Lecture 14: Dense Linear Algebra

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Where we are

- This week: *dense* linear algebra
- Next week: *sparse* linear algebra

Numerical linear algebra in a nutshell

- Basic problems
  - Linear systems: $Ax = b$
  - Least squares: minimize $\|Ax - b\|_2^2$
  - Eigenvalues: $Ax = \lambda x$
- Basic paradigm: matrix factorization
  - $A = LU$, $A = LL^T$
  - $A = QR$
  - $A = V \Lambda V^{-1}$, $A = QTQ^T$
  - $A = U \Sigma V^T$
- Factorization $\equiv$ switch to basis that makes problem easy

Numerical linear algebra in a nutshell

Two flavors: dense and sparse

- Dense == common structures, no complicated indexing
  - General dense (all entries nonzero)
  - Banded (zero below/above some diagonal)
  - Symmetric/Hermitian
  - Standard, robust algorithms (LAPACK)
- Sparse == stuff not stored in dense form!
  - Maybe few nonzeros (e.g. compressed sparse row formats)
  - May be implicit (e.g. via finite differencing)
  - May be "dense", but with compact repn (e.g. via FFT)
  - Most algorithms are iterative; wider variety, more subtle
  - Build on dense ideas

History

BLAS 1 (1973–1977)

- Standard library of 15 ops (mostly) on vectors
  - Up to four versions of each: S/D/C/Z
  - Example: DAXPY
    - Double precision (real)
    - Computes $Ax + y$
  - Goals
    - Raise level of programming abstraction
    - Robust implementation (e.g. avoid over/underflow)
    - Portable interface, efficient machine-specific implementation
  - BLAS 1 == $O(n^1)$ ops on $O(n^1)$ data
  - Used in LINPACK (and EISPACK?)

History

BLAS 2 (1984–1986)

- Standard library of 25 ops (mostly) on matrix/vector pairs
  - Different data types and matrix types
  - Example: DGEMV
    - Double precision
    - GEneral matrix
    - Matrix-Vector product
- Goals
  - BLAS1 insufficient
  - BLAS2 for better vectorization (when vector machines roamed)
- BLAS2 == $O(n^2)$ ops on $O(n^2)$ data

History

BLAS 3 (1987–1988)

- Standard library of 9 ops (mostly) on matrix/matrix
  - Different data types and matrix types
  - Example: DGEMM
    - Double precision
    - GEneral matrix
    - Matrix-Matrix product
  - BLAS3 == $O(n^3)$ ops on $O(n^2)$ data
- Goals
  - Efficient cache utilization!

BLAS goes on

- `http://www.netlib.org/blas`
- CBLAS interface standardized
- Lots of implementations (MKL, Veclib, ATLAS, Goto, ...)
- Still new developments (XBLAS, tuning for GPUs, ...)

Why BLAS?

Consider Gaussian elimination.

LU for 2×2:

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ c/a & 1 \end{bmatrix} \begin{bmatrix} a & b \\ 0 & d - bc/a \end{bmatrix}$$

Block elimination

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} = \begin{bmatrix} I & 0 \\ CA^{-1} & I \end{bmatrix} \begin{bmatrix} A & B \\ 0 & D - CA^{-1}B \end{bmatrix}$$

Block LU

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} = \begin{bmatrix} L_{11} & 0 \\ L_{12} & L_{22} \end{bmatrix} \begin{bmatrix} U_{11} & U_{12} \\ 0 & U_{22} \end{bmatrix} = \begin{bmatrix} L_{11}U_{11} & L_{11}U_{12} \\ L_{12}U_{11} & L_{21}U_{12} + L_{22}U_{22} \end{bmatrix}$$

Why BLAS?

Block LU

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} = \begin{bmatrix} L_{11} & 0 \\ L_{12} & L_{22} \end{bmatrix} \begin{bmatrix} U_{11} & U_{12} \\ 0 & U_{22} \end{bmatrix} = \begin{bmatrix} L_{11}U_{11} & L_{11}U_{12} \\ L_{12}U_{11} & L_{21}U_{12} + L_{22}U_{22} \end{bmatrix}$$

Think of A as $k \times k$, k moderate:

```
[L11,U11] = small_lu(A);    % Small block LU
U12 = L11\B;                % Triangular solve
L12 = C/U11;                % "
S   = D-L21*U12;            % Rank m update
[L22,U22] = lu(S);          % Finish factoring
```

Three level-3 BLAS calls!

