Lecture 10:
Linear Algebra Algorithms

Jack Dongarra, U of Tennessee

Slides are adapted from Jim Demmel, UCB's Lecture on Linear Algebra Algorithms

Outline

° Motivation for Dense Linear Algebra
  • Ax=b: Computational Electromagnetics
  • Ax = l x: Quantum Chemistry

° 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 matrix-matrix multiplication

° Parallel Gaussian Elimination

° ScaLAPACK library overview

° Eigenvalue problem

Parallelism in Sparse Matrix-vector multiplication

° y = A*x, where A is sparse and n x n

° Questions
  • which processors store
    - y[i], x[i], and A[i,j]
  • which processors compute
    - y[i] = sum (from 1 to n) A[i,j] * x[j]
      = (row i of A) . x … a sparse dot product

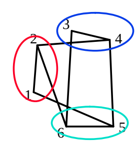
° Partitioning
  • Partition index set {1,…,n} = N1 u N2 u … u Np
  • For all i in Nk, Processor k stores y[i], x[i], and row i of A
  • For all i in Nk, Processor k computes y[i] = (row i of A) . x
    - "owner computes" rule: Processor k compute the y[i]s it owns

° Goals of partitioning
  • balance load (how is load measured?)
  • balance storage (how much does each processor store?)
  • minimize communication (how much is communicated?)

Graph Partitioning and Sparse Matrices

° Relationship between matrix and graph

	1	2	3	4	5	6
1	1	1			1	
2	1	1		1		1
3			1	1		1
4		1	1	1	1	
5	1			1	1	1
6		1	1		1	1

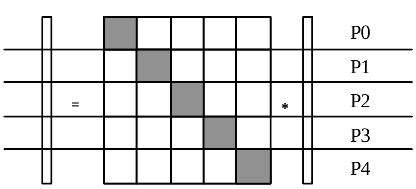


° A "good" partition of the graph has
  • equal (weighted) number of nodes in each part (load and storage balance)
  • minimum number of edges crossing between (minimize communication)

° Can reorder the rows/columns of the matrix by putting all the nodes in one partition together

More on Matrix Reordering via Graph Partitioning

° "Ideal" matrix structure for parallelism: (nearly) block diagonal
  • p (number of processors) blocks
  • few non-zeros outside these blocks, since these require communication



What about implicit methods and eigenproblems?

° Direct methods (Gaussian elimination)
  • Called LU Decomposition, because we factor A = L*U
  • Future lectures will consider both dense and sparse cases
  • More complicated than sparse-matrix vector multiplication

° Iterative solvers
  • Will discuss several of these in future
    - Jacobi, Successive overrelaxiation (SOR) , Conjugate Gradients (CG), Multigrid,...
  • Most have sparse-matrix-vector multiplication in kernel

° Eigenproblems
  • Future lectures will discuss dense and sparse cases
  • Also depend on sparse-matrix-vector multiplication, direct methods

° Graph partitioning

Partial Differential Equations
PDEs

Continuous Variables, Continuous Parameters

Examples of such systems include

- **Heat flow:** Temperature(position, time)
- **Diffusion:** Concentration(position, time)
- **Electrostatic or Gravitational Potential:** Potential(position)
- **Fluid flow:** Velocity,Pressure,Density(position,time)
- **Quantum mechanics:** Wave-function(position,time)
- **Elasticity:** Stress,Strain(position,time)

Example: Deriving the Heat Equation

Consider a simple problem

- A bar of uniform material, insulated except at ends
- Let $u(x,t)$ be the temperature at position x at time t
- Heat travels from x-h to x+h at rate proportional to:

$$\frac{d\,u(x,t)}{dt} = C * \frac{(u(x-h,t)-u(x,t))/h - (u(x,t)- u(x+h,t))/h}{h}$$

- As $h \to 0$, we get the heat equation:

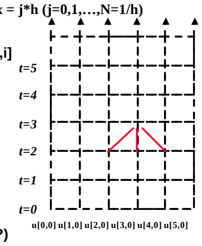
$$\frac{d\,u(x,t)}{dt} = C * \frac{d^2\,u(x,t)}{dx^2}$$

Explicit Solution of the Heat Equation

- For simplicity, assume $C=1$
- Discretize both time and position
- Use finite differences with u[j,i] as the heat at
  - time t= i*dt (i = 0,1,2,…) and position x = j*h (j=0,1,…,N=1/h)
  - initial conditions on u[j,0]
  - boundary conditions on u[0,i] and u[N,i]
- At each timestep i = 0,1,2,...

```
For j=0 to N
   u[j,i+1]= z*u[j-1,i]+ (1-2*z)*u[j,i]+
             z*u[j+1,i]
```

