CS601: Software Development for Scientific Computing

Autumn 2023

Week5: Matrix Computations with Dense Matrices, Library functions

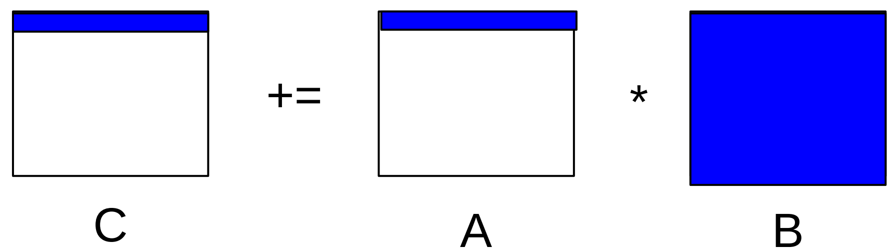
Computational Intensity – Matrix-Matrix Product

- Words moved = $n^3+3n^2 = n^3+O(n^2)$
- Number of arithmetic operations = $2n^3$ (from slide 35)
- computational intensity $q \approx 2n^3/n^3 = 2$. (computation to communication ratio)

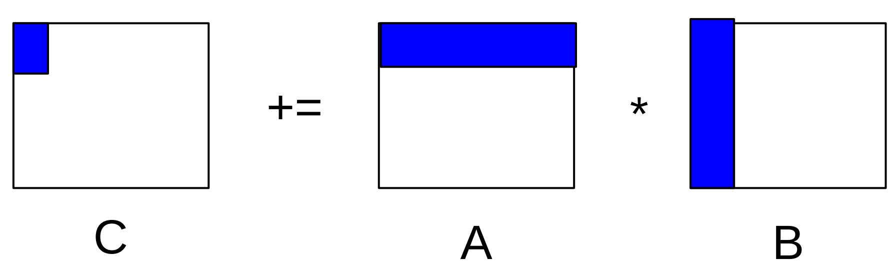
- Can we do better?

Insight - Data reuse

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

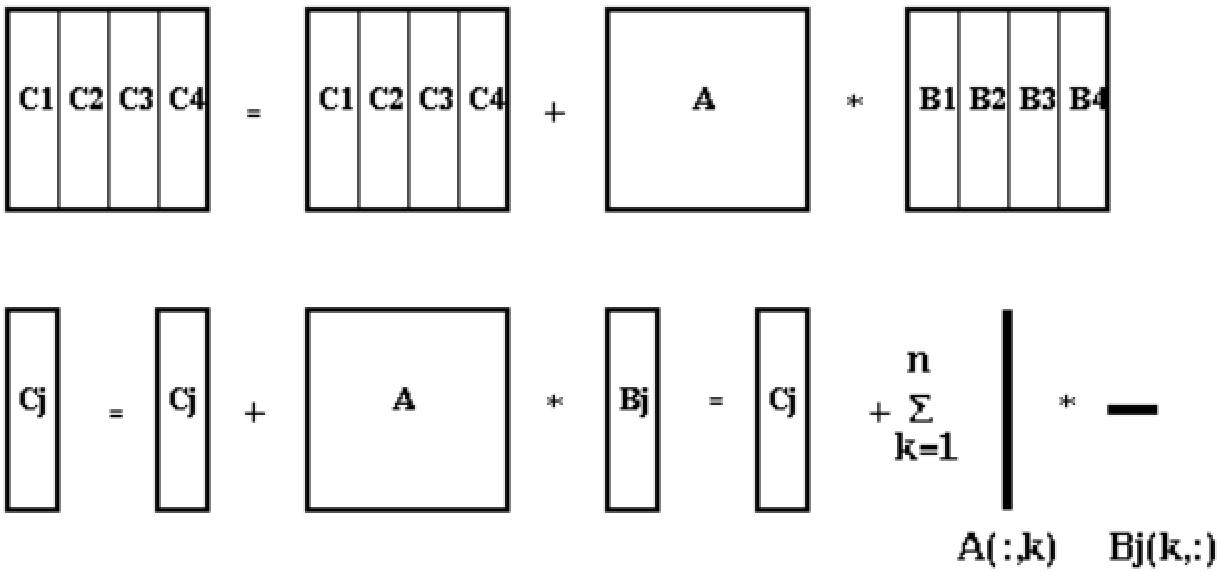


- How many memory accesses needed to compute a tile of C of size 64x64?



