Parallel Algorithms for Dense Matrices

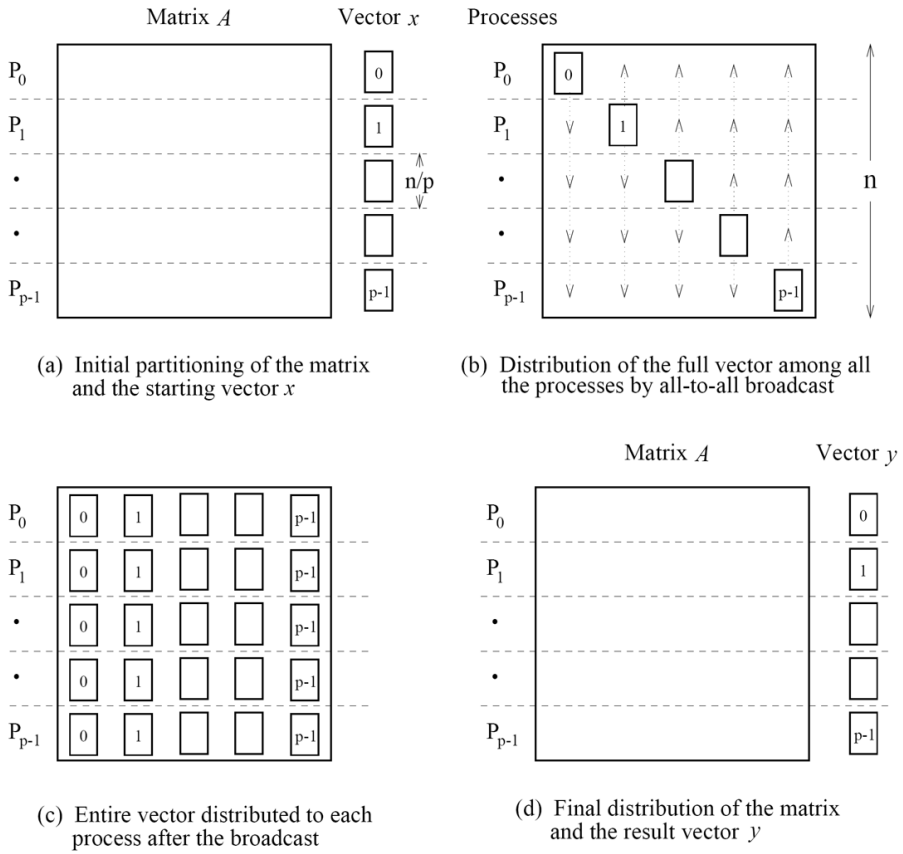
CS121 Parallel Computing

Spring 2020

Dense matrices

- Dense matrices are ones where most elements are nonzero.
- Dense matrices are used in many optimization problems, and physics and chemistry based simulations.
- Many dense matrix operations are compute bound. This, plus their highly regular structure, allows dense matrix operations to be highly optimized.
- High performance parallel implementations provided by LAPACK, ScaLAPACK, HPL, etc.
- We'll look at algorithms for matrix-vector multiplication, matrix-matrix multiplication and equation solving (Gaussian elimination).

1D matrix-vector multiplication



(a) Initial partitioning of the matrix and the starting vector x

(b) Distribution of the full vector among all the processes by all-to-all broadcast

