Outline

- Motivation, overview for Dense Linear Algebra
- Review Gaussian Elimination (GE) for solving Ax=b
- Optimizing GE for caches on sequential machines
  - using matrix-matrix multiplication (BLAS)
- LAPACK library overview and performance
- Data layouts on parallel machines
- Parallel Gaussian Elimination
- ScaLAPACK library overview
- Eigenvalue problems
- Current Research

Motivation (1)

3 Basic Linear Algebra Problems

1. Linear Equations: Solve $Ax=b$ for x
2. Least Squares: Find x that minimizes $||r||_2 \equiv \sqrt{\Sigma\, r_i^2}$ where $r=Ax-b$
   - Statistics: Fitting data with simple functions

3a. Eigenvalues: Find λ and x where $Ax = \lambda x$

- Vibration analysis, e.g., earthquakes, circuits

3b. Singular Value Decomposition: $A^TAx=\sigma^2x$

- Data fitting, Information retrieval

Lots of variations depending on structure of A

- A symmetric, positive definite, banded, …

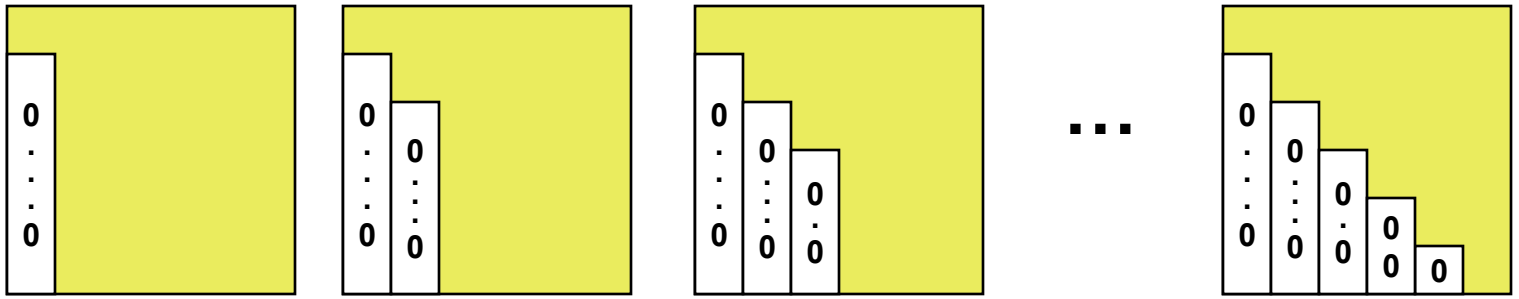
Motivation (2)

- **Why dense A, as opposed to sparse A?**
  - Many large matrices are sparse, but …
  - Dense algorithms easier to understand
  - Some applications yields large dense matrices
  - LINPACK Benchmark (www.top500.org)
    - "How fast is your computer?" = "How fast can you solve dense Ax=b?"
  - Large sparse matrix algorithms often yield smaller (but still large) dense problems

Gaussian Elimination (GE) for solving Ax=b

- Add multiples of each row to later rows to make A upper triangular
- Solve resulting triangular system Ux = c by substitution

```
… for each column i
… zero it out below the diagonal by adding multiples of row i to later rows
for i = 1 to n-1
    … for each row j below row i
    for j = i+1 to n
        … add a multiple of row i to row j
        tmp = A(j,i);
        for k = i to n
            A(j,k) = A(j,k) - (tmp/A(i,i)) * A(i,k)
```



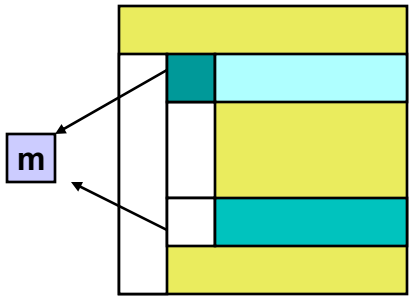
Refine GE Algorithm (1)

- Initial Version

```
… for each column i
… zero it out below the diagonal by adding multiples of row i to later rows
for i = 1 to n-1
    … for each row j below row i
    for j = i+1 to n
        … add a multiple of row i to row j
        tmp = A(j,i);
        for k = i to n
            A(j,k) = A(j,k) - (tmp/A(i,i)) * A(i,k)
```

- Remove computation of constant tmp/A(i,i) from inner loop.

```
for i = 1 to n-1
    for j = i+1 to n
        m = A(j,i)/A(i,i)
        for k = i to n
            A(j,k) = A(j,k) - m * A(i,k)
```



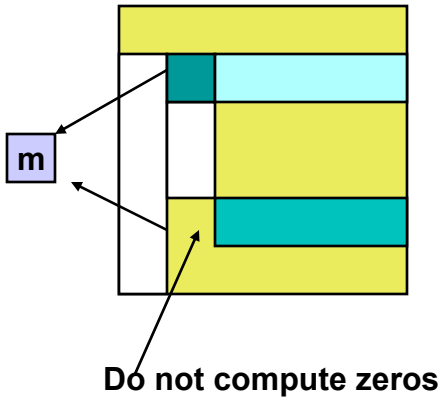
Refine GE Algorithm (2)

- Last version

```
for i = 1 to n-1
    for j = i+1 to n
        m = A(j,i)/A(i,i)
        for k = i to n
            A(j,k) = A(j,k) - m * A(i,k)
```

- Don't compute what we already know: zeros below diagonal in column i

```
for i = 1 to n-1
    for j = i+1 to n
        m = A(j,i)/A(i,i)
        for k = i+1 to n
            A(j,k) = A(j,k) - m * A(i,k)
```



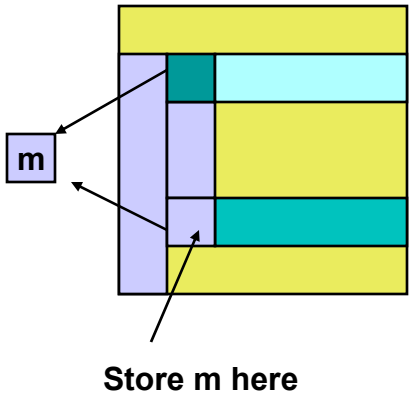
Refine GE Algorithm (3)

- Last version

```
for i = 1 to n-1
    for j = i+1 to n
        m = A(j,i)/A(i,i)
        for k = i+1 to n
            A(j,k) = A(j,k) - m * A(i,k)
```

- Store multipliers m below diagonal in zeroed entries for later use

```
for i = 1 to n-1
    for j = i+1 to n
        A(j,i) = A(j,i)/A(i,i)
        for k = i+1 to n
            A(j,k) = A(j,k) - A(j,i) * A(i,k)
```



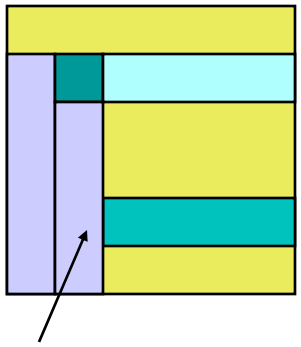
Refine GE Algorithm (4)

