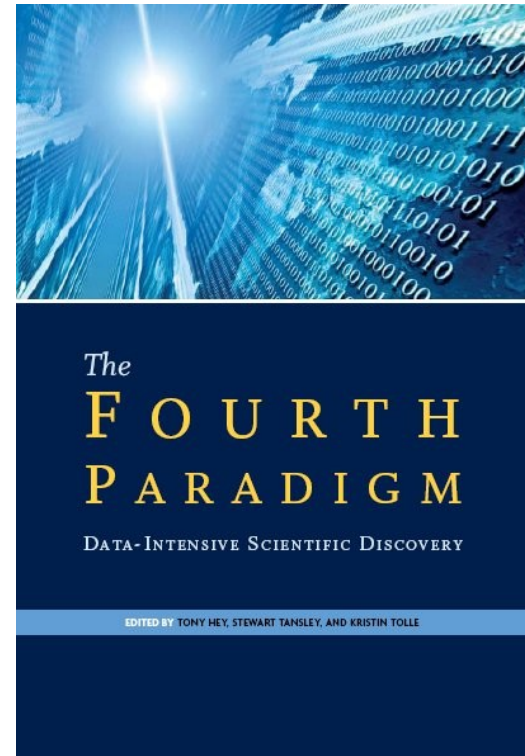


# Matrix multiplication

# Computational Science

## Paradigms in science

1. Theory
2. Experiments
3. Large scale computer simulations
  - Construct mathematical models
  - Implement as computer programs
  - Simulate on computers
4. Massive data sets



All types of computational science sooner or later boil down to numerical computations

# Elementary computations

<b>BLAS: Basic Linear Algebra Subprograms</b>	Data	Work
Level 1: $\mathbf{y} = \alpha \mathbf{x} + \mathbf{y}$ where $\mathbf{x}$ and $\mathbf{y}$ are $n$ -dimensional vectors	$O(n)$	$O(n)$
Level 2: $\mathbf{y} = \alpha \mathbf{A} \mathbf{x} + \beta \mathbf{y}$ where $\mathbf{A}$ is an $n \times n$ matrix	$O(n^2)$	$O(n^2)$
Level 3: $\mathbf{C} = \alpha \mathbf{A} \mathbf{B} + \beta \mathbf{C}$ where $\mathbf{B}$ and $\mathbf{C}$ are $n \times n$ matrices	$O(n^2)$	$O(n^3)$

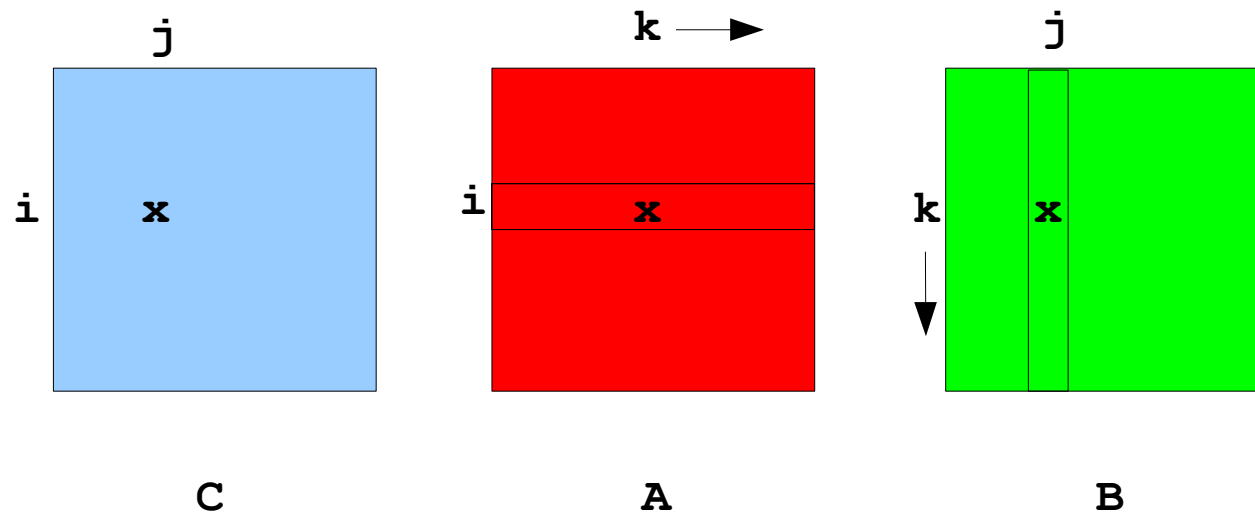
Building blocks when solving various problems in numerical linear algebra:

- Systems of linear equations
- Linear least squares
- Eigenvalue problems
- Singular value decompositions

Also similar computations for *sparse* data sets

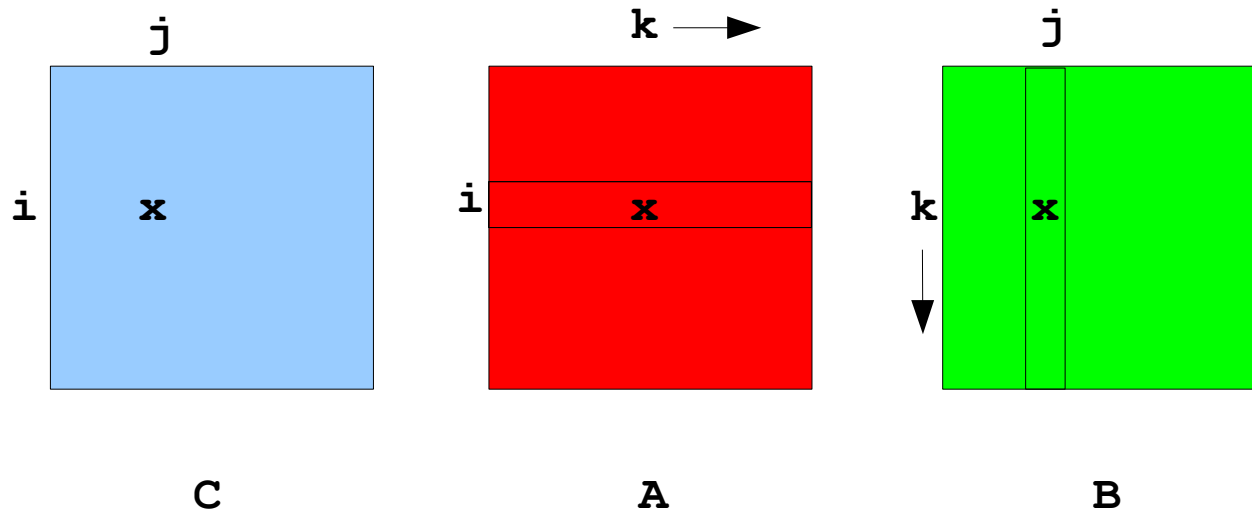
# BLAS 3: Matrix Multiplication

Compute  $C = A * B$  where  $A$ ,  $B$ , and  $C$  are  $n \times n$  real valued matrices