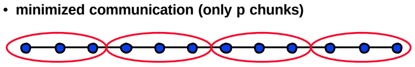
where z = dt/h²



- This corresponds to
  - matrix vector multiply (what is matrix?)
  - nearest neighbors on grid

Parallelism in Explicit Method for PDEs

- Partitioning the space (x) into p largest chunks
  - good load balance (assuming large number of points relative to p)
  - minimized communication (only p chunks)



- Generalizes to
  - multiple dimensions
  - arbitrary graphs (= sparse matrices)
- Problem with explicit approach
  - numerical instability
  - solution blows up eventually if z = dt/h > .5
  - need to make the timesteps very small when h is small: dt < .5*h²

Discretization Error

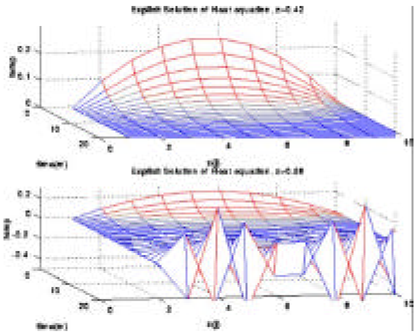
- How accurate will the approximate solution be?
- Beyond the scope of this course.
- The discretization error is

$$e = O(\Delta t) + O[(\Delta x)^2]$$

- The fact that *?t appears to the first power and ?x* to the second power is usually described as the discretization is first-order accurate in time and second-order accurate in space.
- For the discretization to be stable *?t and ?x* must satisfy the relationship

$$\Delta t \le \frac{1}{2}(\Delta x)^2$$

Instability in solving the heat equation explicitly



13

Implicit Methods

- The previous method was called explicit because the value of u[j,i+1] at the next time level are obtained by an explicit formula in terms of the values at the previous time level.

  u[j,i+1]= z*u[j-1,i] + (1-2*z)*u[j,i] + z*u[j+1,i]

- Consider the difference approximation

  u[j,i+1] - u[j,i] = z*(u[j+1,i+1] -2*u[j,i+1] + u[j-1,i+1]

- Similar in form but has the important difference that the values of u_j on the right are now evaluated at the *i+1*[th] time level rather than at the *i*[th].
- Must solve equations to advance to the next time level.

14

Implicit Solution

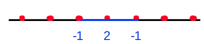
- As with many (stiff) ODEs, need an implicit method
- This turns into solving the following equation

  (I + (z/2)*T) * u[:,i+1]= (I - (z/2)*T) *u[:,i]

- Here *I* is the identity matrix and *T* is:

$$T = \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix}$$

Graph and "stencil"



- I.e., essentially solving Poisson's equation in 1D

u[j,i+1] - u[j,i] = z *(u[j+1,i+1] -2*u[j,i+1] + u[j-1,i+1]

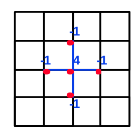
15

2D Implicit Method

- Similar to the 1D case, but the matrix *T* is now

$$T = \left(\begin{array}{ccc|ccc|ccc} 4 & -1 & & -1 & & & & & \\ -1 & 4 & -1 & & -1 & & & & \\ & -1 & 4 & & & -1 & & & \\ \hline -1 & & & 4 & -1 & & -1 & & \\ & -1 & & -1 & 4 & -1 & & -1 & \\ & & -1 & & -1 & 4 & & & -1 \\ \hline & & & -1 & & & 4 & -1 & \\ & & & & -1 & & -1 & 4 & -1 \\ & & & & & -1 & & -1 & 4 \end{array}\right)$$

Graph and "stencil"



- Multiplying by this matrix (as in the explicit case) is simply nearest neighbor computation on 2D grid
- To solve this system, there are several techniques

16

Algorithms for 2D Poisson Equation with N unknowns

Algorithm	Serial	PRAM	Memory	#Procs
Dense LU	N^3	N	N^2	N^2
Band LU	N^2	N	$N^{3/2}$	N
Jacobi	N^2	N	N	N
Explicit Inv.	N^2	log N	N^2	N^2
Conj.Grad.	$N^{3/2}$	$N^{1/2}$ *log N	N	N
RB SOR	$N^{3/2}$	$N^{1/2}$	N	N
Sparse LU	$N^{3/2}$	$N^{1/2}$	N*log N	N
FFT	N*log N	log N	N	N
Multigrid	N	$\log^2 N$	N	N
Lower bound	N	log N	N	