Blocked Matrix Multiply

- For N=4:




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


source: http://people.eecs.berkeley.edu/~demmel/cs267/lecture02.html

Blocked Matrix Multiply - Example

$$\begin{array}{cccc} C_1 & C_2 & C_3 & C_4 \\ \multicolumn{4}{c}{\left[\begin{array}{c|c|c|c} c_{11} & c_{12} & c_{!3} & c_{14} \\ c_{21} & c_{22} & c_{23} & c_{24} \\ c_{31} & c_{32} & c_{33} & c_{34} \\ c_{41} & c_{42} & c_{43} & c_{44} \end{array}\right]} \end{array} = \begin{array}{cccc} C_1 & C_2 & C_3 & C_4 \\ \multicolumn{4}{c}{\left[\begin{array}{c|c|c|c} c_{11} & c_{12} & c_{!3} & c_{14} \\ c_{21} & c_{22} & c_{23} & c_{24} \\ c_{31} & c_{32} & c_{33} & c_{34} \\ c_{41} & c_{42} & c_{43} & c_{44} \end{array}\right]} \end{array} + \begin{array}{c} \text{A} \\ \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} \end{array} \begin{array}{cccc} B_1 & B_2 & B_3 & B_4 \\ \multicolumn{4}{c}{\left[\begin{array}{c|c|c|c} b_{11} & b_{12} & b_{13} & b_{14} \\ b_{21} & b_{22} & b_{23} & b_{24} \\ b_{31} & b_{32} & b_{33} & b_{34} \\ b_{41} & b_{42} & b_{43} & b_{44} \end{array}\right]} \end{array}$$

```
for k=1 to n
```

j=1

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

....

```
for k=1 to n
```

j=4

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

Blocked Matrix Multiply - Example

$$\begin{array}{c} \begin{array}{cccc} C_1 & C_2 & C_3 & C_4 \end{array} \\ \begin{bmatrix} c_{11} & c_{12} & c_{!3} & c_{14} \\ c_{21} & c_{22} & c_{23} & c_{24} \\ c_{31} & c_{32} & c_{33} & c_{34} \\ c_{41} & c_{42} & c_{43} & c_{44} \end{bmatrix} \end{array} = \begin{array}{c} \begin{array}{cccc} C_1 & C_2 & C_3 & C_4 \end{array} \\ \begin{bmatrix} c_{11} & c_{12} & c_{!3} & c_{14} \\ c_{21} & c_{22} & c_{23} & c_{24} \\ c_{31} & c_{32} & c_{33} & c_{34} \\ c_{41} & c_{42} & c_{43} & c_{44} \end{bmatrix} \end{array} + \begin{array}{c} \text{A} \\ \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} \end{array} \begin{array}{c} \begin{array}{cccc} B_1 & B_2 & B_3 & B_4 \end{array} \\ \begin{bmatrix} b_{11} & b_{12} & b_{13} & b_{14} \\ b_{21} & b_{22} & b_{23} & b_{24} \\ b_{31} & b_{32} & b_{33} & b_{34} \\ b_{41} & b_{42} & b_{43} & b_{44} \end{bmatrix} \end{array}$$

```
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=1

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

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

$$\begin{array}{cccc} C_1 & C_2 & C_3 & C_4 \end{array} \quad \begin{array}{cccc} C_1 & C_2 & C_3 & C_4 \end{array} \quad \text{A} \quad \begin{array}{cccc} B_1 & B_2 & B_3 & B_4 \end{array}$$

$$\begin{bmatrix} \boxed{\begin{matrix} c_{11} \\ c_{21} \\ c_{31} \\ c_{41} \end{matrix}} & \begin{matrix} c_{12} \\ c_{22} \\ c_{32} \\ c_{42} \end{matrix} & \begin{matrix} c_{!3} \\ c_{23} \\ c_{33} \\ c_{43} \end{matrix} & \begin{matrix} c_{14} \\ c_{24} \\ c_{34} \\ c_{44} \end{matrix} \end{bmatrix} = \begin{bmatrix} \boxed{\begin{matrix} c_{11} \\ c_{21} \\ c_{31} \\ c_{41} \end{matrix}} & \begin{matrix} c_{12} \\ c_{22} \\ c_{32} \\ c_{42} \end{matrix} & \begin{matrix} c_{!3} \\ c_{23} \\ c_{33} \\ c_{43} \end{matrix} & \begin{matrix} c_{14} \\ c_{24} \\ c_{34} \\ c_{44} \end{matrix} \end{bmatrix} + \begin{bmatrix} a_{11} & \boxed{\begin{matrix} a_{12} \\ a_{22} \\ a_{32} \\ a_{42} \end{matrix}} & \begin{matrix} a_{13} \\ a_{23} \\ a_{33} \\ a_{43} \end{matrix} & \begin{matrix} a_{14} \\ a_{24} \\ a_{34} \\ a_{44} \end{matrix} \\ a_{21} & & & \\ a_{31} & & & \\ a_{41} & & & \end{bmatrix} \begin{bmatrix} \boxed{\begin{matrix} b_{11} \\ b_{21} \\ b_{31} \\ b_{41} \end{matrix}} & \begin{matrix} b_{12} \\ b_{22} \\ b_{32} \\ b_{42} \end{matrix} & \begin{matrix} b_{13} \\ b_{23} \\ b_{33} \\ b_{43} \end{matrix} & \begin{matrix} b_{14} \\ b_{24} \\ b_{34} \\ b_{44} \end{matrix} \end{bmatrix}$$

