over the network, then $\Omega(n^2 / P^{2/3})$ words must be written to NVM !

- Parallel LU: choice of best algorithm depends on hardware parameters

| | #words interprocessor comm. | #writes NVM |
|---|---|---|
| Left-looking | $O((n^3 \log^2 P) / (P M^{1/2}))$ | $O(n^2 / P)$ |
| Right-looking | $O((n^2 \log P) / P^{1/2})$ | $O((n^2 \log^2 P) / P^{1/2})$ |