Dense Matrix Algorithms (Chapter 8)

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B2-206

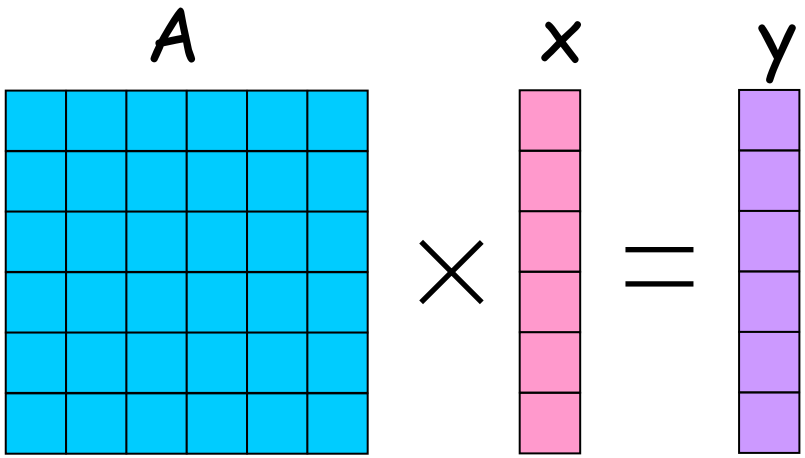
Dense Matrix Algorithm

- Dense or full matrices: few known zeros.
  - Other algorithms for sparse matrix.
- Square matrices for pedagogical purposes only – can be generalized.
- Natural to have data decomposition.
  - 3.2.2 input/output/intermediate data.
  - 3.4.1 mapping schemes based on data partitioning.

Today

- Matrix*Vector
- Matrix*Matrix
- Solving systems of linear equations.

Matrix*Vector – Recall

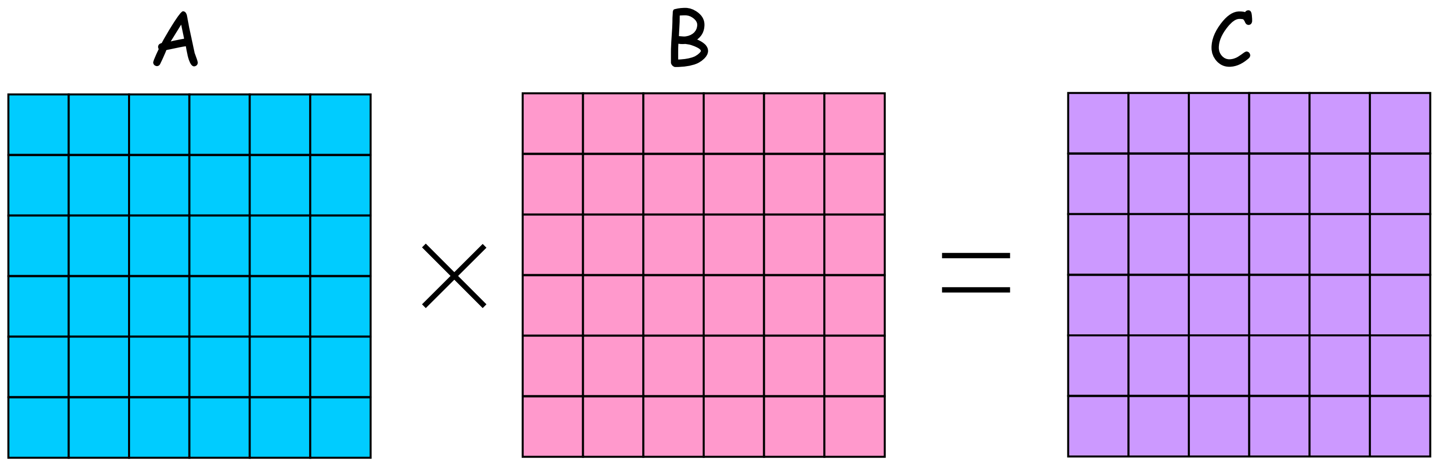


$$y_i = \sum_{k=1}^{n} a_{ik} x_k$$

Serial algorithm:
n^2 multiplications and addition.

W = n^2

Matrix*Matrix – Recall



$$c_{ij} = \sum_{k=1}^{n} a_{ik} b_{kj}$$

Serial algorithm:
n^3 multiplications and addition.

W = n^3

Matrix*Vector – Serial Algorithm

$$y_i = \sum_{k=1}^{n} a_{ik} x_k \longrightarrow$$

```
procedure MAT_Vec(A,x,y)
    for i := 0 to n-1 do
        y[i] := 0
        for k := 0 to n-1 do
            y[i] := y[i] + A[i,k]*x[k]
        done
    done
endproc
```

How to parallelize?

Matrix*Matrix – Serial Algorithm

$$c_{ij} = \sum_{k=1}^{n} a_{ik} b_{kj} \rightarrow$$

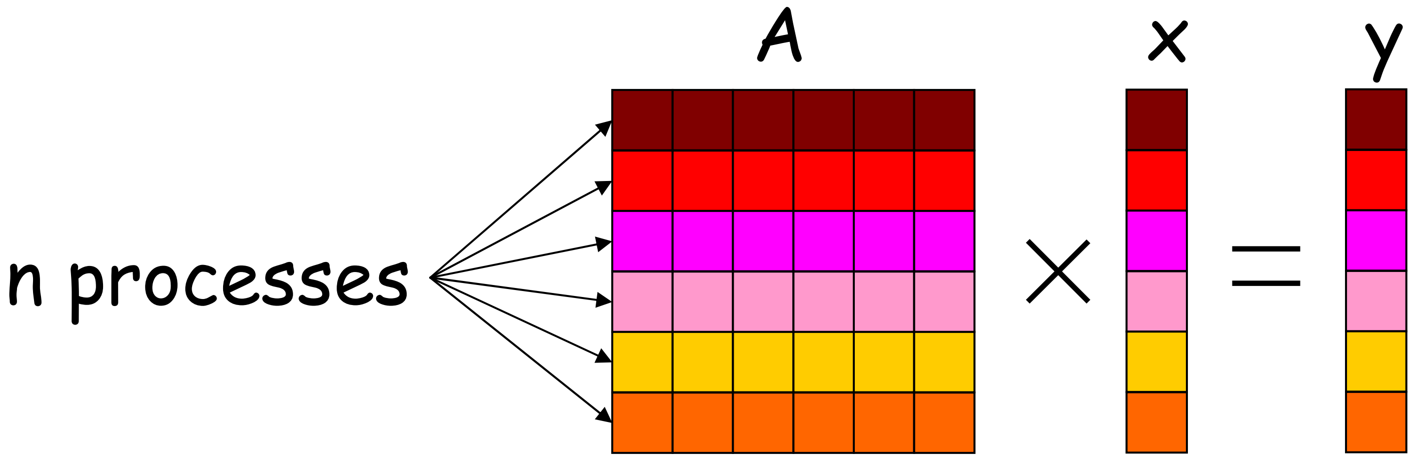
```
procedure MAT_MULT(A,B,C)
    for i := 0 to n-1 do
        for j := 0 to n-1 do
            C[i,j] := 0
            for k := 0 to n-1 do
                C[i,j] := C[i,j] + A[i,k]*B[k,j]
            done
        done
    done
endproc
```

How to parallelize?