- Last version

```
for i = 1 to n-1
    for j = i+1 to n
        A(j,i) = A(j,i)/A(i,i)
        for k = i+1 to n
            A(j,k) = A(j,k) - A(j,i) * A(i,k)
```

- Split Loop

```
for i = 1 to n-1
    for j = i+1 to n
        A(j,i) = A(j,i)/A(i,i)
    for j = i+1 to n
        for k = i+1 to n
            A(j,k) = A(j,k) - A(j,i) * A(i,k)
```



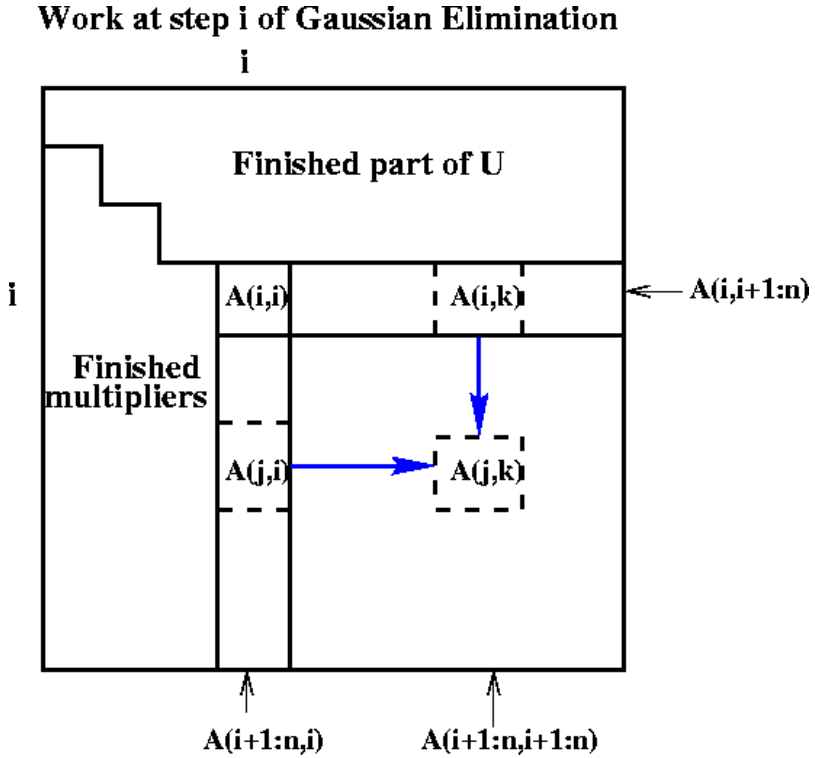
Store all m's here before updating rest of matrix

Refine GE Algorithm (5)

- Last version

```
for i = 1 to n-1
    for j = i+1 to n
        A(j,i) = A(j,i)/A(i,i)
    for j = i+1 to n
        for k = i+1 to n
            A(j,k) = A(j,k) - A(j,i) * A(i,k)
```

- Express using matrix operations (BLAS)




```
for i = 1 to n-1
    A(i+1:n,i) = A(i+1:n,i) * ( 1 / A(i,i) )
    A(i+1:n,i+1:n) = A(i+1:n , i+1:n )
                   - A(i+1:n , i) * A(i , i+1:n)
```

What GE really computes

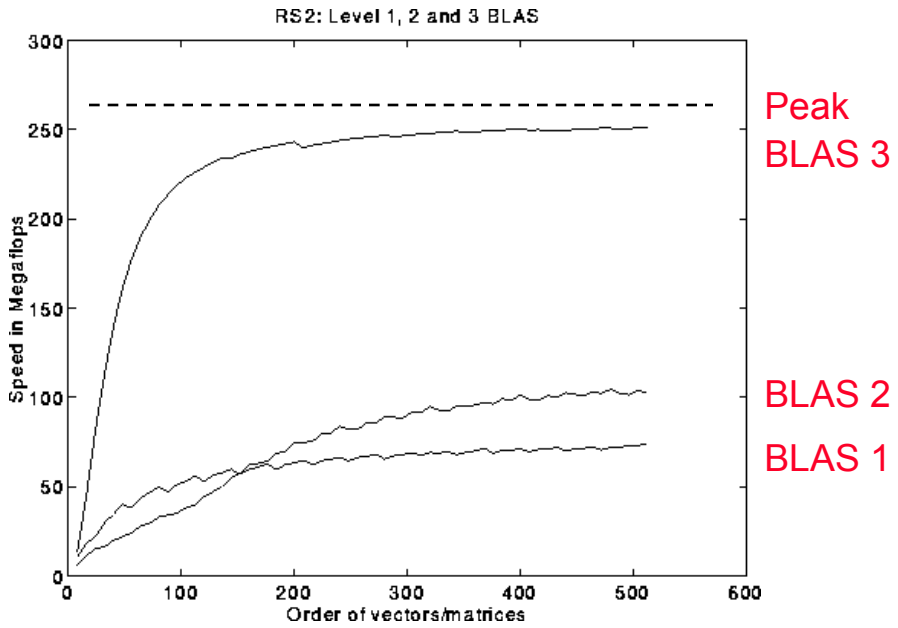
```
for i = 1 to n-1
    A(i+1:n,i) = A(i+1:n,i) / A(i,i)
    A(i+1:n,i+1:n) = A(i+1:n , i+1:n ) - A(i+1:n , i) * A(i , i+1:n)
```

- Call the strictly lower triangular matrix of multipliers M, and let L = I+M
- Call the upper triangle of the final matrix U
- *Lemma (LU Factorization):* If the above algorithm terminates (does not divide by zero) then A = L*U
- Solving A*x=b using GE
  - Factorize A = L*U using GE (cost = 2/3 n^3 flops)
  - Solve L*y = b for y, using substitution (cost = n^2 flops)
  - Solve U*x = y for x, using substitution (cost = n^2 flops)
- Thus A*x = (L*U)*x = L*(U*x) = L*y = b as desired

Problems with basic GE algorithm

- What if some A(i,i) is zero? Or very small?
  - Result may not exist, or be "unstable", so need to pivot
- Current computation all BLAS 1 or BLAS 2, but we know that BLAS 3 (matrix multiply) is fastest (earlier lectures…)

```
for i = 1 to n-1
    A(i+1:n,i) = A(i+1:n,i) / A(i,i)          … BLAS 1 (scale a vector)
    A(i+1:n,i+1:n) = A(i+1:n , i+1:n )  … BLAS 2 (rank-1 update)
            - A(i+1:n , i) * A(i , i+1:n)
```



Pivoting in Gaussian Elimination

- A = [0 1] fails completely because can't divide by A(1,1)=0
  [1 0]
- But solving Ax=b should be easy!
- When diagonal A(i,i) is tiny (not just zero), algorithm may terminate but get completely wrong answer
  - Numerical instability
  - Roundoff error is cause
- Cure: Pivot (swap rows of A) so A(i,i) large

