CS 5220

GEMV, GEMM, and LU

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Matrix multiply

Simple $y = Ax$ involves two indices:

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

Sums can go in any order!

Matrix vector product

Organize $y = Ax$ around rows or columns:

```
% 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!

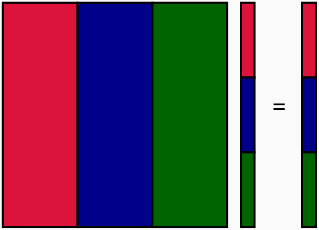
Parallel matvec: 1D row-blocked

Broadcast x, compute rows independently.

Parallel matvec: 1D row-blocked


```
Allgather(xlocal, xall)
ylocal = Alocal * xall
```

Parallel matvec: 1D col-blocked

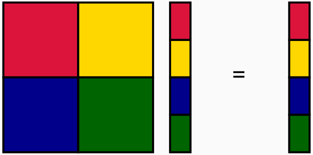


Compute partial matvecs and reduce.

Parallel matvec: 1D col-blocked


```
z = Alocal * xlocal
for j = 1:p
    Reduce(sum, z[i], ylocal at proc i)
end
```

Parallel matvec: 2D blocked

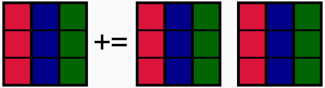


- Involves broadcast *and* reduction
- … but with subsets of processors

Parallel matmul

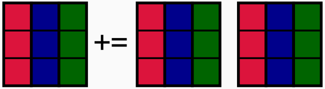
- Basic operation: $C = C + AB$
- Computation: $2n^3$ flops
- Goal: $2n^3/p$ flops per processor, minimal communication
- Two main contenders: SUMMA and Cannon

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 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).

```
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

Recall outer product organization:

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

Outer product algorithm

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

SUMMA + “pass it around?”

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

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

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

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

Speedup and efficiency

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	$\left(1 + O\left(\frac{\sqrt{p}}{n}\right)\right)^{-1}$

Assuming no overlap of communication and computation.

LU

Reminder: Evolution of LU

On board… or not.

$$\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 10 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 4 \\ 13 \\ 22 \end{bmatrix}$$

LU by example

$$\begin{bmatrix} 1 & 0 & 0 \\ -4 & 1 & 0 \\ -7 & 0 & 1 \end{bmatrix} \left(\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 10 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 4 \\ 13 \\ 22 \end{bmatrix} \right)$$

LU by example

$$\begin{bmatrix}1 & 2 & 3\\ 0 & -3 & -6\\ 0 & -6 & -11\end{bmatrix}\begin{bmatrix}x\\ y\\ z\end{bmatrix} = \begin{bmatrix}4\\ -3\\ -6\end{bmatrix}$$

LU by example

$$\begin{bmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & -2 & 1\end{bmatrix}\left(\begin{bmatrix}1 & 2 & 3\\ 0 & -3 & -6\\ 0 & -6 & -11\end{bmatrix}\begin{bmatrix}x\\ y\\ z\end{bmatrix}=\begin{bmatrix}4\\ -3\\ -6\end{bmatrix}\right)$$

LU by example

$$\begin{bmatrix} 1 & 2 & 3 \\ 0 & -3 & -6 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 4 \\ -3 \\ 0 \end{bmatrix}$$

LU by example

$$\begin{bmatrix} 1 & 0 & 0 \\ 4 & 1 & 0 \\ 7 & 2 & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 & 3 \\ 0 & -3 & -6 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 10 \end{bmatrix}$$

Simple LU

Overwrite A with L and U

```
for j = 1:n-1
  for i = j+1:n
    A(i,j) = A(i,j) / A(j,j);    % Compute multiplier
    for k = j+1:n
      A(i,k) -= A(i,j) * A(j,k); % Update row
    end
  end
end
```

Simple LU

Overwrite A with L and U

```
for j = 1:n-1
  A(j+1:n,j) = A(j+1:n,j)/A(j,j);          % Compute multipliers
  A(j+1:n,j+1:n) -= A(j+1:n,j) * A(j, j+1:n);  % Trailing update
end
```

Pivoting

Stability is a problem! Compute $PA = LU$

```
p = 1:n;
for j = 1:n-1
  [~,jpiv] = max(abs(A(j+1:n,j)));              % Find pivot
 A([j, j+jpiv-1],:) = A([j+jpiv-1, j]);      % Swap pivot row
 p([j, j+jpiv-1],:) = p([j+jpiv-1, j]);      % Save pivot info
 A(j+1:n,j) = A(j+1:n,j)/A(j,j);             % Compute multipliers
 A(j+1:n,j+1:n) -= A(j+1:n,j) * A(j, j+1:n);  % Trailing update
end
```

