

CS601: Software Development for Scientific Computing

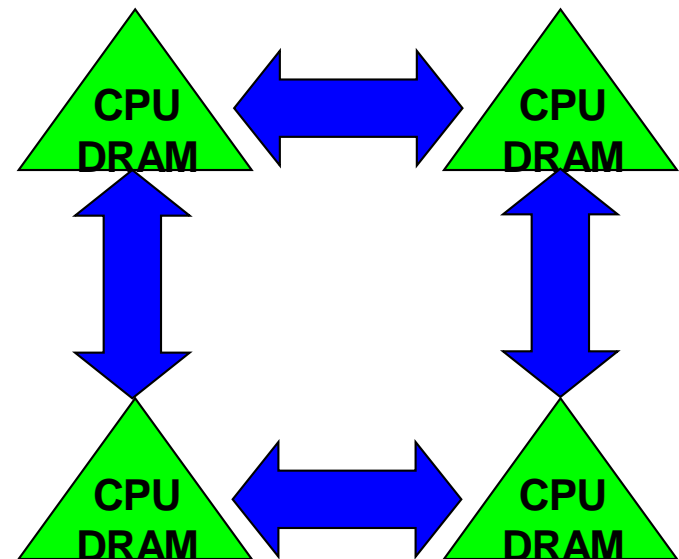
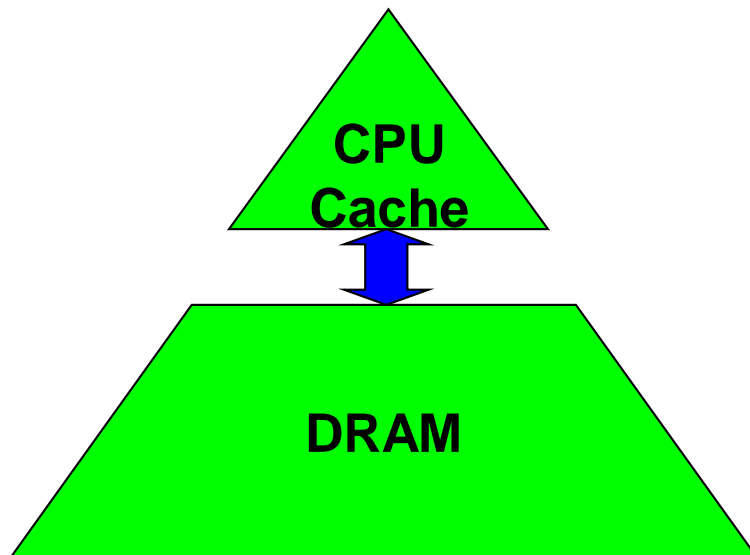
Autumn 2024

Week6: Matrix Computations with Dense Matrices
(contd.)

Costs Involved

Algorithms have two costs:

1. Arithmetic (FLOPS)
2. Communication: moving data between
 - levels of a **memory hierarchy** (sequential case)
 - **processors over a network** (parallel case).



Computational Intensity

- Connection between computation and communication cost
- Average number of operations performed per data element (word) read/written from slow memory
 - E.g. Read/written m words from memory. Perform f operations on m words.
 - Computational Intensity $q = f/m$ (*flops per word*).
- Goal: we want to *maximize* the computational intensity
 - We want to minimize words moved (read/written)
 - We want to minimize messages sent

What is the computational intensity, q , for:
axpy?

Matrix-Vector product?

Matrix-Matrix product?

Computational Intensity - axpy

Note: a slightly changed variant of axpy. There are n scalars (x_i) here.

$$\begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{bmatrix} + [x_1 \quad x_2 \quad \dots \quad x_n]^T \cdot * \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{bmatrix} + \begin{bmatrix} x_1 \times y_1 \\ x_2 \times y_2 \\ \vdots \\ x_n \times y_n \end{bmatrix}$$

*. * indicates component-wise multiplication*

```
Read(x) //read x from slow memory
```

```
Read(y) //read y from slow memory
```

```
Read(c) //read c from slow memory
```

```
for i=1 to n
```

```
    c[i] = c[i] + x[i]*y[i] //do arithmetic on data read
```

```
Write(c) //write c back to slow memory
```

- Number of memory operations = $4n$ (assuming one word of storage for each component (x_i, y_i, c_i) of vectors x, y, c resp.)
- Number of arithmetic operations = $2n$ (one addition and one multiplication per row.)
- **$q=2n/4n = 1/2$**