Matrix*Vector – Row-wise 1-D Partitioning

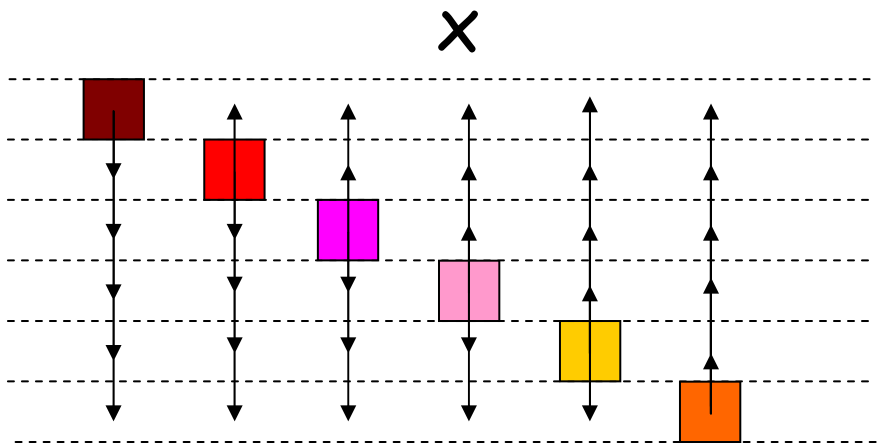
- Initial distribution:
  - Each process has a row of the $n*n$ matrix.
  - Each process has an element of the $n*1$ vector.
  - Each process is responsible for computing one element of the result.

Matrix*Vector – 1-D

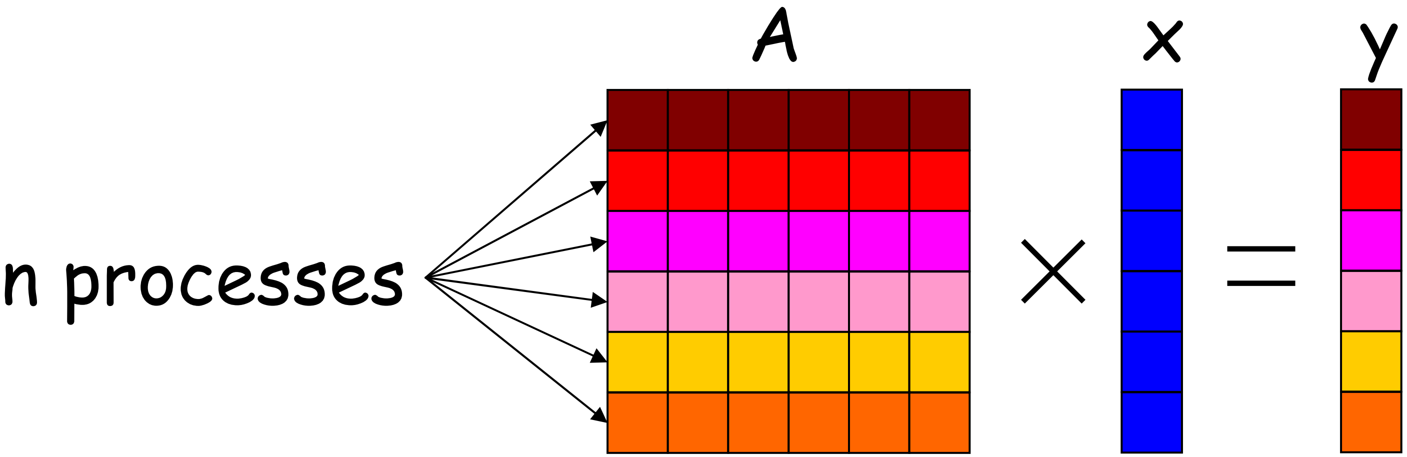


But every process needs the entire vector
⇒ all-to-all broadcast.

All-to-All Broadcast

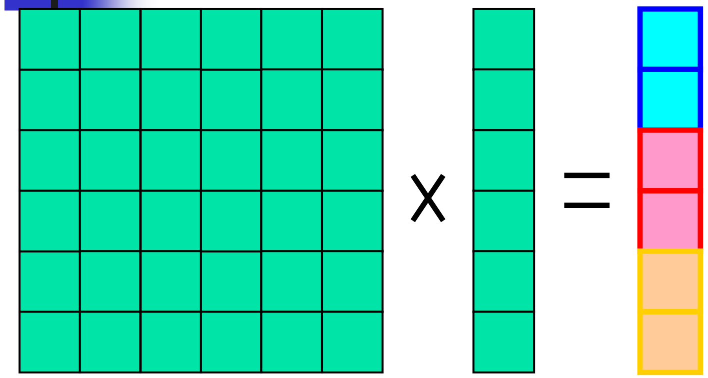


Parallel Computation



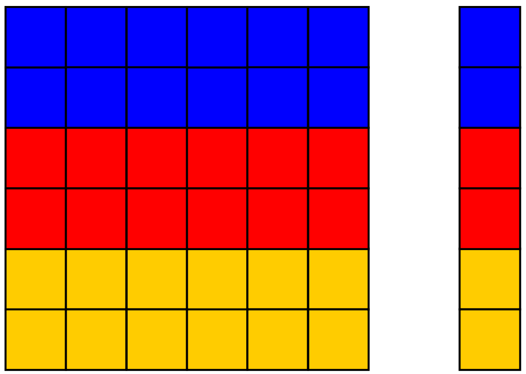
$$y_i = \sum_{k=1}^{n} a_{ik} x_k$$ in parallel on the n processes.