- Two triangular solves
- One rank-k update

LAPACK

LAPACK (1989–present):
`http://www.netlib.org/lapack`

- Supercedes earlier LINPACK and EISPACK
- High performance through BLAS
  - Parallel to the extent BLAS are parallel (on SMP)
  - Linear systems and least squares are nearly 100% BLAS 3
  - Eigenproblems, SVD — only about 50% BLAS 3
- Careful error bounds on everything
- Lots of variants for different structures

ScaLAPACK

ScaLAPACK (1995–present):

`http://www.netlib.org/scalapack`

- MPI implementations
- Only a small subset of LAPACK functionality

Why is ScaLAPACK not all of LAPACK?

Consider what LAPACK contains...

Decoding LAPACK names

- F77 $\implies$ limited characters per name
- General scheme:
  - Data type (double/single/double complex/single complex)
  - Matrix type (general/symmetric, banded/not banded)
  - Operation type
- Example: DGETRF
  - Double precision
  - GEneral matrix
  - TRiangular Factorization
- Example: DSYEVX
  - Double precision
  - General SYmmetric matrix
  - EigenValue computation, eXpert driver

Structures

- General: general (GE), banded (GB), pair (GG), tridiag (GT)
- Symmetric: general (SY), banded (SB), packed (SP), tridiag (ST)
- Hermitian: general (HE), banded (HB), packed (HP)
- Positive definite (PO), packed (PP), tridiagonal (PT)
- Orthogonal (OR), orthogonal packed (OP)
- Unitary (UN), unitary packed (UP)
- Hessenberg (HS), Hessenberg pair (HG)
- Triangular (TR), packed (TP), banded (TB), pair (TG)
- Bidiagonal (BD)

LAPACK routine types

- Linear systems (general, symmetric, SPD)
- Least squares (overdetermined, underdetermined, constrained, weighted)
- Symmetric eigenvalues and vectors
  - Standard: $Ax = \lambda x$
  - Generalized: $Ax = \lambda Bx$
- Nonsymmetric eigenproblems
  - Schur form: $A = QTQ^T$
  - Eigenvalues/vectors
  - Invariant subspaces
  - Generalized variants
- SVD (standard/generalized)
- Different interfaces
  - Simple drivers
  - Expert drivers with error bounds, extra precision, etc
  - Low-level routines
  - ... and ongoing discussions! (e.g. about C interfaces)

Matrix vector product

Simple $y = Ax$ involves two indices

$$y_i = \sum_j A_{ij} x_j$$

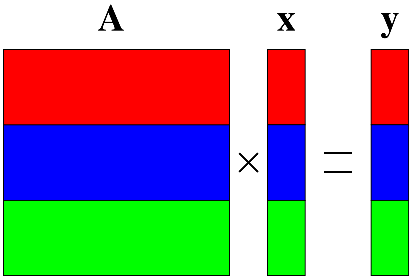
Can organize around either one:

```
% Row-oriented
for i = 1:n
  y(i) = A(i,:)*x;
end

% Col-oriented
y = 0;
for j = 1:n
  y = y + A(:,j)*x(j);
end
```

... or deal with index space in other ways!