Computational Intensity – matrix-vector

- Assume $m=r=n =n$

$$\begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_m \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_m \end{bmatrix} + \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1r} \\ a_{21} & a_{22} & \cdots & a_{2r} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mr} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_r \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_m \end{bmatrix} + \begin{bmatrix} a_{11}x_1 + a_{12}x_2 + \cdots + a_{1r}x_r \\ a_{21}x_1 + a_{22}x_2 + \cdots + a_{2r}x_r \\ \vdots \\ a_{m1}x_1 + a_{m2}x_2 + \cdots + a_{mr}x_r \end{bmatrix}$$

- Number of memory operations = $n^2 + 3n = n^2 + O(n)$
- Number of arithmetic operations = $2n^2$
- $q \approx 2n^2/n^2 = 2$

Communication Cost – Matrix-Matrix Product

//Assume A, B, C are all nxn

```
for i=1 to n
  for j=1 to n
    for k=1 to n
      C(i,j)=C(i,j) + A(i,k)*B(k,j)
```

- loop k=1 to n: read C(i,j) into fast memory and update in fast memory
- End of loop k=1 to n: write C(i,j) back to slow memory

- n^2 words read: each row of A read once for each i.
- Assume that row i of A stays in fast memory during j=2, .. J=n
- Reading a row i of A

n^2 words read and n^2 words written (each entry of C read/written to memory once).
= $2 n^2$ words read/written

- Reading column j of B
- Suppose there is space in fast memory to hold only one column of B (in addition to one row of A and 1 element of C), then every column of B is read in **inner two loops**.
- Each column of B read n times including **outer i loop** = n^3 words read

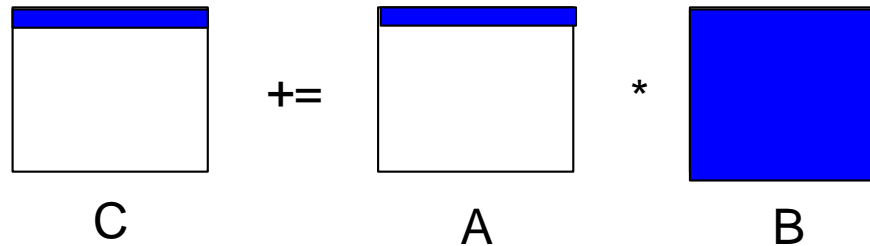
total cost = $3 n^2 + n^3$ (if the cache size is $n+n+1$)

Computational Intensity – Matrix-Matrix Product

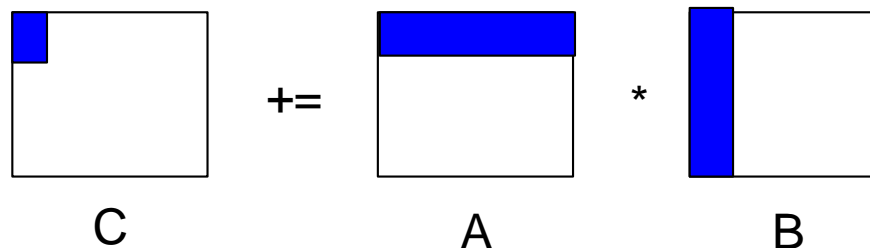
- Words moved = $n^3 + 3n^2 = n^3 + O(n^2)$
- Number of arithmetic operations = $2n^3$
- computational intensity $q \approx 2n^3/n^3 = 2$. (computation to communication ratio)
- Can we do better?

Insight - Data reuse

- How many memory accesses needed to compute a row of C, where 4096x4096 are the sizes of matrices.



- How many memory accesses needed to compute a tile of C of size 64x64?



Blocked Matrix Multiply

- For $N=4$:

$$\begin{bmatrix} C1 & C2 & C3 & C4 \end{bmatrix} = \begin{bmatrix} C1 & C2 & C3 & C4 \end{bmatrix} + \begin{bmatrix} A \end{bmatrix} * \begin{bmatrix} B1 & B2 & B3 & B4 \end{bmatrix}$$

$$\begin{bmatrix} Cj \end{bmatrix} = \begin{bmatrix} Cj \end{bmatrix} + \begin{bmatrix} A \end{bmatrix} * \begin{bmatrix} Bj \end{bmatrix} = \begin{bmatrix} Cj \end{bmatrix} + \sum_{k=1}^n \begin{bmatrix} A(:,k) \end{bmatrix} * \begin{bmatrix} Bj(k,:) \end{bmatrix}$$

```
for j=1 to N
  for k=1 to n
    Cj=Cj + A(*,k) * Bj(k,*)
```

