Recursive Blocked Algorithms and Hybrid Data Structures for Dense Matrix Computations

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High Performance Computing Center North (HPC2N)

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HPC2N – "HPC to North"

- National center for Scientific and Parallel Computing

New super cluster (installed 2004-06-07):
- 392 proc (64 bit, AMD Opteron)
- 1.5 TB memory
- Myrinet
- ~ 1.3 Tflops/s HP-Linpack
- Most powerful computer in Sweden
- Funded by the Wallenberg Foundation (KAW)

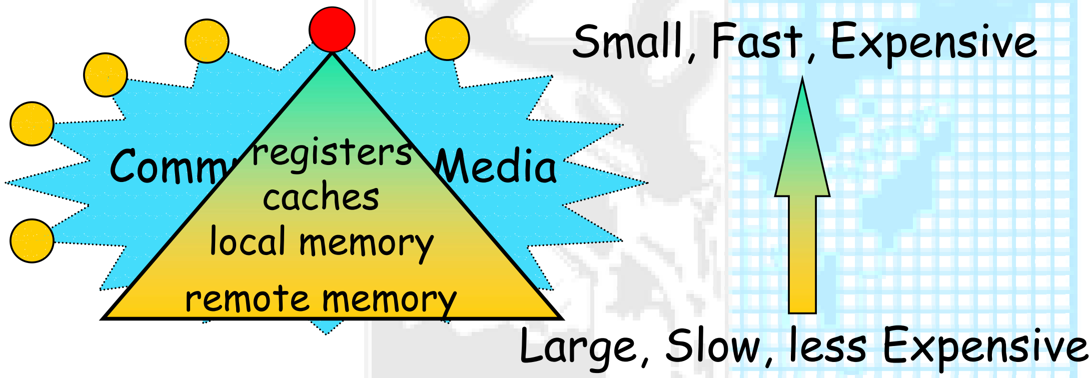
- Funded by the Swedish Research Council and its meta-center SNIC

Matrix Computations

- Fundamental and ubiquitous in computational science and its vast application areas
- Library software – optimized building blocks for fundamental operations
  - BLAS, (Sca)LAPACK, SLICOT (see also NETLIB)
  - ESSL and other vendors
  - Portability and efficiency
- Continuing demand for new and improved algorithms and software along with the computer evolution

"Data transport" in memory hierarchies

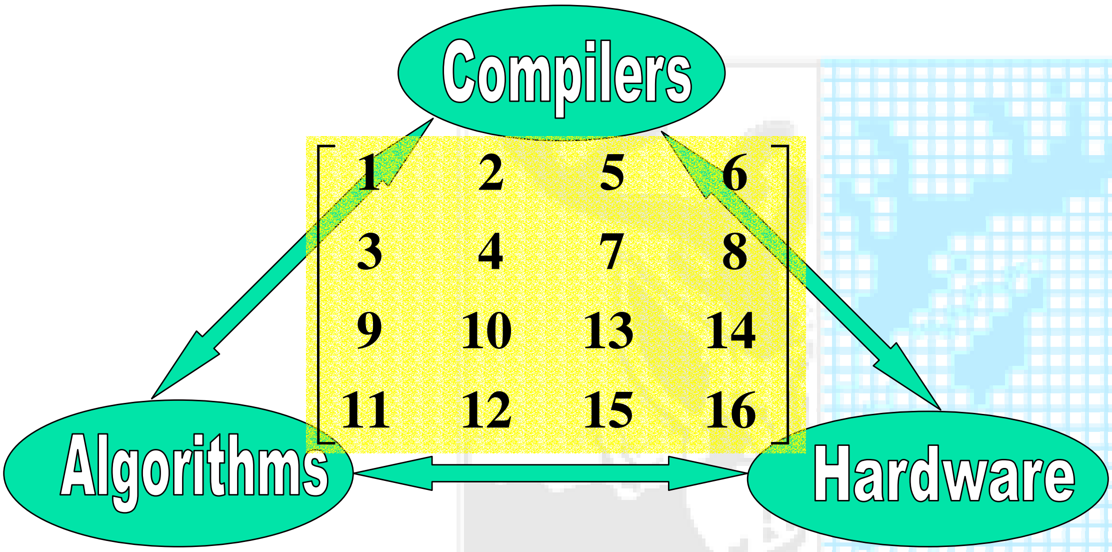
- of today's computer systems
  - PC - cluster - supercomputer



Management of deep memory hierarchies

- Architecture evolution: HPC systems with multiple SMP nodes, several levels of caches, more functional units per CPU
- Key to performance: understand the algorithm and architecture interaction
- Hierarchical blocking

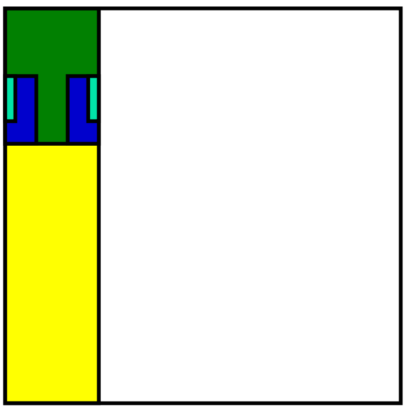
The fundamental AHC triangle



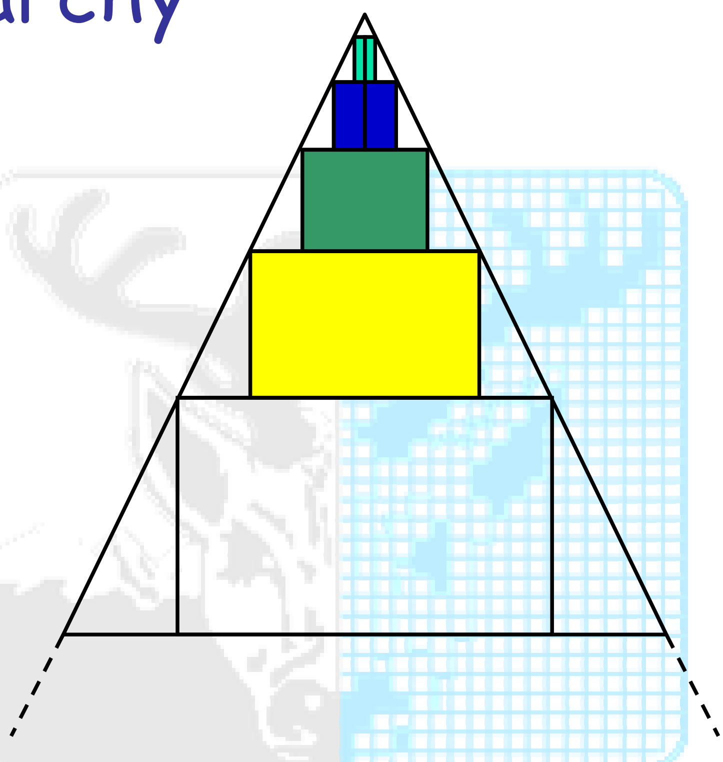
Outline

- Hierarchical blocking: motivation and implications
- Recursive blocked templates and algorithms
- Recursive blocked data structures
- Case studies:
  - General matrix multiply and add (GEMM)
  - Packed Cholesky factorization
  - QR factorization and linear systems
  - Triangular matrix equations and condition estimation
- Some related and complementary work
- Work in progress: periodic matrix equations
- Concluding remarks