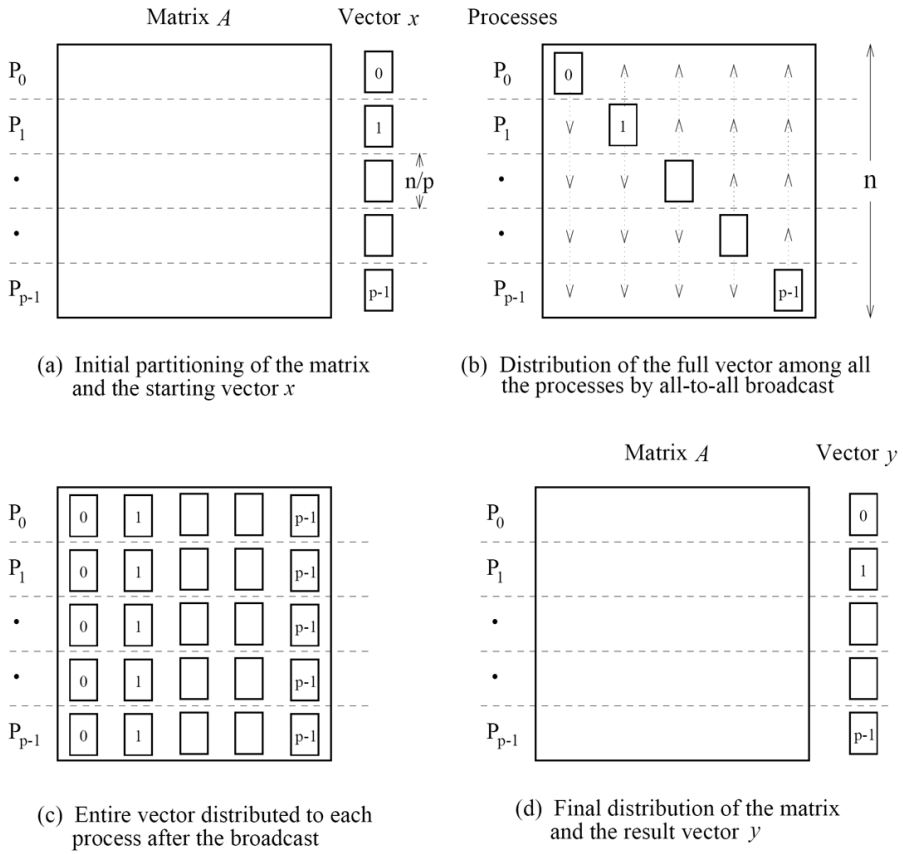
(c) Entire vector distributed to each process after the broadcast

(d) Final distribution of the matrix and the result vector y

Source: Introduction to Parallel Computing, Grama et al

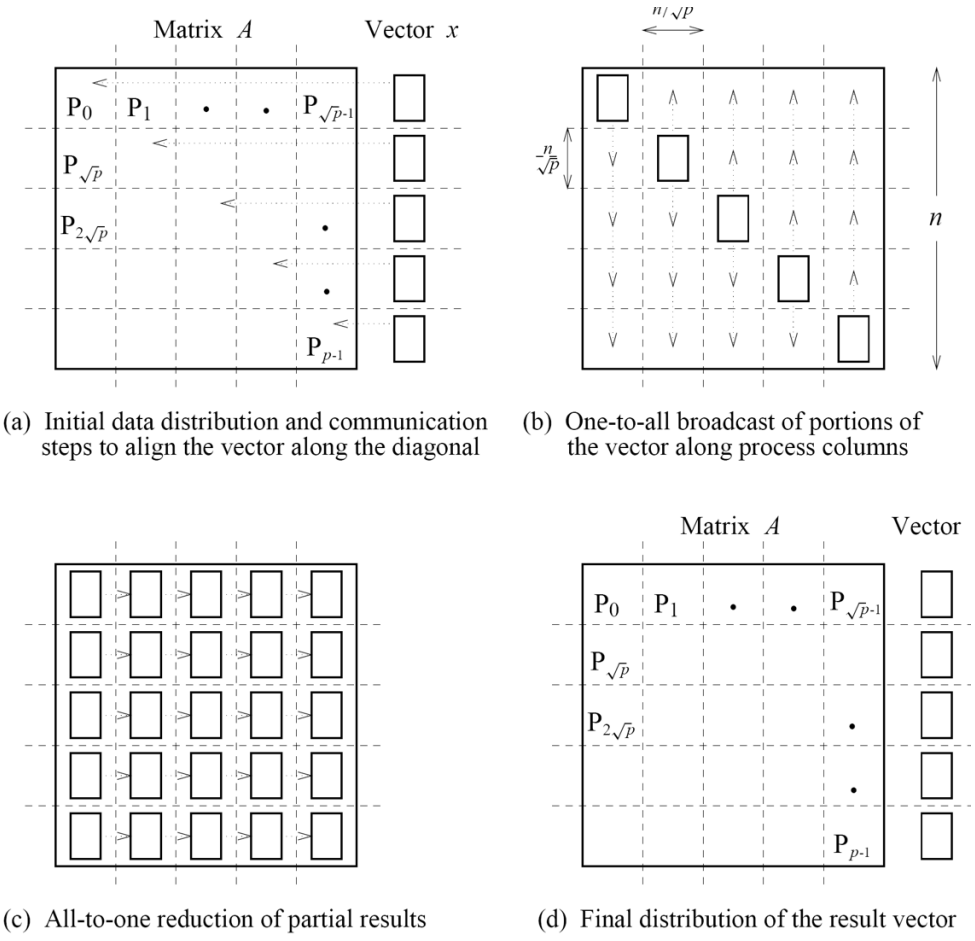
- Consider an n x n matrix A and an n x 1 vector x partitioned across $p \leq n$ processors.
  - Initially each process stores n/p rows of A and n/p values of x.
- Each process needs the entire vector to multiply by its rows.
  - In step (b), do all-to-all broadcast of the processors' vector segments.
- Each process multiplies the vector by its rows.
  - Each process ends up with n/p values of the output.