PRAM is an idealized parallel model with zero cost communication

(see next slide for explanation)

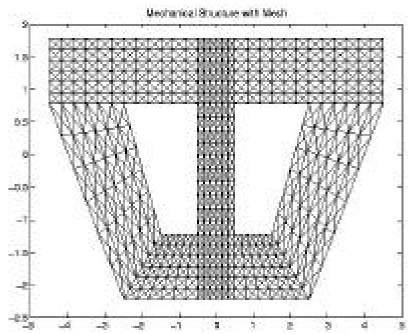
17

Short explanations of algorithms on previous slide

- Sorted in two orders (roughly):
  - from slowest to fastest on sequential machines
  - from most general (works on any matrix) to most specialized (works on matrices "like" T)
- Dense LU: Gaussian elimination; works on any N-by-N matrix
- Band LU: exploit fact that T is nonzero only on sqrt(N) diagonals nearest main diagonal, so faster
- Jacobi: essentially does matrix-vector multiply by T in inner loop of iterative algorithm
- Explicit Inverse: assume we want to solve many systems with T, so we can precompute and store inv(T) "for free", and just multiply by it
  - It's still expensive!
- Conjugate Gradients: uses matrix-vector multiplication, like Jacobi, but exploits mathematical properties of T that Jacobi does not
- Red-Black SOR (Successive Overrelaxation): Variation of Jacobi that exploits yet different mathematical properties of T
  - Used in Multigrid
- Sparse LU: Gaussian elimination exploiting particular zero structure of T
- FFT (Fast Fourier Transform): works only on matrices *very* like T
- Multigrid: also works on matrices like T, that come from elliptic PDEs
- Lower Bound: serial (time to print answer); parallel (time to combine N inputs)

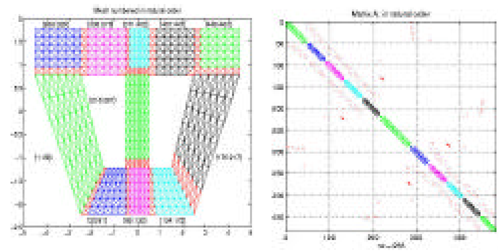
18

Composite mesh from a mechanical structure



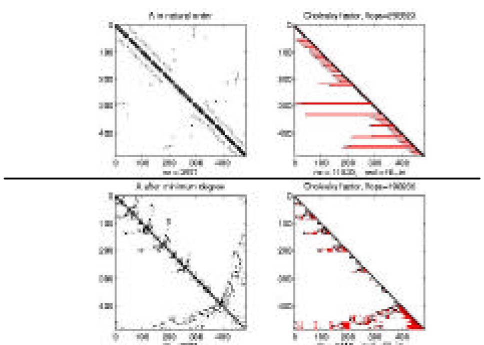
19

Converting the mesh to a matrix



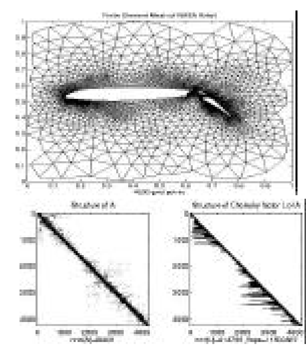
20

Effects of Ordering Rows and Columns on Gaussian Elimination



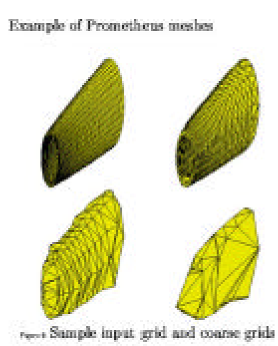
21

Irregular mesh: NASA Airfoil in 2D (direct solution)



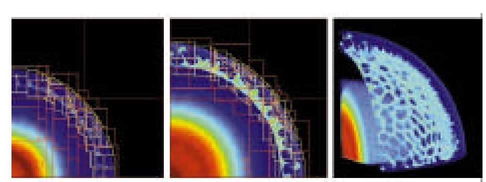
22

Irregular mesh: Tapered Tube (multigrid)



23

Adaptive Mesh Refinement (AMR)



- Adaptive mesh around an explosion
- John Bell and Phil Colella at LBL (see class web page for URL)
- Goal of Titanium is to make these algorithms easier to implement in parallel

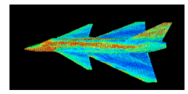
24

Computational Electromagnetics

- 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), and
  - Finite differences (time domain)

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)

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

Results for Parallel Implementation on Delta

Task	Time (hours)
Fill	9.20
Factor	8.25
Solve	2 .17
Field Calc.	0.12

The problem solved was for a matrix of size 48,672. (The world record in 1991.)