```
for k=1 to n
```

j=1

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

k=2

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

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

$$\begin{array}{c} \begin{array}{cccc} C_1 & C_2 & C_3 & C_4 \end{array} \\ \begin{bmatrix} c_{11} & c_{12} & c_{!3} & c_{14} \\ c_{21} & c_{22} & c_{23} & c_{24} \\ c_{31} & c_{32} & c_{33} & c_{34} \\ c_{41} & c_{42} & c_{43} & c_{44} \end{bmatrix} \end{array} = \begin{array}{c} \begin{array}{cccc} C_1 & C_2 & C_3 & C_4 \end{array} \\ \begin{bmatrix} c_{11} & c_{12} & c_{!3} & c_{14} \\ c_{21} & c_{22} & c_{23} & c_{24} \\ c_{31} & c_{32} & c_{33} & c_{34} \\ c_{41} & c_{42} & c_{43} & c_{44} \end{bmatrix} \end{array} + \begin{array}{c} \text{A} \\ \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} \end{array} \begin{array}{c} \begin{array}{cccc} B_1 & B_2 & B_3 & B_4 \end{array} \\ \begin{bmatrix} b_{11} & b_{12} & b_{13} & b_{14} \\ b_{21} & b_{22} & b_{23} & b_{24} \\ b_{31} & b_{32} & b_{33} & b_{34} \\ b_{41} & b_{42} & b_{43} & b_{44} \end{bmatrix} \end{array}$$

`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

$$\begin{array}{cccc} C_1 & C_2 & C_3 & C_4 \\ \end{array} \qquad \begin{array}{cccc} C_1 & C_2 & C_3 & C_4 \\ \end{array} \qquad \text{A} \qquad \begin{array}{cccc} B_1 & B_2 & B_3 & B_4 \\ \end{array}$$

$$\begin{bmatrix} c_{11} & c_{12} & c_{!3} & c_{14} \\ c_{21} & c_{22} & c_{23} & c_{24} \\ c_{31} & c_{32} & c_{33} & c_{34} \\ c_{41} & c_{42} & c_{43} & c_{44} \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{!3} & c_{14} \\ c_{21} & c_{22} & c_{23} & c_{24} \\ c_{31} & c_{32} & c_{33} & c_{34} \\ c_{41} & c_{42} & c_{43} & c_{44} \end{bmatrix} + \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} \begin{bmatrix} b_{11} & b_{12} & b_{13} & b_{14} \\ b_{21} & b_{22} & b_{23} & b_{24} \\ b_{31} & b_{32} & b_{33} & b_{34} \\ b_{41} & b_{42} & b_{43} & b_{44} \end{bmatrix}$$