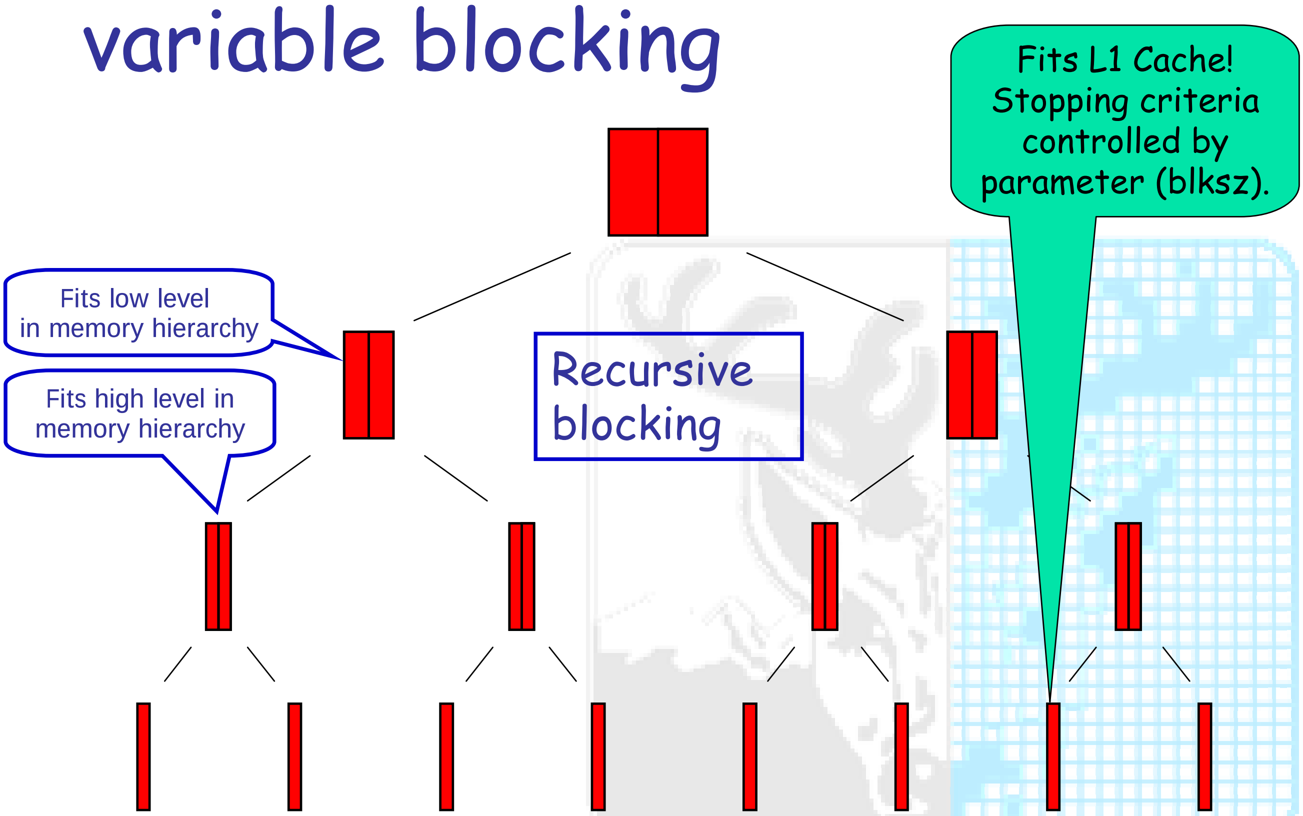
Blocking for a memory hierarchy



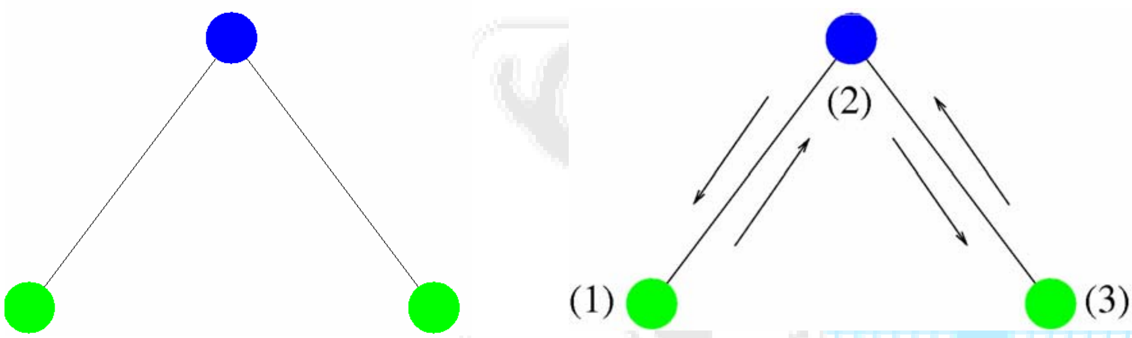
Explicit multi-level blocking



Recursion leads to automatic variable blocking

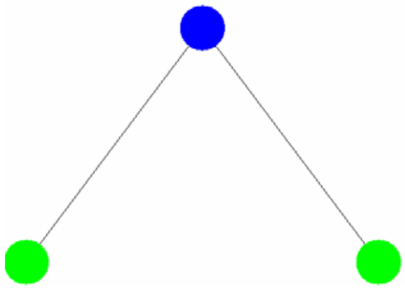


Splittings defining independent and dependent tasks



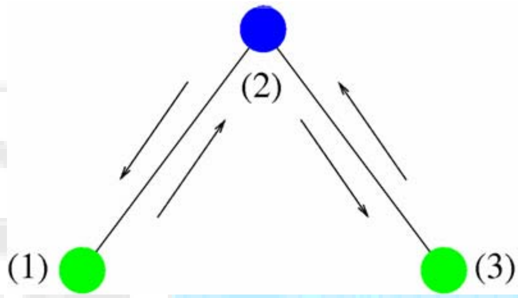
Critical path of subtasks:
(1), (2), (3)

TRSM Operation: AX = C, A mxm upper triangular, C/X mxn



$$A \begin{bmatrix} X_1 & X_2 \end{bmatrix} = \begin{bmatrix} C_1 & C_2 \end{bmatrix}$$

$$AX_1 = C_1,$$
$$AX_2 = C_2.$$



$$\begin{bmatrix} A_{11} & A_{12} \\ & A_{22} \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} = \begin{bmatrix} C_1 \\ C_2 \end{bmatrix}$$

$$A_{11}X_1 = C_1 - A_{12}X_2,$$
$$A_{22}X_2 = C_2.$$

Case Study 1

General matrix multiply and add (GEMM)