Current Records for Solving Dense Systems

Year	System Size	Machine	# Procs	Gflops	(Peak)
1950's	O(100)				
1995	128,600	Intel Paragon	6768	281	(338)
1996	215,000	Intel ASCI Red	7264	1068	(1453)
1998	148,000	Cray T3E	1488	1127	(1786)
1998	235,000	Intel ASCI Red	9152	1338	(1830)
1999	374,000	SGI ASCI Blue	5040	1608	(2520)
1999	362,880	Intel ASCI Red	9632	2379	(3207)
2000	430,000	IBM ASCI White	8192	4928	(12000)
2002	1,075,200	NEC Earth Sim	5120	35860	(41000)

source: Alan Edelman http://www-math.mit.edu/~edelman/records.html
LINPACK Benchmark: http://www.netlib.org/performance/html/PDSreports.html

Computational Chemistry

- Seek energy levels of a molecule, crystal, etc.
  - Solve Schroedinger's Equation for energy levels = eigenvalues
  - Discretize to get $Ax = \lambda Bx$, solve for eigenvalues λ and eigenvectors x
  - A and B large, symmetric or Hermitian matrices (B positive definite)
  - May want some or all eigenvalues/eigenvectors
- MP-Quest (Sandia NL)
  - Si and sapphire crystals of up to 3072 atoms
  - Local Density Approximation to Schroedinger Equation
  - A and B up to n=40000, 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 Glops peak),
  - Eigensolver ran at 684 Gflops
  - www.cs.berkeley.edu/~stanley/gbell/index.html
  - Runner-up for Gordon Bell Prize at Supercomputing 98

EISPACK and LINPACK

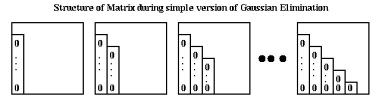
- EISPACK
  - Design for the algebraic eigenvalue problem, $Ax = \lambda x$ and $Ax = \lambda Bx$.
  - work of J. Wilkinson and colleagues in the 70's.
  - Fortran 77 software based on translation of ALGOL.
- LINPACK
  - Design for the solving systems of equations, Ax = b.
  - Fortran 77 software using the Level 1 BLAS.

Review of 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
      for k = i to n
         A(j,k) = A(j,k) - (A(j,i)/A(i,i)) * A(i,k)
```

Structure of Matrix during simple version of Gaussian Elimination



After i=1 After i=2 After i=3 After i=n-1

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

- Remove computation of constant A(j,i)/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)
```

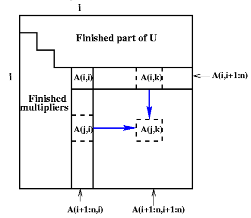

Refine GE Algorithm (4)

° **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)
```

° **Express using matrix operations (BLAS)**

Work at step i of Gaussian Elimination




```
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)
```


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

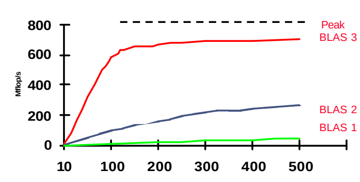
° **What if some A(i,i) is zero? Or very small?**

- 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 (Lecture 2)**

```
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)
```

IBM RS/6000 Power 3 (200 MHz, 800 Mflop/s Peak)



Pivoting in Gaussian Elimination

° A = [0 1]   fails completely, even though A is "easy"
      [1 0]

° Illustrate problems in 3-decimal digit arithmetic:

```
A = [ 1e-4  1 ]   and   b = [ 1 ],  correct answer to 3 places is x = [ 1 ]
    [   1   1 ]             [ 2 ]                                     [ 1 ]
```

° Result of LU decomposition is

```
L = [ 1           0 ]  = [ 1      0 ]          … No roundoff error yet
    [ fl(1/1e-4)  1 ]    [ 1e4    1 ]

U = [ 1e-4        1        ]  = [ 1e-4     1  ]   … Error in 4th decimal place
    [ 0     fl(1-1e4*1)    ]    [ 0     -1e4  ]

Check if A = L*U = [ 1e-4   1 ]                   … (2,2) entry entirely wrong
                   [   1    0 ]
```

° Algorithm "forgets" (2,2) entry, gets same L and U for all |A(2,2)|<5
  ° Numerical instability
  ° Computed solution x totally inaccurate

° Cure: Pivot (swap rows of A) so entries of L and U bounded

Gaussian Elimination with Partial Pivoting (GEPP)

° **Partial Pivoting: swap rows so that each multiplier**
|L(i,j)| = |A(j,i)/A(i,i)| <= 1

```
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**

° **Since each entry of |L(i,j)| <= 1, this algorithm is considered numerically stable**

° **For details see LAPACK code at www.netlib.org/lapack/single/sgetf2.f**

History of Block Partitioned Algorithms

- Early algorithms involved use of small main memory using tapes as secondary storage.
- Recent work centers on use of vector registers, level 1 and 2 cache, main memory, and "out of core" memory.