Example Matrix*Vector (Program 6.4)

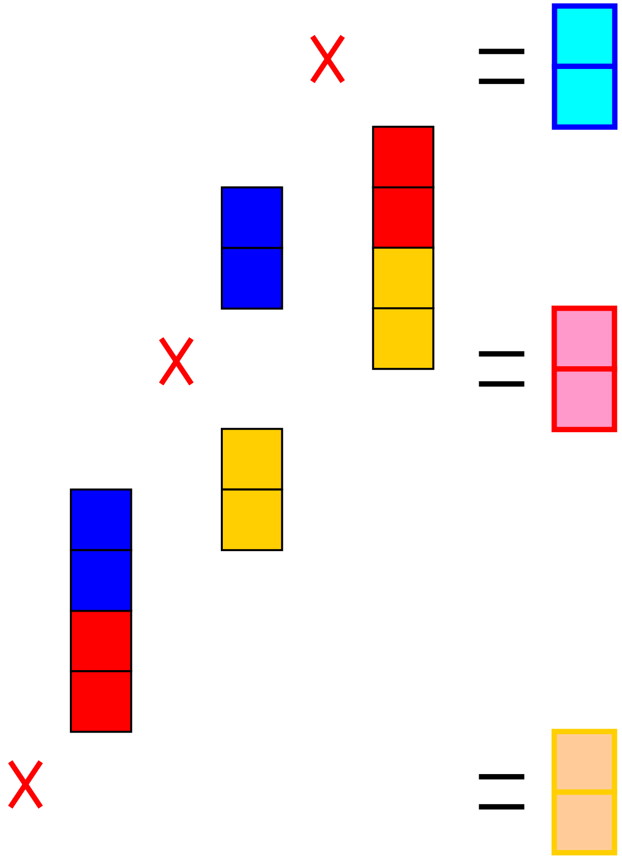


Allgather (All-to-all broadcast)

Partition on rows.



Multiply



Analysis

- All-to-all broadcast & multiplications in $\Theta(n)$.
- For n processes $W=n^2=nT_P$.
  $\Rightarrow$ The algorithm is cost-optimal.

A parallel system is cost-optimal iff $pT_P=\Theta(W)$.

Performance Metrics

- Efficiency $E=S/p$.
  - Measure time spent in doing useful work.
  - Previous sum example: $E = \Theta(1/\log n)$.
- Cost $C=pT_P$.
  - A.k.a. work or processor-time product.
  - Note: $E=T_S/C$.
  - Cost optimal if E is a constant.

Using Fewer Processes

- Brent's scheduling principle: It's possible.
- Using p processes:
  - n/p rows per process.
  - Communication time = $t_s \log p + t_w (n/p)(p-1)$ $\sim t_s \log p + t_w n = \Theta(n)$.
  - Computation: n*n/p.
    $\Rightarrow pT_P = \Theta(n^2) = W \Rightarrow$ It is cost optimal.

Scalability – Recall

- Efficiency increases with the size of the problem.
- Efficiency decreases with the number of processors.
- Scalability measures the ability to increase speedup in function of *p*.

Isoefficiency Function

- For scalable systems efficiency can be kept constant if T_0/W is kept constant.

For a target E
$$E = \frac{1}{1 + T_o(W,p)/W},$$

Keep this constant
$$\frac{T_o(W,p)}{W} = \frac{1-E}{E},$$

Isoefficiency function
$$W = \frac{E}{1-E} T_o(W,p).$$

$$\boxed{W = KT_0(W,p)}$$

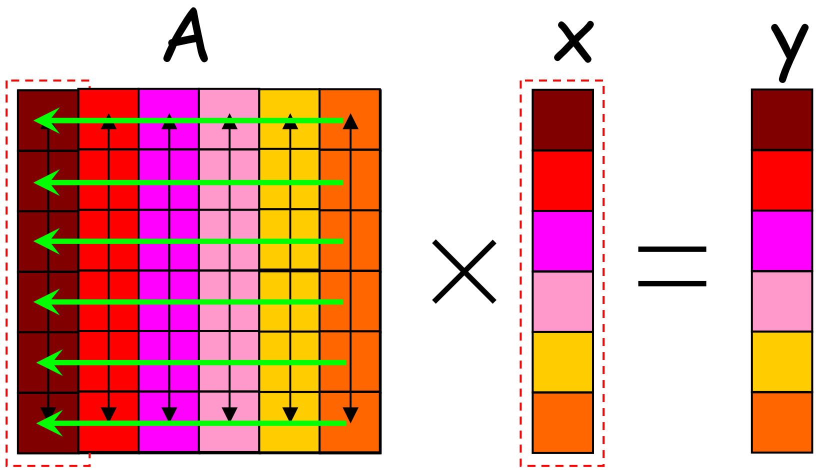
Is Our Algorithm Scalable?

- $T_0 = pT_P - W \Rightarrow T_0 = t_s p \log p + t_w np$.
- We want to determine $W = KT_0$. Try with both terms separately:
  - $W = Kt_s p \log p$.
  - $W = Kt_w np = n^2 \Rightarrow W = (Kt_w p)^2$.
  - Bound from concurrency: $p = O(n) \Rightarrow W = \Omega(p^2)$.
  - $W = \Theta(p^2)$: asymptotic isoefficiency function. Rate to increase the problem size (in function of p) to maintain a fixed efficiency: $p = \Theta(n)$.

Matrix*Vector – 2-D

- Matrix $n*n$ partitioned on $n*n$ processes.
- Vector $n*1$ distributed in the last (or 1st column).
- Similarly we want fewer processes: blocks of $(n/\sqrt{p})^2$ elements.