1D matrix-vector multiplication



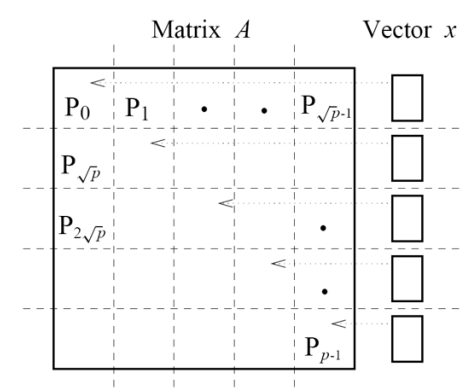
- Assume an underlying hypercube architecture.
- Compute time for each process is $\frac{n^2}{p}$.
- Communication time for all-to-all broadcast is $t_s \log p + t_w n$.
- Overhead by all p processors from communication is $t_s p \log p + t_w n\, p$.
- Total amount of work is n^2.
- For isoefficiency, need $n^2 = \Omega(t_s p \log p + t_w n\, p)$.
  - This is satisfied for $p = O(n)$.

2D matrix-vector multiplication

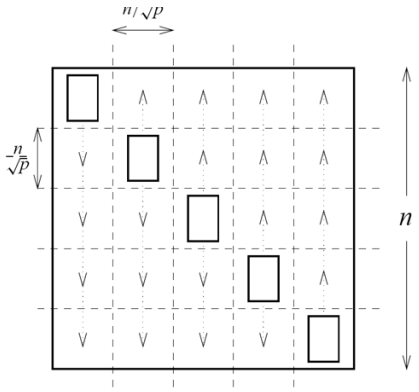


- Consider a logical 2D mesh of p processes, each initially with a $(n/\sqrt{p}) \times (n/\sqrt{p})$ portion of the matrix.
- The vector is stored only in the last column. Each process in last column has $(n/\sqrt{p})$ vector values.
- In (a), each process in last column sends its vector elements to a process on the diagonal.
- In (b), each diagonal process does a one-to-all broadcast of the vector chunk.
- In (c), each process multiplies its row chunks by its vector chunks, producing $(n/\sqrt{p})$ partial values. Then each row of processes does a reduction of the partial values to the last process in the row.
- The output is stored in the last column of processes.

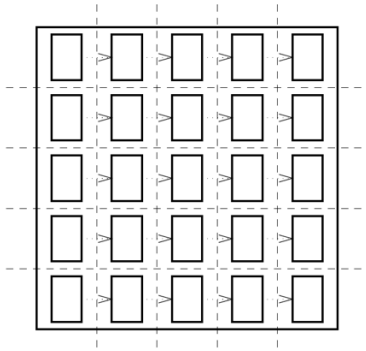
2D matrix-vector multiplication



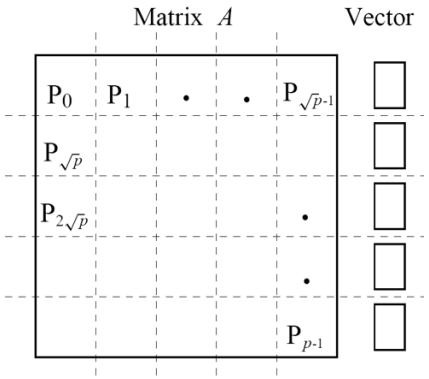
(a) Initial data distribution and communication steps to align the vector along the diagonal