43

Blocked Partitioned Algorithms

- LU Factorization
- Cholesky factorization
- Symmetric indefinite factorization
- Matrix inversion
- QR, QL, RQ, LQ factorizations
- Form Q or Q^TC
- Orthogonal reduction to:
  - (upper) Hessenberg form
  - symmetric tridiagonal form
  - bidiagonal form
- Block QR iteration for nonsymmetric eigenvalue problems

44

Converting BLAS2 to BLAS3 in GEPP

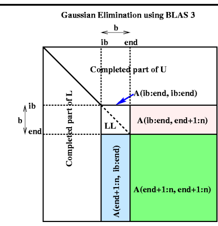
- Blocking
  - Used to optimize matrix-multiplication
  - Harder here because of data dependencies in GEPP
- Delayed Updates
  - Save updates to "trailing matrix" from several consecutive BLAS2 updates
  - Apply many saved updates simultaneously in one BLAS3 operation
- Same idea works for much of dense linear algebra
  - Open questions remain
- Need to choose a block size b
  - Algorithm will save and apply b updates
  - b must be small enough so that active submatrix consisting of b columns of A fits in cache
  - b must be large enough to make BLAS3 fast

45

Blocked GEPP (www.netlib.org/lapack/single/sgetrf.f)

```
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
```

(For a correctness proof, see on- lines notes.)



46

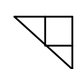
LAPACK

- Linear Algebra library in Fortran 77
  - Solution of systems of equations
  - Solution of eigenvalue problems
- Combine algorithms from LINPACK and EISPACK into a single package
- Efficient on a wide range of computers
  - RISC, Vector, SMPs
- User interface similar to LINPACK
  - Single, Double, Complex, Double Complex
- Built on the Level 1, 2, and 3 BLAS

47

Derivation of Blocked Algorithms
Cholesky Factorization A = U^TU

$$\begin{pmatrix} A_{11} & a_j & A_{13} \\ a_j^T & a_{jj} & a_j^T \\ A_{13}^T & a_j & A_{33} \end{pmatrix} = \begin{pmatrix} U_{11}^T & 0 & 0 \\ u_j^T & u_{jj} & 0 \\ U_{13}^T & m_j & U_{33}^T \end{pmatrix} \begin{pmatrix} U_{11} & u_j & U_{13} \\ 0 & u_{jj} & m_j^T \\ 0 & 0 & U_{33} \end{pmatrix}$$



Equating coefficient of the j[th] column, we obtain

$$a_j = U_{11}^T u_j$$
$$a_{jj} = u_j^T u_j + u_{jj}^2$$

Hence, if U_{11} has already been computed, we can compute u_j and u_{jj} from the equations:

$$U_{11}^T u_j = a_j$$
$$u_{jj}^2 = a_{jj} - u_j^T u_j$$

48

LINPACK Implementation

- Here is the body of the LINPACK routine SPOFA which implements the method:

```
      DO 30 J = 1, N
         INFO = J
         S = 0.0E0
         JM1 = J - 1
         IF( JM1.LT.1 ) GO TO 20
         DO 10 K = 1, JM1
            T = A( K, J ) - SDOT( K -1, A( 1, K ), 1,A( 1, J ), 1 )
            T = T / A( K, K )
            A( K, J ) = T
            S = S + T*T
   10    CONTINUE
   20    CONTINUE
         S = A( J, J ) - S
C     ...EXIT
         IF( S.LE.0.0E0 ) GO TO 40
         A( J, J ) = SQRT( S )
   30 CONTINUE
```

49

LAPACK Implementation

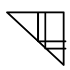
```
      DO 10 J = 1, N
         CALL STRSV( 'Upper', 'Transpose', 'Non-Unit', J-1, A, LDA, A( 1, J ), 1 )
         S = A( J, J ) - SDOT( J-1, A( 1, J ), 1, A( 1, J ), 1 )
         IF( S.LE.ZERO ) GO TO 20
         A( J, J ) = SQRT( S )
   10 CONTINUE
```

- This change by itself is sufficient to significantly improve the performance on a number of machines.
- From 238 to 312 Mflop/s for a matrix of order 500 on a Pentium 4-1.7 GHz.
- However on peak is 1,700 Mflop/s.
- Suggest further work needed.