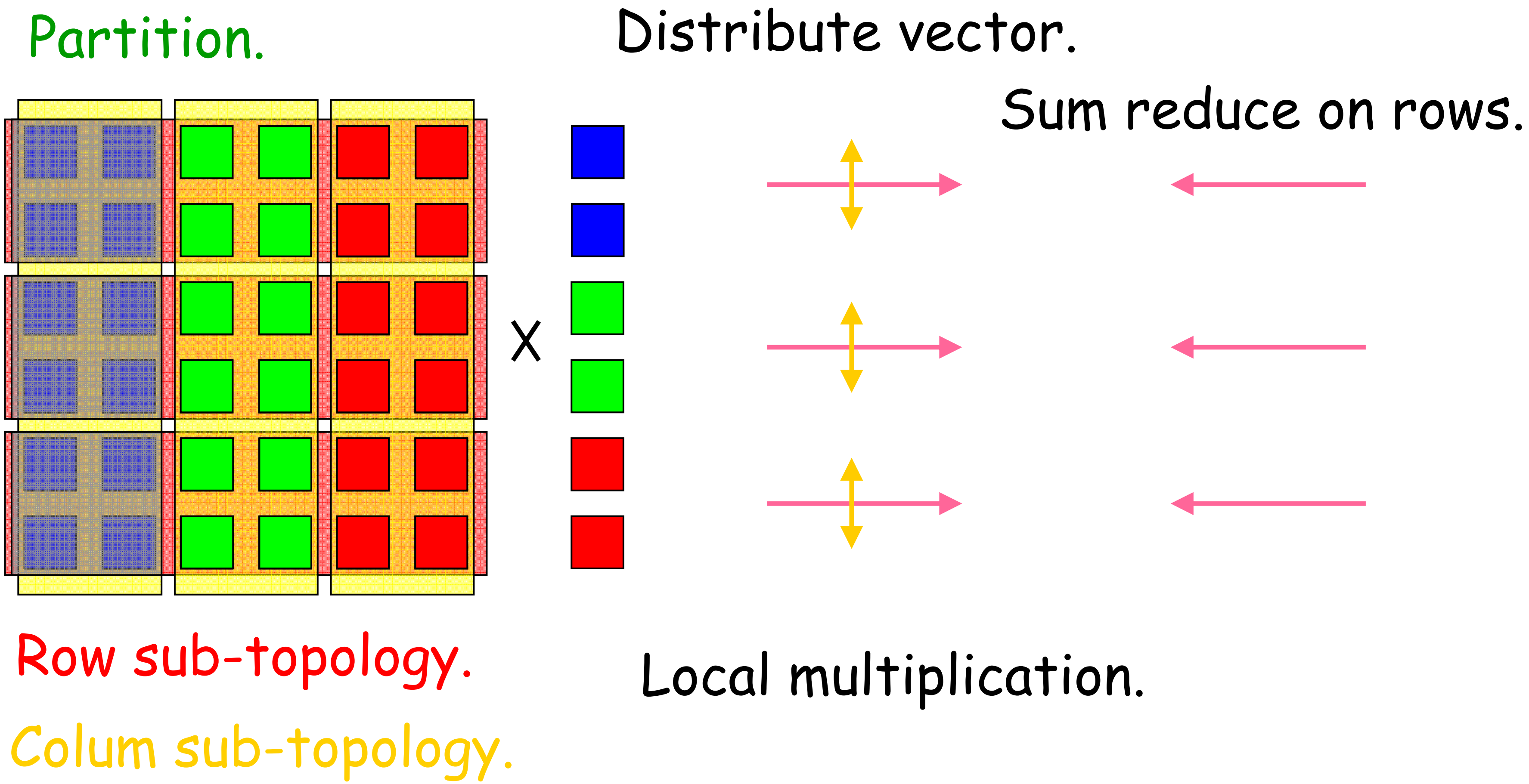
Matrix*Vector – 2-D



Processes in column i need element of the vector in row i.

1. Distribute on diagonal.
2. One-to-all broadcast on columns.
3. Multiplication.
4. All-to-one reduction (+).

Example Matrix*Vector (Program 6.8)



Which one is better? 1-D or 2-D?

Analysis

- Communications:
  - one-to-one $\Theta(1)$ +
  - one-to-all broadcast $\Theta(\log n)$ +
  - all-to-one reduction $\Theta(\log n)$.
- + multiplications $\Theta(1)$.
- $T_P = \Theta(n^2 \log n) \Rightarrow$ not cost-optimal.
- Brent's scheduling principle?

Using Fewer Processes

- Blocks of $(n/\sqrt{p})^2$ elements. Costs:
  - one to one in $t_s+t_w n/\sqrt{p}$ +
  - one-to-all broadcast in $(t_s+t_w n/\sqrt{p}) \log \sqrt{p}$ +
  - all-to-one reduction in $(t_s+t_w n/\sqrt{p}) \log \sqrt{p}$ +
  - computations in $(n/\sqrt{p})^2$.
- Total ~ $n^2/p+t_s \log p+(t_w n/\sqrt{p}) \log p$.
- $pT_P=\Theta(n^2) \Rightarrow$ cost-optimal.

Scalability Analysis

- $T_0 = pT_P - W = t_s \log p + t_w n\sqrt{p} \log p$.
- As before, isoefficiency analysis:
  - $W = Kt_s p \log p$.
  - $W = Kt_w n\sqrt{p} \log p = n^2 \Rightarrow W = (Kt_w \sqrt{p} \log p)^2$.
  - Bound from concurrency: $p = O(n^2) \Rightarrow W = \Omega(p)$.
  - $W = \Theta(p \log^2 p)$.
- $p = f(n)$? $p \log^2 p = \Theta(n^2)$ … $p = \Theta(n^2 / \log^2 n)$.

Which One Is Better?

- 1-D: $T_P \sim n^2/p + t_s \log p + t_w n$.
- 2-D: $T_P \sim n^2/p + t_s \log p + (t_w n/\sqrt{p}) \log p$.

- 1-D: $W = \Theta(p^2)$.
- 2-D: $W = \Theta(p \log^2 p)$.

- Degree of concurrency…

Block Matrix*Matrix

```
procedure  BLOCK_MAT_MULT(A,B,C)
    for i := 0 to q-1 do
        for j := 0 to q-1 do
            C[i,j] := 0
            for k := 0 to q-1 do
                C[i,j] := C[i,j] + A[i,k]*B[k,j]
            done
        done
    done
endproc
```

q*q blocks of (n/q)*(n/q) submatrices.
Still n^3 additions & multiplications.

A Simple Parallel Algorithm

- Map the algorithm to $p=q^2$ processes.
- We need all A[i,k] and B[k,j] to compute the C[i,j].
- Steps:
  - All-to-all broadcast of A[i,k] on rows.
  - All-to-all broadcast of B[k,j] on columns.
  - Local multiplications.