Recursive splittings for GEMM:

$$C \leftarrow \beta \mathrm{op}(C) + \alpha \mathrm{op}(A)\mathrm{op}(B)$$

Split	m × n	m × k	k × n

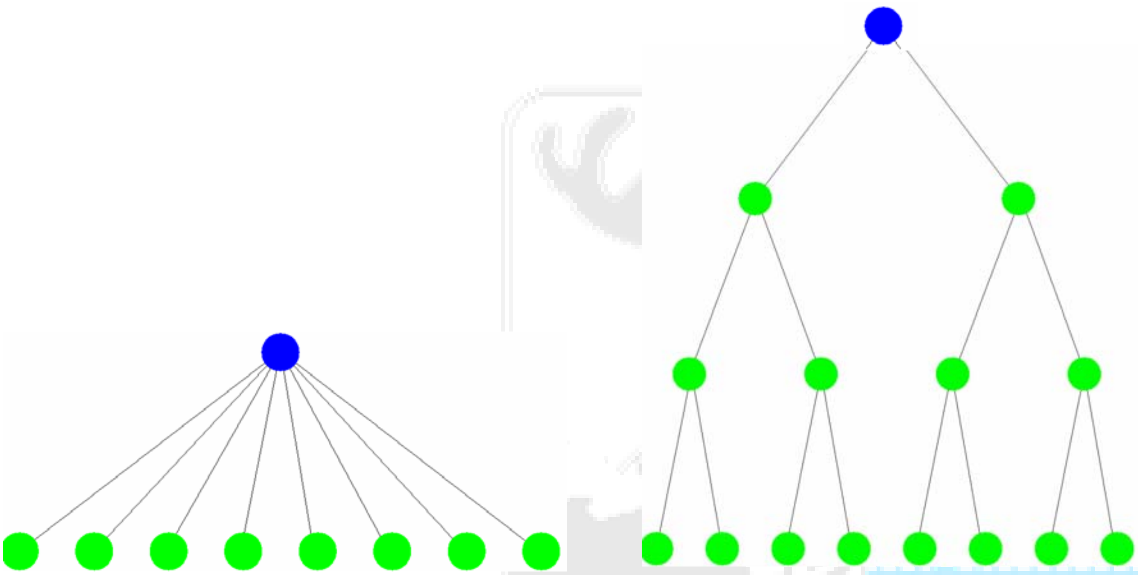
m, n, k
$$\begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix} + \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix} =$$

m
$$= \begin{bmatrix} \begin{bmatrix} C_{11} & C_{12} \end{bmatrix} + \begin{bmatrix} A_{11} & A_{12} \end{bmatrix} \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix} \\ \begin{bmatrix} C_{21} & C_{22} \end{bmatrix} + \begin{bmatrix} A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix} \end{bmatrix} =$$

n
$$= \left[\begin{bmatrix} C_{11} \\ C_{21} \end{bmatrix} + \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} B_{11} \\ B_{21} \end{bmatrix}, \quad \begin{bmatrix} C_{12} \\ C_{22} \end{bmatrix} + \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} B_{12} \\ B_{22} \end{bmatrix} \right] =$$

k
$$= \begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix} + \begin{bmatrix} A_{11} \\ A_{21} \end{bmatrix} \begin{bmatrix} B_{11} & B_{12} \end{bmatrix} + \begin{bmatrix} A_{12} \\ A_{22} \end{bmatrix} \begin{bmatrix} B_{21} & B_{22} \end{bmatrix}$$

Recursive splitting - by breadth or by depth



GEMM recursive blocked template - splitting by depth

```
C = rgemm( A, B, C, blksz)
If m, n, and k <= blksz
   C = opt_gemm( A, B, C) % optimized GEMM kernel!

elseif m = max(m, n, k) % split m: m2 = m/2
   C(1:m2, :)     = rgemm( A(1:m2, :), B, C(1:m2, :), blksz)
   C(m2+1:m, :) = rgemm( A(m2+1:m, :), B, C(m2+1:m, :), blksz)

elseif n = max(n,k)        % split n: n2 = n/2, k
   C(:,1:n2)       = rgemm( A, B(:,1:n2), C(:,1:n2), blksz)
   C(:,n2+1:n)    = rgemm( A, B(:,n2+1:n), C(:,n2+1:n), blksz)

else                                      % split k: k2 = k/2,
   C  = rgemm(A(:,1:n2), B(1:m2, :), C, blksz)
   C  = rgemm(A(:,n2+1:n), B(m2+1:m, :), C, blksz)
```

When to end the recursive splitting?

Locality of reference

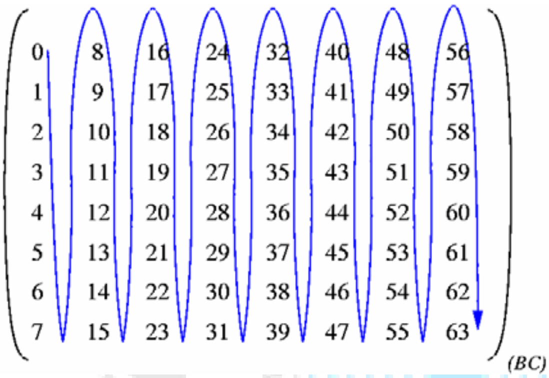
- Recursive blocked algorithms mainly improve on the temporal locality
- Further performance improvements by matching the data structure with the algorithm (and vice versa)
- Recursive blocked data structures improve on the spatial locality

Blocked data formats

$q = 8$

$p = 8$

$$\begin{bmatrix} A_{11} & A_{12} & \cdots & A_{18} \\ A_{21} & \ddots & & A_{28} \\ \vdots & & & \vdots \\ A_{81} & A_{82} & \cdots & A_{88} \end{bmatrix} \sim$$



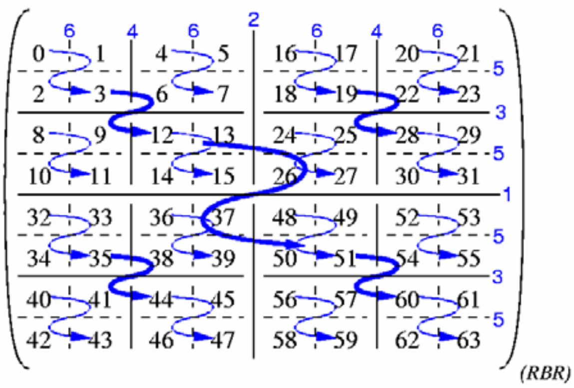
Blocks A_{ij} of size $mb \times nb$ can be ordered in $(pq)!$ different ways

Recursive blocked row format

$q = 8$

$p = 8$

$$\begin{bmatrix} A_{11} & A_{12} & \cdots & A_{18} \\ A_{21} & \ddots & & A_{28} \\ \vdots & & & \vdots \\ A_{81} & A_{82} & \cdots & A_{88} \end{bmatrix} \sim$$



Recursive ordering: a 1-dim tour through a 2-dim object (Hilbert space filling heuristics)

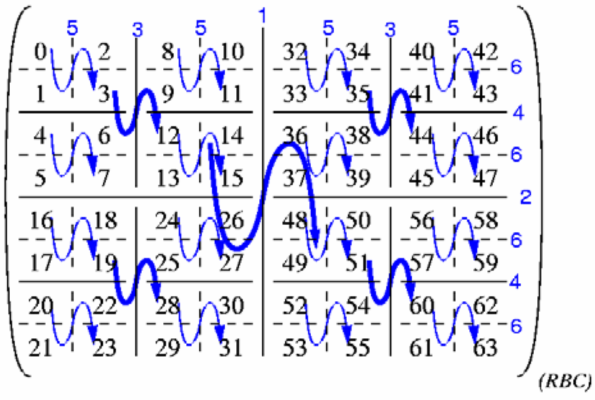
RBR <-> Z-Morton ordering

Recursive blocked column format

q = 8

p = 8

$$\begin{bmatrix} A_{11} & A_{12} & \cdots & A_{18} \\ A_{21} & \ddots & & A_{28} \\ \vdots & & & \vdots \\ A_{81} & A_{82} & \cdots & A_{88} \end{bmatrix} \sim$$