(b) One-to-all broadcast of portions of the vector along process columns



(c) All-to-one reduction of partial results



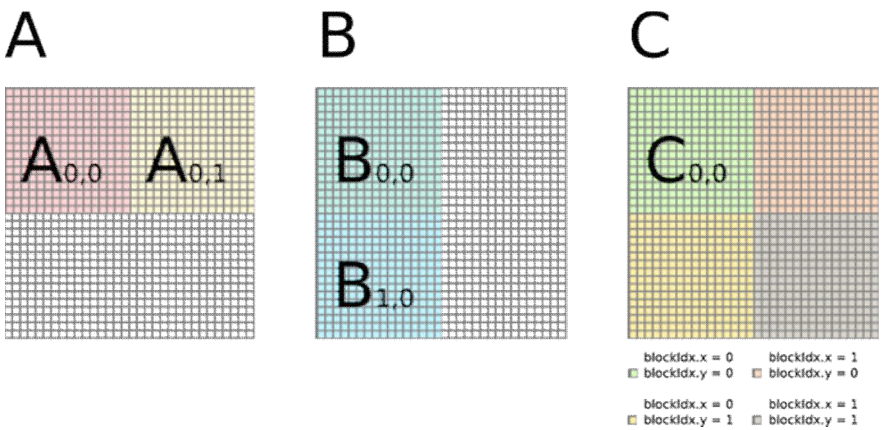
(d) Final distribution of the result vector

- Each process stores n^2/p matrix values, and does one multiplication and one addition for each value. So the total computation is $O(n^2/p)$.
- Communication time
  - (a) $t_s + t_w\, n/\sqrt{p}$.
  - (b) and (c) $(t_s + t_w\, n/\sqrt{p})\log(\sqrt{p})$.
- Total time per process is $O\left(\frac{n^2}{p} + \log p + \frac{n}{\sqrt{p}}\log p\right)$.
- Communication overhead is $p\log p + n\sqrt{p}\log p$.
- Isoefficiency requires $n^2 = \Omega(\text{overhead})$
  - So $n^2 = \Omega(n\sqrt{p}\log p)$, so $n = \Omega(\sqrt{p}\log p)$, so $n^2 = \Omega(p\log^2 p)$.
  - So need $p = O(\frac{n^2}{\log^2 p})$.
- 2D matrix-vector multiplication is more scalable than 1D.

Matrix-matrix multiplication

```
1.  procedure MAT_MULT (A, B, C)
2.  begin
3.      for i := 0 to n − 1 do
4.          for j := 0 to n − 1 do
5.              begin
6.                  C[i, j] := 0;
7.                  for k := 0 to n − 1 do
8.                      C[i, j] := C[i, j] + A[i, k] × B[k, j];
9.              endfor;
10. end MAT_MULT
```

```
1.  procedure BLOCK_MAT_MULT (A, B, C)
2.  begin
3.      for i := 0 to q − 1 do
4.          for j := 0 to q − 1 do
5.              begin
6.                  Initialize all elements of C_{i,j} to zero;
7.                  for k := 0 to q − 1 do
8.                      C_{i,j} := C_{i,j} + A_{i,k} × B_{k,j};
9.              endfor;
10. end BLOCK_MAT_MULT
```



- Matrix multiplication can be done element by element, or by breaking the matrices into blocks and multiplying block by block.
- We partition A and B into $\sqrt{p} \times \sqrt{p}$ blocks, each of size $(n/\sqrt{p}) \times (n/\sqrt{p})$.
- Suppose p processes form a $\sqrt{p} \times \sqrt{p}$ mesh.
- Each process stores the corresponding block from A and B.
- Each $C_{i,j}$ requires $A_{i,k}$ and $B_{k,j}$ for $1 \leq k \leq \sqrt{p}$.
  - So row i processes do all-to-all broadcast of their A blocks, and column j processes do all-to-all broadcast of their B blocks.
- Each process (i,j) ends up with $C_{i,j}$ stored locally.

