CS601: Software Development for Scientific Computing

Autumn 2023

Week5: Matrix Computations with Dense Matrices, Library functions

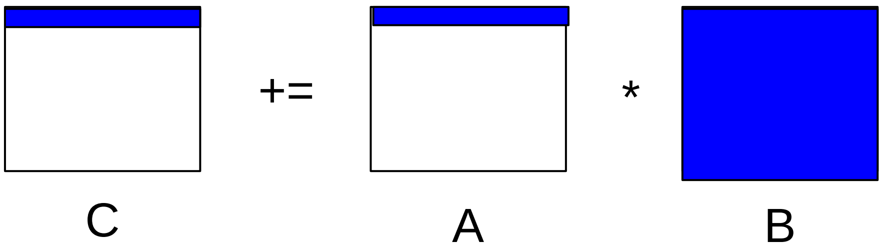
Computational Intensity – Matrix-Matrix Product

- 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)

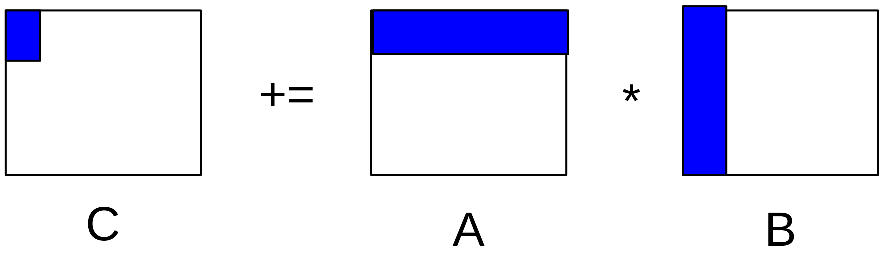
- Can we do better?

Insight - Data reuse

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

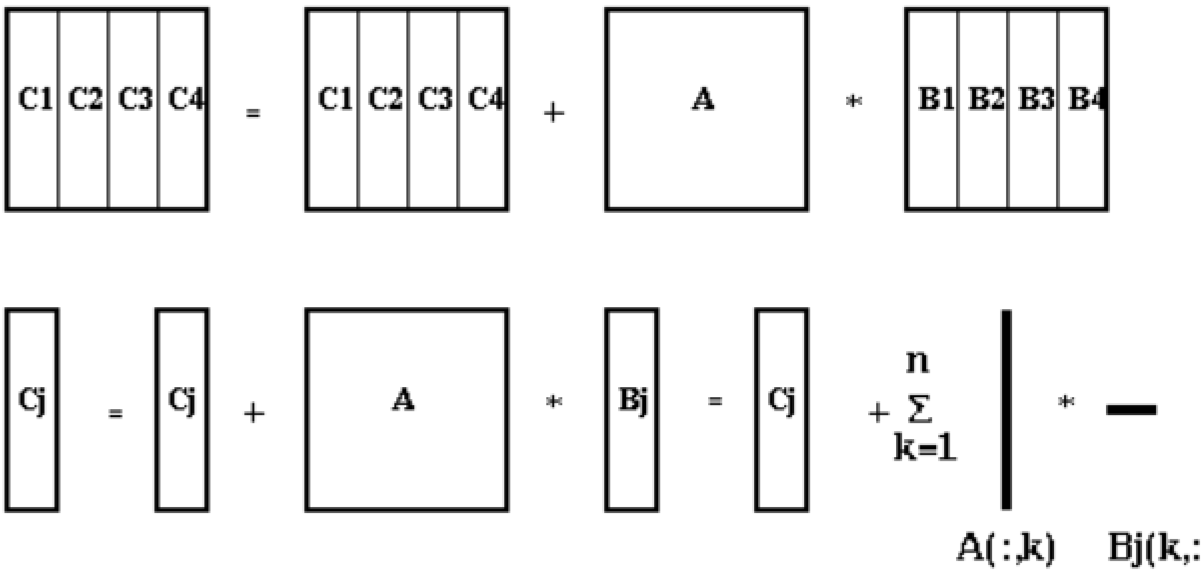


- How many memory accesses needed to compute a tile of C of size 64x64?