Blocking

Think in a way that uses level 3 BLAS

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} = \begin{bmatrix} L_{11} & 0 \\ L_{21} & L_{22} \end{bmatrix} \begin{bmatrix} U_{11} & U_{12} \\ 0 & U_{22} \end{bmatrix}$$

Blocking

Think in a way that uses level 3 BLAS

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} = \begin{bmatrix} L_{11}U_{11} & L_{11}U_{12} \\ L_{21}U_{11} & L_{21}U_{12} + L_{22}U_{22} \end{bmatrix}$$

Blocking

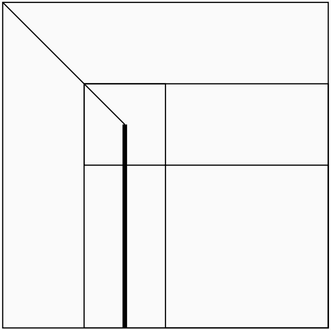
Think in a way that uses level 3 BLAS

$$\begin{aligned} L_{11}U_{11} &= A_{11} \\ U_{12} &= L_{11}^{-1}A_{12} \\ L_{21} &= A_{21}U_{11}^{-1} \\ L_{22}U_{22} &= A_{22} - L_{21}U_{12} \end{aligned}$$

Enter pictures

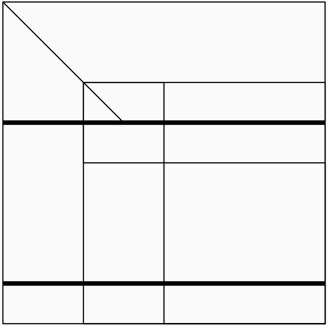
- Still haven't showed how to do pivoting!
- Easier to draw diagrams from here
- Take 6210 or 4220 if you want more on LU!

Blocked GEPP



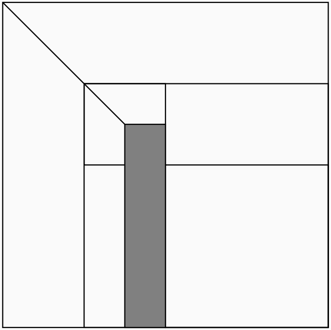
Find pivot

Blocked GEPP



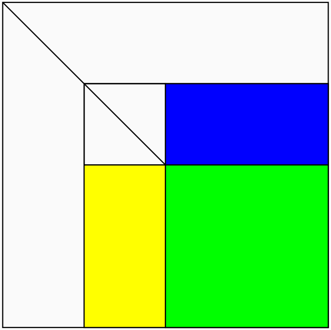
Swap pivot row

Blocked GEPP



Update within block column

Blocked GEPP



Delayed update (at end of block)

Big idea

- *Delayed update* strategy lets us do LU fast
    - Could have also delayed application of pivots
- Same idea with other one-sided factorizations (QR)
- Decent multi-core speedup with parallel BLAS!

  ... assuming n sufficiently large.

Issues left over (block size?)...

Explicit parallelization of GE

What to do:

- *Decompose* into work chunks
- *Assign* work to threads in a balanced way
- *Orchestrate* communication + synchronization
- *Map* which processors execute which threads

Possible matrix layouts

How should we share the matrix across ranks?

1D col blocked

$$\begin{bmatrix} 0 & 0 & 0 & 1 & 1 & 1 & 2 & 2 & 2 \\ 0 & 0 & 0 & 1 & 1 & 1 & 2 & 2 & 2 \\ 0 & 0 & 0 & 1 & 1 & 1 & 2 & 2 & 2 \\ 0 & 0 & 0 & 1 & 1 & 1 & 2 & 2 & 2 \\ 0 & 0 & 0 & 1 & 1 & 1 & 2 & 2 & 2 \\ 0 & 0 & 0 & 1 & 1 & 1 & 2 & 2 & 2 \\ 0 & 0 & 0 & 1 & 1 & 1 & 2 & 2 & 2 \\ 0 & 0 & 0 & 1 & 1 & 1 & 2 & 2 & 2 \\ 0 & 0 & 0 & 1 & 1 & 1 & 2 & 2 & 2 \end{bmatrix}$$

