Lecture 16: Dense Linear Algebra II

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Review: 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

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)

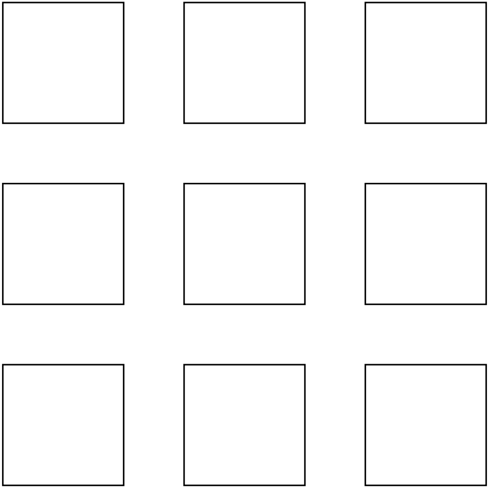
```
for k = 0:s-1
  for each i in parallel
    broadcast A(i,k) to row
  for each j in parallel
    broadcast A(k,j) to col
  On processor (i,j), C(i,j) += A(i,k)*B(k,j);
end
```

If we have tree along each row/column, then

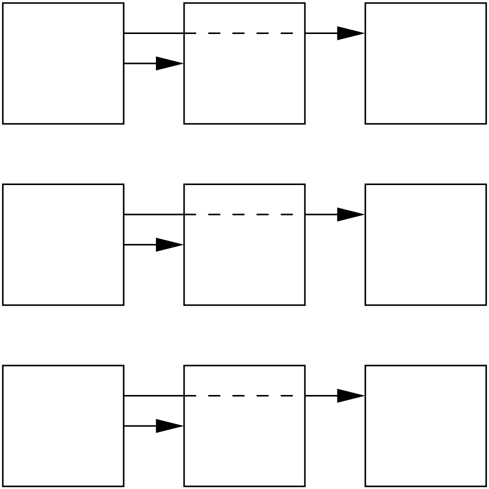
- $\log(s)$ messages per broadcast
- $\alpha + \beta n^2/s^2$ per message
- $2\log(s)(\alpha s + \beta n^2/s)$ total communication
- Compare to 1D ring: $(p-1)\alpha + (1-1/p)n^2\beta$

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

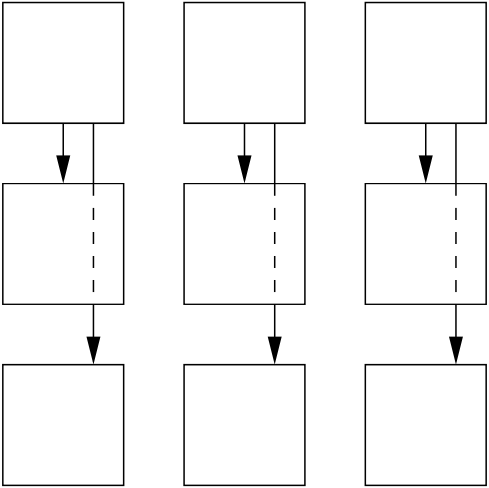
SUMMA



SUMMA



SUMMA



Parallel outer product (SUMMA)

If we have tree along each row/column, then

- $\log(s)$ messages per broadcast
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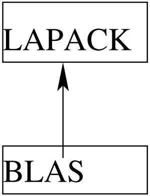
Assuming communication and computation can potentially overlap *completely*, what does the speedup curve look like?

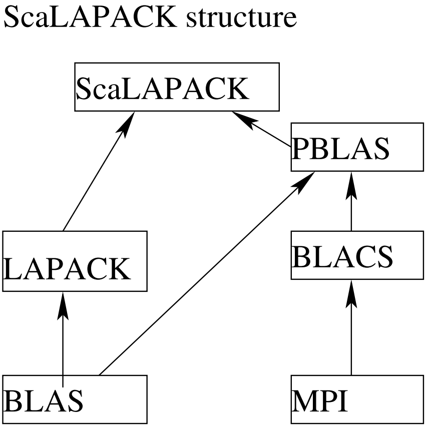
Reminder: Why matrix multiply?

LAPACK structure



Build fast serial linear algebra (LAPACK) on top of BLAS 3.

Reminder: Why matrix multiply?

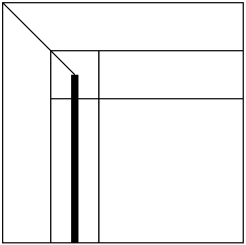


ScaLAPACK builds additional layers on same idea.