Analysis

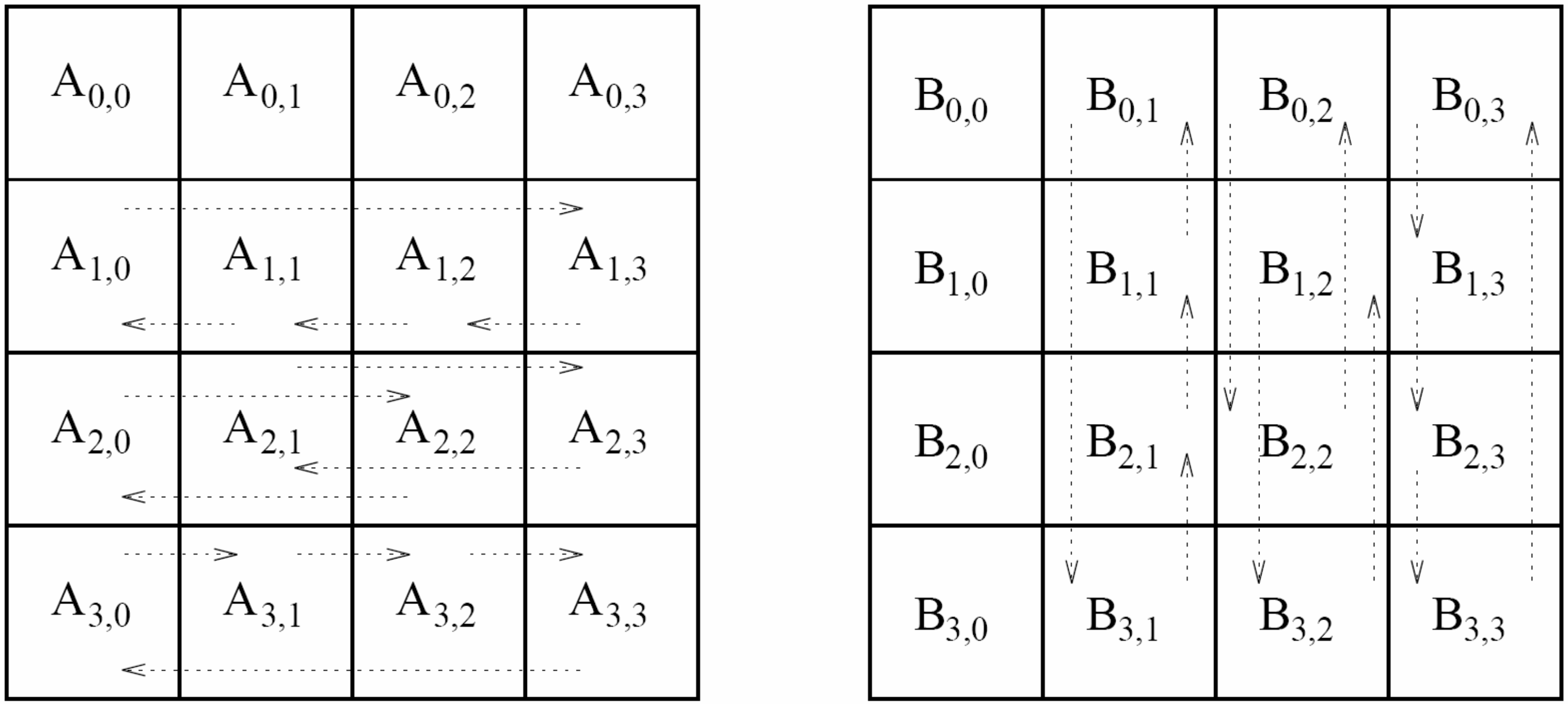
- Costs:
  - all-to-all $\sqrt{p}$ broadcasts of n^2/p elements $= t_s \log\sqrt{p} + t_w(n^2/p)(\sqrt{p}-1)$ *2
  - + computations = $\sqrt{p}$ multiplications of $(n/\sqrt{p})*(n/\sqrt{p})$ matrices cost n^3/p.
  - $pT_P=\Theta(n^3)$ for $p=O(n^2) \Rightarrow$ cost-optimal.
  - Isoefficiency $W=\Theta(p^{3/2})$.
- Drawback: memory requirement in $n^2\sqrt{p}$.

Better?

Cannon's Algorithm

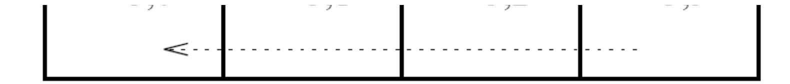
- Idea: re-schedule computations to avoid contention.
  - Processes on rows i hold a different A[i,k].
  - Processes on columns j hold a different B[k,j].
  - Rotate the matrices $\Rightarrow$ we need only 2 sub-matrices per process at any time.
    $\Rightarrow$ memory efficient in $O(n^2)$.