Gaussian Elimination with Partial Pivoting (GEPP)

- Partial Pivoting: swap rows so that A(i,i) is largest in column

```
for i = 1 to n-1
    find and record k where |A(k,i)| = max{i <= j <= n} |A(j,i)|
        … i.e. largest entry in rest of column i
    if |A(k,i)| = 0
        exit with a warning that A is singular, or nearly so
    elseif  k != i
        swap rows i and k of A
    end if
    A(i+1:n,i) = A(i+1:n,i) / A(i,i)        … each quotient lies in [-1,1]
    A(i+1:n,i+1:n) = A(i+1:n , i+1:n ) - A(i+1:n , i) * A(i , i+1:n)
```

- *Lemma*: This algorithm computes A = P*L*U, where P is a permutation matrix.
- This algorithm is numerically stable in practice
- For details see LAPACK code at
  http://www.netlib.org/lapack/single/sgetf2.f

Parallelizing Gaussian Elimination

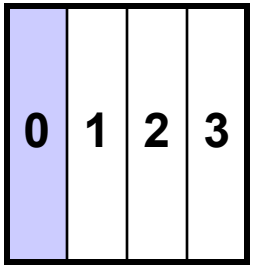
- Parallelization steps
  - Decomposition: identify enough parallel work, but not too much
  - Assignment: load balance work among threads
  - Orchestrate: communication and synchronization
  - Mapping: which processors execute which threads
- Decomposition
  - In BLAS 2 algorithm nearly each flop in inner loop can be done in parallel, so with n^2 processors, need 3n parallel steps

```
for i = 1 to n-1
    A(i+1:n,i) = A(i+1:n,i) / A(i,i)          … BLAS 1 (scale a vector)
    A(i+1:n,i+1:n) = A(i+1:n , i+1:n )  … BLAS 2 (rank-1 update)
                - A(i+1:n , i) * A(i , i+1:n)
```

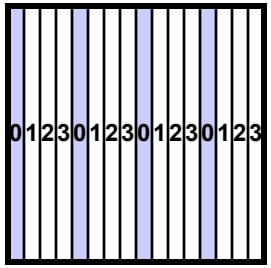
  - This is too fine-grained, prefer calls to local matmuls instead
  - Need to use parallel matrix multiplication
- Assignment
  - Which processors are responsible for which submatrices?

Different Data Layouts for Parallel GE

Bad load balance:
P0 idle after first
n/4 steps



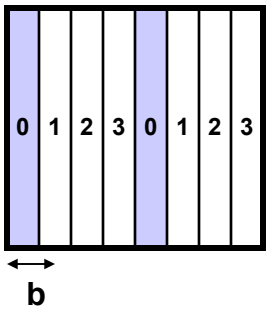
1) 1D Column Blocked Layout



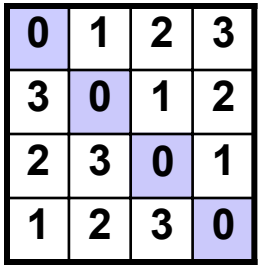
Load balanced, but
can't easily use
BLAS2 or BLAS3

2) 1D Column Cyclic Layout

Can trade load balance
and BLAS2/3
performance by
choosing b, but
factorization of block
column is a bottleneck



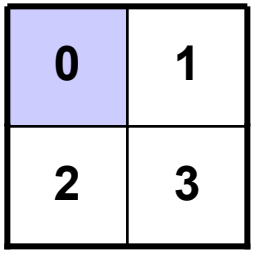
3) 1D Column Block Cyclic Layout



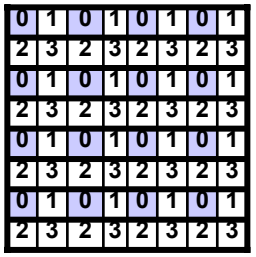
Complicated
addressing

4) Block Skewed Layout

Bad load balance:
P0-P2 idle after
first n/2 steps



5) 2D Row and Column Blocked Layout



The winner!

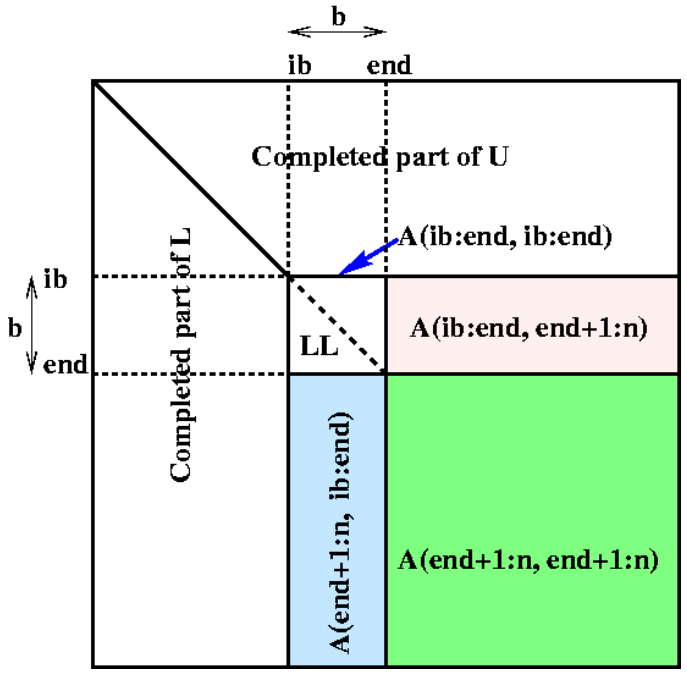
6) 2D Row and Column
Block Cyclic Layout

Review: BLAS 3 (Blocked) GEPP

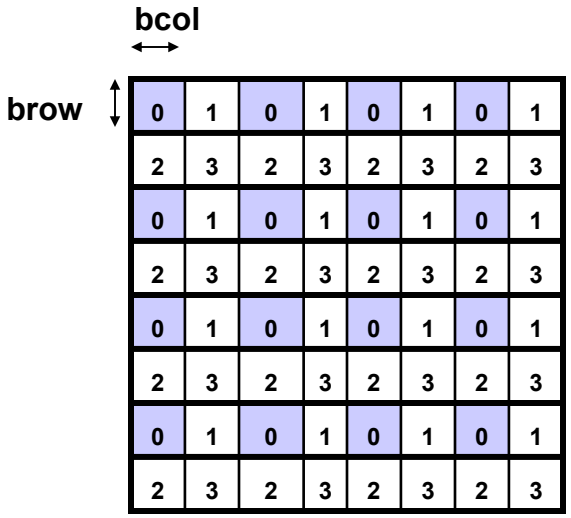
```
for   ib = 1 to n-1 step b     … Process matrix b columns at a time
    end = ib + b-1             … Point to end of block of b columns
    apply BLAS2 version of GEPP to  get A(ib:n , ib:end) = P' * L' * U'
    … let LL denote the strict lower triangular part of A(ib:end , ib:end) + I
    A(ib:end , end+1:n) = LL^-1 * A(ib:end , end+1:n)        … update next b rows of U
    A(end+1:n , end+1:n ) = A(end+1:n , end+1:n )
              - A(end+1:n , ib:end) * A(ib:end , end+1:n)
                                … apply delayed updates with single matrix-multiply
                                … with inner dimension b
```

