CS601: Software Development for Scientific Computing

Autumn 2021

Week14:

Matrix Algebra

Course Progress..

- Last week: FMM, PA4, Matrix Algebra
  - FMM ideas - applying 3-step approximation (decomposition), optimizing (reuse computation), better approximation (multipole expansion), Cost.
  - PA4 discussion
  - Matrix algebra
    - Overview: matrix-matrix multiplication (motivation), program representation of a matrix, storage layout and performance implications.
- This week: Matrix algebra contd.

Matrix Multiplication

- Three fundamental ways to think of the computation
  1. Dot product

$$\begin{bmatrix}1 & 2\\3 & 4\end{bmatrix}\times\begin{bmatrix}5 & 6\\7 & 8\end{bmatrix}=\begin{bmatrix}1.5+2.7 & 1.6+2.8\\3.5+4.7 & 3.6+4.8\end{bmatrix}$$

  2. Linear combination of the columns of the left matrix

$$\begin{bmatrix}1 & 2\\3 & 4\end{bmatrix}\times\begin{bmatrix}5 & 6\\7 & 8\end{bmatrix}=\begin{bmatrix}5\begin{bmatrix}1\\3\end{bmatrix}+7\begin{bmatrix}2\\4\end{bmatrix} & 6\begin{bmatrix}1\\3\end{bmatrix}+8\begin{bmatrix}2\\4\end{bmatrix}\end{bmatrix}$$

  3. Sum of outer products

$$\begin{bmatrix}1 & 2\\3 & 4\end{bmatrix}\times\begin{bmatrix}5 & 6\\7 & 8\end{bmatrix}=\begin{bmatrix}\begin{bmatrix}1\\3\end{bmatrix}\begin{bmatrix}5 & 6\end{bmatrix} + \begin{bmatrix}2\\4\end{bmatrix}\begin{bmatrix}7 & 8\end{bmatrix}\end{bmatrix}$$

Dot Product

- Vector $x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$, Vector $y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$ $\mathrm{x_i}, \mathrm{y_i} \in \mathbb{R}$
- $x^T = [x_1 \quad x_2 \quad .. \quad x_n]$
- Dot Product or Inner Product: $c = x^T y$ $\mathrm{x}^{\mathrm{T}} \in \mathbb{R}^{1\times n}, y \in \mathbb{R}^{n\times 1}, c\ is\ scalar$

$$[x_1 \quad x_2 \quad .. \quad x_n] \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = [x_1 y_1 + x_2 y_2 + .. + x_n y_n]$$

- E.g. $[1 \quad 2 \quad 3] \begin{bmatrix} 4 \\ 5 \\ 6 \end{bmatrix} = [1 \times 4 + 2 \times 5 + 3 \times 6] = 32$

AXPY

- Computing the more common (a times x plus y): $y = y + ax$
- $\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} y \\ y_2 \\ \vdots \\ y_n \end{bmatrix} + a \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$

```
..
for i=1 to n
   c[i] = c[i] +  x[i]*y[i]
..
```

- Cost? n multiplications and n additions = **`2n`** `or` **`O(n)`**

Matrix Vector Product

- Computing Matrix-Vector product: $c = c + Ax,\ A \in \mathbb{R}^{m\times r}, x \in \mathbb{R}^{r\times 1}$

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

- Rewriting Matrix-Vector product using dot products:

$$\begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_m \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_m \end{bmatrix} + \begin{bmatrix} a_{11} & a_{12} & .. & a_{1r} \\ a_{21} & a_{22} & .. & a_{2r} \\ & \vdots & & \\ a_{m1} & a_{m2} & .. & a_{mr} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_r \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_m \end{bmatrix} + \begin{bmatrix} a_1^T x \\ a_2^T x \\ \vdots \\ a_m^T x \end{bmatrix}$$

- Cost? m rows involving dot products and having the form $c_i = c_i + x^T y$ (Per row cost = `2r` `(because` $a_i, x \in \mathbb{R}^r$`)`, Total cost = **`2mr`** `or` **`O(mr))`**