1D col cyclic

$$\begin{bmatrix} 0 & 1 & 2 & 0 & 1 & 2 & 0 & 1 & 2 \\ 0 & 1 & 2 & 0 & 1 & 2 & 0 & 1 & 2 \\ 0 & 1 & 2 & 0 & 1 & 2 & 0 & 1 & 2 \\ 0 & 1 & 2 & 0 & 1 & 2 & 0 & 1 & 2 \\ 0 & 1 & 2 & 0 & 1 & 2 & 0 & 1 & 2 \\ 0 & 1 & 2 & 0 & 1 & 2 & 0 & 1 & 2 \\ 0 & 1 & 2 & 0 & 1 & 2 & 0 & 1 & 2 \\ 0 & 1 & 2 & 0 & 1 & 2 & 0 & 1 & 2 \\ 0 & 1 & 2 & 0 & 1 & 2 & 0 & 1 & 2 \end{bmatrix}$$

1D col block cyclic

$$\begin{bmatrix} 0 & 0 & 1 & 1 & 2 & 2 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 2 & 2 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 2 & 2 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 2 & 2 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 2 & 2 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 2 & 2 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 2 & 2 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 2 & 2 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 2 & 2 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 2 & 2 & 0 & 0 & 1 & 1 \end{bmatrix}$$

Block skewed

$$\begin{bmatrix} 0 & 0 & 0 & 1 & 1 & 1 & 2 & 2 & 2 \\ 0 & 0 & 0 & 1 & 1 & 1 & 2 & 2 & 2 \\ 0 & 0 & 0 & 1 & 1 & 1 & 2 & 2 & 2 \\ 2 & 2 & 2 & 0 & 0 & 0 & 1 & 1 & 1 \\ 2 & 2 & 2 & 0 & 0 & 0 & 1 & 1 & 1 \\ 2 & 2 & 2 & 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 2 & 2 & 2 & 0 & 0 & 0 \\ 1 & 1 & 1 & 2 & 2 & 2 & 0 & 0 & 0 \\ 1 & 1 & 1 & 2 & 2 & 2 & 0 & 0 & 0 \end{bmatrix}$$

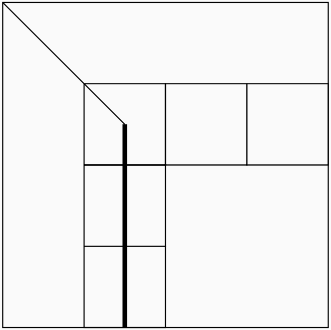
2D block cyclic

$$\begin{bmatrix} 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 2 & 2 & 3 & 3 & 2 & 2 & 3 & 3 \\ 2 & 2 & 3 & 3 & 2 & 2 & 3 & 3 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 2 & 2 & 3 & 3 & 2 & 2 & 3 & 3 \\ 2 & 2 & 3 & 3 & 2 & 2 & 3 & 3 \end{bmatrix}$$

Possible matrix layouts

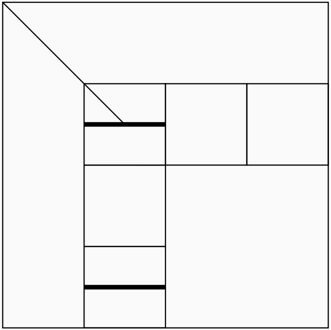
- 1D col blocked: bad load balance
- 1D col cyclic: hard to use BLAS2/3
- 1D col block cyclic: factoring col a bottleneck
- Block skewed (a la Cannon): just complicated
- 2D row/col block: bad load balance
- 2D row/col block cyclic: win!

Distributed GEPP

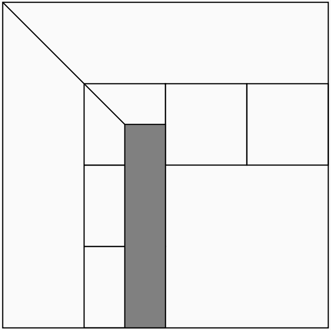


Find pivot (column broadcast)