BLAS 3

Gaussian Elimination using BLAS 3



Row and Column Block Cyclic Layout



- processors and matrix blocks are distributed in a 2d array
  - prow-by-pcol array of processors
  - brow-by-bcol matrix blocks
- pcol-fold parallelism in any column, and calls to the BLAS2 and BLAS3 on matrices of size brow-by-bcol
- serial bottleneck is eased
- prow ≠ pcol possible, even desirable
- brow ≠ bcol more complicated

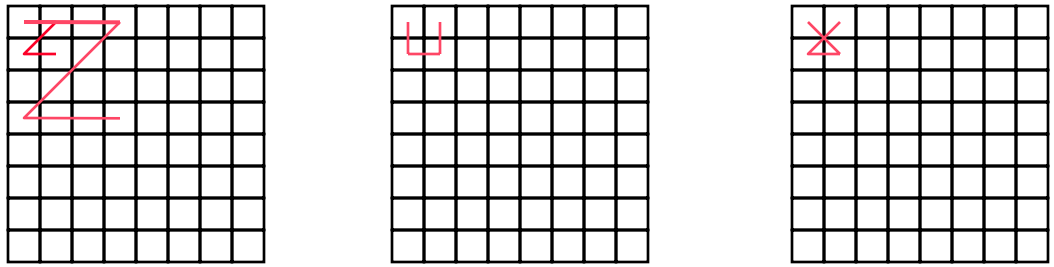
Distributed GE with a 2D Block Cyclic Layout

- block sizes b = bcol = brow in the algorithm and in the layout are all equal
- shaded regions indicate processors busy with computation or communication.
- unnecessary to have a barrier between each step of the algorithm, e.g. steps 9, 10, and 11 can be pipelined

Extra Slides

Recursive Algorithms

- Still uses delayed updates, but organized differently
  - (formulas on board)
- Can exploit recursive data layouts
  - 3x speedups on least squares for tall, thin matrices



- Theoretically optimal memory hierarchy performance
- See references at
  - "Recursive Block Algorithms and Hybrid Data Structures," Elmroth, Gustavson, Jonsson, Kagstrom, SIAM Review, 2004
  - http://www.cs.umu.se/research/parallel/recursion/

Gaussian Elimination via a Recursive Algorithm

F. Gustavson and S. Toledo

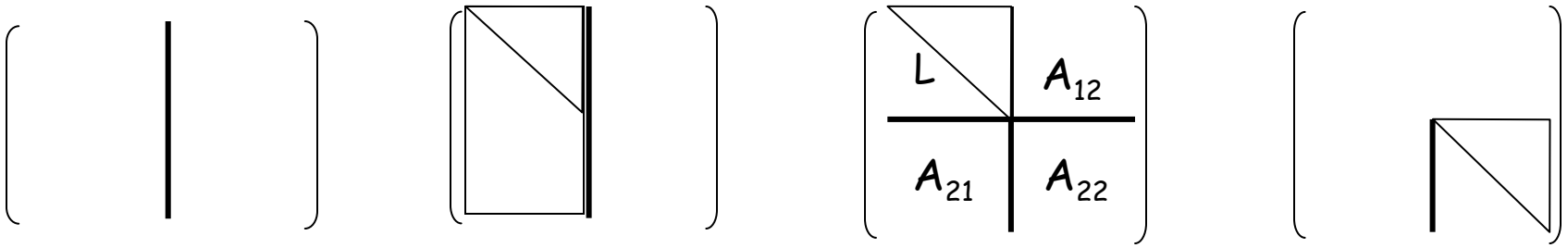
LU Algorithm:

1: Split matrix into two rectangles (m x n/2)
if only 1 column, scale by reciprocal of pivot & return

2: Apply LU Algorithm to the left part

3: Apply transformations to right part
(triangular solve $A_{12} = L^{-1}A_{12}$ and
matrix multiplication $A_{22}=A_{22} - A_{21}*A_{12}$)