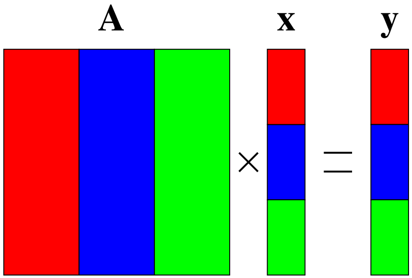
Parallel matvec: 1D row-blocked



Receive broadcast x_0, x_1, x_2 into local x_0, x_1, x_2; then

$$
\begin{aligned}
&\text{On P0:} \quad A_{00}x_0 + A_{01}x_1 + A_{02}x_2 = y_0 \\
&\text{On P1:} \quad A_{10}x_0 + A_{11}x_1 + A_{12}x_2 = y_1 \\
&\text{On P2:} \quad A_{20}x_0 + A_{21}x_1 + A_{22}x_2 = y_2
\end{aligned}
$$

Parallel matvec: 1D col-blocked

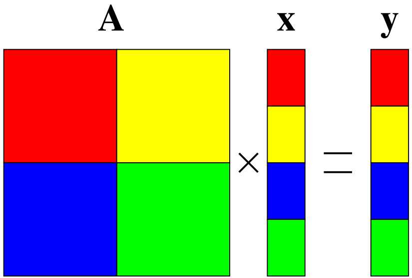


Independently compute

$$z^{(0)} = \begin{bmatrix} A_{00} \\ A_{10} \\ A_{20} \end{bmatrix} x_0 \qquad z^{(1)} = \begin{bmatrix} A_{00} \\ A_{10} \\ A_{20} \end{bmatrix} x_1 \qquad z^{(2)} = \begin{bmatrix} A_{00} \\ A_{10} \\ A_{20} \end{bmatrix} x_2$$

and perform reduction: $y = z^{(0)} + z^{(1)} + z^{(2)}$.

Parallel matvec: 2D blocked



- Involves broadcast *and* reduction
- ... but with subsets of processors

Parallel matvec: 2D blocked

Broadcast x_0, x_1 to local copies x_0, x_1 at P0 and P2
Broadcast x_2, x_3 to local copies x_2, x_3 at P1 and P3

In parallel, compute

$$\begin{bmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = \begin{bmatrix} z_0^{(0)} \\ z_1^{(0)} \end{bmatrix} \qquad \begin{bmatrix} A_{02} & A_{03} \\ A_{12} & A_{13} \end{bmatrix} \begin{bmatrix} x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} z_0^{(1)} \\ z_1^{(1)} \end{bmatrix}$$

$$\begin{bmatrix} A_{20} & A_{21} \\ A_{30} & A_{31} \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = \begin{bmatrix} z_2^{(3)} \\ z_3^{(3)} \end{bmatrix} \qquad \begin{bmatrix} A_{20} & A_{21} \\ A_{30} & A_{31} \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = \begin{bmatrix} z_2^{(3)} \\ z_3^{(3)} \end{bmatrix}$$

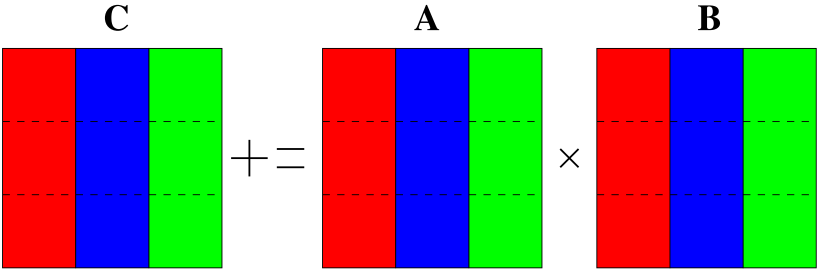
Reduce across rows:

$$\begin{bmatrix} y_0 \\ y_1 \end{bmatrix} = \begin{bmatrix} z_0^{(0)} \\ z_1^{(0)} \end{bmatrix} + \begin{bmatrix} z_0^{(1)} \\ z_1^{(1)} \end{bmatrix} \qquad \begin{bmatrix} y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} z_2^{(2)} \\ z_3^{(2)} \end{bmatrix} + \begin{bmatrix} z_2^{(3)} \\ z_3^{(3)} \end{bmatrix}$$

Parallel matmul

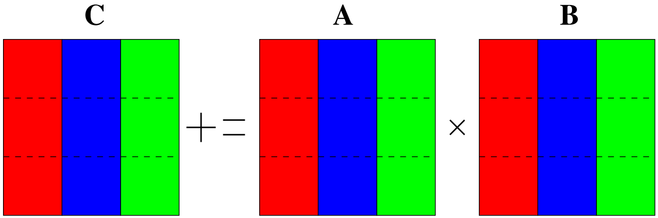
- Basic operation: $C = C + AB$
- Computation: $2n^3$ flops
- Goal: $2n^3/p$ flops per processor, minimal communication