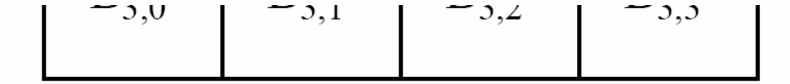
Align A & B



(a) Initial alignment of A

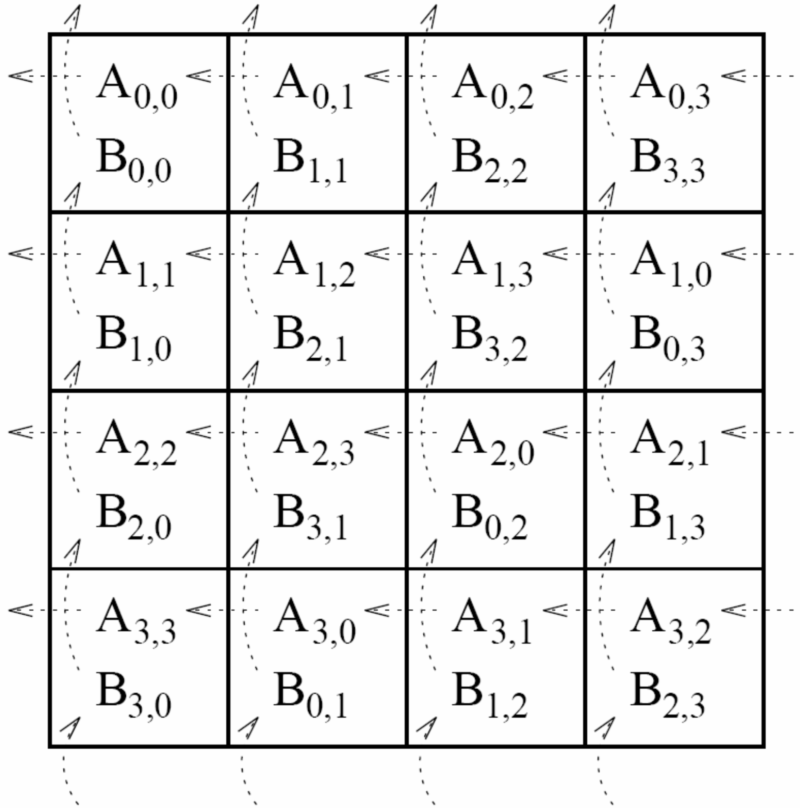
(b) Initial alignment of B



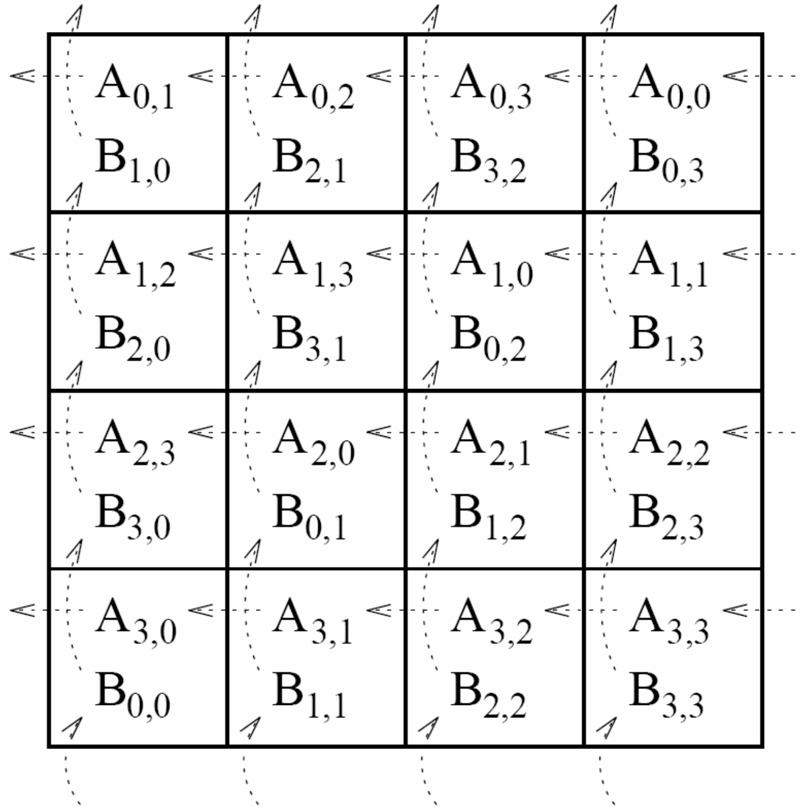


(a) Initial alignment of A

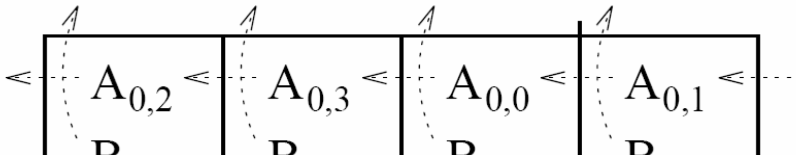
(b) Initial alignment of B

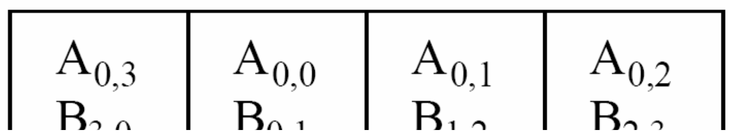


(c) A and B after initial alignment

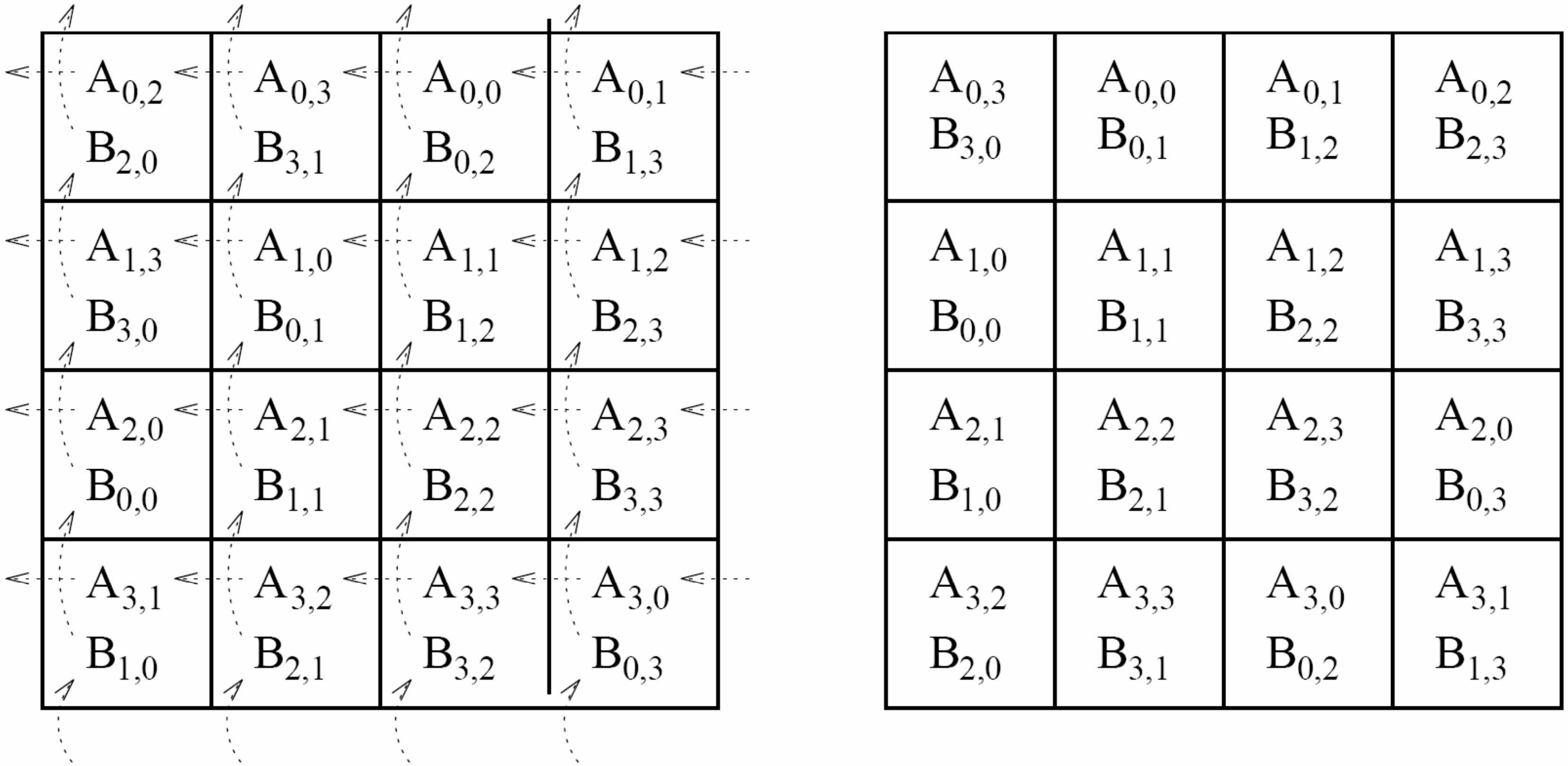


(d) Submatrix locations after first shift





(c) A and B after initial alignment (d) Submatrix locations after first shift



(e) Submatrix locations after second shift (f) Submatrix locations after third shift