# BLAS 3: Matrix Multiplication

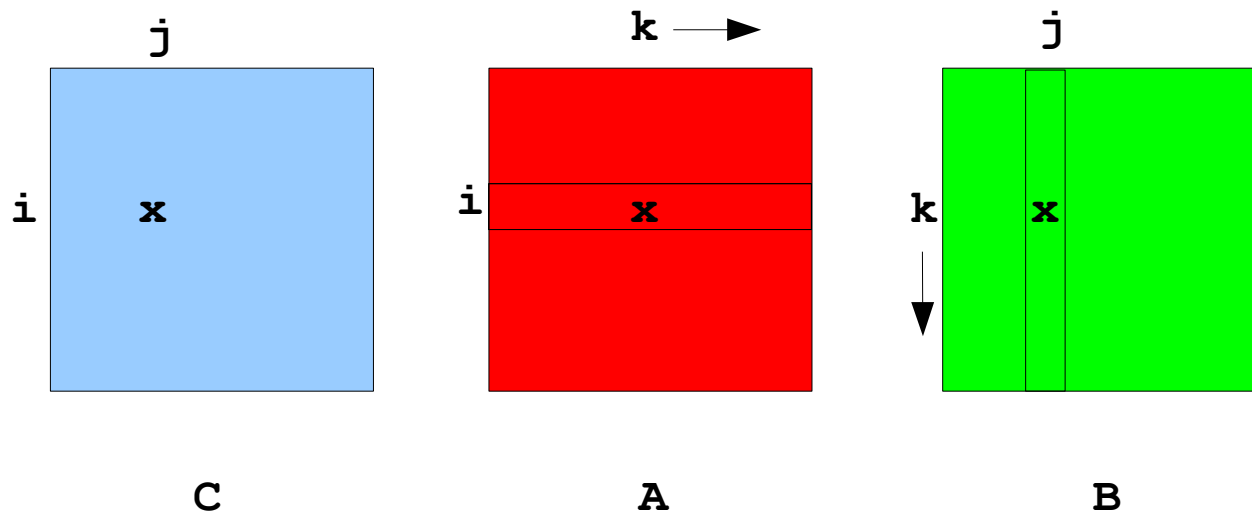
Compute  $C = A * B$  where  $A$ ,  $B$ , and  $C$  are  $n \times n$  real valued matrices



```
for i=0,...,n-1
  for j=0,...,n-1 {
    c[i][j] = 0.0
    for k=0,...,n-1
      c[i][j] += a[i][k] * b[k][j]
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```

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      c[i][j] += a[i][k] * b[k][j]
  }
```

Requires  $3n^2$  data elements and  $n^2 (2n - 1)$  flops

Running time:  $\Theta(n^3)$

# The evolution of matrix multiplication algorithms

- Straightforward:  $n^3$
- Strassen (1968):  $n^{\lg(7)} \approx n^{2.8074}$
- Coppersmith–Winograd (1990):  $n^{2.375477}$
- Stothers (2010):  $n^{2.3736897}$ 
  - Williams (2011):  $n^{2.3728642}$
  - Le Gall (2014):  $n^{2.3728639}$

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## In practice:

- Algorithms with lower complexity than Strassen are **slow**
- Sub-cubic algorithms require much **memory**



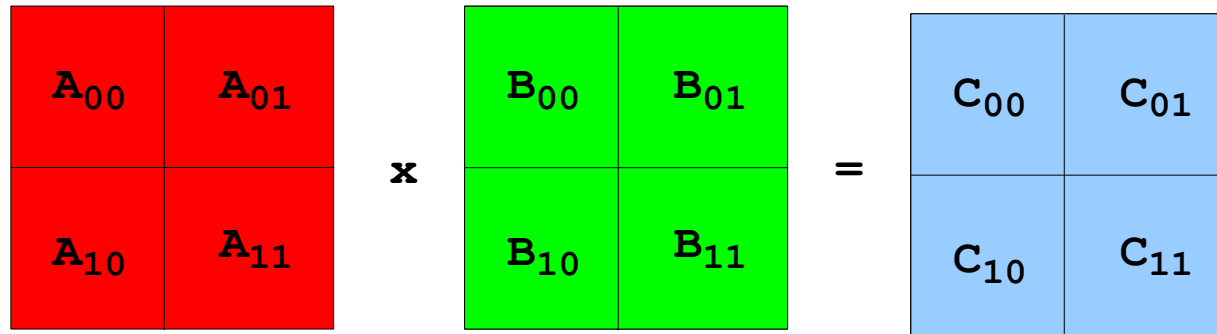
# Strassen's algorithm

$$\begin{array}{|c|c|} \hline A_{00} & A_{01} \\ \hline A_{10} & A_{11} \\ \hline \end{array} \times \begin{array}{|c|c|} \hline B_{00} & B_{01} \\ \hline B_{10} & B_{11} \\ \hline \end{array} = \begin{array}{|c|c|} \hline C_{00} & C_{01} \\ \hline C_{10} & C_{11} \\ \hline \end{array}$$

```

Algorithm Strassen(A, B, n) {
    if (n==1) return A*B
    P1 = Strassen(A00+A11, B00+B11, n/2)
    P2 = Strassen(A10+A11, B00, n/2)
    P3 = Strassen(A00, B01-B11, n/2)
    P4 = Strassen(A11, B10-B00, n/2)
    P5 = Strassen(A00+A01, B11, n/2)
    P6 = Strassen(A10-A00, B00+B01, n/2)
    P7 = Strassen(A01-A11, B10+B11, n/2)
    C00 = P1+P4-P5+P7
    C01 = P3+P5
    C10 = P2+P4
    C11 = P1-P2+P3+P6
    return C
}
    
```

# Strassen's algorithm



**Algorithm** Strassen(**A**, **B**, **n**) {

    if (**n**==1) return **A**\***B**

**P**<sub>1</sub> = Strassen (**A**<sub>00</sub>+**A**<sub>11</sub>, **B**<sub>00</sub>+**B**<sub>11</sub>, **n**/2)

**P**<sub>2</sub> = Strassen (**A**<sub>10</sub>+**A**<sub>11</sub>, **B**<sub>00</sub>, **n**/2)

**P**<sub>3</sub> = Strassen (**A**<sub>00</sub>, **B**<sub>01</sub>-**B**<sub>11</sub>, **n**/2)

**P**<sub>4</sub> = Strassen (**A**<sub>11</sub>, **B**<sub>10</sub>-**B**<sub>00</sub>, **n**/2)

**P**<sub>5</sub> = Strassen (**A**<sub>00</sub>+**A**<sub>01</sub>, **B**<sub>11</sub>, **n**/2)

**P**<sub>6</sub> = Strassen (**A**<sub>10</sub>-**A**<sub>00</sub>, **B**<sub>00</sub>+**B**<sub>01</sub>, **n**/2)

**P**<sub>7</sub> = Strassen (**A**<sub>01</sub>-**A**<sub>11</sub>, **B**<sub>10</sub>+**B**<sub>11</sub>, **n**/2)

**C**<sub>00</sub> = **P**<sub>1</sub>+**P**<sub>4</sub>-**P**<sub>5</sub>+**P**<sub>7</sub>

**C**<sub>01</sub> = **P**<sub>3</sub>+**P**<sub>5</sub>

**C**<sub>10</sub> = **P**<sub>2</sub>+**P**<sub>4</sub>

**C**<sub>11</sub> = **P**<sub>1</sub>-**P**<sub>2</sub>+**P**<sub>3</sub>+**P**<sub>6</sub>

    return **C**

}

**Running time:**  $f(n) =$

number of additions and multiplications

**Recursion:**  $f(n) = 7f(n/2) + k*n^2$

**Yields:**  $f \in \Theta(n^{\lg 7})$

# Straightforward algorithm in OpenMP

```
for i=0,...,n-1
  for j=0,...,n-1 {
    c[i][j] = 0.0
    for k=0,...,n-1
      c[i][j] += a[i][k] * b[k][j]
  }
```

# Straightforward algorithm in OpenMP

```
#pragma omp parallel for private(j,k)
for i=0,...,n-1
  for j=0,...,n-1 {
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  }
```

## Speedup:

- Wrt sequential straightforward:  $n^3 / (n^3/p) = p$  (perfect speedup!)