Matrix-matrix multiplication

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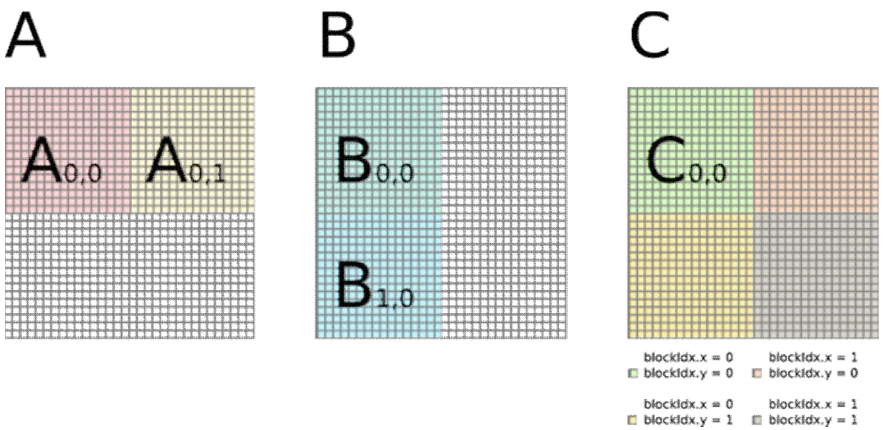
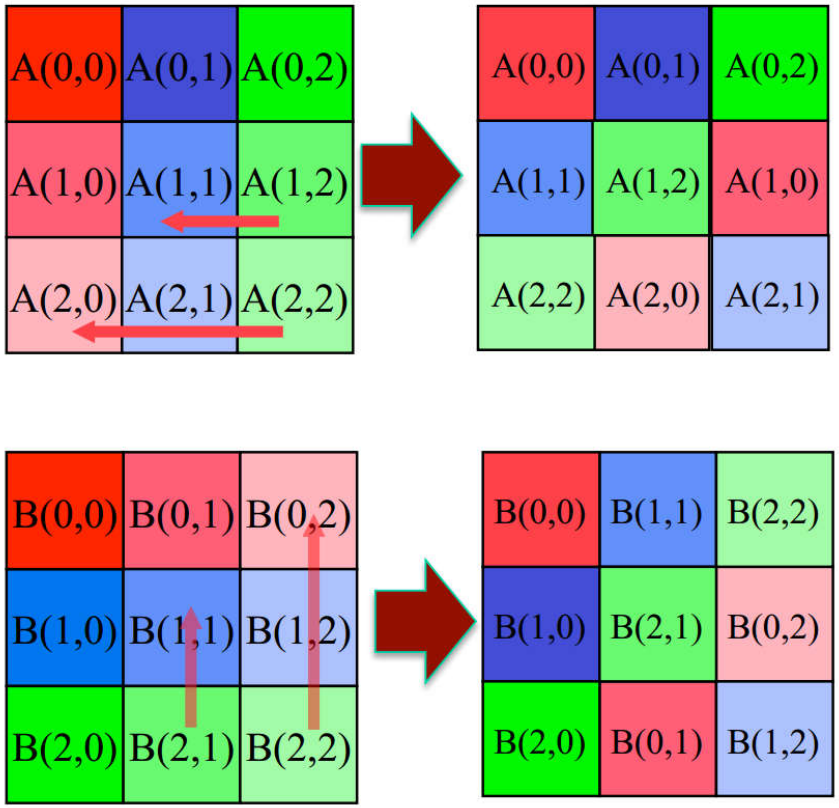
```



- Each process does $\sqrt{p}$ multiplications of $(n/\sqrt{p}) \times (n/\sqrt{p})$ matrices.
  - Compute cost is $\left(\frac{n}{\sqrt{p}}\right)^3 \sqrt{p} = \frac{n^3}{p}$.
- Each row or column of $\sqrt{p}$ processes does all-to-all broadcast of $\frac{n^2}{p}$ amount of data.
  - Communication time is $O(\log \sqrt{p} + \frac{n^2}{p}\sqrt{p})$.
- Total work is $O(n^3)$, and total overhead is $O(p \log \sqrt{p} + n^2\sqrt{p})$.
- Isoefficiency requires $n^3 = \Omega(n^2\sqrt{p})$, so need $p = O(n^2)$.
- One problem with this algorithm is that each process needs to store $\sqrt{p}$ copies of $(n/\sqrt{p}) \times (n/\sqrt{p})$ matrices.
  - So memory use per process is $n^2/\sqrt{p}$, and total memory use for all processes is $n^2\sqrt{p}$.
  - This is $\sqrt{p}$ factor more than for the sequential algorithm.