Matrix-Matrix Product

- Computing Matrix-Matrix product $C = C + AB, A \in \mathbb{R}^{m\times r}, B \in \mathbb{R}^{r\times n}, C \in \mathbb{R}^{m\times n}$

$$\begin{bmatrix} c_{11} & c_{12} & \cdots & c_{1n} \\ c_{21} & c_{22} & \cdots & c_{2n} \\ & \vdots & & \\ c_{m1} & c_{m2} & \cdots & c_{mn} \end{bmatrix} = \underset{m\downarrow\ \xrightarrow{n}}{\begin{bmatrix} c_{11} & c_{12} & \cdots & c_{1n} \\ c_{21} & c_{22} & \cdots & c_{2n} \\ & \vdots & & \\ c_{m1} & c_{m2} & \cdots & c_{mn} \end{bmatrix}} + \underset{m\downarrow\ \xrightarrow{r}}{\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1r} \\ a_{21} & a_{22} & \cdots & a_{2r} \\ & \vdots & & \\ a_{m1} & a_{m2} & \cdots & a_{mr} \end{bmatrix}} \underset{r\downarrow\ \xrightarrow{n}}{\begin{bmatrix} b_{11} & b_{12} & \cdots & b_{1n} \\ b_{21} & b_{22} & \cdots & b_{2n} \\ & \vdots & & \\ b_{r1} & b_{r2} & \cdots & b_{rn} \end{bmatrix}}$$

- Consider the AB part first.

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1r} \\ a_{21} & a_{22} & \cdots & a_{2r} \\ & \vdots & & \\ a_{m1} & a_{m2} & \cdots & a_{mr} \end{bmatrix} \begin{bmatrix} b_{11} & b_{12} & \cdots & b_{1n} \\ b_{21} & b_{22} & \cdots & b_{2n} \\ & \vdots & & \\ b_{r1} & b_{r2} & \cdots & b_{rn} \end{bmatrix}$$

Matrix-Matrix Product

$$\overset{A}{\begin{bmatrix} a_{11} & a_{12} & .. & a_{1r} \\ a_{21} & a_{22} & .. & a_{2r} \\ & \vdots & & \\ a_{m1} & a_{m2} & .. & a_{mr} \end{bmatrix}} \overset{B}{\begin{bmatrix} b_{11} & b_{12} & .. & b_{1n} \\ b_{21} & b_{22} & .. & b_{2n} \\ & \vdots & & \\ b_{r1} & b_{r2} & .. & b_{rn} \end{bmatrix}}$$

$$= \begin{bmatrix} a_{11}b_{11} + a_{12}b_{21} + .. + a_{1r}x_{r1} & . & . & a_{11}b_{1n} + a_{12}b_{2n} + .. + a_{1r}x_{rn} \\ . & & & \\ a_{m1}b_{11} + a_{m2}b_{21} + .. + a_{mr}x_{r1} & . & . & a_{m1}b_{1n} + a_{m2}b_{2n} + .. + a_{mr}x_{rn} \end{bmatrix}$$

$$= \begin{bmatrix} a_1^T b_1 & . & . & a_1^T b_n \\ . & . & & \\ a_m^T b_1 & . & . & a_m^T b_n \end{bmatrix}$$

$a_i^T \in \mathbb{R}^{1 \times r}, b_j \in \mathbb{R}^{r \times 1}$

i ranges from 1 to m

j ranges from 1 to n

Matrix-Matrix Product using Dot Product Formulation

- Pseudocode - Matrix-Matrix product: $C = C + AB,\ A \in \mathbb{R}^{m \times r}, B \in \mathbb{R}^{r \times n}, C \in \mathbb{R}^{m \times n}$

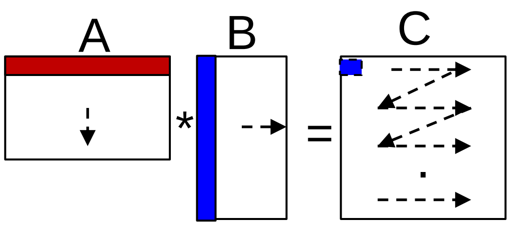
```
..
for i=1 to m
    for j=1 to n
        //compute updates involving dot products
```

$$c_{ij} = c_{ij} + a_i^T b_j$$

- Expanded:

```
..
for i=1 to m
    for j=1 to n
        for k=1 to r
```

$$c_{ij} = c_{ij} + a_{ik} b_{kj}$$



Elements of C matrix are computed from top to bottom, left to right. Per element computation, you need a row of A and a column of B.