4: Apply LU Algorithm to right part

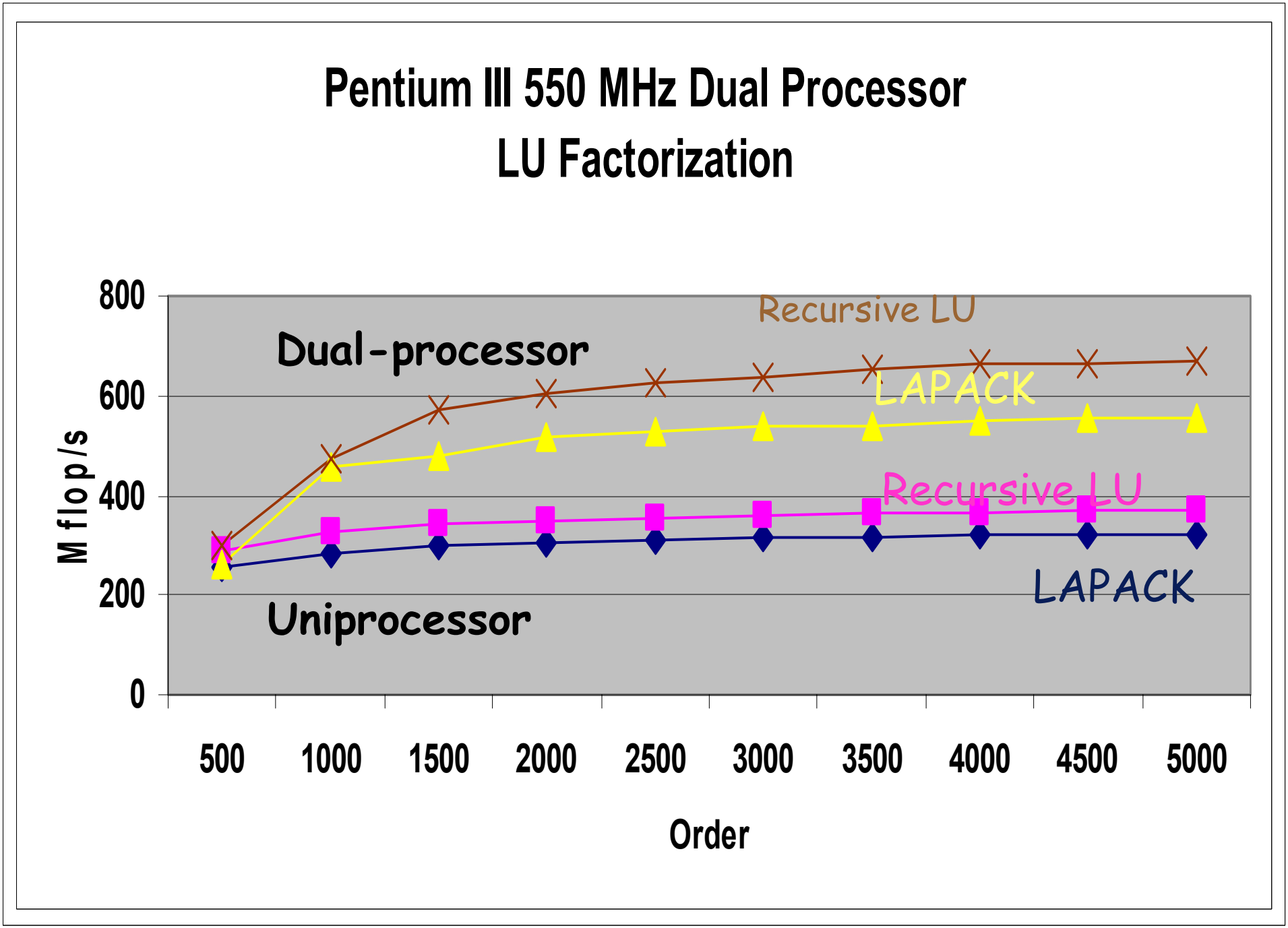


Most of the work in the matrix multiply
Matrices of size n/2, n/4, n/8, …

Source: Jack Dongarra

Recursive Factorizations

- Just as accurate as conventional method
- Same number of operations
- Automatic variable-size blocking
  - Level 1 and 3 BLAS only !
- Simplicity of expression
- Potential for efficiency while being “cache oblivious”
  - But shouldn’t recur down to single columns!
- The recursive formulation is just a rearrangement of the point-wise LINPACK algorithm
- The standard error analysis applies (assuming the matrix operations are computed the “conventional” way).



Source: Jack Dongarra

Recursive Algorithms – Limits

- Two kinds of dense matrix compositions
- One Sided
  - Sequence of simple operations applied on left of matrix
  - Gaussian Elimination: A = L*U or A = P*L*U
    - Symmetric Gaussian Elimination: $A = L*D*L^T$
    - Cholesky: $A = L*L^T$
  - QR Decomposition for Least Squares: A = Q*R
  - Can be nearly 100% BLAS 3
  - Susceptible to recursive algorithms
- Two Sided
  - Sequence of simple operations applied on both sides, alternating
  - Eigenvalue algorithms, SVD
  - At least ~25% BLAS 2
  - Seem impervious to recursive approach?
  - Some recent progress on SVD (25% vs 50% BLAS2)

Out of "Core" Algorithms

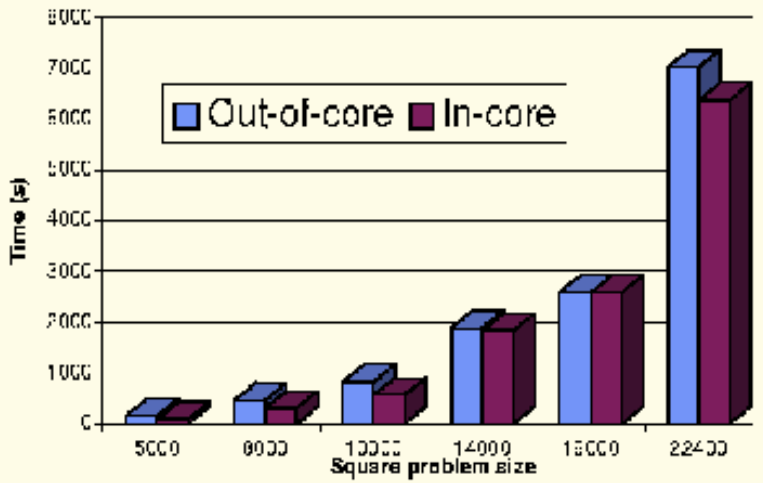
Out-of-Core Performance Results for Least Squares

- Prototype code for Out-of-Core extension
- Linear solvers based on "Left-looking" variants of LU, QR, and Cholesky factorization
- Portable I/O interface for reading/writing ScaLA-PACK matrices

Out-of-core means matrix lives on disk; too big for main memory

Much harder to hide latency of disk

QR much easier than LU because no pivoting needed for QR



Source: Jack Dongarra

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With the cooperation of
Cray, IBM, Convex, DEC, Fujitsu, NEC, NAG, IMSL

Upcoming related talks

- SIAM Conference on Parallel Processing in Scientific Computing
  - San Francisco, Feb 22-24
  - http://www.siam.org/meetings/pp06/index.htm
  - Applications, Algorithms, Software, Hardware
  - 3 Minisymposia on Dense Linear Algebra on Friday 2/24
    - MS41, MS47(*), MS56
- Scientific Computing Seminar,
  - "An O(n log n) tridiagonal eigensolver", Jonathan Moussa
  - Wednesday, Feb 15, 11-12, 380 Soda
- Special Seminar
  - Towards Combinatorial Preconditioners for Finite-Elements Problems", Prof. Sivan Toledo, Technion
  - Tuesday, Feb 21, 1-2pm, 373 Soda

QR (Least Squares)

Scales well,
nearly full machine speed

Performance of ScaLAPACK QR (Least squares)

Efficiency = MFlops(PDGELS)/MFlops(PDGEMM)					
Machine	Procs	Block Size	N		
			2000	4000	10000
Cray T3E	4	32	.54	.61	
	16		.46	.55	.60
	64		.26	.47	.54
IBM SP2	4	50	.51		
	16		.29	.51	
	64		.19	.36	.54
Intel XP/S GP Paragon	4	32	.61		
	16		.43	.63	
	64		.22	.48	.62
Berkeley NOW	4	32	.51	.77	
	32		.49	.66	.71
	64		.37	.60	.72

Time(PDGELS)/Time(PDGEMM)					
Machine	Procs	Block Size	N		
			2000	4000	10000
Cray T3E	4	32	1.2	1.1	
	16		1.5	1.2	1.1
	64		2.6	1.4	1.2
IBM SP2	4	50	1.3		
	16		2.3	1.3	
	64		3.6	1.8	1.2
Intel XP/S GP Paragon	4	32	1.1		
	16		1.6	1.1	
	64		3.0	1.4	1.1
Berkeley NOW	4	32	1.3	.9	
	32		1.4	1.0	.9
	64		1.8	1.1	.9

Performance of Symmetric Eigensolvers

Current algorithm:
Faster than initial algorithm
Occasional numerical instability
New, faster and more stable algorithm planned

Time(PDSYEVX)/Time(PDGEMM)
(bisection + inverse iteration)

Machine	Procs	Block Size	N	
			2000	4000
Cray T3E	4	32	10	
	16		13	10
	64		29	14
IBB SP2	16	50	24	
	64		40	29
Intel XP/S GP	16	32	22	
Paragon	64		34	20
Berkeley NOW	16	32	20	
	32		24	52