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

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

```
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

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

`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

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

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

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

j=1

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

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

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

```
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=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

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

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

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

j=2

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

- 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

$$C = \begin{bmatrix} C_{11} & C_{12} & .. & C_{1r} \\ C_{21} & C_{22} & .. & C_{2r} \\ & \vdots & & \\ C_{q1} & C_{q2} & .. & C_{qr} \end{bmatrix}$$

r q

$$A = \begin{bmatrix} A_{11} & A_{12} & .. & A_{1p} \\ A_{21} & A_{22} & .. & A_{2p} \\ & \vdots & & \\ A_{q1} & A_{q2} & .. & A_{qp} \end{bmatrix}$$

q p

$$B = \begin{bmatrix} B_{11} & B_{12} & .. & B_{1r} \\ B_{21} & B_{22} & .. & B_{2r} \\ & \vdots & & \\ B_{p1} & B_{p2} & .. & B_{pr} \end{bmatrix}$$

r p

- $A, B, C \in \mathbb{R}^{n\times n}$
- 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 $\frac{n}{q}\times\frac{n}{r} + \frac{n}{q}\times\frac{n}{p} + \frac{n}{p}\times\frac{n}{r} \le M$

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: $M << 3n^2$ 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 A11*B11 - better spatial locality. There is also better temporal locality. How?

Efficiency Considerations

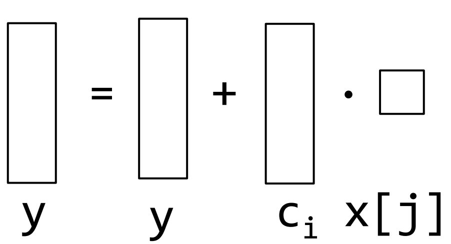
- Storage layout
- Data movement overhead
- Cache details (size)
- Parallel functional Units (Vector units)

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*

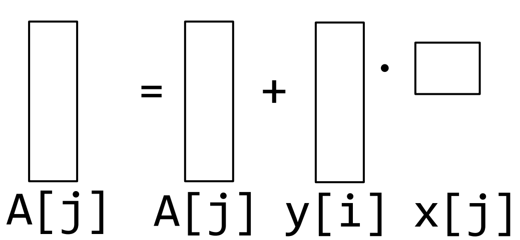
gaxpy

```
// 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
```



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
```



Parallel Functional Units

- IBM's RS/6000 and Fused Multiply Add (FMA)
  - Fuses multiply and an add into one functional unit (c=c+a*b)
  - The functional unit consists of 3 independent subunits
    - Pipelining
  - Example:

```
sum=0.0
for (i=0;i<n;i++)
  sum=sum+a[i]*b[i]
```

  - Suppose the FMA unit takes 3 cycles to complete, how many cycles do you need to execute the above code snippet?
  - With loop unrolled 4 times? Assume n is divisible by 4.

Exercise: Storage Layout Considerations

- Assume column-order storage for A, B, and C. Which implementation scheme for matmul is better? Why?

<u>ijk</u> **vs.** **<u>jki</u>**

```
for i=1 to m
    for j=1 to n
        for k=1 to r
             c[i][j]=c[i][j]+
                a[i][k]*b[k][j]
```