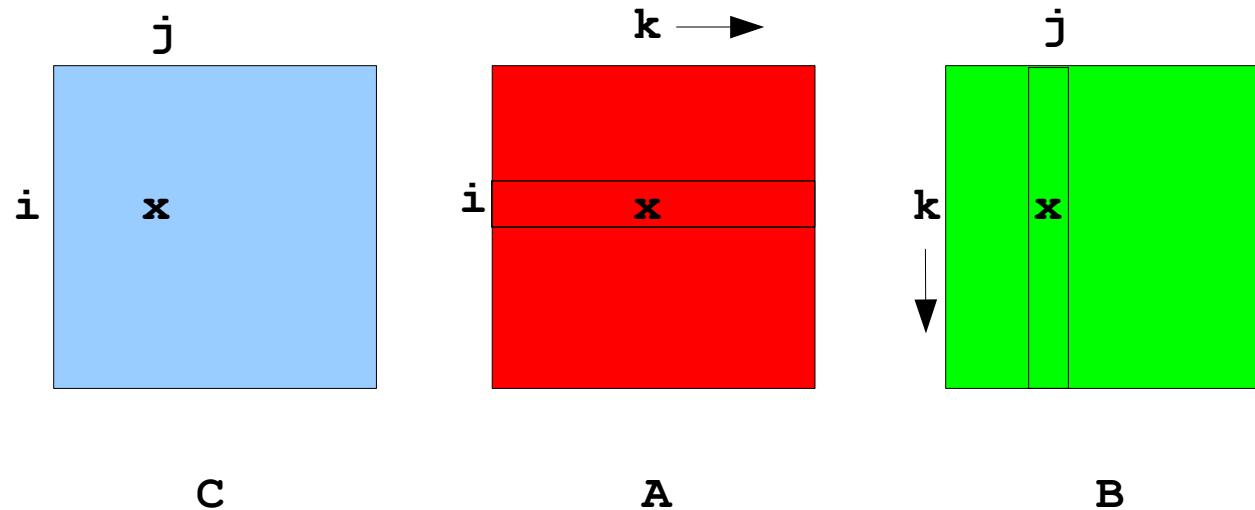
# Straightforward algorithm in OpenMP

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```

## Speedup:

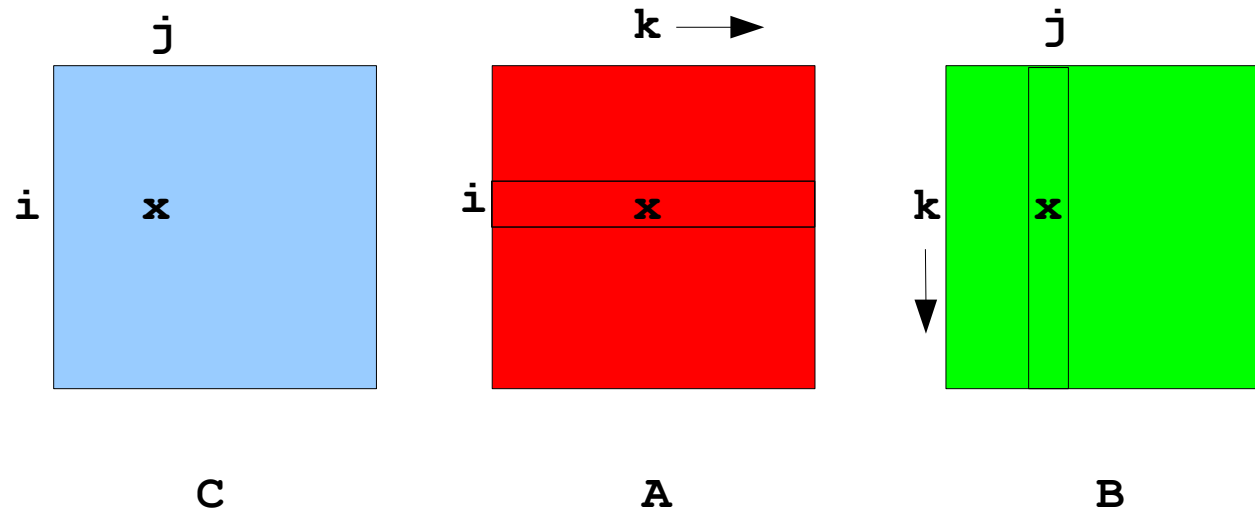
- Wrt sequential straightforward:  $n^3 / (n^3/p) = p$  (perfect speedup!)
- Wrt sequential Strassen:  $n^{1.58} / (n^3/p) = pn^{1.58-3} \rightarrow 0$  as  $n \rightarrow \infty$

# Matrix multiplication in OpenMP



```
#pragma omp parallel for private(j,k)
for i=0,...,n-1
  for j=0,...,n-1 {
    c[i][j] = 0.0
    for k=0,...,n-1
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  }
```

# Matrix multiplication in OpenMP

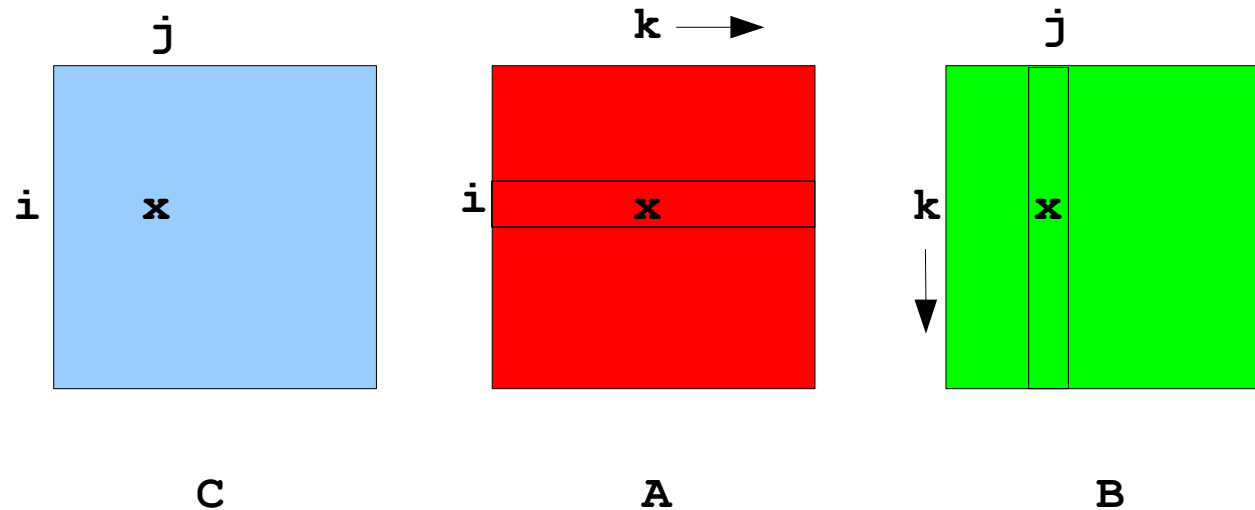


```
#pragma omp parallel for private(j,k)
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  for j=0,...,n-1 {
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    for k=0,...,n-1
      c[i][j] += a[i][k] * b[k][j]
  }
```

Rows of B move in and out of cache!