Initial algorithm:
Numerically stable
Easily parallelized
Slow: will abandon

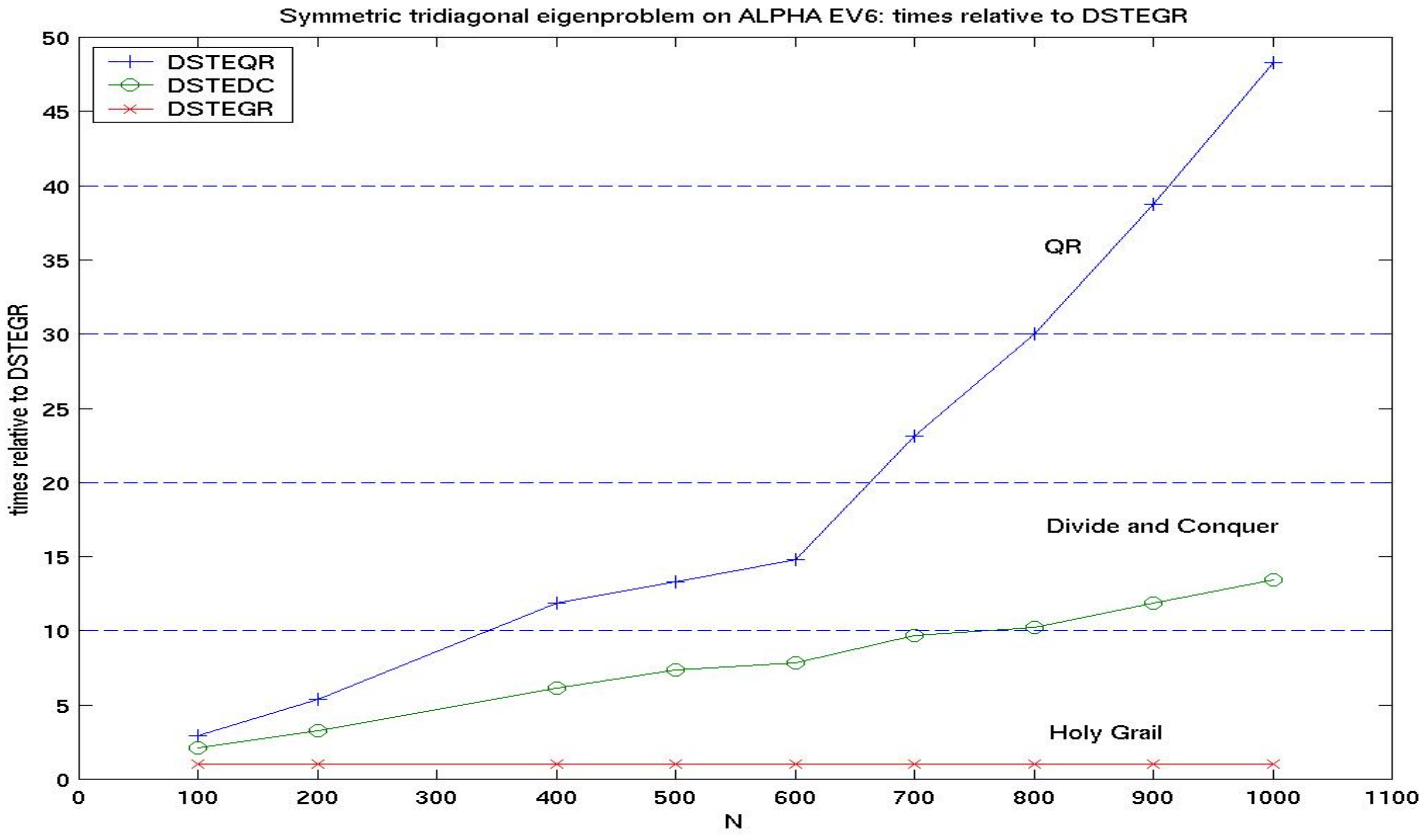
Time(PDSYEV)/Time(PDGEMM)
(QR iteration)

Machine	Procs	Block Size	N	
			2000	4000
Cray T3E	4	32	35	
	16		37	35
	64		57	41
IBM SP2	16	50	38	
	64		58	47
Intel XP/S GP	16	32	99	
Paragon	64		193	
Berkeley NOW	16	32	31	
	32		35	55

Scalable Symmetric Eigensolver and SVD

The "Holy Grail" (Parlett, Dhillon, Marques)

Perfect Output complexity (O(n * #vectors)), Embarrassingly parallel, Accurate



To be propagated throughout LAPACK and ScaLAPACK

Performance of SVD (Singular Value Decomposition)

Have good ideas to speedup
Project available!

Time(PDGESVD)/Time(PDGEMM)				
Machine	Procs	Block Size	N	
			2000	4000
Cray T3E	4	32	67	
	16		66	64
	64		93	70
IBM SP2	4	50	97	
	16		60	
	64		81	
Berkeley NOW	4	32	72	
	16		38	16
	32		59	26

Performance of Nonsymmetric Eigensolver (QR iteration)

Hardest of all to parallelize

Time(PDLAHQR)/Time(PDGEMM)				
Machine	Procs	Block Size	N	
			1000	1500
Intel XP/S MP Paragon	16	50	123	97

Scalable Nonsymmetric Eigensolver

- $Ax_i = \lambda_i x_i$, Schur form $A = QTQ^T$
- Parallel HQR
  - Henry, Watkins, Dongarra, Van de Geijn
  - Now in ScaLAPACK
  - Not as scalable as LU: N times as many messages
  - Block-Hankel data layout better in theory, but not in ScaLAPACK
- Sign Function
  - Beavers, Denman, Lin, Zmijewski, Bai, Demmel, Gu, Godunov, Bulgakov, Malyshev
  - $A_{i+1} = (A_i + A_i^{-1})/2 \rightarrow$ shifted projector onto Re $\lambda > 0$
  - Repeat on transformed A to divide-and-conquer spectrum
  - Only uses inversion, so scalable
  - Inverse free version exists (uses QRD)
  - Very high flop count compared to HQR, less stable

Assignment of parallel work in GE

- Think of assigning submatrices to threads, where each thread responsible for updating submatrix it owns
  - "owner computes" rule natural because of locality
- What should submatrices look like to achieve load balance?