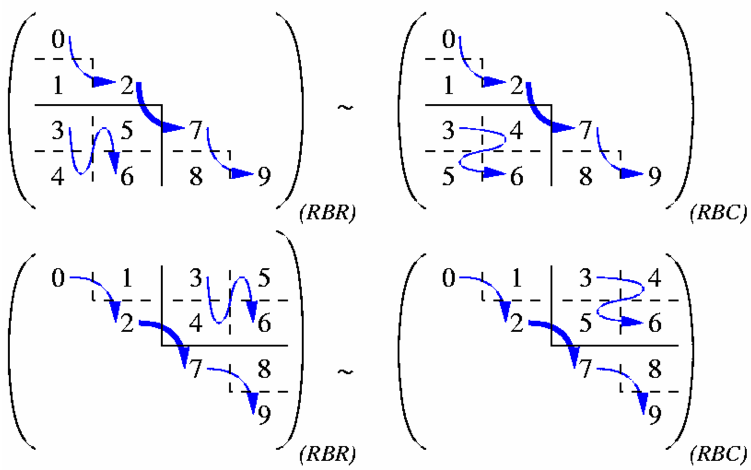


RBC <-> reflected-N-Morton
space filling ordering

Triangular recursive data format

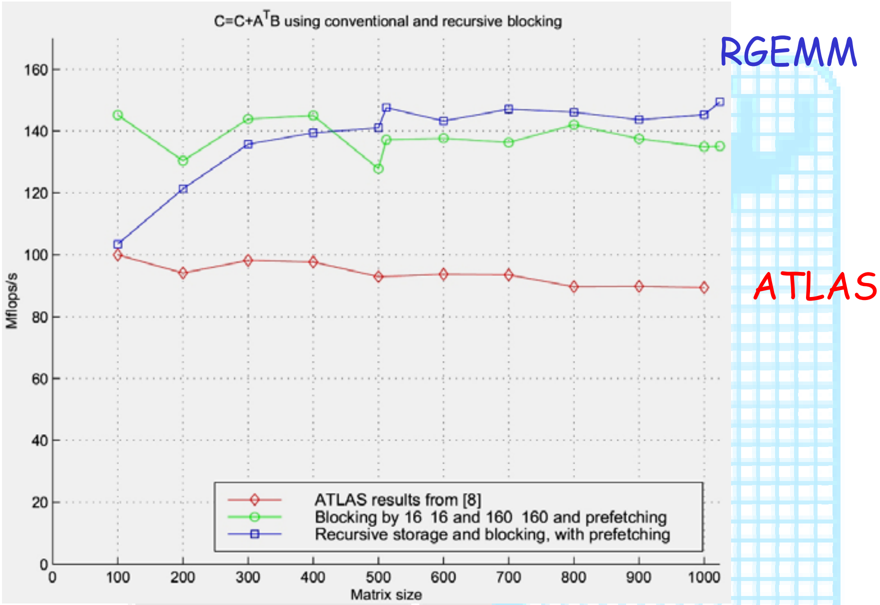
$$\begin{bmatrix} A_{11} & & & \\ A_{21} & \ddots & & \\ \vdots & & & \\ A_{41} & A_{42} & \cdots & A_{44} \end{bmatrix} \sim$$

$$\begin{bmatrix} A_{11} & A_{21} & \cdots & A_{41} \\ & \ddots & & A_{42} \\ & & & \vdots \\ & & & A_{44} \end{bmatrix} \sim$$



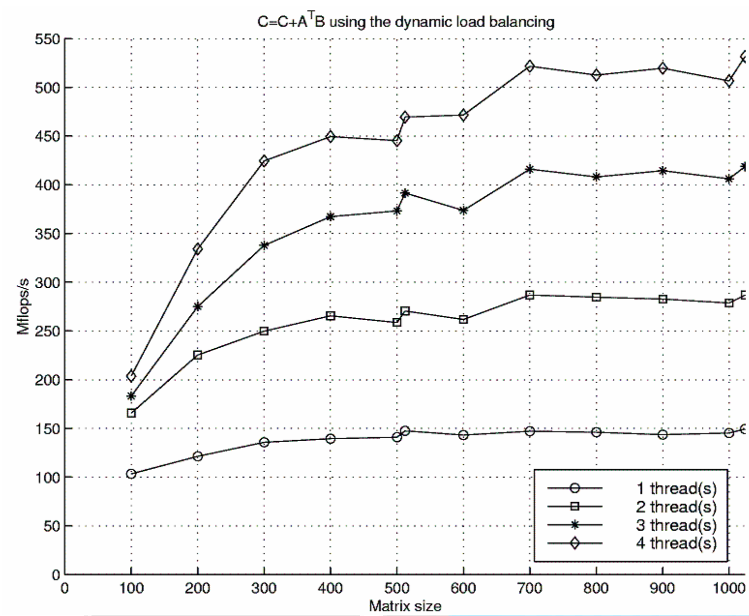
Recursive GEMM: multi-level vs. recursive blocking

IBM PPC604, 112 MHz

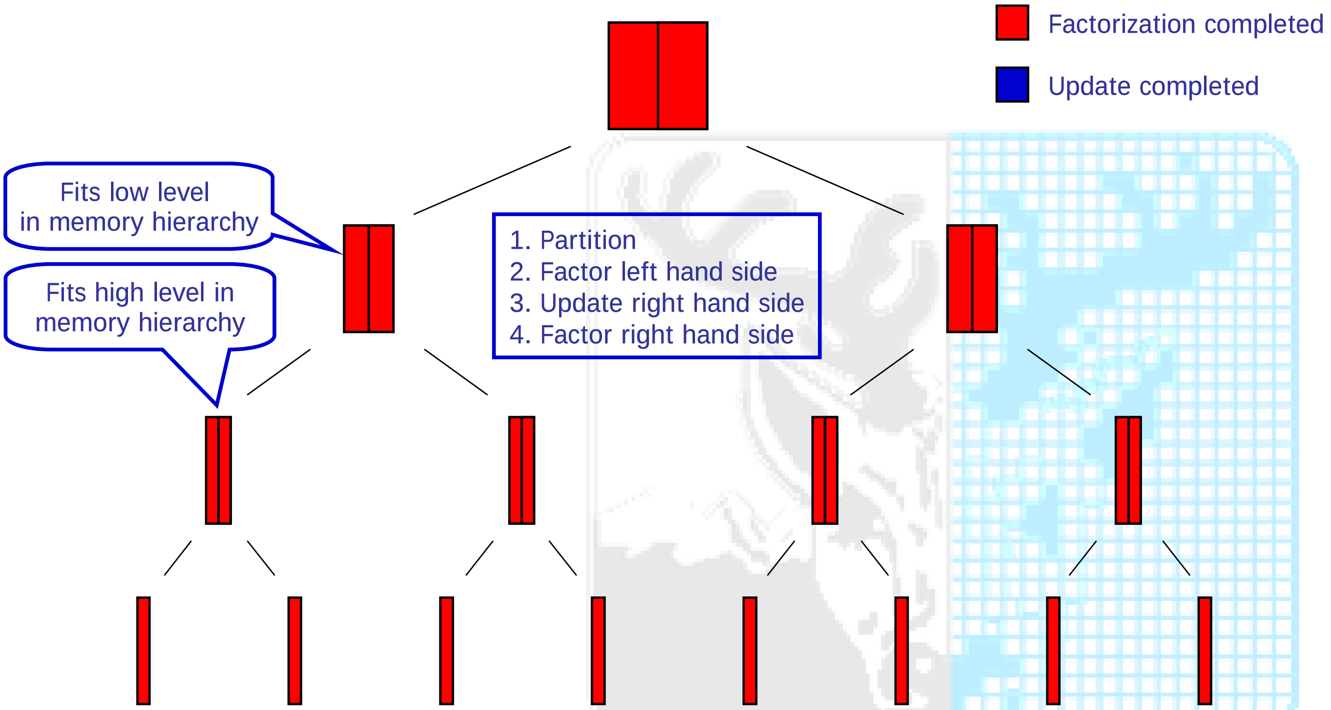


Recursive blocked GEMM and SMP parallelism via threads

IBM PPC604, 4 proc



Recursion template for one-sided matrix factorization



Case Study 2

Cholesky factorization for matrices in packed format

Packed Cholesky factorization

$$A \equiv \begin{bmatrix} A_{11} & A_{21}^T \\ A_{21} & A_{22} \end{bmatrix} = LL^T \equiv \begin{bmatrix} L_{11} & 0 \\ L_{21} & L_{22} \end{bmatrix} \begin{bmatrix} L_{11}^T & L_{21}^T \\ 0 & L_{22} \end{bmatrix}$$