50

Derivation of Blocked Algorithms

$$\begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{12}^T & A_{22} & A_{12} \\ A_{13}^T & A_{12}^T & A_{33} \end{pmatrix} = \begin{pmatrix} U_{11}^T & 0 & 0 \\ U_{12}^T & U_{22}^T & 0 \\ U_{13}^T & U_{23}^T & U_{33}^T \end{pmatrix} \begin{pmatrix} U_{11} & U_{12} & U_{13} \\ 0 & U_{22} & U_{23}^T \\ 0 & 0 & U_{33} \end{pmatrix}$$



Equating coefficient of second block of columns, we obtain

$$A_{12} = U_{11}^T U_{12}$$

$$A_{22} = U_{12}^T U_{12} + U_{22}^T U_{22}$$

Hence, if U_{11} has already been computed, we can compute U_{12} as the solution of the following equations by a call to the Level 3 BLAS routine STRSM:

$$U_{11}^T U_{12} = A_{12}$$

$$U_{22}^T U_{22} = A_{22} - U_{12}^T U_{12}$$

51

LAPACK Blocked Algorithms

```
      DO 10 J = 1, N, NB
         CALL STRSM( 'Left', 'Upper', 'Transpose','Non-Unit', J-1, JB, ONE, A, LDA,
     $               A( 1, J ), LDA )
         CALL SSYRK( 'Upper', 'Transpose', JB, J -1,-ONE, A( 1, J ), LDA, ONE,
     $               A( J, J ), LDA )
         CALL SPOTF2( 'Upper', JB, A( J, J ), LDA, INFO )
         IF( INFO.NE.0 ) GO TO 20
   10 CONTINUE
```

- **On Pentium 4, L3 BLAS squeezes a lot more out of 1 proc**

Intel Pentium 4 1.7 GHz N = 500	Rate of Execution
Linpack variant (L1B)	238 Mflop/s
Level 2 BLAS Variant	312 Mflop/s
Level 3 BLAS Variant	1262 Mflop/s

52

LAPACK Contents

- Combines algorithms from LINPACK and EISPACK into a single package. User interface similar to LINPACK.
- Built on the Level 1, 2 and 3 BLAS, for high performance (manufacturers optimize BLAS)
- LAPACK does not provide routines for structured problems or general sparse matrices (i.e sparse storage formats such as compressed -row, -column, -diagonal, skyline ...).

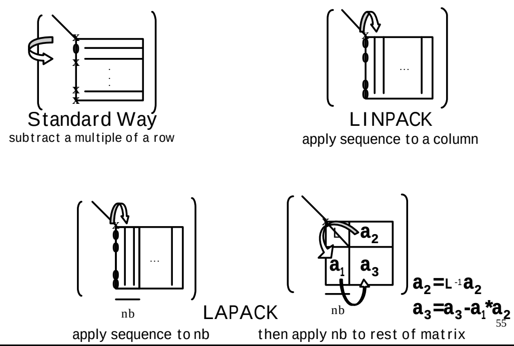
53

LAPACK Ongoing Work

- Add functionality
  - updating/downdating , divide and conquer least squares,bidiagonal bisection, bidiago nal inverse iteration, band SVD, Jacobi methods, ...
- Move to new generation of high performance machines
  - IBM SPs , CRAY T3E, SGI Origin, clusters of workstations
- New challenges
  - New languages: FORTRAN 90, HP FORTRAN, ...
  - (CMMD, MPL, NX ...)
    - many flavors of message passing, need standard (PVM, MPI): BLACS
- Highly varying ratio $\frac{\text{Computational speed}}{\text{Communication speed}}$
- Many ways to layout data,
- Fastest parallel algorithm sometimes less stable numerically.