Matrix-Matrix Product using Dot Product Formulation

- Pseudocode - Matrix-Matrix product: $C = C + AB,\ A \in \mathbb{R}^{m \times r}, B \in \mathbb{R}^{r \times n}, C \in \mathbb{R}^{m \times n}$

```
..
for i=1 to m
    for j=1 to n
        //compute updates involving dot products
```

$$c_{ij} = c_{ij} + a_i^T b_j$$

- Cost?
  - Per dot-product cost = `2r` $(a_i, b_j \in \mathbb{R}^r)$ Total cost = **`2mnr`** `or` **`O(mnr)`**

Common Computational Patterns

Some patterns that we see while doing Matrix-Matrix product:

- Dot Product or Inner Product: $x^T y$ ← Slide 4, Method 1
- Scalar **a** times **x** **p**lus **y**: y=y+ax OR axpy ← Slide 4, Method 2
- Scalar times **x**: αx
- **M**atrix times **x** **p**lus **y**: y=y+Ax ← Slide 4, Method 1
  - generalized axpy OR gaxpy
- Outer product: $C=C+xy^T$ ← Slide 4, Method 3
- **M**atrix times **M**atrix plus Matrix
  - `GEMM` or generalized matrix multiplication

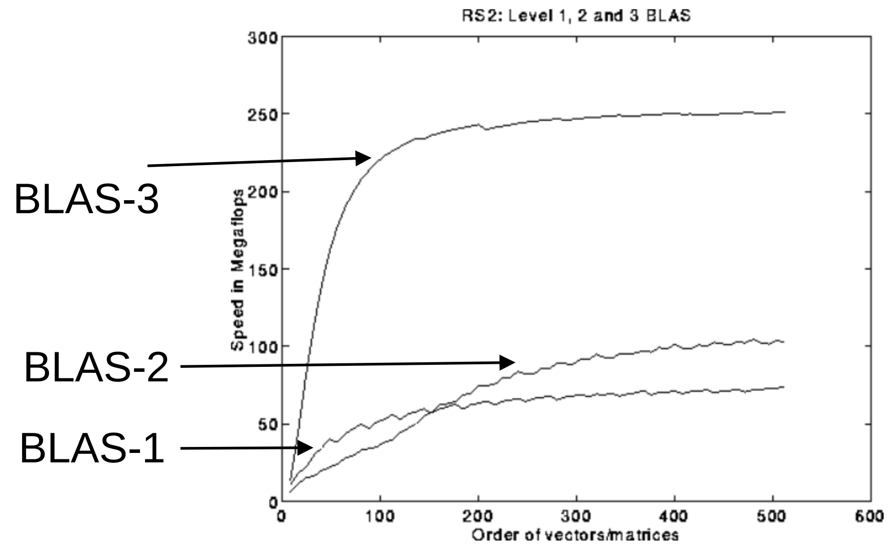
BLAS – Basic Linear Algebra Subroutines

- 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(n³) operations on O(n²) data.**

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



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

Computational Intensity

- 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*).
- We want to *maximize* the computational intensity
- What is q for axpy? Matrix-vector product? Matrix-Matrix product?

Computational Intensity - axpy

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

. 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

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

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

Computational Intensity – matrix-matrix

```
for i=1 to n
//Read row i of A into fast memory
        for j=1 to n
        //Read C(i,j) into fast memory
        //Read column j of B into fast memory
        for k=1 to n
                C(i,j)=C(i,j) + A(i,k)*B(k,j)
        //Write C(i,j) back to slow memory
```

n^2 words read: each row of A read once for each i. Assume that the row read stays in fast memory during the execution of inner two loops.