1D layout



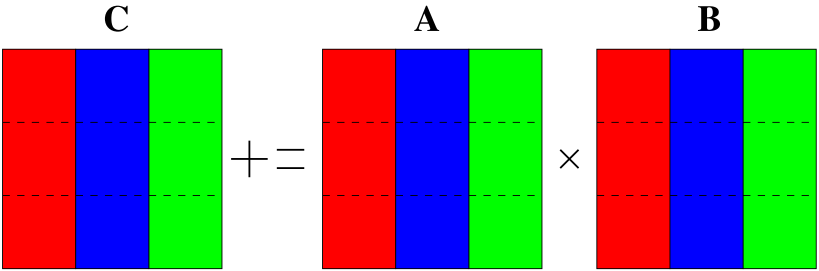
- Block MATLAB notation: $A(:, j)$ means jth block column
- Processor j owns $A(:, j)$, $B(:, j)$, $C(:, j)$
- $C(:, j)$ depends on *all* of A, but only $B(:, j)$
- How do we communicate pieces of A?

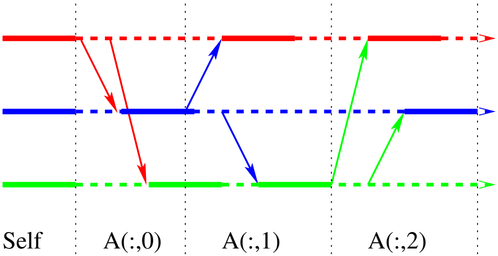
1D layout on bus (no broadcast)



- Everyone computes local contributions first
- P0 sends $A(:,0)$ to each processor j in turn; processor j receives, computes $A(:,0)B(0,j)$
- P1 sends $A(:,1)$ to each processor j in turn; processor j receives, computes $A(:,1)B(1,j)$
- P2 sends $A(:,2)$ to each processor j in turn; processor j receives, computes $A(:,2)B(2,j)$

1D layout on bus (no broadcast)





1D layout on bus (no broadcast)

```
C(:,myproc) += A(:,myproc)*B(myproc,myproc)
for i = 0:p-1
  for j = 0:p-1
    if (i == j)       continue;
    if (myproc == i) i
      send A(:,i) to processor j
    if (myproc == j)
      receive A(:,i) from i
      C(:,myproc) += A(:,i)*B(i,myproc)
    end
  end
end
```

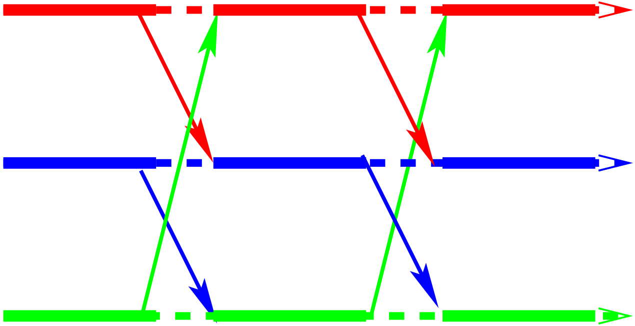
Performance model?

1D layout on bus (no broadcast)

No overlapping communications, so in a simple $\alpha - \beta$ model:

- $p(p-1)$ messages
- Each message involves n^2/p data
- Communication cost: $p(p-1)\alpha + (p-1)n^2\beta$

1D layout on ring



- Every process j can send data to $j + 1$ simultaneously
- Pass slices of A around the ring until everyone sees the whole matrix ($p - 1$ phases).

1D layout on ring

```
tmp = A(myproc)
C(myproc) += tmp*B(myproc,myproc)
for j = 1 to p-1
  sendrecv tmp to myproc+1 mod p,
           from myproc-1 mod p
  C(myproc) += tmp*B(myproc-j mod p, myproc)
```

Performance model?