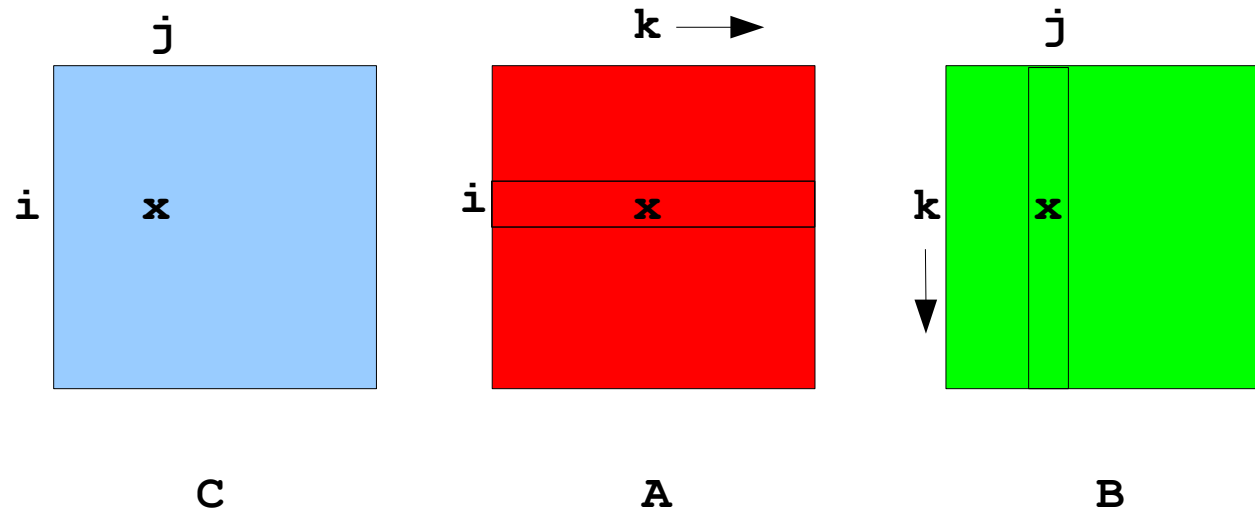


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    for k=0,...,n-1
        for j=0,...,n-1
            c[i][j] += a[i][k] * b[k][j]
}
```

Finish all work with one row in B!

# How fast can two matrices be multiplied?

- Straightforward version with  $n$  threads:  $\Theta(n^2)$

```
for i=0,...,n-1
  for j=0,...,n-1 {
    c[i][j] = 0.0
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- Straightforward version with  $n^2$  threads:
  - Thread  $(i, j)$  computes  $c[i][j]$ :
  - Run through the  $i$ th row of  $A$  and the  $j$ th column of  $B$ :  $\Theta(n)$

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for i=0,...,n-1
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  - Run through the  $i$ th row of  $A$  and the  $j$ th column of  $B$ :  $\Theta(n)$
- Straightforward version with  $n^3$  threads:
  - Thread  $(i, j, k)$  computes  $\text{product} = a[i][k] * b[k][j]$
  - $n^2$  reductions of  $\text{product}$  in parallel :  $(i, j, k) \rightarrow (i, j, 0)$
  - $\Theta(\lg(n))$

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for i=0,...,n-1
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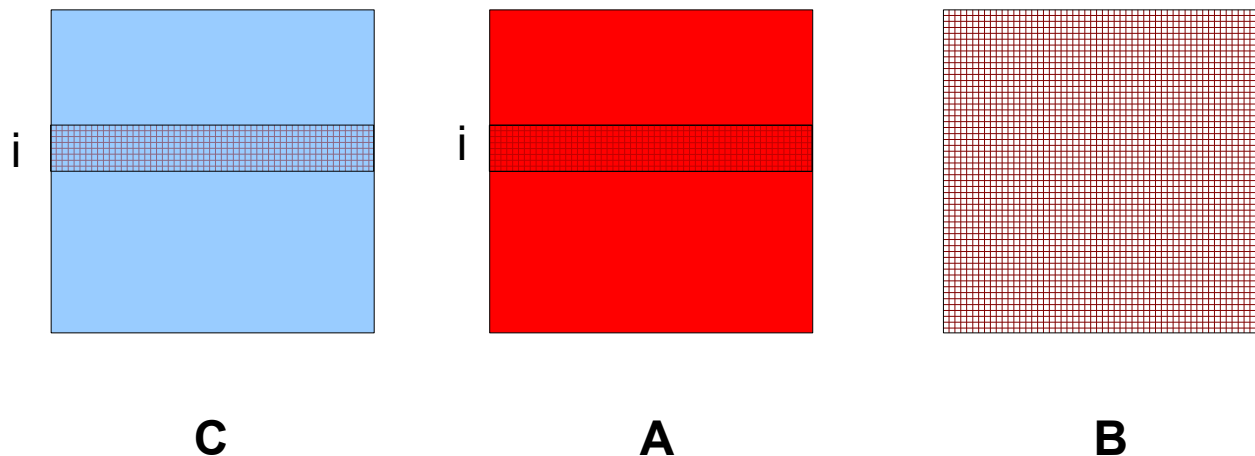
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  - $\Theta(\lg(n))$
- **Theorem** (Moldovan, 1993): Cannot multiply faster than  $\Theta(\lg(n))$

```
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  for j=0,...,n-1 {
    c[i][j] = 0.0
    for k=0,...,n-1
      c[i][j] += a[i][k] * b[k][j]
  }
```

# Matrix multiplication in MPI (or BSP)

Row-wise decomposition (assume  $p=n$ ):

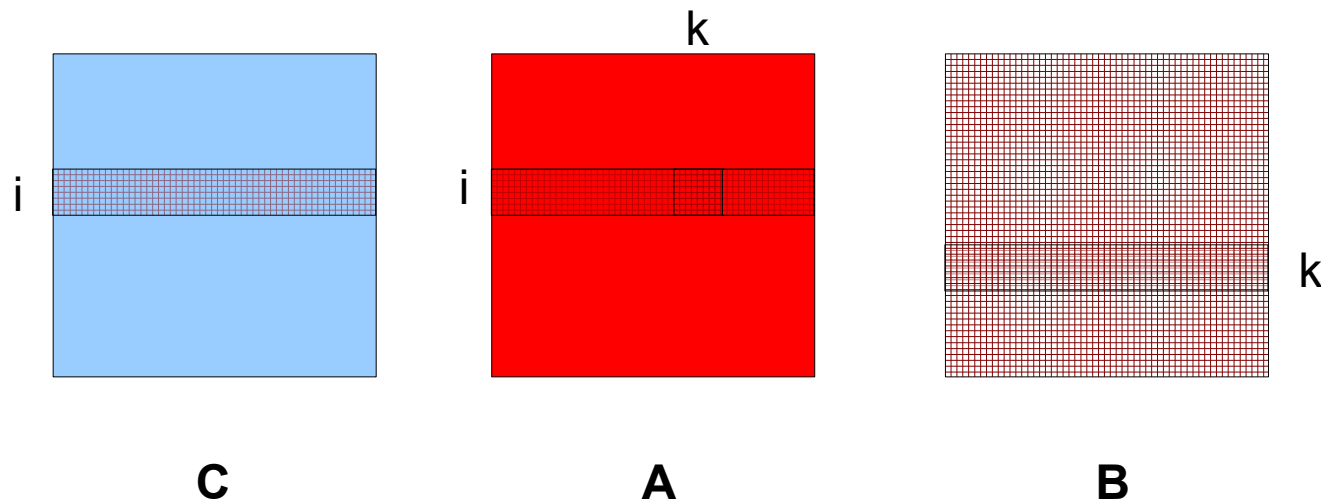
- Process  $i$  holds row  $i$  of matrices  $A$  and  $B$
- Process  $i$  computes the  $i$ th row of  $C$ 
  - Needs access to row  $i$  of  $A$
  - Needs access to all of  $B$
- **Alternative 1**: Broadcast  $B$  to all processes