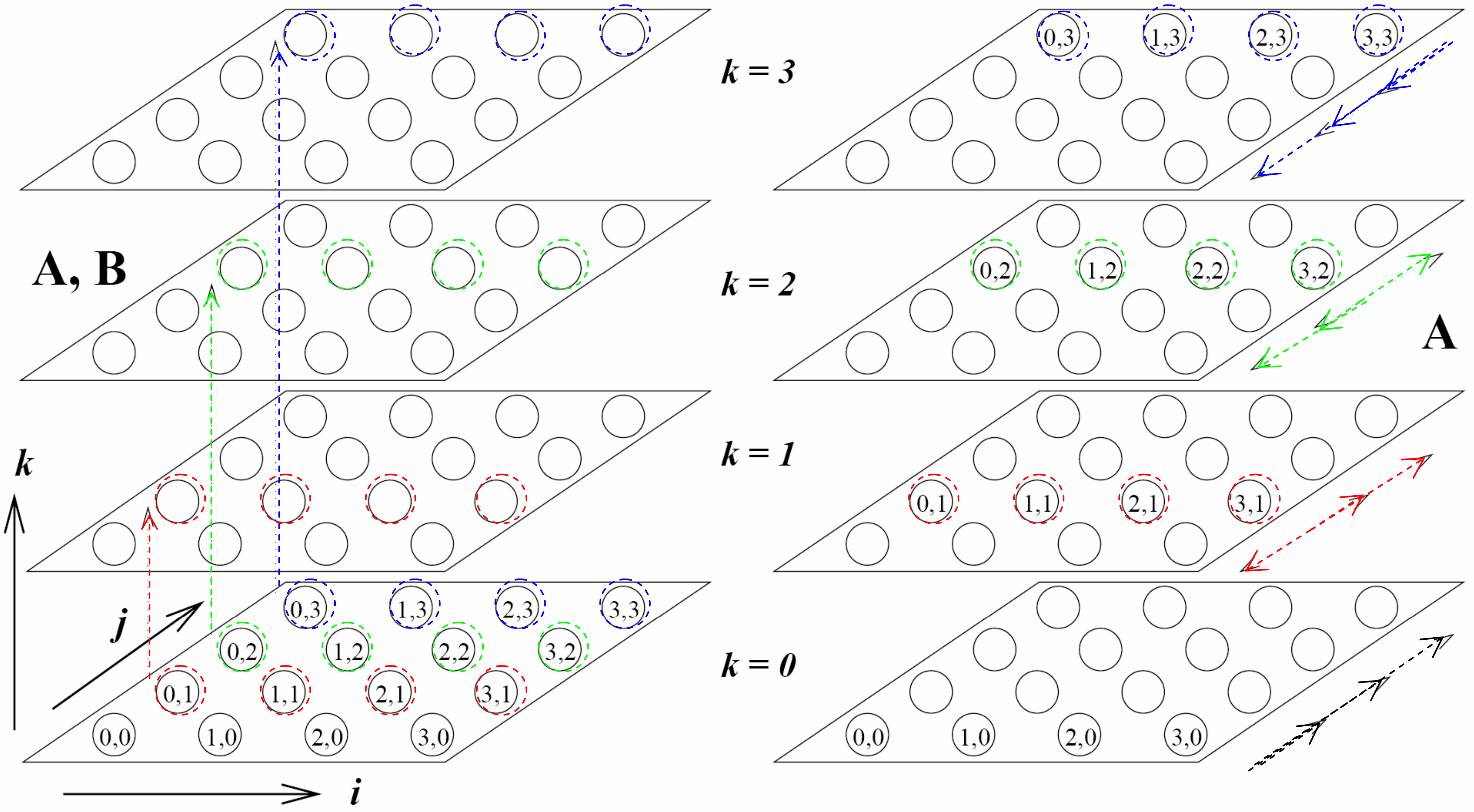
Figure 8.3 The communication steps in Cannon's algorithm on 16 processes.

Analysis

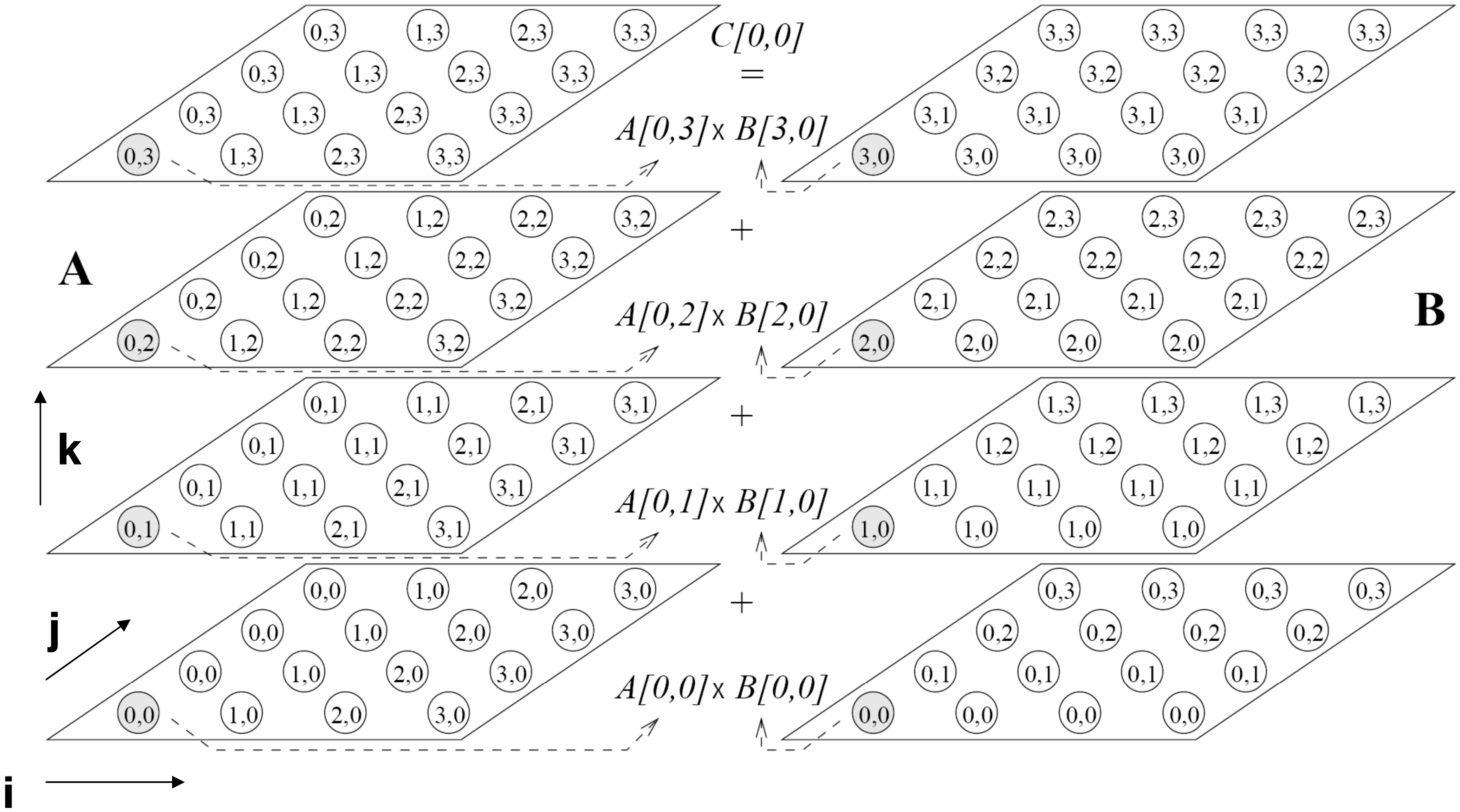
- Costs:
  - 2* (A & B) $\sqrt{p}$-single step shifts = $2(t_s+t_w n^2/p)\sqrt{p}$ +
  - $\sqrt{p}$ multiplications of $(n/\sqrt{p})*(n/\sqrt{p})$ sub-matrices = n^3/p.
  - Cost-optimal, same isoefficiency function as previously.