1D layout on ring

In a simple $\alpha - \beta$ model, at each processor:

- $p - 1$ message sends (and simultaneous receives)
- Each message involves n^2/p data
- Communication cost: $(p - 1)\alpha + (1 - 1/p)n^2\beta$

Outer product algorithm

Serial: Recall outer product organization:

```
for k = 0:s-1
  C += A(:,k)*B(k,:);
end
```

Parallel: Assume $p = s^2$ processors, block $s \times s$ matrices.
For a 2×2 example:

$$\begin{bmatrix} C_{00} & C_{01} \\ C_{10} & C_{11} \end{bmatrix} = \begin{bmatrix} A_{00}B_{00} & A_{00}B_{01} \\ A_{10}B_{00} & A_{10}B_{01} \end{bmatrix} + \begin{bmatrix} A_{01}B_{10} & A_{01}B_{11} \\ A_{11}B_{10} & A_{11}B_{11} \end{bmatrix}$$

- Processor for each $(i, j) \implies$ parallel work for each k!
- Note everyone in row i uses $A(i, k)$ at once,
  and everyone in row j uses $B(k, j)$ at once.

Parallel outer product (SUMMA)

```
for k = 0:s-1
  for each i in parallel
    broadcast A(i,k) to row
  for each j in parallel
    broadcast A(k,j) to col
  On processor (i,j), C(i,j) += A(i,k)*B(k,j);
end
```

If we have tree along each row/column, then

- $\log(s)$ messages per broadcast
- $\alpha + \beta n^2/s^2$ per message
- $2\log(s)(\alpha s + \beta n^2/s)$ total communication
- Compare to 1D ring: $(p-1)\alpha + (1-1/p)n^2\beta$

Note: Same ideas work with block size $b < n/s$

Cannon's algorithm

$$\begin{bmatrix} C_{00} & C_{01} \\ C_{10} & C_{11} \end{bmatrix} = \begin{bmatrix} A_{00}B_{00} & A_{01}B_{11} \\ A_{11}B_{10} & A_{10}B_{01} \end{bmatrix} + \begin{bmatrix} A_{01}B_{10} & A_{00}B_{01} \\ A_{10}B_{00} & A_{11}B_{11} \end{bmatrix}$$

Idea: Reindex products in block matrix multiply

$$\begin{aligned} C(i,j) &= \sum_{k=0}^{p-1} A(i,k)B(k,j) \\ &= \sum_{k=0}^{p-1} A(i,\, k+i+j \mod p)\; B(k+i+j \mod p, j) \end{aligned}$$

For a fixed k, a given block of A (or B) is needed for contribution to *exactly one* $C(i,j)$.

Cannon's algorithm

```
% Move A(i,j) to A(i,i+j)
for i = 0 to s-1
  cycle A(i,:) left by i

% Move B(i,j) to B(i+j,j)
for j = 0 to s-1
  cycle B(:,j) up by j

for k = 0 to s-1
  in parallel;
    C(i,j) = C(i,j) + A(i,j)*B(i,j);
  cycle A(:,i) left by 1
  cycle B(:,j) up by 1
```

Cost of Cannon

- Assume 2D torus topology
- Initial cyclic shifts: $\leq s$ messages each ($\leq 2s$ total)
- For each phase: 2 messages each ($2s$ total)
- Each message is size n^2/s^2
- Communication cost: $4s(\alpha + \beta n^2/s^2) = 4(\alpha s + \beta n^2/s)$
- This communication cost is optimal!
  ... but SUMMA is simpler, more flexible, almost as good

Speedup and efficiency

Recall

$$\text{Speedup} := t_{\text{serial}}/t_{\text{parallel}}$$
$$\text{Efficiency} := \text{Speedup}/p$$

Assuming no overlap of communication and computation, efficiencies are

1D layout	$\left(1 + O\left(\frac{p}{n}\right)\right)^{-1}$
SUMMA	$\left(1 + O\left(\frac{\sqrt{p}\log p}{n}\right)\right)^{-1}$
Cannon	$\left(1 + O\left(\frac{\sqrt{p}}{n}\right)\right)^{-1}$