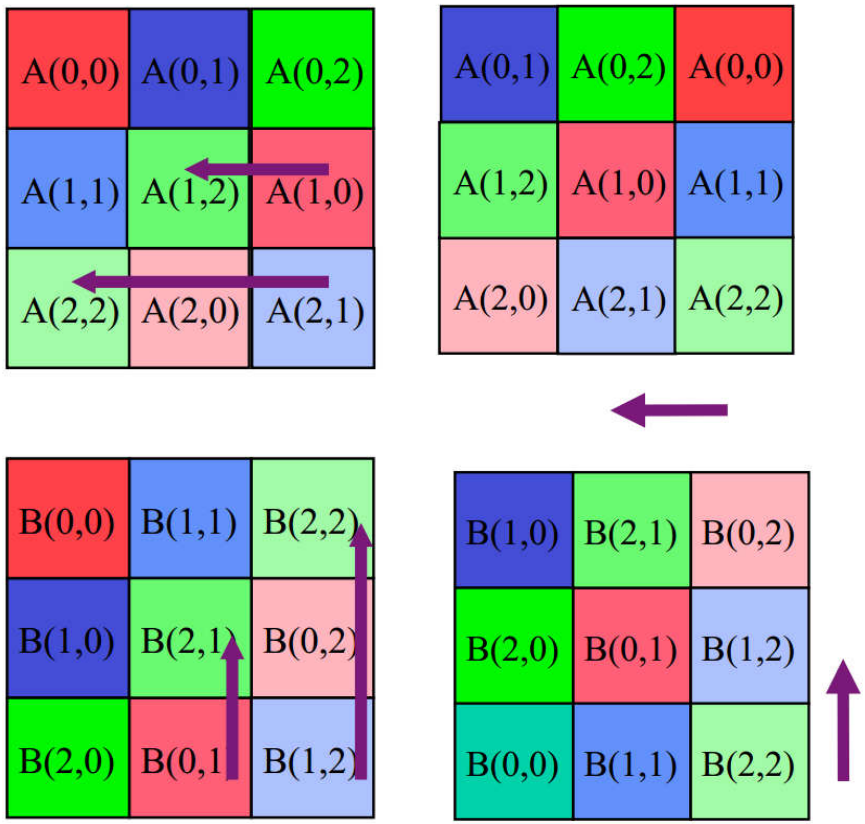
Cannon's matrix-matrix multiplication



Source: http://cseweb.ucsd.edu/classes/fa12/cse260-b/Lectures

- Cannon's algorithm has nearly the same efficiency as the previous algorithm, but uses $O(n^2)$ storage, just like the sequential algorithm.
- It uses the same partitioning as the previous algorithm, but moves some blocks of A and B to other processors.
  - Cyclically shift the i'th row of A to the left by i, and shift the i'th column of B up by i.
- Each C value is formed by multiplying like colored blocks from A and B, then adding up the products, one for each color.
  - Ex $C_{0,1} = A_{0,0}B_{0,1}+A_{0,1}B_{1,1} +A_{0,2}B_{2,1}$, i.e. we add up the red, blue and green products.
- After shifting, for any i, all blocks with the i'th color in A and B lie along the i'th anti-diagonal.
  - So for any (i,j), like colored blocks from $A_{i,:}$ and $B_{:,j}$ are on processor $P_{i,j}$.
  - When these blocks are multiplied, they make up one of the terms of $C_{i,j}$.