# Matrix multiplication in MPI (or BSP)

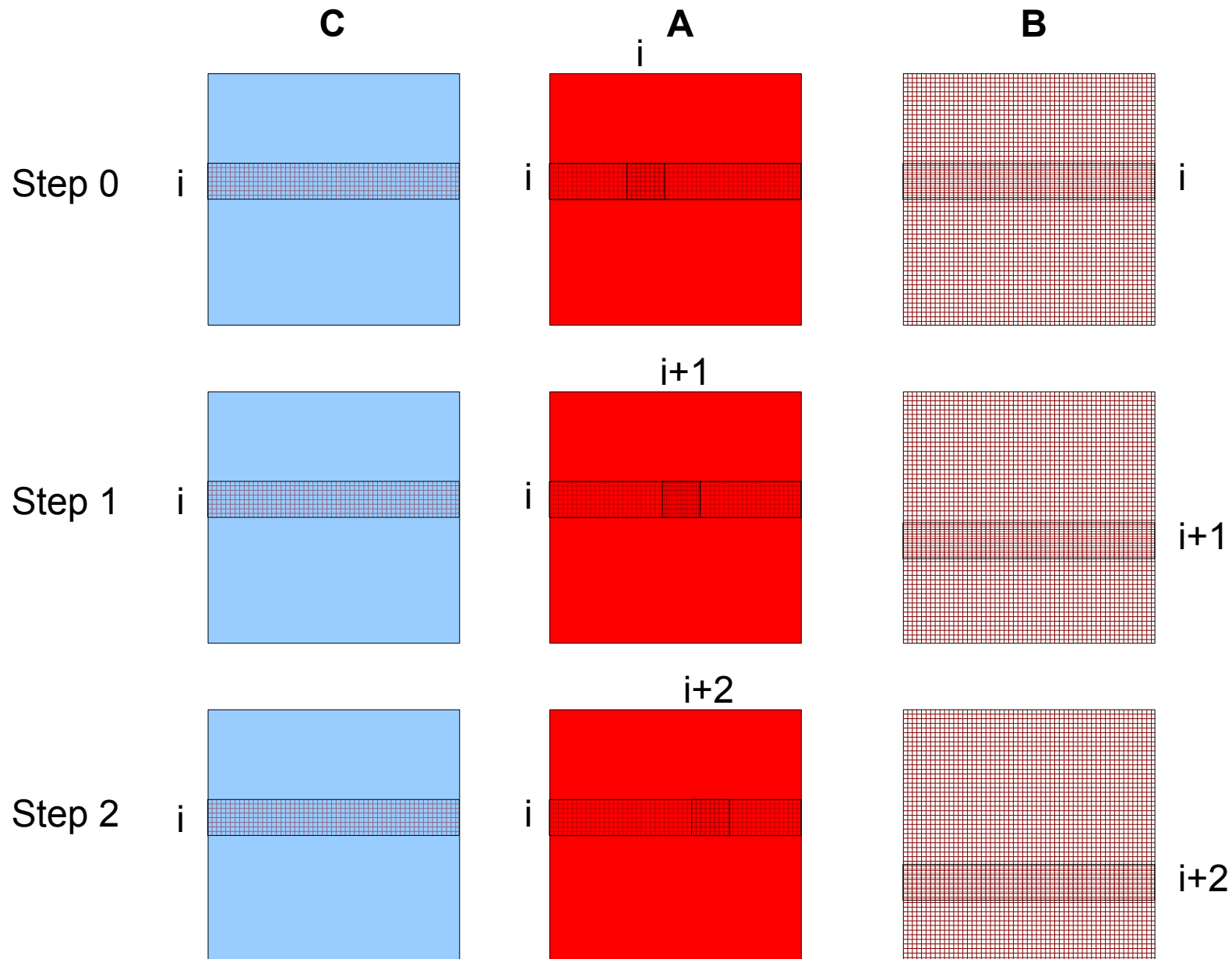
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  - Needs access to row  $i$  of  $A$
  - Needs access to all of  $B$
- **Alternative 1:** Broadcast  $B$  to all processes
- **Alternative 2:** Rotate the rows of  $B$  on the processes
  - Reduces memory usage in each process





# Matrix multiplication in MPI (or BSP)



# Matrix multiplication in MPI (or BSP)

**Idea:** Row  $i$  of  $C = \sum_{0 \leq k < n} (a[k] * \text{row } k \text{ of } B)$

**Algorithm** `MM(A,B,C)` { // Process  $i$  initially holds row  $i$  of  $A$  and  $B$

```
  c[0..n-1] = 0.0; i = process id; k = i  
  repeat  
    for j=0, ..., n-1  
      c[j] += a[k]*b[j]  
      k = (k+1)%n  
      if (k!=i) {  
        send b to process (i-1)%n  
        receive b from process (i+1)%n  
      }  
  until k==i  
}
```

# Matrix multiplication in MPI (or BSP)

When  $p < n$ :

- Process  $i$  holds  $m = n/p$  rows of  $A$
- Process  $i$  computes  $m$  rows of  $C$

# Matrix multiplication in MPI (or BSP)

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- Process  $i$  holds  $m=n/p$  rows of  $A$
- Process  $i$  computes  $m$  rows of  $C$

Running time analysis:

- Computation:
  - each process computes a submatrix with  $m$  rows and  $n$  columns
  - $n^2/p$  elements in total
  - each element takes  $\Theta(n)$  time to compute
  - $T_{\text{comp}} \in \Theta(n^3/p)$

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- Communication:
  - $p$  point-to-point communications of length  $n^2/p$ :  $pt_0 + pt_1 n^2/p = pt_0 + t_1 n^2$
  - $T_{\text{comm}} \in \Theta(p + n^2)$

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- $T_{\text{comp}}/T_{\text{comm}} \in \Theta(n/p)$

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- Communication:
  - $p$  point-to-point communications of length  $n^2/p$ :  $pt_0 + pt_1 n^2/p = pt_0 + t_1 n^2$   
(BSP:  $l = t_0$   $g = t_1$ )
  - $T_{\text{comm}} \in \Theta(p + n^2)$
- $T_{\text{comp}}/T_{\text{comm}} \in \Theta(n/p)$

Observation:

- Process  $i$  needs
  - $n^2/p$  elements from  $A$
  - all  $n^2$  elements from  $B$to compute only  $n^2/p$  elements in  $C$
- Can we compute  $n^2/p$  elements in  $C$  with access to fewer elements from  $B$ ?
  - Is reduced communication

# Block-wise decomposition

$C_{00}$		

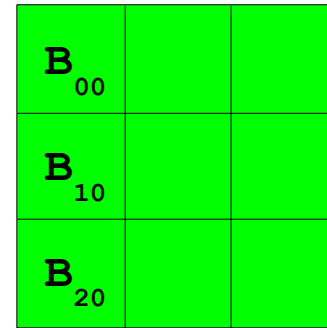
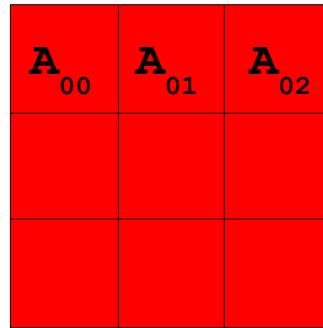
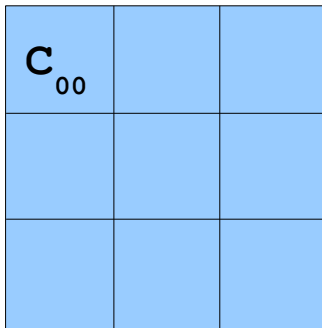
$A_{00}$	$A_{01}$	$A_{02}$

$B_{00}$		
$B_{10}$		
$B_{20}$		

$$C_{00} = (A_{00} * B_{00}) + (A_{01} * B_{10}) + (A_{02} * B_{20})$$



# Block-wise decomposition



$$C_{00} = (A_{00} * B_{00}) + (A_{01} * B_{10}) + (A_{02} * B_{20})$$

**s** = number of row and column blocks

for **i** = 0, ..., **s**-1

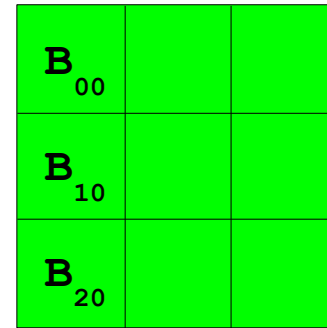
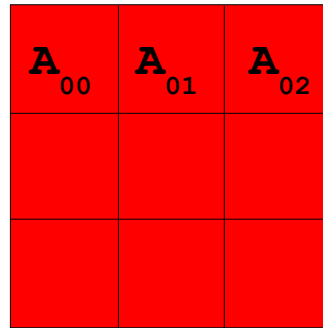
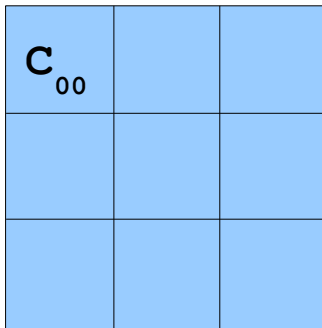
  for **j** = 0, ..., **s**-1