Blocked Matrix Multiply - Example

$$\begin{array}{c} C_1 \quad C_2 \quad C_3 \quad C_4 \\ \left[\begin{array}{c|c|c|c} c_{11} & c_{12} & c_{13} & c_{14} \\ c_{21} & c_{22} & c_{23} & c_{24} \\ c_{31} & c_{32} & c_{33} & c_{34} \\ c_{41} & c_{42} & c_{43} & c_{44} \end{array} \right] = \begin{array}{c} C_1 \quad C_2 \quad C_3 \quad C_4 \\ \left[\begin{array}{c|c|c|c} c_{11} & c_{12} & c_{13} & c_{14} \\ c_{21} & c_{22} & c_{23} & c_{24} \\ c_{31} & c_{32} & c_{33} & c_{34} \\ c_{41} & c_{42} & c_{43} & c_{44} \end{array} \right] + \begin{array}{c} A \\ \left[\begin{array}{c|c|c|c} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{array} \right] \end{array} \begin{array}{c} B_1 \quad B_2 \quad B_3 \quad B_4 \\ \left[\begin{array}{c|c|c|c} b_{11} & b_{12} & b_{13} & b_{14} \\ b_{21} & b_{22} & b_{23} & b_{24} \\ b_{31} & b_{32} & b_{33} & b_{34} \\ b_{41} & b_{42} & b_{43} & b_{44} \end{array} \right] \end{array}
 \end{array}$$

for k=1 to n

$$\begin{array}{c} j=1 \\ \left[\begin{array}{c} c_{11} \\ c_{21} \\ c_{31} \\ c_{41} \end{array} \right] = \left[\begin{array}{c} c_{11} \\ c_{21} \\ c_{31} \\ c_{41} \end{array} \right] + \left[\begin{array}{c|c|c|c} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{array} \right] * \left[\begin{array}{c} b_{11} \\ b_{21} \\ b_{31} \\ b_{41} \end{array} \right]
 \end{array}$$

.....

for k=1 to n

$$\begin{array}{c} j=4 \\ \left[\begin{array}{c} c_{14} \\ c_{24} \\ c_{34} \\ c_{44} \end{array} \right] = \left[\begin{array}{c} c_{14} \\ c_{24} \\ c_{34} \\ c_{44} \end{array} \right] + \left[\begin{array}{c|c|c|c} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{array} \right] * \left[\begin{array}{c} b_{14} \\ b_{24} \\ b_{34} \\ b_{44} \end{array} \right]
 \end{array}$$

Blocked Matrix Multiply - Example

$$\begin{array}{c|c|c|c} C_1 & C_2 & C_3 & C_4 \\ \hline \begin{bmatrix} c_{11} \\ c_{21} \\ c_{31} \\ c_{41} \end{bmatrix} & \begin{bmatrix} c_{12} \\ c_{22} \\ c_{32} \\ c_{42} \end{bmatrix} & \begin{bmatrix} c_{13} \\ c_{23} \\ c_{33} \\ c_{43} \end{bmatrix} & \begin{bmatrix} c_{14} \\ c_{24} \\ c_{34} \\ c_{44} \end{bmatrix} \\ \hline \end{array} = \begin{array}{c|c|c|c} C_1 & C_2 & C_3 & C_4 \\ \hline \begin{bmatrix} c_{11} \\ c_{21} \\ c_{31} \\ c_{41} \end{bmatrix} & \begin{bmatrix} c_{12} \\ c_{22} \\ c_{32} \\ c_{42} \end{bmatrix} & \begin{bmatrix} c_{13} \\ c_{23} \\ c_{33} \\ c_{43} \end{bmatrix} & \begin{bmatrix} c_{14} \\ c_{24} \\ c_{34} \\ c_{44} \end{bmatrix} \\ \hline \end{array} + \begin{array}{c|c|c|c} A & B_1 & B_2 & B_3 & B_4 \\ \hline \begin{bmatrix} a_{11} \\ a_{21} \\ a_{31} \\ a_{41} \end{bmatrix} & \begin{bmatrix} a_{12} \\ a_{22} \\ a_{32} \\ a_{42} \end{bmatrix} & \begin{bmatrix} a_{13} \\ a_{23} \\ a_{33} \\ a_{43} \end{bmatrix} & \begin{bmatrix} a_{14} \\ a_{24} \\ a_{34} \\ a_{44} \end{bmatrix} & \begin{bmatrix} b_{11} \\ b_{21} \\ b_{31} \\ b_{41} \end{bmatrix} & \begin{bmatrix} b_{12} \\ b_{22} \\ b_{32} \\ b_{42} \end{bmatrix} & \begin{bmatrix} b_{13} \\ b_{23} \\ b_{33} \\ b_{43} \end{bmatrix} & \begin{bmatrix} b_{14} \\ b_{24} \\ b_{34} \\ b_{44} \end{bmatrix} \\ \hline \end{array}$$