54

Gaussian Elimination



55

Gaussian Elimination via a Recursive Algorithm

F. Gustavson and S. Toledo

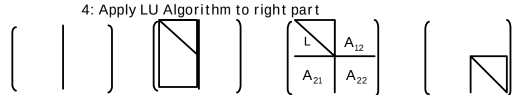
LU Algorithm:

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



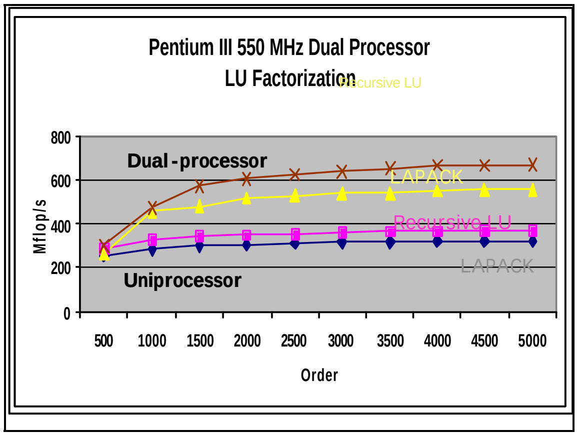
Most of the work in the matrix multiply
Matrices of size n/2, n/4, n/8, …

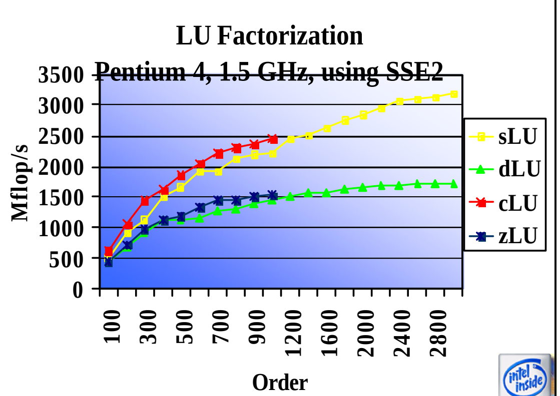
56

Recursive Factorizations

- Just as accurate as conventional method
- Same number of operations
- Automatic variable blocking
  - Level 1 and 3 BLAS only !
- Extreme clarity and simplicity of expression
- Highly efficient
- 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).
- OK for LU, LL^T, & QR
  - Open question on 2-sided algs. eg eigenvalue reduction

57





Challenges in Developing Distributed Memory Libraries

- How to integrate software?
  - Until recently no standards
  - Many parallel languages
  - Various parallel programming models
  - Assumptions about the parallel environment
    - granularity
    - topology
    - overlapping of communication/computation
    - development tools
- Where is the data
  - Who owns it?
  - Opt data distribution
- Who determines data layout
  - Determined by user?
  - Determined by library developer?
  - Allow dynamic data dist.
  - Load balancing

60

ScaLAPACK

- Library of software dealing with dense & banded routines
- Distributed Memory - Message Passing
- MIMD Computers and Networks of Workstations
- Clusters of SMPs

61

Programming Style

- SPMD Fortran 77 with object based design
- Built on various modules
  - PBLAS Interprocessor communication
  - BLACS
    - PVM, MPI, IBM SP, CRI T3, Intel, TMC
    - Provides right level of notation.
  - BLAS
- LAPACK software expertise/quality
  - Software approach
  - Numerical methods

62

Overall Structure of Software

- Object based - Array descriptor
  - Contains information required to establish mapping between a global array entry and its corresponding process and memory location.
  - Provides a flexible framework to easily specify additional data distributions or matrix types.
  - Currently dense, banded, & out-of-core
- Using the concept of context

63

PBLAS

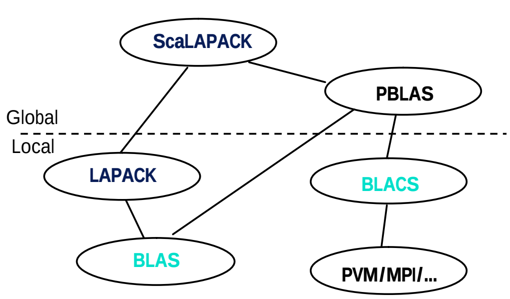
- Similar to the BLAS in functionality and naming.
- Built on the BLAS and BLACS
- Provide global view of matrix

```
CALL DGEXXX   ( M, N, A( IA, JA ), LDA,... )

CALL PDGEXXX( M, N, A, IA, JA, DESCA,... )
```

64

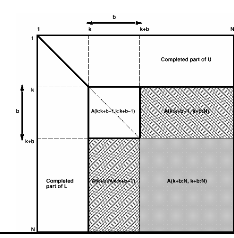
ScaLAPACK Structure



65

Choosing a Data Distribution

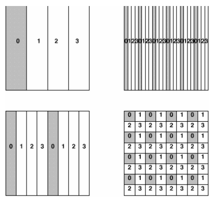
- Main issues are:
  - Load balancing
  - Use of the Level 3 BLAS