**C<sub>ij</sub>** = 0.0

    for **k** = 0, ..., **s**-1

**C<sub>ij</sub>** += **A<sub>ik</sub>** \* **B<sub>kj</sub>** // Matrix multiplication

# Block-wise decomposition



$$C_{00} = (A_{00} * B_{00}) + (A_{01} * B_{10}) + (A_{02} * B_{20})$$

$s$  = number of row and column blocks

for  $i = 0, \dots, s-1$

for  $j = 0, \dots, s-1$

$C_{ij} = 0.0$

for  $k = 0, \dots, s-1$

$C_{ij} += A_{ik} * B_{kj}$  // Matrix multiplication

- assume  $p=s^2$  is a square number
- process  $(i, j)$  to compute  $C_{ij}$
- $m = n/s$  = rows and columns in a block
- each block multiplication requires  $\sim 2m^3$  flops.

# Block-wise decomposition

$C_{00}$		

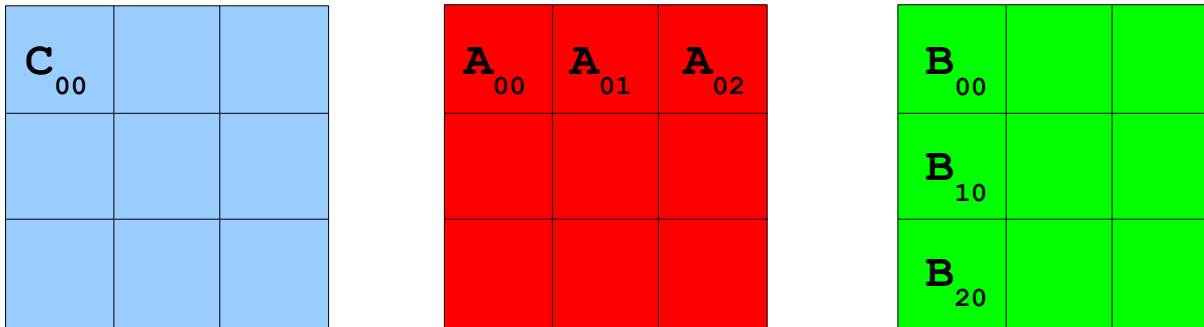
$A_{00}$	$A_{01}$	$A_{02}$

$B_{00}$		
$B_{10}$		
$B_{20}$		

$$C_{00} = (A_{00} * B_{00}) + (A_{01} * B_{10}) + (A_{02} * B_{20})$$

- [Idea \(Canon's algorithm\)](#): Rotate **A**- and **B**-blocks between the processes

# Block-wise decomposition



$$C_{00} = (A_{00} * B_{00}) + (A_{01} * B_{10}) + (A_{02} * B_{20})$$

- **Idea (Canon's algorithm):** Rotate **A**- and **B**-blocks between the processes
- To what **A**- and **B**-blocks does process  $(i, j)$  need access?
  - **A**-blocks with row index  $i$ :  $A_{i0}, A_{i1}, \dots, A_{i,s-1}$
  - **B**-blocks with column index  $j$ :  $B_{0j}, B_{1j}, \dots, B_{s-1,j}$
  - Synchronization: Get  $A_{ik}$  and  $B_{kj}$  simultaneously

# Block-wise decomposition

$C_{00}$		

$A_{00}$	$A_{01}$	$A_{02}$

$B_{00}$		
$B_{10}$		
$B_{20}$		

$$C_{00} = (A_{00} * B_{00}) + (A_{01} * B_{10}) + (A_{02} * B_{20})$$

- **Idea (Canon's algorithm):** Rotate **A**- and **B**-blocks between the processes
- To what **A**- and **B**-blocks does process  $(i, j)$  need access?
  - **A**-blocks with row index  $i$ :  $A_{i0}, A_{i1}, \dots, A_{i,s-1}$
  - **B**-blocks with column index  $j$ :  $B_{0j}, B_{1j}, \dots, B_{s-1,j}$
  - Synchronization: Get  $A_{ik}$  and  $B_{kj}$  simultaneously
- What processes need access to  $A_{ij}$ ?
  - $C_{i*}$ : All processes with row id  $i$ :  $(i, 0), (i, 1), \dots, (i, s-1)$
- What processes need access to  $B_{ij}$ ?
  - $C_{*j}$ : All processes with column id  $j$ :  $(0, j), (1, j), \dots, (s-1, j)$

# Block-wise decomposition

$C_{00}$		

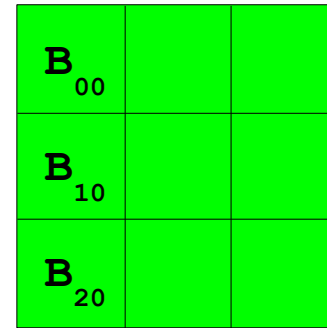
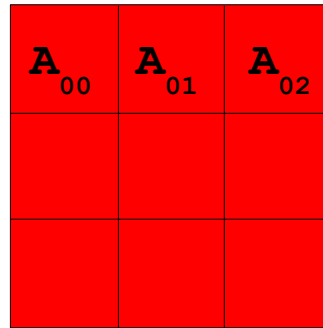
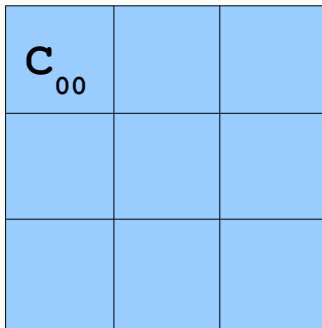
$A_{00}$	$A_{01}$	$A_{02}$

$B_{00}$		
$B_{10}$		
$B_{20}$		

$$C_{00} = (A_{00} * B_{00}) + (A_{01} * B_{10}) + (A_{02} * B_{20})$$

- [Idea \(Canon's algorithm\)](#): Rotate **A**- and **B**-blocks on the processes
- Order is irrelevant for summation  $C_{ij} = \sum_k (A_{ik} * B_{kj})$

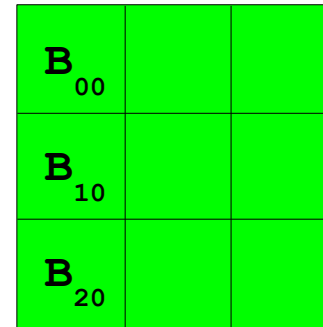
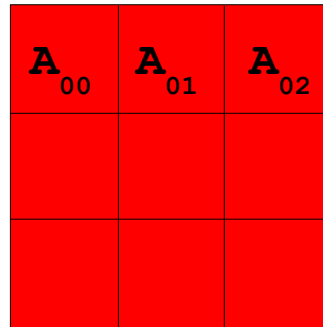
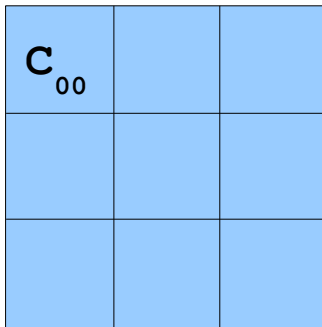
# Block-wise decomposition



$$C_{00} = (A_{00} * B_{00}) + (A_{01} * B_{10}) + (A_{02} * B_{20})$$

- **Idea (Canon's algorithm):** Rotate **A**- and **B**-blocks on the processes
- Order is irrelevant for summation  $C_{ij} = \sum_k (A_{ik} * B_{kj})$
- Start at  $k=0$ :  $C_{ij} = A_{i0} * B_{0j} + A_{i1} * B_{1j} + \dots + A_{i,s-1} * B_{s-1,j}$ 
  - **Bad!** All procs  $(i, 0), (i, 1), (i, 2), \dots, (i, s-1)$  need  $A_{i0}$  early!