for k=1 to n



j=1

$$\begin{bmatrix} c_{11} \\ c_{21} \\ c_{31} \\ c_{41} \end{bmatrix} = \begin{bmatrix} c_{11} \\ c_{21} \\ c_{31} \\ c_{41} \end{bmatrix} + \begin{bmatrix} a_{11} \\ a_{21} \\ a_{31} \\ a_{41} \end{bmatrix} \begin{bmatrix} a_{12} & a_{13} & a_{14} \\ a_{22} & a_{23} & a_{24} \\ a_{32} & a_{33} & a_{34} \\ a_{42} & a_{43} & a_{44} \end{bmatrix} * \begin{bmatrix} b_{11} \\ b_{21} \\ b_{31} \\ b_{41} \end{bmatrix}$$

k=1

$$\begin{bmatrix} c_{11} \\ c_{21} \\ c_{31} \\ c_{41} \end{bmatrix} = \begin{bmatrix} c_{11} \\ c_{21} \\ c_{31} \\ c_{41} \end{bmatrix} + \begin{bmatrix} a_{11} \\ a_{21} \\ a_{31} \\ a_{41} \end{bmatrix} * [b_{11}] \quad \leftarrow \text{First row of } B_1$$

$$= \begin{bmatrix} c_{11} \\ c_{21} \\ c_{31} \\ c_{41} \end{bmatrix} = \begin{bmatrix} c_{11} \\ c_{21} \\ c_{31} \\ c_{41} \end{bmatrix} + \begin{bmatrix} a_{11}b_{11} \\ a_{21}b_{11} \\ a_{31}b_{11} \\ a_{41}b_{11} \end{bmatrix}$$

-  What is required to be in fast memory
-  What is operated upon

Blocked Matrix Multiply - Example

$$\begin{bmatrix} C_1 & C_2 & C_3 & C_4 \\ \begin{bmatrix} c_{11} \\ c_{21} \\ c_{31} \\ c_{41} \end{bmatrix} & \begin{bmatrix} c_{12} \\ c_{22} \\ c_{32} \\ c_{42} \end{bmatrix} & \begin{bmatrix} c_{13} \\ c_{23} \\ c_{33} \\ c_{43} \end{bmatrix} & \begin{bmatrix} c_{14} \\ c_{24} \\ c_{34} \\ c_{44} \end{bmatrix} \end{bmatrix} = \begin{bmatrix} C_1 & C_2 & C_3 & C_4 \\ \begin{bmatrix} c_{11} \\ c_{21} \\ c_{31} \\ c_{41} \end{bmatrix} & \begin{bmatrix} c_{12} \\ c_{22} \\ c_{32} \\ c_{42} \end{bmatrix} & \begin{bmatrix} c_{13} \\ c_{23} \\ c_{33} \\ c_{43} \end{bmatrix} & \begin{bmatrix} c_{14} \\ c_{24} \\ c_{34} \\ c_{44} \end{bmatrix} \end{bmatrix} + \begin{bmatrix} A & B_1 & B_2 & B_3 & B_4 \\ \begin{bmatrix} a_{11} \\ a_{21} \\ a_{31} \\ a_{41} \end{bmatrix} & \begin{bmatrix} a_{12} \\ a_{22} \\ a_{32} \\ a_{42} \end{bmatrix} & \begin{bmatrix} a_{13} \\ a_{23} \\ a_{33} \\ a_{43} \end{bmatrix} & \begin{bmatrix} a_{14} \\ a_{24} \\ a_{34} \\ a_{44} \end{bmatrix} & \begin{bmatrix} b_{11} \\ b_{21} \\ b_{31} \\ b_{41} \end{bmatrix} & \begin{bmatrix} b_{12} \\ b_{22} \\ b_{32} \\ b_{42} \end{bmatrix} & \begin{bmatrix} b_{13} \\ b_{23} \\ b_{33} \\ b_{43} \end{bmatrix} & \begin{bmatrix} b_{14} \\ b_{24} \\ b_{34} \\ b_{44} \end{bmatrix} \end{bmatrix}$$