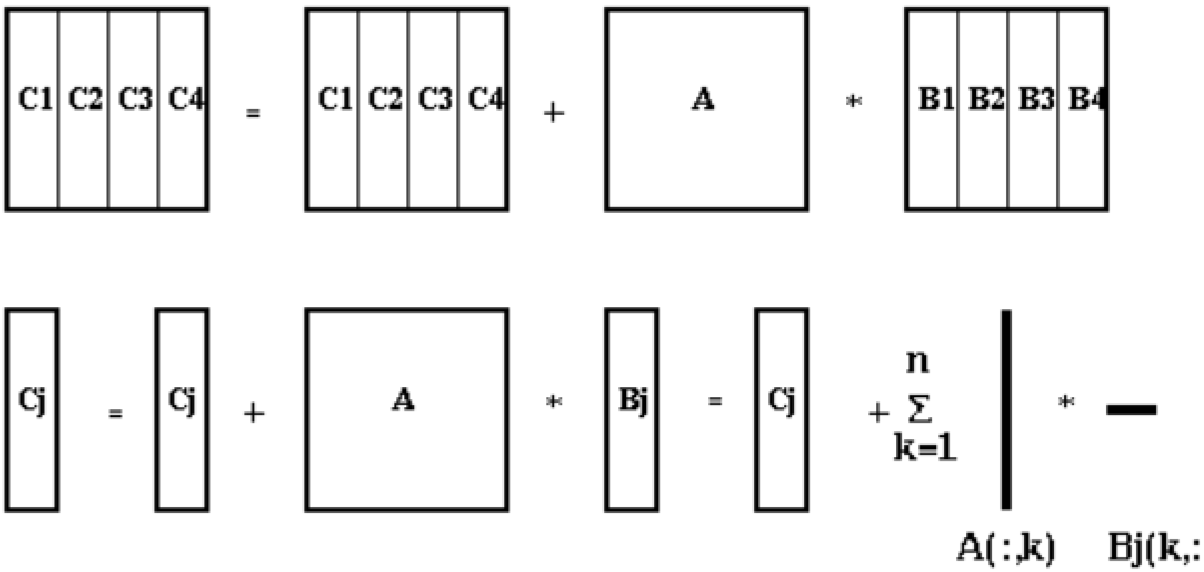
n^3 words read: each column of B read n^2 times

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

- Number of memory operations = $n^3 + 3n^2 = n^3 + O(n^2)$
- Number of arithmetic operations = $2n^3$
- $\boldsymbol{q \approx 2n^3/n^3 \ = \ 2.}$ *Same as matrix-vector?*
- What if the fast memory has space to hold entire B matrix, a row of A matrix, and one element of C matrix?

Blocked Matrix Multiply

- For N=4:




```
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
   Cj=Cj + A(*,k) * Bj(k,*)
   //Write Cj back to slow memory
```


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

Blocked Matrix Multiply - Example

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

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

j=1

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

....

```
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

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

```
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=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

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

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

```
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=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

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

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

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

j=1

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

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

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

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

j=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

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

$\downarrow$ q $\rightarrow$ r $\qquad$ $\downarrow$ q $\rightarrow$ p $\qquad$ $\downarrow$ p $\rightarrow$ 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?

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.

Efficiency Considerations

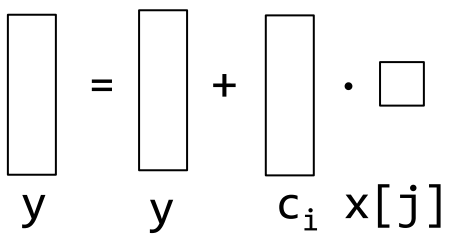
- Cache details (size)
- Data movement overhead
- Storage layout
- Parallel functional Units (Vector units)

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*

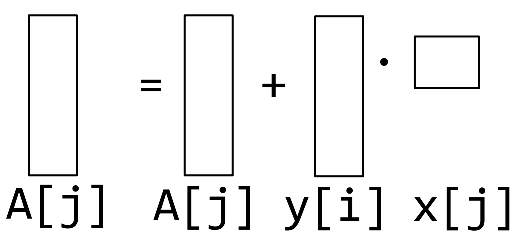
gaxpy

```
// 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_ix[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
```



Storage Layout Considerations

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

ijk vs. **jki**

```
for i=1 to m
    for j=1 to n
        for j=1 to n
             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]
```

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

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

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.

Matrix Structure and Efficiency

- Sparse Matrices
  - E.g. banded matrices
  - Diagonal
  - Tridiagonal etc.
- Symmetric Matrices

Admit optimizations w.r.t.

- Storage
- Computation