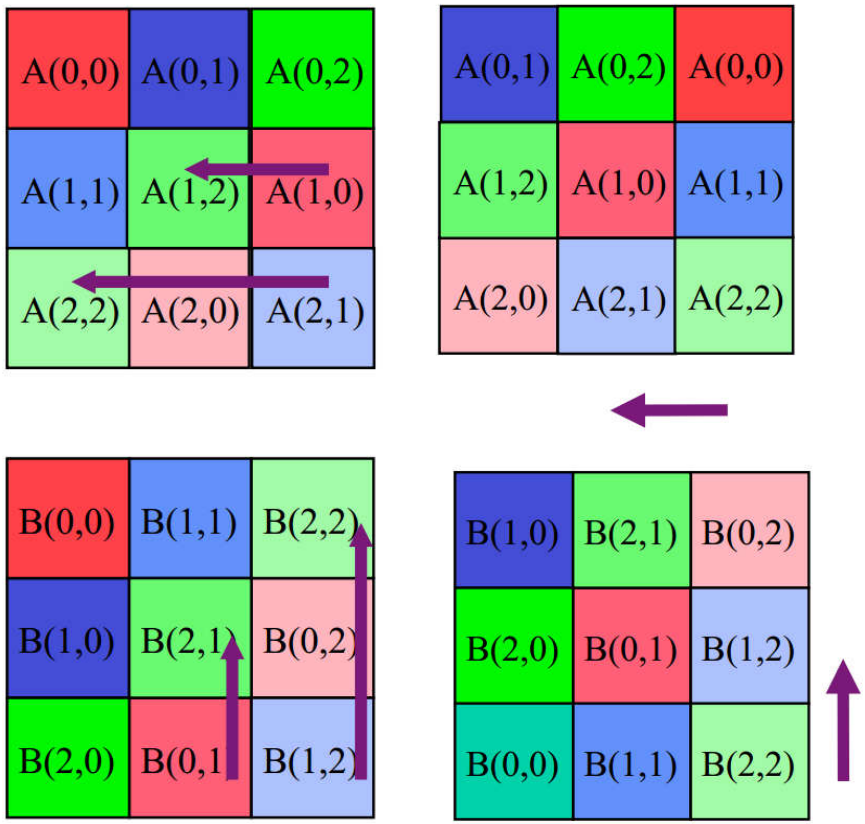
Cannon's matrix-matrix multiplication



Step 0 Step 1

- After the initial shifting, run for $\sqrt{p} - 1$ more stages.
  - In every stage, shift A blocks left by 1, and B blocks up by 1.
- Each processor $P_{i,j}$ still has like colored blocks from A and B.
- Blocks from A stay in same rows and blocks from B stay in same columns.
- So product of the blocks makes up another term in $C_{i,j}$.
- After $\sqrt{p}$ stages, $P_{i,j}$ contains $C_{i,j}$, for all i and j.

Cannon's matrix-matrix multiplication

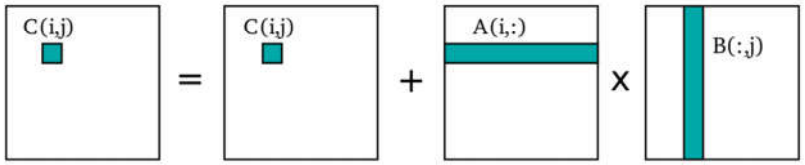


Step 0 Step 1

- Each process only stores one block at a time. So total storage at any time is $O(n^2)$.
- Each process does $O\left(\frac{n^3}{p}\right)$ amount of computation.
- Each of the $\sqrt{p}$ shifts costs each processor $O\left(t_s + \frac{t_w n^2}{p}\right)$ communication.
- Total overhead is $O(p^{\frac{3}{2}} + n^2\sqrt{p})$.
- Isoefficiency requires $p = O(n^2)$.

SUMMA multiplication