for k=1 to n

$$\begin{matrix} j=1 \\ \begin{bmatrix} c_{11} \\ c_{21} \\ c_{31} \\ c_{41} \end{bmatrix} \end{matrix} = \begin{bmatrix} c_{11} \\ c_{21} \\ c_{31} \\ c_{41} \end{bmatrix} + \begin{bmatrix} a_{11} \\ a_{21} \\ a_{31} \\ a_{41} \end{bmatrix} \begin{bmatrix} a_{12} \\ a_{22} \\ a_{32} \\ a_{42} \end{bmatrix} \begin{bmatrix} a_{13} & a_{14} \\ a_{23} & a_{24} \\ a_{33} & a_{34} \\ a_{43} & a_{44} \end{bmatrix} * \begin{bmatrix} b_{11} \\ b_{21} \\ b_{31} \\ b_{41} \end{bmatrix}$$

$$\begin{matrix} k=2 \\ \begin{bmatrix} c_{11} \\ c_{21} \\ c_{31} \\ c_{41} \end{bmatrix} \end{matrix} = \begin{bmatrix} a_{11}b_{11} \\ a_{21}b_{11} \\ a_{31}b_{11} \\ a_{41}b_{11} \end{bmatrix} + \begin{bmatrix} a_{12} \\ a_{22} \\ a_{32} \\ a_{42} \end{bmatrix} * [b_{21}]$$

← Second row of B_1

Comes from partial
sum for C_1 computed
for k=1 (previous
slide)

$$\begin{bmatrix} c_{11} \\ c_{21} \\ c_{31} \\ c_{41} \end{bmatrix} = \begin{bmatrix} a_{11}b_{11} \\ a_{21}b_{11} \\ a_{31}b_{11} \\ a_{41}b_{11} \end{bmatrix} + \begin{bmatrix} a_{12}b_{21} \\ a_{22}b_{21} \\ a_{32}b_{21} \\ a_{42}b_{21} \end{bmatrix}$$

Blocked Matrix Multiply - Example

$$\begin{array}{c|c|c|c} C_1 & C_2 & C_3 & C_4 \\ \hline \begin{bmatrix} c_{11} \\ c_{21} \\ c_{31} \\ c_{41} \end{bmatrix} & \begin{bmatrix} c_{12} \\ c_{22} \\ c_{32} \\ c_{42} \end{bmatrix} & \begin{bmatrix} c_{13} \\ c_{23} \\ c_{33} \\ c_{43} \end{bmatrix} & \begin{bmatrix} c_{14} \\ c_{24} \\ c_{34} \\ c_{44} \end{bmatrix} \\ \hline \end{array} = \begin{array}{c|c|c|c} C_1 & C_2 & C_3 & C_4 \\ \hline \begin{bmatrix} c_{11} \\ c_{21} \\ c_{31} \\ c_{41} \end{bmatrix} & \begin{bmatrix} c_{12} \\ c_{22} \\ c_{32} \\ c_{42} \end{bmatrix} & \begin{bmatrix} c_{13} \\ c_{23} \\ c_{33} \\ c_{43} \end{bmatrix} & \begin{bmatrix} c_{14} \\ c_{24} \\ c_{34} \\ c_{44} \end{bmatrix} \\ \hline \end{array} + \begin{array}{c|c|c|c} A & & & \\ \hline \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} & & & \\ \hline \end{array} \begin{array}{c|c|c|c} B_1 & B_2 & B_3 & B_4 \\ \hline \begin{bmatrix} b_{11} \\ b_{21} \\ b_{31} \\ b_{41} \end{bmatrix} & \begin{bmatrix} b_{12} \\ b_{22} \\ b_{32} \\ b_{42} \end{bmatrix} & \begin{bmatrix} b_{13} \\ b_{23} \\ b_{33} \\ b_{43} \end{bmatrix} & \begin{bmatrix} b_{14} \\ b_{24} \\ b_{34} \\ b_{44} \end{bmatrix} \\ \hline \end{array}$$

for k=1 to n

j=1

$$\begin{bmatrix} c_{11} \\ c_{21} \\ c_{31} \\ c_{41} \end{bmatrix} = \begin{bmatrix} c_{11} \\ c_{21} \\ c_{31} \\ c_{41} \end{bmatrix} + \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} * \begin{bmatrix} b_{11} \\ b_{21} \\ b_{31} \\ b_{41} \end{bmatrix}$$

k=3

$$\begin{bmatrix} c_{11} \\ c_{21} \\ c_{31} \\ c_{41} \end{bmatrix} = \begin{bmatrix} a_{11}b_{11} + a_{12}b_{21} \\ a_{21}b_{11} + a_{22}b_{21} \\ a_{31}b_{11} + a_{32}b_{21} \\ a_{41}b_{11} + a_{42}b_{21} \end{bmatrix} + \begin{bmatrix} a_{13} \\ a_{23} \\ a_{33} \\ a_{43} \end{bmatrix} * [b_{31}]$$