Computational Electromagnetics (MOM)

The main steps in the solution process are

- **Fill:** computing the matrix elements of A
- **Factor:** factoring the dense matrix A
- **Solve:** solving for one or more excitations b
- **Field Calc:** computing the fields scattered from the object

Analysis of MOM for Parallel Implementation

Task	Work	Parallelism	Parallel Speed
Fill	O(n**2)	embarrassing	low
→ Factor	O(n**3)	moderately diff.	very high
Solve	O(n**2)	moderately diff.	high
Field Calc.	O(n)	embarrassing	high

BLAS2 version of GE with Partial Pivoting (GEPP)

```
for i = 1 to n-1
    find and record k where |A(k,i)| = max{i <= j <= n} |A(j,i)|
          … i.e. largest entry in rest of column i
    if |A(k,i)| = 0
        exit with a warning that A is singular, or nearly so
    elseif  k != i
        swap rows i and k of A
    end if
    A(i+1:n,i) = A(i+1:n,i) / A(i,i)
                 … each quotient lies in [-1,1]
                 … BLAS 1
    A(i+1:n,i+1:n) = A(i+1:n , i+1:n ) - A(i+1:n , i) * A(i , i+1:n)
                 … BLAS 2, most work in this line
```

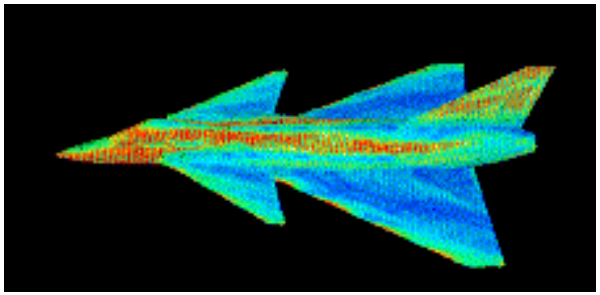
Computational Electromagnetics – Solve Ax=b

- Developed during 1980s, driven by defense applications
- Determine the RCS (radar cross section) of airplane
- Reduce signature of plane (stealth technology)
- Other applications are antenna design, medical equipment
- Two fundamental numerical approaches:
  - MOM methods of moments (frequency domain)
    - Large dense matrices
  - Finite differences (time domain)
    - Even larger sparse matrices

Computational Electromagnetics

- Discretize surface into triangular facets using standard modeling tools

- Amplitude of currents on surface are unknowns



- Integral equation is discretized into a set of linear equations

image: NW Univ. Comp. Electromagnetics Laboratory http://nueml.ece.nwu.edu/

Computational Electromagnetics (MOM)

After discretization the integral equation has the form

$$A\ x = b$$

where

A is the (dense) impedance matrix,

x is the unknown vector of amplitudes, and

b is the excitation vector.

(see Cwik, Patterson, and Scott, Electromagnetic Scattering on the Intel Touchstone Delta, IEEE Supercomputing '92, pp 538 - 542)

Results for Parallel Implementation on Intel Delta

Task	Time (hours)
Fill (compute n^2 matrix entries)	9.20
(embarrassingly parallel but slow)	
Factor (Gaussian Elimination, $O(n^3)$)	8.25
(good parallelism with right algorithm)	
Solve ($O(n^2)$)	2 .17
(reasonable parallelism with right algorithm)	
Field Calc. (O(n))	0.12
(embarrassingly parallel and fast)	

The problem solved was for a matrix of size 48,672.
2.6 Gflops for Factor - The world record in 1991.

Computational Chemistry – Ax = λ x

- Seek energy levels of a molecule, crystal, etc.
  - Solve Schroedinger's Equation for energy levels = eigenvalues
  - Discretize to get Ax = λBx, solve for eigenvalues λ and eigenvectors x
  - A and B large Hermitian matrices (B positive definite)
- MP-Quest (Sandia NL)
  - Si and sapphire crystals of up to 3072 atoms
  - A and B up to n=40000, complex Hermitian
  - Need all eigenvalues and eigenvectors
  - Need to iterate up to 20 times (for self-consistency)
- Implemented on Intel ASCI Red
  - 9200 Pentium Pro 200 processors (4600 Duals, a CLUMP)
  - Overall application ran at 605 Gflops (out of 1800 Gflops peak),
  - Eigensolver ran at 684 Gflops
  - www.cs.berkeley.edu/~stanley/gbell/index.html
  - Runner-up for Gordon Bell Prize at Supercomputing 98

LAPACK and ScaLAPACK

	LAPACK	ScaLAPACK
Machines	Workstations, Vector, SMP	Distributed Memory, DSM
Based on	BLAS	BLAS, BLACS
Functionality	Linear Systems Least Squares Eigenproblems	Linear Systems Least Squares Eigenproblems (less than LAPACK)
Matrix types	Dense, band	Dense, band, out-of-core
Error Bounds	Complete	A few
Languages	F77 or C	F77 and C
Interfaces to	C++, F90	HPF
Manual?	Yes	Yes
Where?	www.netlib.org/lapack	www.netlib.org/scalapack

Parallelism in ScaLAPACK

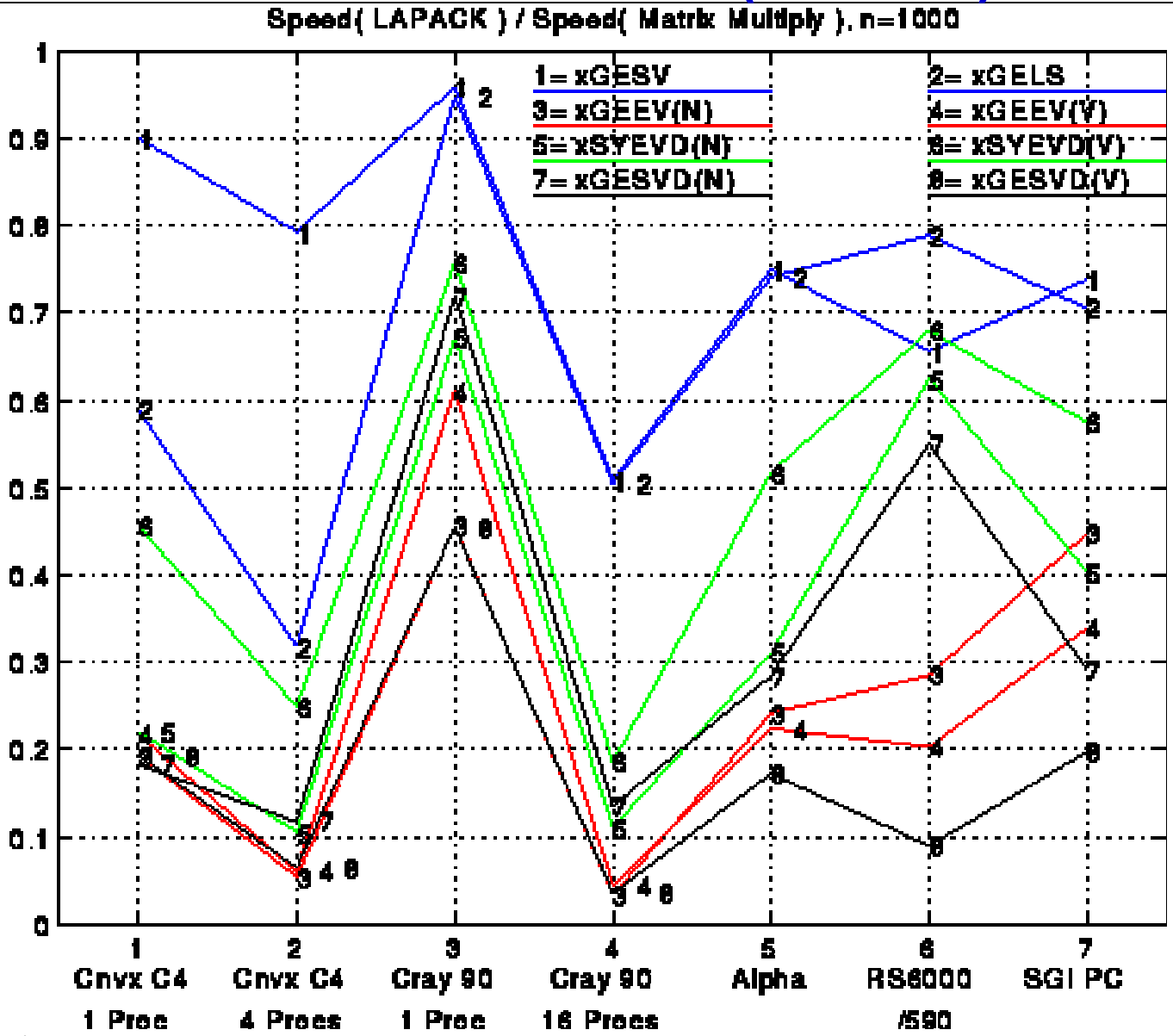
- Level 3 BLAS block operations
  - All the reduction routines
- Pipelining
  - QR Iteration, Triangular Solvers, classic factorizations
- Redundant computations
  - Condition estimators
- Static work assignment
  - Bisection
- Task parallelism
  - Sign function eigenvalue computations
- Divide and Conquer
  - Tridiagonal and band solvers, symmetric eigenvalue problem and Sign function
- Cyclic reduction
  - Reduced system in the band solver