```
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=4

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

Fourth row of B_1

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

Blocked Matrix Multiply - Example

$$\begin{array}{c} \begin{array}{cccc} C_1 & C_2 & C_3 & C_4 \end{array} \\ \left[\begin{array}{c|c|c|c} c_{11} & c_{12} & c_{!3} & c_{14} \\ c_{21} & c_{22} & c_{23} & c_{24} \\ c_{31} & c_{32} & c_{33} & c_{34} \\ c_{41} & c_{42} & c_{43} & c_{44} \end{array}\right] \end{array} = \begin{array}{c} \begin{array}{cccc} C_1 & C_2 & C_3 & C_4 \end{array} \\ \left[\begin{array}{c|c|c|c} c_{11} & c_{12} & c_{!3} & c_{14} \\ c_{21} & c_{22} & c_{23} & c_{24} \\ c_{31} & c_{32} & c_{33} & c_{34} \\ c_{41} & c_{42} & c_{43} & c_{44} \end{array}\right] \end{array} + \begin{array}{c} \text{A} \\ \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} \end{array} \begin{array}{c} \begin{array}{cccc} B_1 & B_2 & B_3 & B_4 \end{array} \\ \left[\begin{array}{c|c|c|c} b_{11} & b_{12} & b_{13} & b_{14} \\ b_{21} & b_{22} & b_{23} & b_{24} \\ b_{31} & b_{32} & b_{33} & b_{34} \\ b_{41} & b_{42} & b_{43} & b_{44} \end{array}\right] \end{array}$$

j=2

`for k=1 to n`

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

- `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
//Read entire Cj into fast memory
  for k=1 to n
   //Read column k of A into fast memory
   C(*,j)=C(*,j) + A(*,k)*Bj(k,*) //outer-product
        //Write Cj back to slow memory
```

n^2 words read: each column of B read once.

Nn^2 words read: each column of A read N times

$2n^2$ words read: read/write each entry of C to memory once.

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

Blocked Matrix Multiply - General

$$C = \begin{bmatrix} C_{11} & C_{12} & .. & C_{1r} \\ C_{21} & C_{22} & .. & C_{2r} \\ & \vdots & & \\ C_{q1} & C_{q2} & .. & C_{qr} \end{bmatrix} \qquad A = \begin{bmatrix} A_{11} & A_{12} & .. & A_{1p} \\ A_{21} & A_{22} & .. & A_{2p} \\ & \vdots & & \\ A_{q1} & A_{q2} & .. & A_{qp} \end{bmatrix} \qquad B = \begin{bmatrix} B_{11} & B_{12} & .. & B_{1r} \\ B_{21} & B_{22} & .. & B_{2r} \\ & \vdots & & \\ B_{p1} & B_{p2} & .. & B_{pr} \end{bmatrix}$$

C: $\downarrow q$, $\xrightarrow{r}$ $\qquad$ A: $\downarrow q$, $\xrightarrow{p}$ $\qquad$ B: $\downarrow p$, $\xrightarrow{r}$

- $A, B, C \in \mathbb{R}^{n \times n}$
- We wish to update C block-by-block: $C_{ij} = C_{ij} + \Sigma_{k=1}^{p} A_{ik}B_{kj}$
  - 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 $\frac{n}{q} \times \frac{n}{r} + \frac{n}{q} \times \frac{n}{p} + \frac{n}{p} \times \frac{n}{r} \leq M$
  - $q_{opt} = p_{opt} = r_{opt} \approx \sqrt{\frac{n^2}{3M}}$
- 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?