← Third row of B_1

$$= \begin{bmatrix} c_{11} \\ c_{21} \\ c_{31} \\ c_{41} \end{bmatrix} = \begin{bmatrix} a_{11}b_{11} + a_{12}b_{21} \\ a_{21}b_{11} + a_{22}b_{21} \\ a_{31}b_{11} + a_{32}b_{21} \\ a_{41}b_{11} + a_{42}b_{21} \end{bmatrix} + \begin{bmatrix} a_{13}b_{31} \\ a_{23}b_{31} \\ a_{33}b_{31} \\ a_{43}b_{31} \end{bmatrix}$$

Blocked Matrix Multiply - Example

$$\begin{array}{c|c|c|c} C_1 & C_2 & C_3 & C_4 \\ \hline \begin{bmatrix} c_{11} \\ c_{21} \\ c_{31} \\ c_{41} \end{bmatrix} & \begin{bmatrix} c_{12} \\ c_{22} \\ c_{32} \\ c_{42} \end{bmatrix} & \begin{bmatrix} c_{13} \\ c_{23} \\ c_{33} \\ c_{43} \end{bmatrix} & \begin{bmatrix} c_{14} \\ c_{24} \\ c_{34} \\ c_{44} \end{bmatrix} \\ \hline \end{array} = \begin{array}{c|c|c|c} C_1 & C_2 & C_3 & C_4 \\ \hline \begin{bmatrix} c_{11} \\ c_{21} \\ c_{31} \\ c_{41} \end{bmatrix} & \begin{bmatrix} c_{12} \\ c_{22} \\ c_{32} \\ c_{42} \end{bmatrix} & \begin{bmatrix} c_{13} \\ c_{23} \\ c_{33} \\ c_{43} \end{bmatrix} & \begin{bmatrix} c_{14} \\ c_{24} \\ c_{34} \\ c_{44} \end{bmatrix} \\ \hline \end{array} + \begin{array}{c|c|c|c} A & & & \\ \hline \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} & & & \\ \hline \end{array} \begin{array}{c|c|c|c} B_1 & B_2 & B_3 & B_4 \\ \hline \begin{bmatrix} b_{11} \\ b_{21} \\ b_{31} \\ b_{41} \end{bmatrix} & \begin{bmatrix} b_{12} \\ b_{22} \\ b_{32} \\ b_{42} \end{bmatrix} & \begin{bmatrix} b_{13} \\ b_{23} \\ b_{33} \\ b_{43} \end{bmatrix} & \begin{bmatrix} b_{14} \\ b_{24} \\ b_{34} \\ b_{44} \end{bmatrix} \\ \hline \end{array}$$

for k=1 to n

j=1

$$\begin{bmatrix} c_{11} \\ c_{21} \\ c_{31} \\ c_{41} \end{bmatrix} = \begin{bmatrix} c_{11} \\ c_{21} \\ c_{31} \\ c_{41} \end{bmatrix} + \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} * \begin{bmatrix} b_{11} \\ b_{21} \\ b_{31} \\ b_{41} \end{bmatrix}$$

Fourth row of B_1

k=4

$$\begin{bmatrix} c_{11} \\ c_{21} \\ c_{31} \\ c_{41} \end{bmatrix} = \begin{bmatrix} a_{11}b_{11} + a_{12}b_{21} + a_{13}b_{31} \\ a_{21}b_{11} + a_{22}b_{21} + a_{23}b_{31} \\ a_{31}b_{11} + a_{32}b_{21} + a_{33}b_{31} \\ a_{41}b_{11} + a_{42}b_{21} + a_{43}b_{31} \end{bmatrix} + \begin{bmatrix} a_{14} \\ a_{24} \\ a_{34} \\ a_{44} \end{bmatrix} * [b_{41}]$$

$$= \begin{bmatrix} c_{11} \\ c_{21} \\ c_{31} \\ c_{41} \end{bmatrix} = \begin{bmatrix} a_{11}b_{11} + a_{12}b_{21} + a_{13}b_{31} \\ a_{21}b_{11} + a_{22}b_{21} + a_{23}b_{31} \\ a_{31}b_{11} + a_{32}b_{21} + a_{33}b_{31} \\ a_{41}b_{11} + a_{42}b_{21} + a_{43}b_{31} \end{bmatrix} + \begin{bmatrix} a_{14}b_{41} \\ a_{24}b_{41} \\ a_{34}b_{41} \\ a_{44}b_{41} \end{bmatrix}$$