```
for j=1 to n
    for k=1 to r
        for i=1 to m
         c[i][j]=c[i][j]+
               a[i][k]*b[k][j]
```

Summary: unblocked Matrix Multiplication - Loop Orderings and Properties

Loop Order	Inner Loop	Inner Two Loops	Inner Loop Data Access
i j k	dot	Vector x Matrix	A by row, B by column
j k i	saxpy	gaxpy	A by column, C by column
k j i	saxpy	Outer product	A by column, C by column
j i k			
i k j			
k i j			

Ref: Matrix Computations, 4th Ed., Golub and Van Loan

Linear Algebra in Scientific Computing

- Not just matrix multiplication (matmul!)
- Solving system of equations: Ax=b (e.g. using Gaussian Elimination)
- Computing Least Squares: choose x to minimize $||Ax-b||_2$
  - Overdetermined or underdetermined; Unconstrained, constrained, or weighted
- Computing Eigenvalues and Eigenvectors of Matrices (Symmetric and Unsymmetric)
    - Standard ($Ax = \lambda x$), Generalized ($Ax=\lambda Bx$)
- Representing Different matrix structures
  - Real, complex; Symmetric, Hermitian, positive definite; dense, triangular, banded …
- Capturing level of detail
  - error bounds, extra-precision, other options

Linear Algebra Software

- **Goals**: programmer productivity, readability, robustness, portability, machine efficiency
- Examples
  - EISPACK (for computing eigenvalue problems)
  - BLAS
  - LAPACK
  - Many more..
- Contain subroutines / functions that implement high-level mathematical operations described in the previous slide

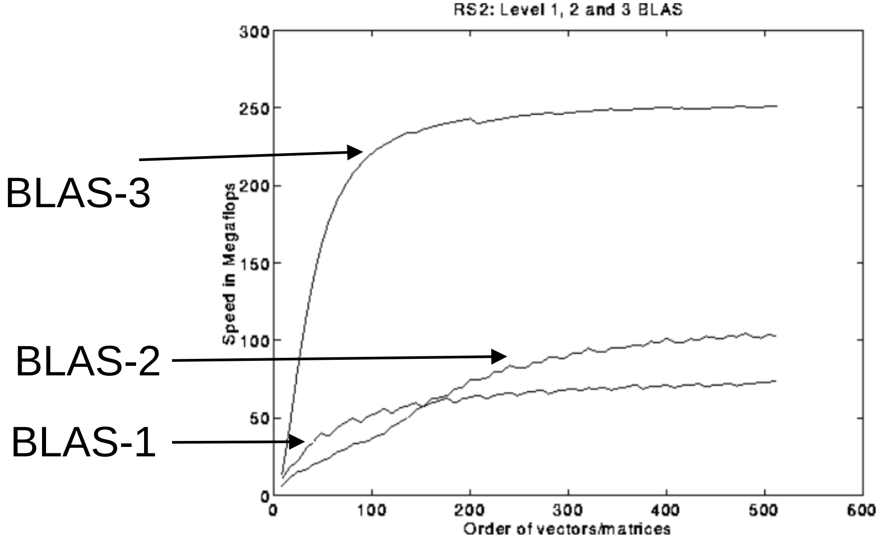
BLAS – Basic Linear Algebra Subroutines

- Level-1 or BLAS-1 (46 operations, routines operating on vectors mostly)
  - axpy, dot product, rotation, scale, etc.
  - 4 versions each: **S**ingle-precision, **d**ouble-precision, **c**omplex, complex-double (**z**)
  - E.g. saxpy, daxpy, caxpy etc.
  - **Do O(n) operations on O(n) data.**
- Level-2 or BLAS-2 (25 operations, routines operating on matrix-vectors mostly)
  - E.g. GEMV ($\alpha A.x + \beta y$), GER (Rank-1 update $A = A + y.x^T$), Triangular solve ($y = T.x, T\ is\ a\ triangular\ matrix$) etc.
  - 4 versions each, **do $O(n^2)$ operations on $O(n^2)$ data.**

BLAS – Basic Linear Algebra Subroutines

- Level-3 or BLAS-3 (9 basic operations, routines operating on matrix-matrix mostly)
  - GEMM ($C = \alpha A.B + \beta C$),
  - Multiple triangular solve ($Y = TX$, T is triangular, X is rectangular)
  - **Do $O(n^3)$ operations on $O(n^2)$ data.**

- *Why categorize as BLAS-1, BLAS-2, BLAS-3?*
  - *Performance*



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