66

Possible Data Layouts

- 1D block and cyclic column distributions



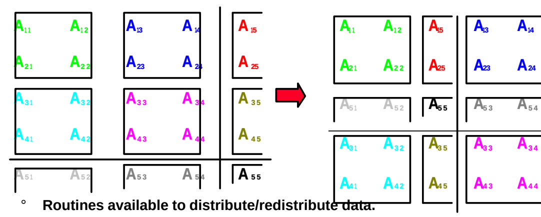
- 1D block-cycle column and 2D block-cyclic distribution
- 2D block-cyclic used in ScaLAPACK for dense matrices

Distribution and Storage

- Matrix is block-partitioned & maps blocks
- Distributed 2-D block- cyclic scheme

5x5 matrix partitioned in 2x2 blocks

2x2 process grid point of view



- Routines available to distribute/redistribute data.

Parallelism in ScaLAPACK

- Level 3 BLAS block operations
  - All the reduction routines
- Pipelining
  - QR Algorithm, 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
- Data parallelism
  - Sign function

ScaLAPACK - What's Included

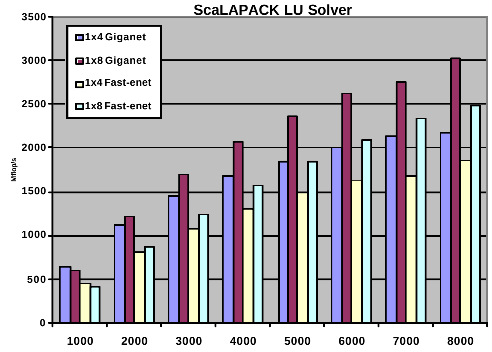
Problem type Ax=b	SDrv	EDrv	Factor	Solve	Inv	Cond Est	Iter Refin
Triangular				X	X	X	X
SPD	X	X	X	X	X	X	X
SPD Banded	X		X	X			
SPD Tridiagonal	X		X	X			
General	X	X	X	X	X	X	X
General Banded	X		X	X			
General Tridiagonal	X		X	X			
Least squares	X		X	X			
GQR			X				
GRQ			X				
$Ax = \lambda x$ or $Ax = \lambda Bx$	SDrv	Edrv	Reduct	Solution			
Symmetric (2 types)	X	X	X	X			
General (2 types)			X	X			
Generalized BSPD		X	X	X			
SVD			X	X			

- Timing and Testing routines for almost all
- This is a large component of the package
- Prebuilt libraries available for SP, PGON, HPPA, DEC, Sun, RS6K

Heterogeneous Computing

- Software intended to be used in this context
- Communication of ft. pt. numbers between processors
- Machine precision and other machine specific parameters
- Iterative convergence across clusters of processors
- Defensive programming required

T0 Dual (500 MHz Alpha EV5/6)
Fast & Gigabit Ethernet
ScaLAPACK LU Solver

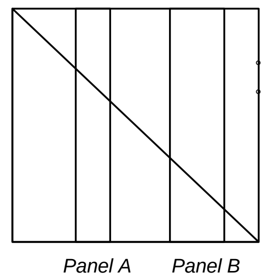


Out of Core Approach

- High-level I/O Interface
- ScaLAPACK uses a `Right-looking' variant for LU, QR and Cholesky factorizations.
- A `Left-looking' variant is used for Out-of-core factorization to reduce I/O traffic.
- Requires two in-core column panels.
- Imposes another level in the memory hierarchy.

73

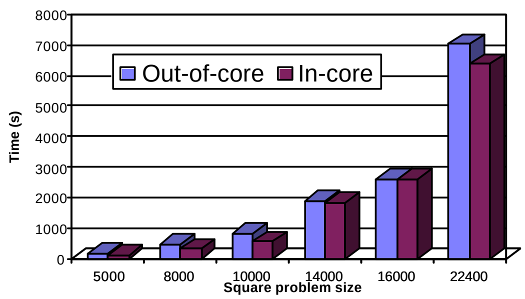
Out of Core Algorithm



- Hybrid approach
- Algorithm is ``Left-Looking'' in nature, but uses ``Right-Looking'' (ScaLAPACK) on Panel B
- Latency Tolerant
- Model for deep memory hierarchy algorithms

74

QR Factorization on 64 processors Intel Paragon



References

- http://www.netlib.org
- http://www.netlib.org/lapack
- http://www.netlib.org/scalapack
- http://www.netlib.org/lapack/lawns
- http://www.netlib.org/atlas
- http://www.netlib.org/papi/
- http://www.netlib.org/netsolve/
- http://www.netlib.org/lapack90
- http://www.nhse.org

- lapack@cs.utk.edu
- scalapack@cs.utk.edu

76