Blocked Matrix Multiply - Example

$$\begin{bmatrix} C_1 & C_2 & C_3 & C_4 \\ \begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} \\ c_{21} & c_{22} & c_{23} & c_{24} \\ c_{31} & c_{32} & c_{33} & c_{34} \\ c_{41} & c_{42} & c_{43} & c_{44} \end{bmatrix} \end{bmatrix} = \begin{bmatrix} C_1 & C_2 & C_3 & C_4 \\ \begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} \\ c_{21} & c_{22} & c_{23} & c_{24} \\ c_{31} & c_{32} & c_{33} & c_{34} \\ c_{41} & c_{42} & c_{43} & c_{44} \end{bmatrix} \end{bmatrix} + \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} \begin{bmatrix} B_1 & B_2 & B_3 & B_4 \\ \begin{bmatrix} b_{11} & b_{12} & b_{13} & b_{14} \\ b_{21} & b_{22} & b_{23} & b_{24} \\ b_{31} & b_{32} & b_{33} & b_{34} \\ b_{41} & b_{42} & b_{43} & b_{44} \end{bmatrix} \end{bmatrix}$$

for k=1 to n

$$\begin{matrix} j=2 \\ \begin{bmatrix} c_{12} \\ c_{22} \\ c_{32} \\ c_{42} \end{bmatrix} \end{matrix} = \begin{bmatrix} c_{12} \\ c_{22} \\ c_{32} \\ c_{42} \end{bmatrix} + \begin{bmatrix} a_{11} \\ a_{21} \\ a_{31} \\ a_{41} \end{bmatrix} \begin{bmatrix} a_{12} & a_{13} & a_{14} \\ a_{22} & a_{23} & a_{24} \\ a_{32} & a_{33} & a_{34} \\ a_{42} & a_{43} & a_{44} \end{bmatrix} * \begin{bmatrix} b_{12} \\ b_{22} \\ b_{32} \\ b_{42} \end{bmatrix}$$

- And so on..
- At any point, you need C_j , B_j , and one column of A to be in fast memory

Computational Intensity - Blocked Matrix Multiply

```
for j=1 to N
  //Read entire Bj into fast memory →  $n^2$  words read: each column of B read once.
  //Read entire Cj into fast memory
  for k=1 to n
    //Read column k of A into fast memory →  $Nn^2$  words read: each column of A read N times
    C(*,j)=C(*,j) + A(*,k)*Bj(k,*) //outer-product
    //Write Cj back to slow memory →  $2n^2$  words read: read/write each entry of C to memory once.
```

- Number of arithmetic operations = $2n^3$
- $q = 2n^3 / (N + 3)n^2 = 2n/N$. **Good!**

Blocked Matrix Multiply - General

$$\begin{array}{ccc}
 C & A & B \\
 \begin{bmatrix} C_{11} & C_{12} & \dots & C_{1r} \\ C_{21} & C_{22} & \dots & C_{2r} \\ \vdots & \vdots & \ddots & \vdots \\ C_{q1} & C_{q2} & \dots & C_{qr} \end{bmatrix} & \begin{bmatrix} A_{11} & A_{12} & \dots & A_{1p} \\ A_{21} & A_{22} & \dots & A_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ A_{q1} & A_{q2} & \dots & A_{qp} \end{bmatrix} & \begin{bmatrix} B_{11} & B_{12} & \dots & B_{1r} \\ B_{21} & B_{22} & \dots & B_{2r} \\ \vdots & \vdots & \ddots & \vdots \\ B_{p1} & B_{p2} & \dots & B_{pr} \end{bmatrix} \\
 \begin{array}{c} \downarrow \rightarrow \\ q \quad r \end{array} & \begin{array}{c} \downarrow \rightarrow \\ q \quad p \end{array} & \begin{array}{c} \downarrow \rightarrow \\ p \quad r \end{array}
 \end{array}$$

- $A, B, C \in \mathbb{R}^{n \times n}$
- We wish to update C block-by-block: $C_{ij} = C_{ij} + \sum_{k=1}^p A_{ik} B_{kj}$
 - Assume that blocks of A , B , and C fit in cache. C_{ij} is roughly n/q by n/r , A_{ij} is roughly n/q by n/p , B_{ij} is roughly n/p by n/r .
 - But how to choose block parameters p, q, r such that assumption holds for a cache of size M ?
 - i.e. given the constraint that $\frac{n}{q} \times \frac{n}{r} + \frac{n}{q} \times \frac{n}{p} + \frac{n}{p} \times \frac{n}{r} \leq M$

Blocked Matrix Multiply - General

- Maximize $\frac{2n^3}{qrp}$ subject to $\frac{n}{q} \times \frac{n}{r} + \frac{n}{q} \times \frac{n}{p} + \frac{n}{p} \times \frac{n}{r} \leq M$
 - $q_{opt} = p_{opt} = r_{opt} \approx \sqrt{\frac{n^2}{3M}}$

Assumption: $M \ll 3n^2$ and cache can hold M floating point numbers

- Each block should roughly be a square matrix and occupy one third of the cache size
- Can we design algorithms that are independent of cache size?