Standard approach (typified by LAPACK):

- Packed storage -> cannot use standard level 3 BLAS (e.g., DGEMM)
- Possible to produce packed level 3 BLAS routines at a great programming cost
- Run at level 2 performance, i.e., much below full storage routines.
- Minimum storage: 1/2n(n+1) elements

Packed recursive blocked data

1	2	4	7	11	16	22
	3	5	8	12	17	23
		6	9	13	18	24
			10	14	19	25
				15	20	26
					21	27
						28

Packed upper

1	2	3	7	10	13	16
	4	5	8	11	14	17
		6	9	12	15	18
			19	20	22	24
				21	23	25
					26	27
						28

Packed recursive upper

FIG. 3.1. *Memory indices for 7×7 upper triangular matrix stored in traditional packed format and recursive packed format.*

- Divide into two isosceles triangles T1, T2 and rectangle R
- Divide triangles recursively down to element level
- Store in order: T1, R, T2
- Rectangles stored in full format ➔
  Possible to use full storage level 3 BLAS

Cholesky recursive blocked template

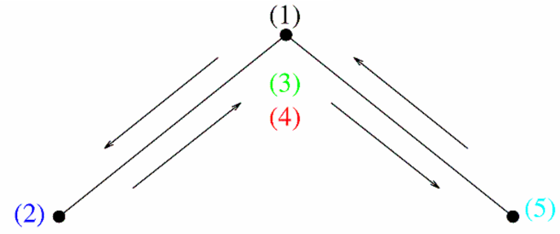
$$A = \begin{pmatrix} A_{11} & A_{21}^T \\ A_{21} & A_{22} \end{pmatrix} = LL^T = \begin{pmatrix} L_{11} & 0 \\ L_{21} & L_{22} \end{pmatrix} \begin{pmatrix} L_{11}^T & L_{21}^T \\ 0 & L_{22} \end{pmatrix} \quad (1)$$

$$\text{Factor}: \; A_{11} = L_{11}L_{11}^T. \quad (2)$$

$$\text{TRSM}: \; L_{21}L_{11}^T = A_{21}. \quad (3)$$

$$\text{SYRK}: \; \tilde{A}_{22} = A_{22} - L_{21}L_{21}^T \quad (4)$$

$$\text{Factor}: \; \tilde{A}_{22} = L_{22}L_{22}^T \quad (5)$$



TRSM recursive blocked template

Similar formulation for SYRK

$$XA^T = B \quad \text{or} \quad (6)$$

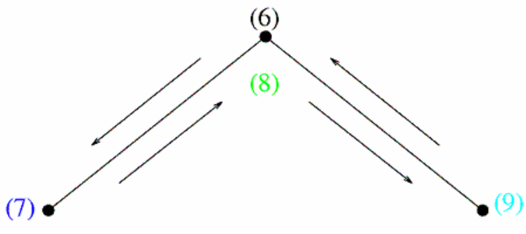
$$m\{(\overbrace{X_1}^{k_1} \; \overbrace{X_2}^{k_2}) \begin{pmatrix} A_{11}^T & A_{21}^T \\ 0 & A_{22}^T \end{pmatrix} = m\{(\overbrace{B_1}^{k_1} \; \overbrace{B_2}^{k_2}) = B$$

If we break Equation (6) into its component pieces we get

$$\text{TRSM}: \; X_1A_{11}^T = B_1 \quad (7)$$

$$\text{GEMM}: \; \tilde{B}_2 = B_2 - X_1A_{21}^T \quad (8)$$

$$\text{TRSM}: \; X_2A_{22}^T = \tilde{B}_2 \quad (9)$$

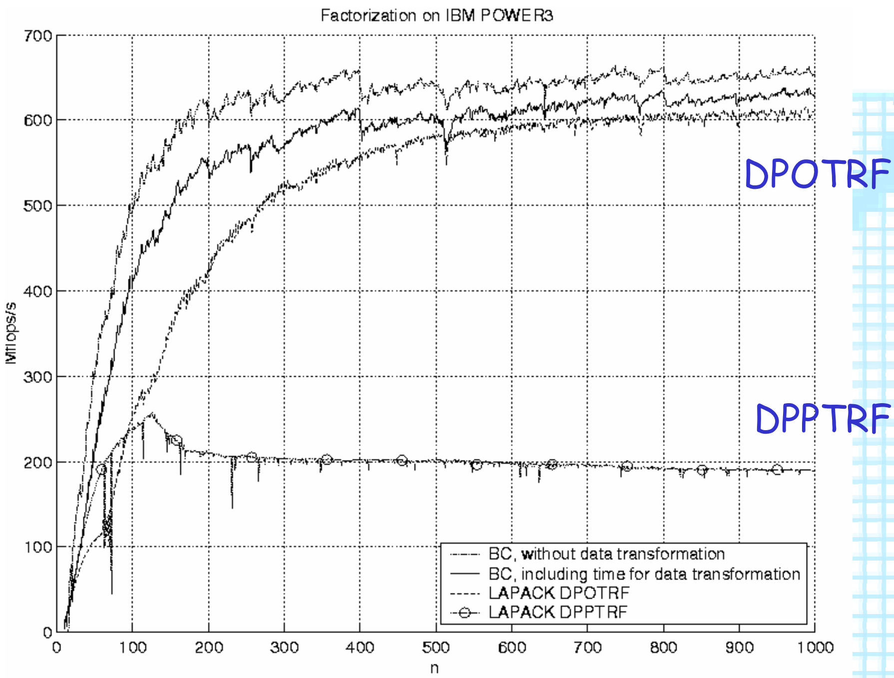


Packed recursive blocked Cholesky highlights

- Recursive blocked algorithm + recursive packed data layout => can make use of high performance level 3 BLAS routines (e.g., DGEMM)
- Use minimal storage for matrix A
- Temporary workspace = $1/8n^2$ elements (~25%)
- Leaf problems (< blksz) are solved using superscalar kernels (Cholesky, TRSM, SYRK)

Recursive blocked Cholesky vs. LAPACK – (rec.) packed format

Runs at level 3 performance – at least!