# Block-wise decomposition

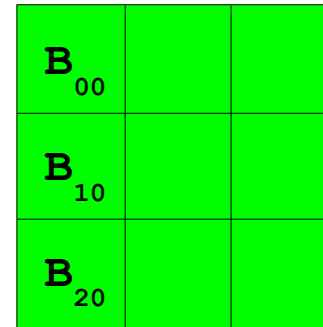
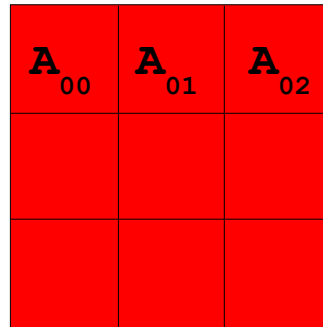
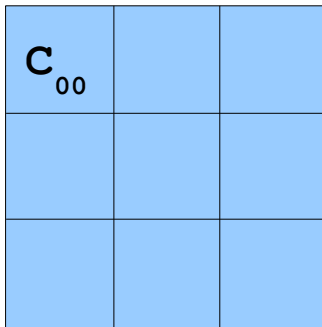


$$C_{00} = (A_{00} * B_{00}) + (A_{01} * B_{10}) + (A_{02} * B_{20})$$

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  - **Bad!** All procs  $(i, 0), (i, 1), (i, 2), \dots, (i, s-1)$  need  $A_{i0}$  early!
- Start at  $k=i$ :  $C_{ij} = A_{ii} * B_{ij} + A_{i,i+1} * B_{i+1,j} + \dots + A_{i,s-1} * B_{s-1,j}$   
 $+ A_{i0} * B_{0j} + A_{i1} * B_{1j} + \dots + A_{i,i-1} * B_{i-1,j}$ 
  - **Bad!** All procs  $(i, 0), (i, 1), (i, 2), \dots, (i, s-1)$  need  $A_{ii}$  early!



# Block-wise decomposition



$$C_{00} = (A_{00} * B_{00}) + (A_{01} * B_{10}) + (A_{02} * B_{20})$$

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- Order is irrelevant for summation  $C_{ij} = \sum_k (A_{ik} * B_{kj})$
- Start at  $k=0$ :  $C_{ij} = A_{i0} * B_{0j} + A_{i1} * B_{1j} + \dots + A_{i,s-1} * B_{s-1,j}$ 
  - **Bad!** All procs  $(i, 0), (i, 1), (i, 2), \dots, (i, s-1)$  need  $A_{i0}$  early!
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 $+ A_{i0} * B_{0j} + A_{i1} * B_{1j} + \dots + A_{i,i-1} * B_{i-1,j}$ 
  - **Bad!** All procs  $(i, 0), (i, 1), (i, 2), \dots, (i, s-1)$  need  $A_{ii}$  early!
- Summation order must depend on both  $i$  and  $j$

# Block-wise decomposition

$C_{00}$		

$A_{00}$	$A_{01}$	$A_{02}$

$B_{00}$		
$B_{10}$		
$B_{20}$		

$$C_{00} = (A_{00} * B_{00}) + (A_{01} * B_{10}) + (A_{02} * B_{20})$$

- [Idea \(Canon's algorithm\)](#): Rotate **A**- and **B**-blocks on the processes
- Order is irrelevant for summation  $C_{ij} = \sum_k (A_{ik} * B_{kj})$

	k=0	k=1	k=2
First	k=1	k=2	k=0
summation			
index value	k=2	k=0	k=1

# Block-wise decomposition

$C_{00}$		

$A_{00}$	$A_{01}$	$A_{02}$

$B_{00}$		
$B_{10}$		
$B_{20}$		

$$C_{00} = (A_{00} * B_{00}) + (A_{01} * B_{10}) + (A_{02} * B_{20})$$

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- Order is irrelevant for summation  $C_{ij} = \sum_k (A_{ik} * B_{kj})$

	k=0	k=1	k=2
First	k=1	k=2	k=0
summation			
index value	k=2	k=0	k=1

Start at  $k = (i+j) \% s$

# Block-wise decomposition

$C_{00}$		

$A_{00}$	$A_{01}$	$A_{02}$

$B_{00}$		
$B_{10}$		
$B_{20}$		

$$C_{00} = (A_{00} * B_{00}) + (A_{01} * B_{10}) + (A_{02} * B_{20})$$

- [Idea \(Canon's algorithm\)](#): Rotate **A**- and **B**-blocks on the processes
- Order is irrelevant for summation  $C_{ij} = \sum_k (A_{ik} * B_{kj})$