Recursive Matrix Multiply

- Cache-oblivious algorithm
 - No matter what the size of the cache is, the algorithm performs at a near-optimal level
- Divide-conquer approach

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \times \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix} = \begin{bmatrix} A_{11}B_{11} + A_{12}B_{21} & A_{11}B_{12} + A_{12}B_{22} \\ A_{21}B_{11} + A_{22}B_{21} & A_{21}B_{12} + A_{22}B_{22} \end{bmatrix}$$

- Apply the formula recursively to $A_{11}B_{11}$ etc.
 - Works neat when n is a power of 2.
- What layout format is preferred for this algorithm?
 - Row-major or Col-major? Neither.

Recursive Matrix Multiply

- Cache-oblivious Data structure

$$\begin{bmatrix} 1 & 2 & 5 & 6 & 17 & 18 & 21 & 22 \\ 3 & 4 & 7 & 8 & 19 & 20 & 23 & 24 \\ 9 & 10 & 13 & 14 & 25 & 26 & 29 & 30 \\ 11 & 12 & 15 & 16 & 27 & 28 & 31 & 32 \\ 33 & 34 & 37 & 38 & 49 & 50 & 53 & 54 \\ 35 & 36 & 39 & 40 & 51 & 52 & 55 & 56 \\ 41 & 42 & 45 & 46 & 57 & 58 & 61 & 62 \\ 43 & 44 & 47 & 48 & 59 & 60 & 63 & 64 \end{bmatrix}.$$

- Matrix entries are stored in the order shown
 - E.g. row-major would have 1-8 in the first row, followed by 9-16 in the second and so on.

Recursive Matrix Multiply

- Illustration: Cache-oblivious Data structure

a11	a12	a13	a14	a15	a16	a17	a18
a21	a22	a23	a24	a25	a26	a27	a28
a31	a32	a33	a34	a35	a36	a37	a38
a41	a42	a43	a44	a45	a46	a47	a48
a51	a52	a53	a54	a55	a56	a57	a58
a61	a62	a63	a64	a65	a66	a67	a68
a71	a72	a73	a74	a75	a76	a77	a78
a81	a82	a83	a84	a85	a86	a87	a88

Matrix A

Row-major layout:

a11	a12	a13	a14	a15	a16	a17	a18	...
-----	-----	-----	-----	-----	-----	-----	-----	-----

addr:0x100 0x104 0x108 0x10C 0x110 0x114 0x118 0x11C

Col-major layout:

a11	a21	a31	a41	a51	a61	a71	a81	...
-----	-----	-----	-----	-----	-----	-----	-----	-----

addr:0x100 0x104 0x108 0x10C 0x110 0x114 0x118 0x11C

Z-order layout:

a11	a12	a21	a22	a13	a14	a23	a24	...
-----	-----	-----	-----	-----	-----	-----	-----	-----

addr:0x100 0x104 0x108 0x10C 0x110 0x114 0x118 0x11C

Why this is better for recursive divide-conquer algorithm?

Reading a11 gets you nearby elements in memory that are actually needed immediately to compute $A_{11} * B_{11}$ - better spatial locality. There is also better temporal locality. How?

Efficiency Considerations

- Storage layout
- Data movement overhead
- Cache details (size)
- Parallel functional Units (Vector units)

Data Movement Overhead - Example

- gaxpy ($y = y + Ax$) vs. Outer product ($A = A + yx^T$)
- What is the data movement overhead? *assume a vector of dimension n can be read with one memory read*

gaxpy

```
// Read y into fast memory
// Read x into fast memory
for i=1 to n
    //Read column  $c_i$  of A into fast memory
    for j=1 to n
         $y[j] = y[j] + c_i x[j]$ 
//Write y into slow memory
```

$$\mathbf{y} = \mathbf{y} + \mathbf{c}_i \cdot \mathbf{x}[j]$$

Outer product

```
// Read y into fast memory
// Read x into fast memory
for j=1 to n
    //Read a column of A into fast memory
    for i=1 to n
         $A[i,j] = A[i,j] + y[i]x[j]$ 
    //Write  $A[*,j]$  into slow memory
```

$$A[j] = A[j] + y[i] \cdot x[j]$$