Distributed GEPP

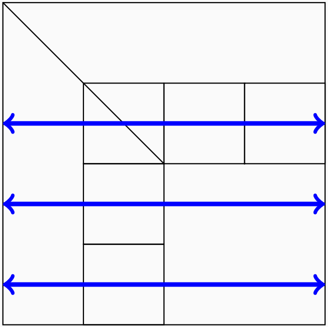


Swap pivot row within block column + broadcast pivot



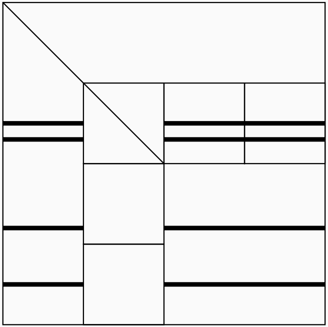
Update within block column

Distributed GEPP

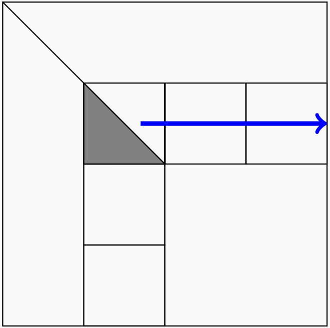


At end of block, broadcast swap info along rows

Distributed GEPP

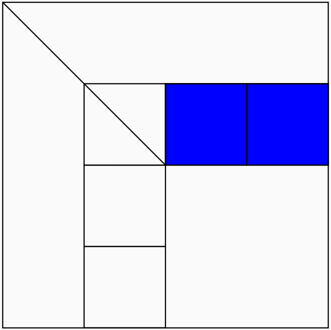


Apply all row swaps to other columns



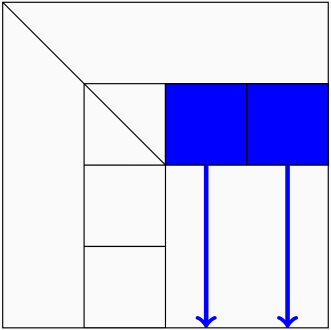
Broadcast block L_{II} right

Distributed GEPP



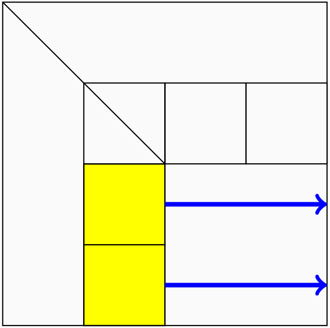
Update remainder of block row

Distributed GEPP



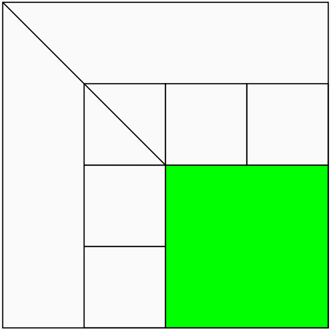
Broadcast rest of block row down

Distributed GEPP



Broadcast rest of block col right

Distributed GEPP



Update of trailing submatrix

Cost of ScaLAPACK GEPP

Communication costs:

- Lower bound: $O(n^2/\sqrt{P})$ words, $O(\sqrt{P})$ messages
- ScaLAPACK:
  - $O(n^2 \log P/\sqrt{P})$ words sent
  - $O(n \log p)$ messages
  - Problem: reduction to find pivot in each column
- Tournaments for stability without partial pivoting

If you don't care about dense LU?

Let's review some ideas in a different setting...

Goal: All pairs shortest path lengths.

Idea: Dynamic programming! Define

$$d_{ij}^{(k)} = \text{shortest path } i \text{ to } j \text{ with intermediates in } \{1, \ldots, k\}.$$

Then

$$d_{ij}^{(k)} = \min\left(d_{ij}^{(k-1)}, d_{ik}^{(k-1)} + d_{kj}^{(k-1)}\right)$$

and $d_{ij}^{(n)}$ is the desired shortest path length.

Floyd's algorithm for all-pairs shortest paths:

```
for k=1:n
  for i = 1:n
    for j = 1:n
      D(i,j) = min(D(i,j), D(i,k)+D(k,j));
```

Unpivoted Gaussian elimination (overwriting A):

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

The same and different

- The same: $O(n^3)$ time, $O(n^2)$ space
- The same: can't move k loop (data dependencies)
  - … at least, can't without care!
  - Different from matrix multiplication
- The same: $x_{ij}^{(k)} = f\left(x_{ij}^{(k-1)}, g\left(x_{ik}^{(k-1)}, x_{kj}^{(k-1)}\right)\right)$
  - Same basic dependency pattern in updates!
  - Similar algebraic relations satisfied
- Different: Update to full matrix vs trailing submatrix

How far can we get?

How would we write

- Cache-efficient (blocked) *serial* implementation?
- Message-passing *parallel* implementation?

The full picture could make a fun class project...

Onward!

Next up: Sparse linear algebra and iterative solvers!