Reminder: Evolution of LU

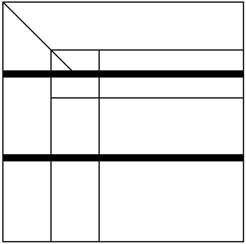
On board...

Blocked GEPP



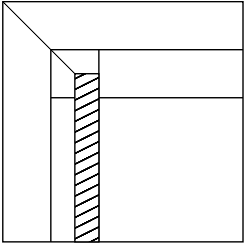
Find pivot

Blocked GEPP



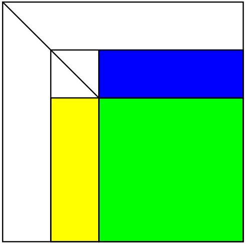
Swap pivot row

Blocked GEPP



Update within block

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)
- Can get decent multi-core speedup with parallel BLAS!
  ... assuming n sufficiently large.

There are still some issues left over (block size? pivoting?)...

Explicit parallelization of GE

What to do:

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

Possible matrix layouts

1D column blocked: bad load balance

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

Possible matrix layouts

1D column cyclic: hard to use BLAS2/3

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

Possible matrix layouts

1D column block cyclic: block column factorization a bottleneck

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

Possible matrix layouts

Block skewed: indexing gets messy

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

Possible matrix layouts

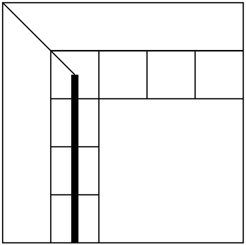
2D block cyclic:

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

Possible matrix layouts

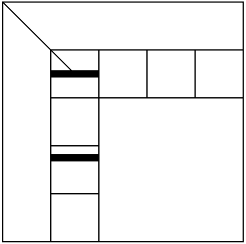
- 1D column blocked: bad load balance
- 1D column cyclic: hard to use BLAS2/3
- 1D column block cyclic: factoring column is a bottleneck
- Block skewed (a la Cannon): just complicated
- 2D row/column block: bad load balance
- 2D row/column block cyclic: win!

Distributed GEPP



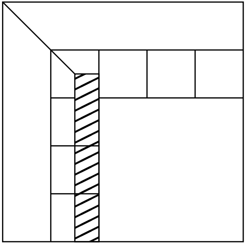
Find pivot (column broadcast)

Distributed GEPP



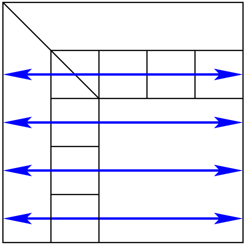
Swap pivot row within block column + broadcast pivot

Distributed GEPP



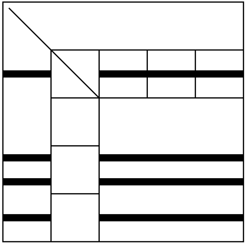
Update within block column

Distributed GEPP



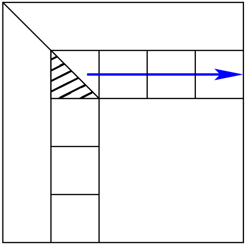
At end of block, broadcast swap info along rows

Distributed GEPP



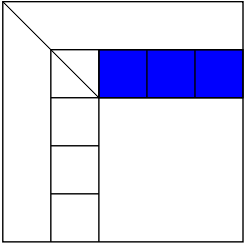
Apply all row swaps to other columns

Distributed GEPP



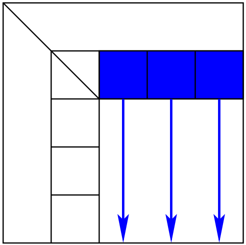
Broadcast block L_{II} right

Distributed GEPP



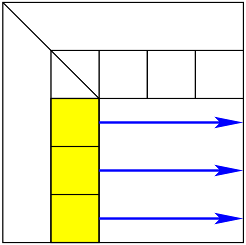
Update remainder of block row

Distributed GEPP



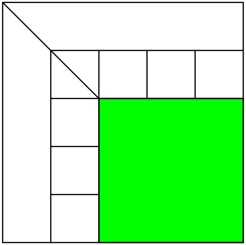
Broadcast rest of block row down

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
- Recent research on stable variants without partial pivoting

What if you don't care about dense Gaussian elimination?
Let's review some ideas in a different setting...

Floyd-Warshall

Goal: Find shortest path lengths between all node pairs.

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.

The same and different

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 a cache-efficient (blocked) *serial* implementation?
- Write a message-passing *parallel* implementation?

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

Onward!

Next up: Sparse linear algebra and iterative solvers!