The DNS Algorithm

- 3-D partitioning!
- Cube with faces corresponding to A, B, C.
- Internal nodes correspond to multiply operations $P_{i,j,k}$.
  - Multiplications in time $\Theta(1)$.
  - Additions in time $\Theta(\log n)$.
  - Communication…
- Can use up to n^3 processes – better concurrency.



(a) Initial distribution of A and B (b) After moving $A[i,j]$ from $P_{i,j,0}$ to $P_{i,j,j}$



(c) After broadcasting $A[i,j]$ along j axis

(d) Corresponding distribution of B

Figure 8.4 The communication steps in the DNS algorithm while multiplying 4×4 matrices A and B on 64 processes. The shaded processes in part (c) store elements of the first row of A and the shaded processes in part (d) store elements of the first column of B.

Communication Steps

- Move the columns of A & rows of B.
- One-to-all broadcast along j & i axis.
- All-to-one reduction (+) along k axis.
- Communication on groups of n processes, in time $\Theta(\log n)$.
- Not cost optimal for n^3 processes.

Brent's Scheduling Principle

Theorem

If a parallel computation consists of

***k* phases**

taking time $t_1,t_2,\ldots,t_k$

using $a_1,a_2,\ldots,a_k$ processors

in phases $1,2,\ldots,k$

then the computation can be done in time ***O(a/p+t)*** using ***p* processors** where $t=\text{sum}(t_i)$, $a=\text{sum}(a_it_i)$.

Look At One Dimension

- k phases = log$n$.
- t_i = constant time.
- $a_i = n/2, n/4, \ldots, 1$ processors.
- With q processors we can use time $O(\log n + n/p)$.
- Choose $q = O(n/\log n) \rightarrow$ time $O(\log n)$ and this is **optimal**!

$p=q^3$

3-D: use $p=O(n^3/\log^3 n)$

Systems of Linear Equations

$$A \times x = b$$

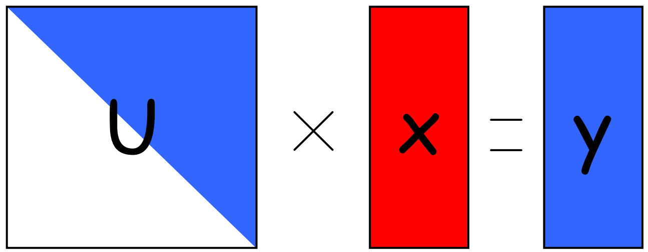
$$a_{0,0}x_0+a_{0,1}x_1+\ldots+a_{0,n-1}x_{n-1}=b_0,$$

$$\ldots$$

$$a_{n-1,0}x_0+a_{n-1,1}x_1+\ldots+a_{n-1,n-1}x_{n-1}=b_{n-1}$$

Solving Systems of Linear Equations

- Step 1: Reduce the original system to



- Step2:
  Solve & back-substitute from x_{n-1} to x_0.

Technical Issues

- Non singular matrices.
- Numerical precision (is the solution numerically stable) $\rightarrow$ permute columns.
  - In particular no division by zero, thanks.
  - Procedure known as Gaussian elimination with partial pivoting.

Gaussian Elimination

```
1.   procedure GAUSSIAN_ELIMINATION (A, b, y)
2.   begin
3.      for k := 0 to n − 1 do                  /* Outer loop */
4.      begin
5.         for j := k + 1 to n − 1 do
6.            A[k, j] := A[k, j]/A[k, k];   /* Division step */
7.         y[k] := b[k]/A[k, k];
8.         A[k, k] := 1;
9.         for i := k + 1 to n − 1 do
10.        begin
11.           for j := k + 1 to n − 1 do
12.              A[i, j] := A[i, j] − A[i, k] × A[k, j]; /* Elimination step */
13.           b[i] := b[i] − A[i, k] × y[k];
14.           A[i, k] := 0;
15.        endfor;          /* Line 9 */
16.     endfor;             /* Line 3 */
17.  end GAUSSIAN_ELIMINATION
```

$W = 2n^3/3$

Parallel Gaussian Elimination

- 1-D partitioning:
  - 1 process/row.
  - Process j computes A[*,j].
  - Cost (+communication) = $\Theta(n^3 \log n)$ not cost optimal.
- All processes work on the same iteration.
  - k+1 iteration starts when k^{th} iteration is complete.
  - Improve: pipelined/asynchronous version.

Pipelined Version

```
1.  procedure GAUSSIAN_ELIMINATION (A, b, y)
2.  begin
3.     for k := 0 to n − 1 do                  /* Outer loop */
4.     begin
5.        for j := k + 1 to n − 1 do
6.           A[k, j] := A[k, j]/A[k, k];   /* Division step */
7.        y[k] := b[k]/A[k, k];
8.        A[k, k] := 1;
9.        for i := k + 1 to n − 1 do
10.       begin
11.          for j := k + 1 to n − 1 do
12.             A[i, j] := A[i, j] − A[i, k] × A[k, j]; /* Elimination step */
13.          b[i] := b[i] − A[i, k] × y[k];
14.          A[i, k] := 0;
15.       endfor;              /* Line 9 */
16.    endfor;                 /* Line 3 */
17. end GAUSSIAN_ELIMINATION
```

P_k forwards & does not wait.

P_js forward & do not wait.

Pipelined Gaussian Elimination

- No log$n$ for communication (no broadcast) and the rest of the computations are the same.
- The pipelined version is cost-optimal.
- Fewer processes:
  - Block 1-D partitioning, loss of efficiency due to idle processes (load balance problem).
  - Cyclic 1-D partitioning better.

Gaussian Elimination – 2-D Partitioning

- Similar as before.
- Pipelined version cost-optimal.
- More scalable than 1-D.

Finally Back-Substitution

```
procedure BACK_SUBSTITUTION (U, x, y)
begin
    for k := n − 1 downto 0 do   /* Main loop */
        begin
            x[k] := y[k];
            for i := k − 1 downto 0 do
                y[i] := y[i] − x[k] × U[i, k];
        endfor;
end BACK_SUBSTITUTION
```

Algorithm 8.5 A serial algorithm for back-substitu
entries of the principal diagonal equal to one, and all

Intrinsically serial algorithm.
Pipelined parallel version not cost optimal.
Does not matter because of lower order of magnitude.