Case Study 3

QR factorization and linear systems

Recursive blocked QR factorization

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = Q \begin{pmatrix} R_{11} & R_{12} \\ 0 & R_{22} \end{pmatrix}$$

1. Divide A mxn in two parts (left & right)

Stopping criteria:
if n < 4 use standard algorithm

2. Factorize left hand side by a recursive call

$$Q_1 \begin{pmatrix} R_{11} \\ 0 \end{pmatrix} = \begin{pmatrix} A_{11} \\ A_{21} \end{pmatrix}$$

3. Update right hand side

$$\begin{pmatrix} R_{12} \\ \tilde{A}_{22} \end{pmatrix} \longleftarrow Q_1^T \begin{pmatrix} A_{12} \\ A_{22} \end{pmatrix}$$

4. Factorize by a recursive call

$$Q_2 R_{22} = \tilde{A}_{22}$$

Aggregating $Q = I - YTY^T$

Given $Q_1 = I - \tau_1 v_1 v_1^T$ and $Q_2 = I - \tau_2 v_2 v_2^T$, then

$$T = \begin{pmatrix} \tau_1 & -\tau_1 v_1^T v_2 \tau_2 \\ 0 & \tau_2 \end{pmatrix} \text{ and } Y = \begin{pmatrix} v_1 & v_2 \end{pmatrix}$$

Two elementary transformations

Given $Q_1 = I - Y_1 T_1 Y_1^T$ and $Q_2 = I - \tau_2 v_2 v_2^T$, then

$$T = \begin{pmatrix} T_1 & -T_1 Y_1^T v_2 \tau_2 \\ 0 & \tau_2 \end{pmatrix} \text{ and } Y = \begin{pmatrix} Y_1 & v_2 \end{pmatrix}$$

One block and one elementary transformation

Column by column using Level 2 operations

Given $Q_1 = I - Y_1 T_1 Y_1^T$ and $Q_2 = I - Y_2 T_2 Y_2^T$, then

$$T = \begin{pmatrix} T_1 & -T_1 Y_1^T Y_2 T_2 \\ 0 & T_2 \end{pmatrix} \text{ and } Y = \begin{pmatrix} Y_1 & Y_2 \end{pmatrix}$$

Two block transformations

Recursively, block by block using Level 3 operations

Recursive blocked QR highlights

- Recursive splitting controlled by nb (splitting point = min(nb, n/2), nb = 32-64)
- Level 3 algorithm for generating $Q = I - YTY^T$ (compact WY) within the recursive blocked algorithm (T triangular of size <= nb)
- Replaces LAPACK level 2 and 3 algorithms

Recursive QR vs. LAPACK

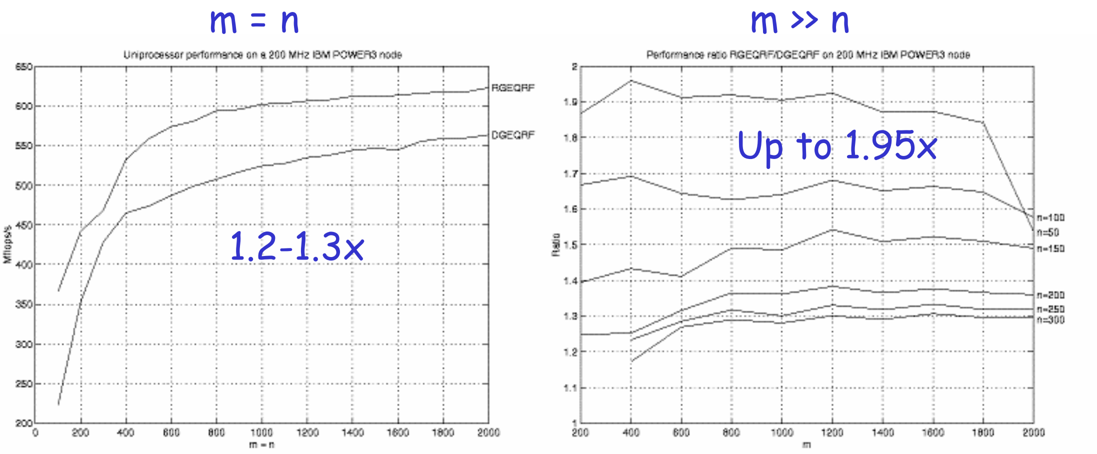


Fig. 4.1 *Performance results in Mflops/s for square matrices (left) and performance ratio for tall, thin matrices (right) for the recursive algorithm RGEQRF and DGEQRF of LAPACK on the 200 MHz IBM Power3.*

Least squares recursive algorithm

X = RGELS(A, B, nb) — GEMM + TRMM + TRSM

If $n \le nb$

1. Factor $A = Q \left[\begin{smallmatrix} R \\ 0 \end{smallmatrix}\right]$; $\tilde{B} \leftarrow Q^T B$; solve $RX = \tilde{B}(1:n,:)$

else

2. Set $A = [\ A_1 \quad A_2\ ]$; $B = \left[\begin{smallmatrix} B_1 \\ B_2 \end{smallmatrix}\right]$ with nb cols in A_1, nb rows in B_1
3. Factor $A_1 = Q_1 \left[\begin{smallmatrix} R_{11} \\ 0 \end{smallmatrix}\right]$
4. Set $\begin{bmatrix} R_{12} & \tilde{B}_1 \\ A_{22} & \tilde{B}_2 \end{bmatrix} \leftarrow Q_1^T [\ A_2 \quad B\ ]$ — GEMM + TRMM
5. X_2 = RGELS($A_{22}, \tilde{B}_2, nb$)
6. Solve $R_{11}X_1 = \tilde{B}_1 - R_{12}X_2$; return $X = \left[\begin{smallmatrix} X_1 \\ X_2 \end{smallmatrix}\right]$ — GEMM + TRSM

endif

Use Recursive QR

Fig. 4.2 *Recursive least squares RGELS algorithm for computing the solution to $AX = B$, where A is $m \times n$ ($m \ge n$).*

Recursive linear systems solvers

Solve op(A)X = B, A m x n - full row (or column) rank (compare LAPACK DGELS):

1. linear least squares solution to $\min \|AX - B\|_F$ $(m \geq n)$;
2. linear least squares solution to $\min \|A^TX - B\|_F$ $(m < n)$;
3. minimum norm solution to $\min \|A^TX - B\|_F$ $(m \geq n)$;
4. minimum norm solution to $\min \|AX - B\|_F$ $(m < n)$.

- RGELS solves P1
- P2 solved as P1 after explicit transposition
- RGELS-like algorithm solves P3
- P4 solved as P3 after explicit transposition

Case Study 4

Triangular matrix equations and condition estimation

Matrix equations

Name	Matrix equation	Acronym
Standard Sylvester (CT)	$AX - XB = C$	SYCT
Standard Lyapunov (CT)	$AX + XA^T = C$	LYCT
Generalized coupled Sylvester	$(AX - YB, DX - YE) = (C, F)$	GCSY
Standard Sylvester (DT)	$AXB^T - X = C$	SYDT
Standard Lyapunov (DT)	$AXA^T - X = C$	LYDT
Generalized Sylvester	$AXB^T - CXD^T = E$	GSYL
Generalized Lyapunov (CT)	$AXE^T + EXA^T = C$	GLYCT
Generalized Lyapunov (DT)	$AXA^T - EXE^T = C$	GLYDT

One-sided (top) and two-sided (bottom)

Block diagonalization and spectral projectors

S block-diagonalized by similarity:

$$\begin{bmatrix} I_m & -R \\ 0 & I_n \end{bmatrix} S \begin{bmatrix} I_m & R \\ 0 & I_n \end{bmatrix} = \begin{bmatrix} A & 0 \\ 0 & B \end{bmatrix} \qquad S = \begin{bmatrix} A & -C \\ 0 & B \end{bmatrix}$$

where R satifies AR – RB = C

Spectral projector associated with (1,1)-block:

$$P = \begin{bmatrix} I_m & R \\ 0 & 0 \end{bmatrix} \qquad \|P\|_2 = (1 + \|R\|_2^2)^{1/2}$$

Computed estimate: $s = 1/\|P\|_F$

Separation of two matrices

$$\text{Sep}[A,B] = \inf_{\|X\|_F=1} \|AX - XB\|_F = \sigma_{\min}(Z),$$
$$\text{where} \quad Z = I_n \otimes A - B^T \otimes I_m.$$

Computing Sep[A,B] costs $O(m^3n^3)$ – impractical!