Winner of TOPS 500 (LINPACK Benchmark)

Year	Machine	Tflops	Factor faster	Peak Tflops	Num Procs	N
2004	Blue Gene / L, IBM	70.7	2.0	91.8	32768	.93M
2002 2003	Earth System Computer, NEC	35.6	4.9	40.8	5104	1.04M
2001	ASCI White, IBM SP Power 3	7.2	1.5	11.1	7424	.52M
2000	ASCI White, IBM SP Power 3	4.9	2.1	11.1	7424	.43M
1999	ASCI Red, Intel PII Xeon	2.4	1.1	3.2	9632	.36M
1998	ASCI Blue, IBM SP 604E	2.1	1.6	3.9	5808	.43M
1997	ASCI Red, Intel Ppro, 200 MHz	1.3	3.6	1.8	9152	.24M
1996	Hitachi CP-PACS	.37	1.3	.6	2048	.10M
1995	Intel Paragon XP/S MP	.28	1	.3	6768	.13M

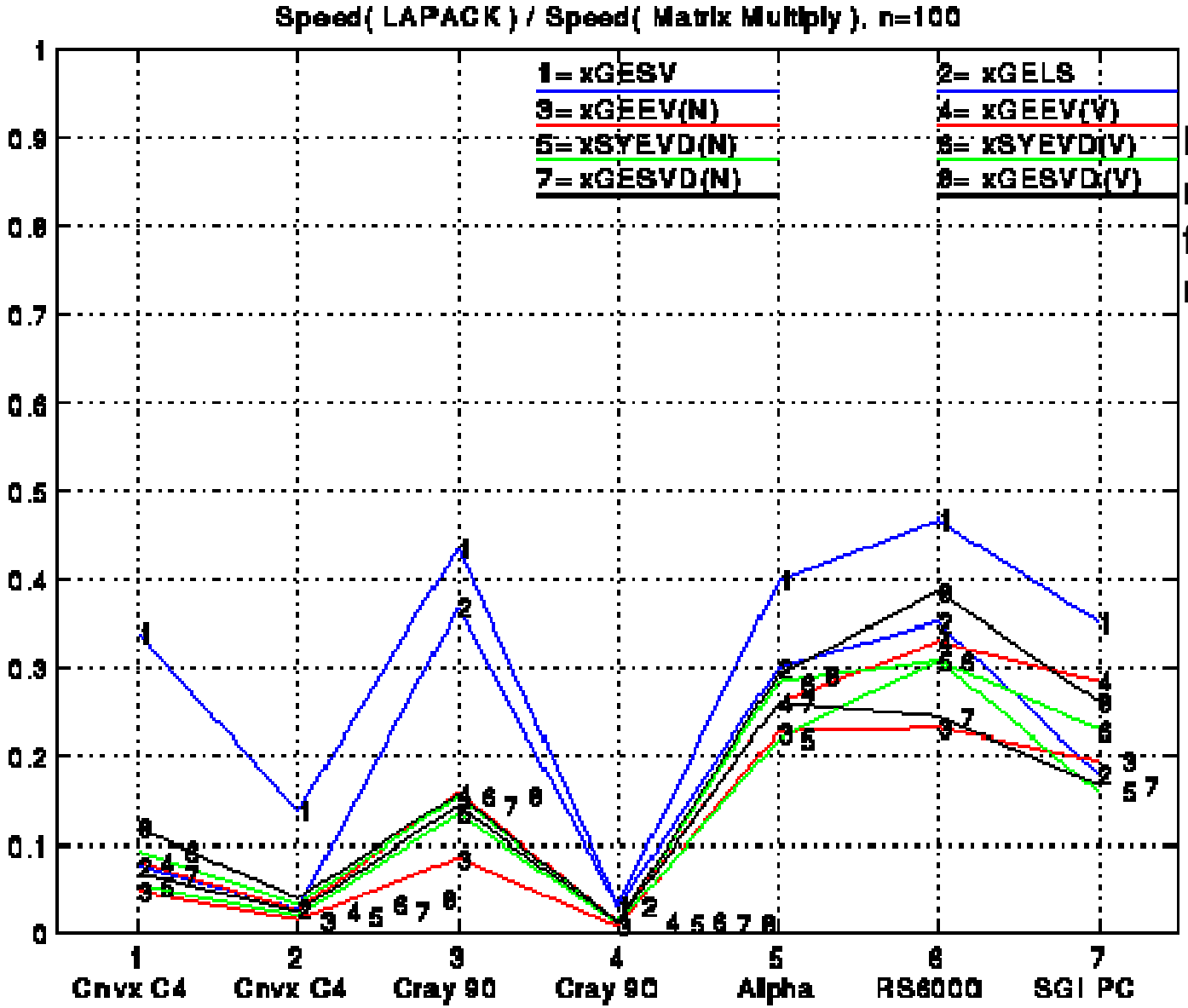
Source: Jack Dongarra (UTK)

Performance of LAPACK (n=1000)



Performance of Eigen-values, SVD, etc.

Performance of LAPACK (n=100)



Efficiency is much lower for a smaller matrix.