First summation index value

k=0	k=1	k=2
k=1	k=2	k=0
k=2	k=0	k=1

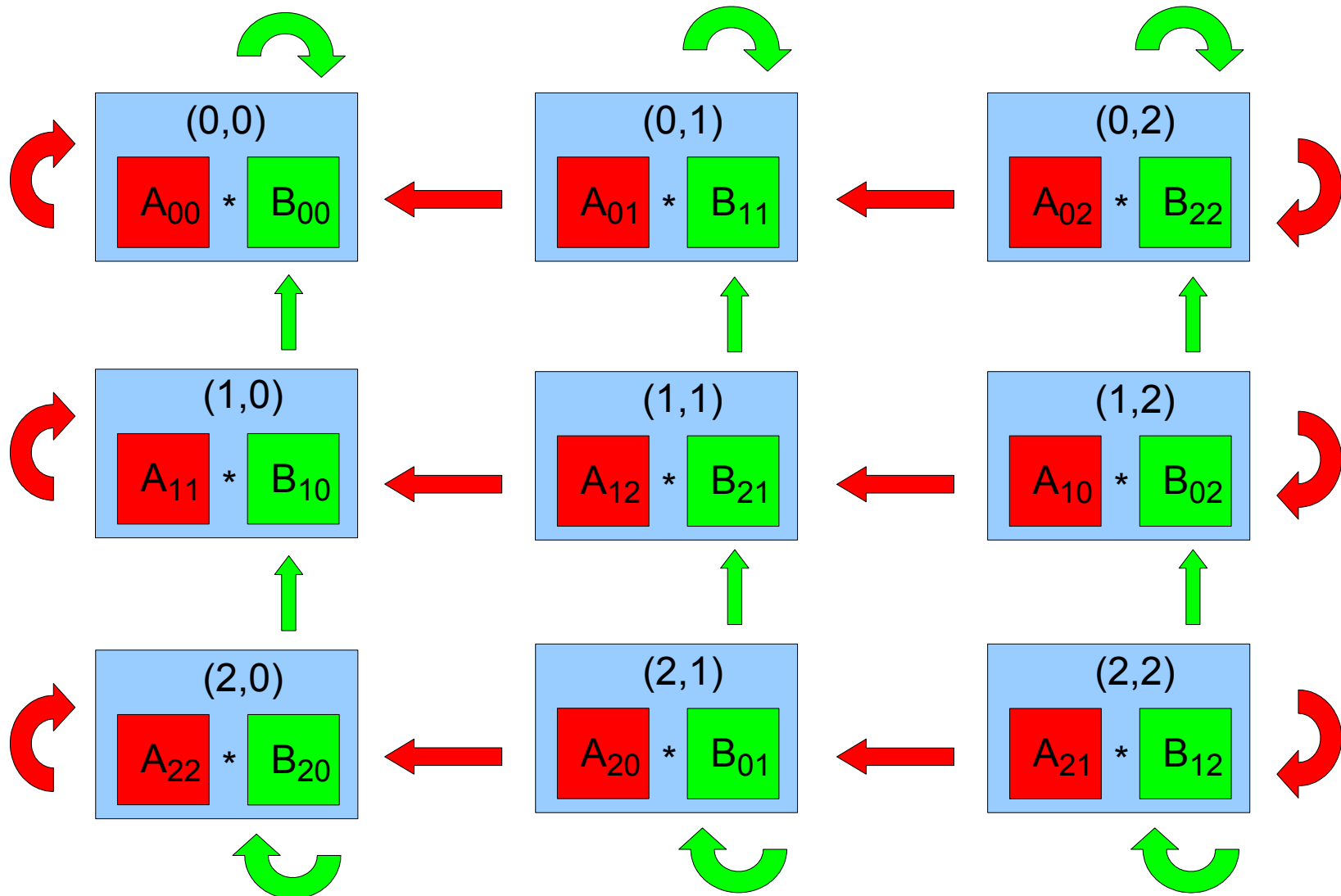
Start at  $k = (i+j) \% s$

Second summation index value

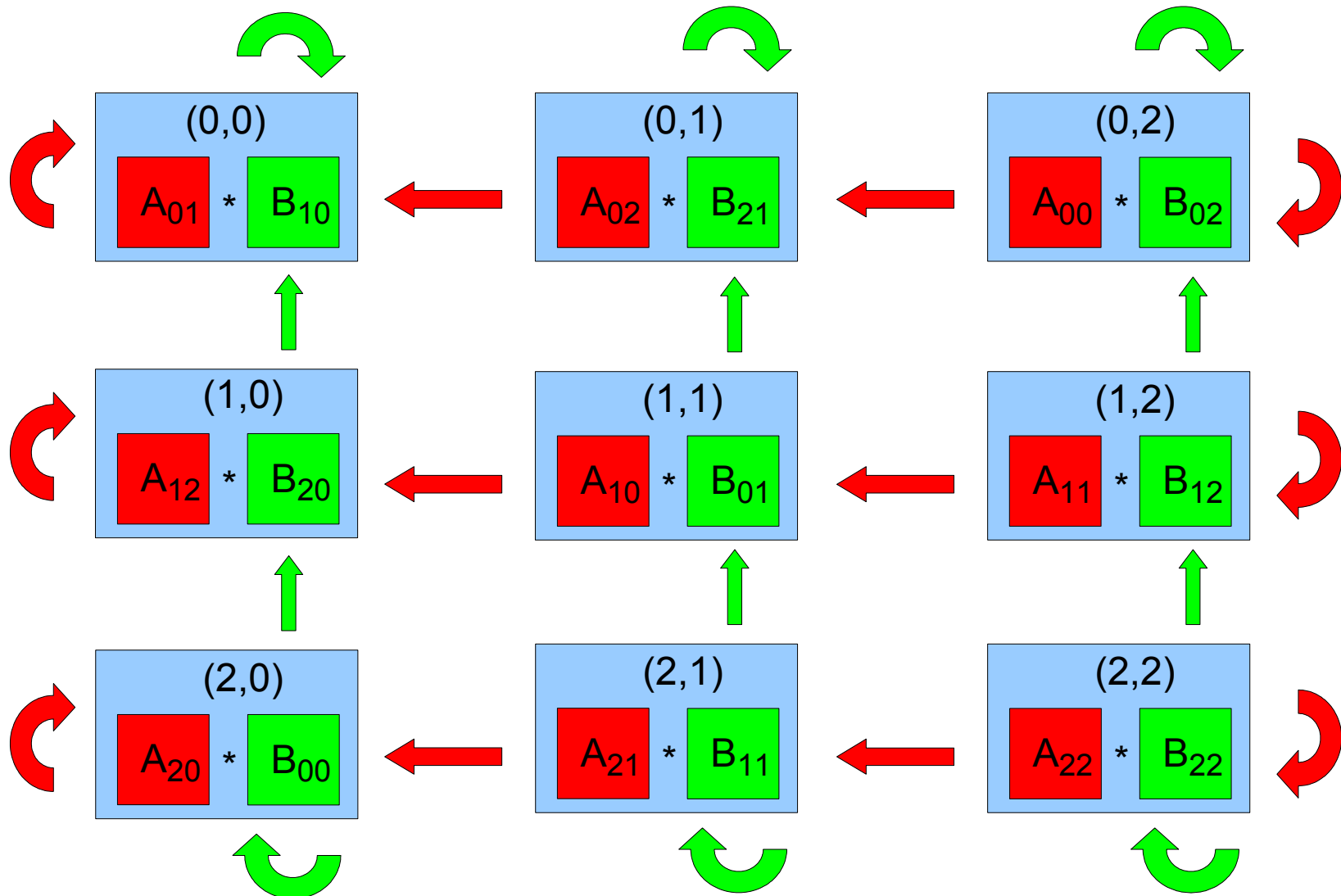
k=1	k=2	k=0
k=2	k=0	k=1
k=0	k=1	k=2

$k = (k+1) \% s$

# Cannon's algorithm: Step 0



# Cannon's algorithm: Step 1



# Canon's algorithm

**Assumption:** Process  $(i, j)$  holds  $\mathbf{A}_{ij}$  and  $\mathbf{B}_{ij}$

# Canon's algorithm

**Assumption:** Process  $(i, j)$  holds  $A_{ij}$  and  $B_{ij}$

**Initialize:**     Rotate  $A_{ij}$   $i$  positions **left**  
                     Rotate  $B_{ij}$   $j$  positions **up**



# Canon's algorithm

**Assumption:** Process  $(i, j)$  holds  $A_{ij}$  and  $B_{ij}$

**Initialize:** Rotate  $A_{ij}$   $i$  positions **left**  
Rotate  $B_{ij}$   $j$  positions **up**

**Compute:** Local matrix multiplication:  $C = A * B$   
Repeat  $\sqrt{p}-1$  times:  
    Send  $A$  to the **left**  
    Send  $B$  **up**  
    Local matrix multiplication:  $C += A * B$

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Repeat  $\sqrt{p}-1$  times:  
    Send  $A$  to the **left**  
    Send  $B$  **up**  
    Local matrix multiplication:  $C += A * B$

**Running time analysis:**

- Computation:  $T_{\text{comp}} \in \Theta((n/\sqrt{p})^3 \sqrt{p}) = \Theta(n^3/p)$
- Communication:  $T_{\text{comm}} = 2\sqrt{p}(t_0 + (n^2/p)t_1) \in \Theta(n^2/\sqrt{p})$
- $T_{\text{comp}}/T_{\text{comm}} \in \Theta(n/\sqrt{p})$

# Canon's algorithm

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**Running time analysis:**

- Computation:  $T_{\text{comp}} \in \Theta((n/p)^3 p) = \Theta(n^3/p)$
- Communication:  $T_{\text{comm}} = 2\sqrt{p}(t_0 + (n^2/p)t_1) \in \Theta(n^2/\sqrt{p})$
- $T_{\text{comp}}/T_{\text{comm}} \in \Theta(n/\sqrt{p})$

**Compared to row-wise decomposition:**

- Communication reduced by a factor  $\sqrt{p}$

# Canon's algorithm

## Technical:

- Process  $(i, j)$  has id  $i*s+j$
- Process  $q$  computes block  $(q/s, q\%s)$
- Process  $q$ 's upstairs neighbor has id  $(q-s) \% p$
- Process  $q$ 's downstairs neighbor has id  $(q+s) \% p$
- Process  $q$ 's right neighbor has id  $q+1$  or  $q-s+1$
- Process  $q$ 's left neighbor has id  $q-1$  or  $q+s-1$