Reliable Sep-estimates of cost $O(m^2n + mn^2)$:

$$\frac{\|x\|_2}{\|y\|_2} = \frac{\|X\|_F}{\|C\|_F} \le \|Z^{-1}\|_2 = \frac{1}{\sigma_{\min}(Z)} = \text{Sep}^{-1},$$

$$(mn)^{-1/2}\|Z^{-1}\|_1 \le \|Z^{-1}\|_2 \le \sqrt{mn}\|Z^{-1}\|_1.$$

Matrix equation Sep-functions

Z-matrix	Sep-function $= \sigma_{\min}(Z_{\_})$
$Z_{\text{SYCT}} = I_n \otimes A - B^T \otimes I_m$	$\inf_{\|X\|_F=1} \|AX - XB\|_F$
$Z_{\text{LYCT}} = I_n \otimes A + A \otimes I_n$	$\inf_{\|X\|_F=1} \|AX - X(-A^T)\|_F$
$Z_{\text{GCSY}} = \begin{bmatrix} I_n \otimes A & -B^T \otimes I_m \\ I_n \otimes D & -E^T \otimes I_m \end{bmatrix}$	$\inf_{\|(X,Y)\|_F=1} \|(AX - YB, DX - YE)\|_F$
$Z_{\text{SYDT}} = B \otimes A - I_n \otimes I_m$	$\inf_{\|X\|_F=1} \|AXB^T - X\|_F$
$Z_{\text{LYDT}} = A \otimes A - I_n \otimes I_n$	$\inf_{\|X\|_F=1} \|AXA^T - X\|_F$
$Z_{\text{GSYL}} = B \otimes A - D \otimes C$	$\inf_{\|X\|_F=1} \|AXB^T - CXD^T\|_F$
$Z_{\text{GLYCT}} = E \otimes A + A \otimes E$	$\inf_{\|X\|_F=1} \|AXE^T - EX(-A^T)\|_F$
$Z_{\text{GLYDT}} = A \otimes A - E \otimes E$	$\inf_{\|X\|_F=1} \|AXA^T - EXE^T\|_F$

$Z\,x = b$, Z is a Kronecker product representation

Sep-function = smallest singular value of Z

Recursive blocked SYCT template

Case 1: 1 <= n <= m/2

$$\begin{bmatrix} A_{11} & A_{12} \\ & A_{22} \end{bmatrix} \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix} - \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix} \begin{bmatrix} B_{11} & B_{12} \\ & B_{22} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix}$$

Case 2: 1 <= m <= n/2

$$\begin{bmatrix} A_{11} & A_{12} \\ & A_{22} \end{bmatrix} \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix} - \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix} \begin{bmatrix} B_{11} & B_{12} \\ & B_{22} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix}$$

Case 3: n/2 < m < 2n

$$\begin{bmatrix} A_{11} & A_{12} \\ & A_{22} \end{bmatrix} \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix} - \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix} \begin{bmatrix} B_{11} & B_{12} \\ & B_{22} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix}$$

Recursive SYCT - Case 3

$$\begin{bmatrix} A_{11} & A_{12} \\ & A_{22} \end{bmatrix} \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix} - \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix} \begin{bmatrix} B_{11} & B_{12} \\ & B_{22} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix}$$

$$\begin{aligned} A_{11}X_{11} - X_{11}B_{11} &= C_{11} - A_{12}X_{21} \\ A_{11}X_{12} - X_{12}B_{22} &= C_{12} - A_{12}X_{22} + X_{11}B_{12} \\ A_{22}X_{21} - X_{21}B_{11} &= C_{21} \\ A_{22}X_{22} - X_{22}B_{22} &= C_{22} + X_{21}B_{12} \end{aligned}$$

Recursive SYCT - Case 3

$$\begin{aligned} A_{11}X_{11} - X_{11}B_{11} &= C_{11} - A_{12}X_{21} \\ A_{11}X_{12} - X_{12}B_{22} &= C_{12} - A_{12}X_{22} + X_{11}B_{12} \\ A_{22}X_{21} - X_{21}B_{11} &= C_{21} \\ A_{22}X_{22} - X_{22}B_{22} &= C_{22} + X_{21}B_{12} \end{aligned}$$

2a, 2b can be executed in parallel as well as 3a,3b

1. SYLV('N', 'N', A_{22}, B_{11}, C_{21})
2a. GEMM('N', 'N', $\alpha = +1$, C_{21}, B_{12}, C_{22})
2b. GEMM('N', 'N', $\alpha = -1$, A_{12}, C_{21}, C_{11})
3a. SYLV('N', 'N', A_{22}, B_{22}, C_{22})
3b. SYLV('N', 'N', A_{11}, B_{11}, C_{11})
4. GEMM('N', 'N', $\alpha = -1$, A_{12}, C_{22}, C_{12})
5. GEMM('N', 'N', $\alpha = +1$, C_{11}, B_{12}, C_{12})
6. SYLV('N', 'N', A_{11}, B_{22}, C_{12})

SYCT and matrix functions

- A triangular => F := f(A) triangular
- f analytic => exists series expansion => A F - F A = 0
- recursive template:

$$\begin{bmatrix} A_{11} & A_{12} \\ & A_{22} \end{bmatrix}\begin{bmatrix} F_{11} & F_{12} \\ & F_{22} \end{bmatrix} - \begin{bmatrix} F_{11} & F_{12} \\ & F_{22} \end{bmatrix}\begin{bmatrix} A_{11} & A_{12} \\ & A_{22} \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$$

$$\Longrightarrow$$

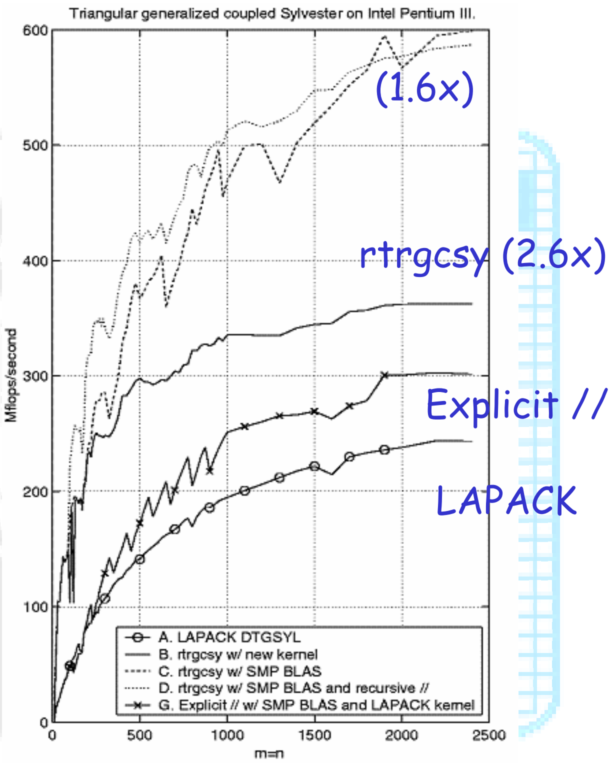
$$\begin{aligned} A_{11}F_{11} - F_{11}A_{11} &= 0 \\ A_{11}F_{12} - F_{12}A_{22} &= F_{11}A_{12} - A_{12}F_{22}, \\ A_{22}F_{22} - F_{22}A_{22} &= 0 \end{aligned}$$

Triangular generalized coupled Sylvester equation - GCSY

AX – YB = C
DX – YE = F

(A, D) and (B, E) in generalized Schur form

Solution (X, Y) over-writes r.h.s. (C, F)



Two-sided matrix equation: GLYDT

- $AXA^T - EXE^T = C$
- $C = C^T$ nxn; (A, E) n x n in gen. Schur form
- Unique sol'n X = X^T ⇔ λ_i of $A - \lambda E$ satisfy $\lambda_i \lambda_j \neq 1$
- Recursive splitting:

$$\begin{bmatrix} A_{11} & A_{12} \\ & A_{22} \end{bmatrix} \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix} \begin{bmatrix} A_{11}^T & \\ A_{12}^T & A_{22}^T \end{bmatrix} -$$

$$\begin{bmatrix} E_{11} & E_{12} \\ & E_{22} \end{bmatrix} \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix} \begin{bmatrix} E_{11}^T & \\ E_{12}^T & E_{22}^T \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix}$$

GLYDT recursion template

$X_{21} = X_{21}^T$ => three GLYDT subequations:

$$
\begin{aligned}
A_{11}X_{11}A_{11}^T - E_{11}X_{11}E_{11}^T &= C_{11} - A_{12}X_{12}^TA_{11}^T - (A_{11}X_{12} + A_{12}X_{22})A_{12}^T \\
&\quad + E_{12}X_{12}^TE_{11}^T + (E_{11}X_{12} + E_{12}X_{22})E_{12}^T, \\
A_{11}X_{12}A_{22}^T - E_{11}X_{12}E_{22}^T &= C_{12} - A_{12}X_{22}A_{22}^T + E_{12}X_{22}E_{22}^T, \\
A_{22}X_{22}A_{22}^T - E_{22}X_{22}E_{22}^T &= C_{22}.
\end{aligned}
$$

Four two-sided updates of C_{11} as two SYR2K ops:

$$
\begin{aligned}
C_{11} &= C_{11} - (A_{11}X_{12})A_{12}^T - A_{12}(A_{11}X_{12})^T \\
C_{11} &= C_{11} + (E_{11}X_{12})E_{12}^T + E_{12}(E_{11}X_{12})^T
\end{aligned}
$$

where $A_{11}X_{12}$ and $E_{11}X_{12}$ are TRMM operations

Two-sided matrix product

$$C = \beta C + \alpha \operatorname{op}(A) X \operatorname{op}(B)^T$$

- A and/or B can be dense or triangular
- One or several of A, B and C can be symmetric
- Extra workspace – size of r.h.s.

Make use of symmetry, e.g., in GLYDT:

$$C_{11} = C_{11} - A_{12}X_{22}A_{12}^T \quad \text{and} \quad C_{11} = C_{11} + E_{12}X_{22}E_{12}^T$$

GLYDT performance with optional condition estimation

Table 5.3 *Timings for solving unreduced two-sided matrix equations (GLYDT) with optional condition estimation. (Job = X, compute solution only; Job = X + Sep, compute solution and Sep-estimation.) Results from 375 MHz IBM Power3.*

	n	SG03AD using SG03AX Total time	SG03AD using SG03AX Solver part	SG03AD using *rtrglydt* Total time	SG03AD using *rtrglydt* Solver part	Speedup	Job
(a)	50	0.0277	49.9 %	0.0185	20.1 %	1.50	X
	100	0.180	51.2 %	0.0967	9.0 %	1.86	X
	250	2.89	46.8 %	1.62	4.7 %	1.79	X
	500	59.0	42.3 %	34.5	1.5 %	1.71	X
	750	303.4	42.0 %	177.5	0.9 %	1.71	X
	1000	646.6	44.6 %	361.8	1.0 %	1.79	X
	50	0.117	87.6 %	0.0263	45.6 %	4.44	X+Sep
	100	0.709	87.3 %	0.152	40.6 %	4.68	X+Sep
	250	9.98	84.5 %	2.08	25.4 %	4.81	X+Sep
	500	178.6	80.9 %	37.8	9.4 %	4.73	X+Sep
	750	924.1	80.9 %	184.4	4.5 %	5.01	X+Sep
	1000	2076.6	82.7 %	391.8	8.4 %	5.30	X+Sep

Up to 1.9x

Up to 5.3x

RECSY library

- Recursive blocked algorithms for solving reduced matrix equations
- Recursion implemented in F90
- SMP versions using OpenMP
- F77 wrappers for LAPACK and SLICOT routines
- www.cs.umu.se/research/parallel/recsy/
- Part of Isak Jonsson's PhD Thesis, Dec 2003

ScaLAPACK-style library

- The methods presented here can be applied to several similar problems.
- Our aim is to construct a ScaLAPACK-style software package of matrix equation solvers for distributed memory machines.
- The triangular solvers will be used in implementing parallel condition estimators for each matrix equation.
- Robert Granat, PhD student

$op(A)X \pm Xop(B) = C$	SYCT	√
$op(A)X + Xop(A^T) = C$	LYCT	√
$op(A)Xop(B) \pm X = C$	SYDT	√
$op(A)Xop(A^T) - X = C$	LYDT	√
$op(A)X \pm Yop(B) = C,$ $op(D)X \pm Yop(E) = F$	GCSY	
$op(A)Xop(B) \pm op(D)Xop(E) = C$	GSYL	
$op(A)Xop(A^T) - op(E)Xop(E^T) = C$	GLYCT	
$op(A)X(E^T) + op(E)Xop(A^T) = C$	GLYDT	

Recursive blocking ...

- creates new algorithms for linear algebra software
- expresses dense linear algebra algorithms entirely in terms of level~3 BLAS like matrix-matrix operations
- introduces an automatic variable blocking that targets every level of a deep memory hierarchy
- can also be used to define hybrid data formats for storing block-partitioned matrices (general, triangular, symmetric, packed)

High-performance software

- implementations are based on data locality and superscalar optimization techniques
- recursive blocked algorithms improve on the temporal data locality
- hybrid data formats improve on the spatial data locality
- portable and generic superscalar kernels ensure that all functional units on the processor(s) are used efficiently

Some related and complementary work

- Recursive algorithms and hybrid data structures
  - Winograd-Strassen'69: Douglas etal'94, ESSL, Demmel-Higham'92 (stability)
  - Quad- and octtrees: Samet'84, Salman-Warner'94 (N-body, Barnes-Hut'84)
  - Cache oblivious algorithms: Leiserson etal'99 (sorting, FFT, A^T)
  - GEMM: Chatterjee etal'02, Valsalam and Skjellum'02, ATLAS-project
  - LU: Toledo'97(dense), Dongarra, Eijkhout Luszczek'01 (sparse)
  - QR: Rabani and Toledo'01 (out-of-core), Frens and Wise'03 (Givens-based)

Some related and complementary work

- Automated generation of library software and compiler technology
  - Empirical optimization:
    PHiPAC – Bilmes, Demmel etal'97,
    ATLAS – Whaley, Petitet and Dongarra'00,
    Sparse kernels – Vuduc, Demmel et al'03
  - FLAME: Gunnels, Goto, Van de Geijn etal'01, '02
  - Compiler blockability: Wolf and Lam'91 (loop transformations), Carr and Lehoucq'97
  - Automatic generation of recursive codes: Ahmed and Pingali'00 (iterative algorithms -> recursive), Yi, Adve and Kennedy'00 (convert loop nests into recursive form)

- Thanks for your attention!

Bo Kågström 2004