```
% inner product approach
for i = 1:I
    for j = 1:J
        for k = 1:K
            C(i,j) = C(i,j) + A(i,k)*B(k,j);
```

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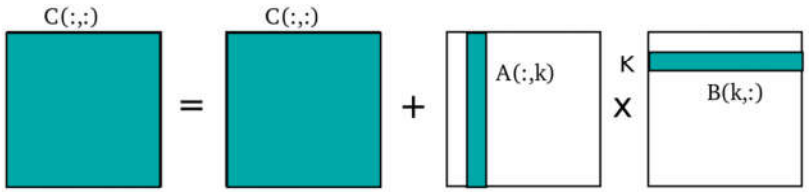
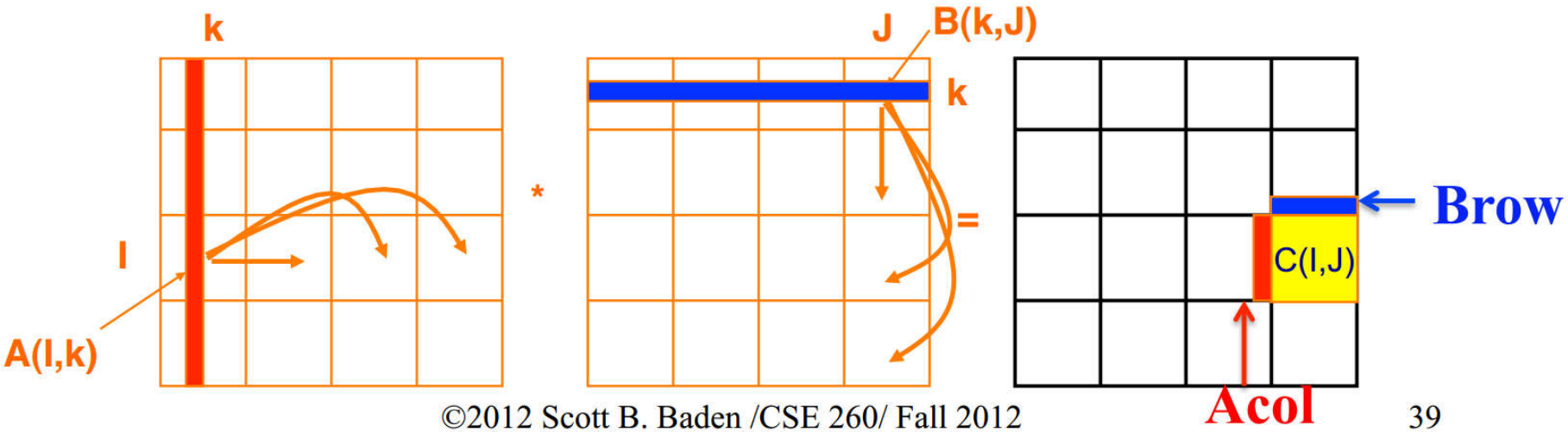


$$\mathbf{u} \otimes \mathbf{v} = \mathbf{u}\mathbf{v}^{\mathrm{T}} = \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} \begin{bmatrix} v_1 & v_2 & v_3 \end{bmatrix} = \begin{bmatrix} u_1 v_1 & u_1 v_2 & u_1 v_3 \\ u_2 v_1 & u_2 v_2 & u_2 v_3 \\ u_3 v_1 & u_3 v_2 & u_3 v_3 \\ u_4 v_1 & u_4 v_2 & u_4 v_3 \end{bmatrix}.$$

- One of the drawbacks of Cannon is that it can only deal with square matrices, and n must be divisible by $\sqrt{p}$.
- SUMMA algorithm overcomes those problems.
  - Our example is still for a square matrix though.
- The basic matrix multiplication algorithm is three nested loops.
  - Fast MM algorithms such as Strassen's work differently.
- The loops can be done in any order.
  - The typical inner product approach is the ijk order.
  - The outer product approach is kij.

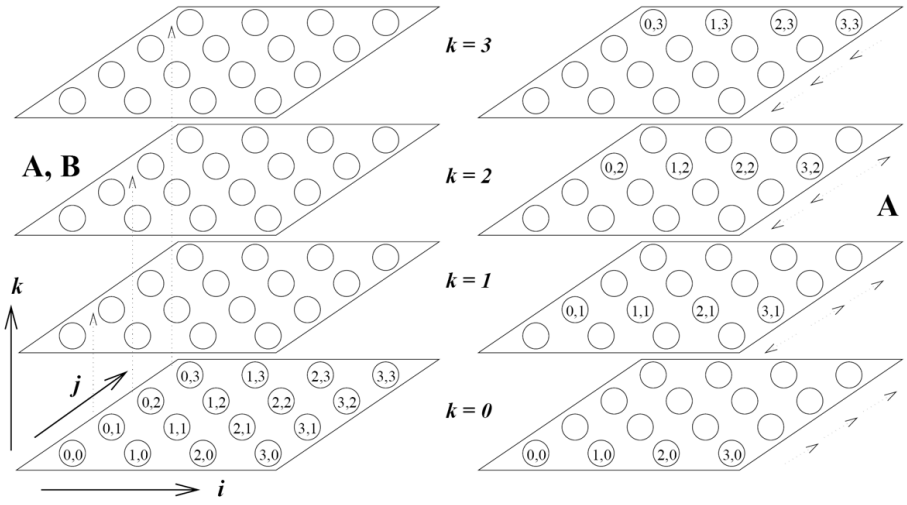
Source: https://patterns.eecs.berkeley.edu/?page_id=158

SUMMA multiplication

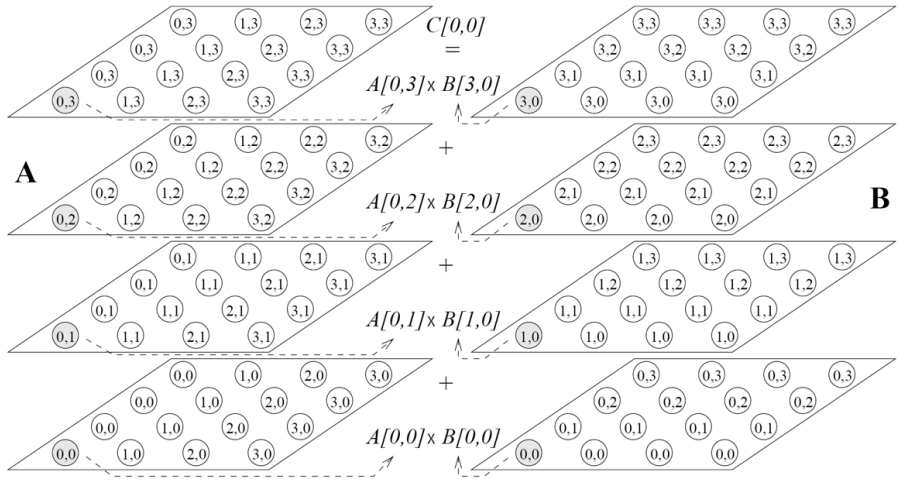


- SUMMA does n outer products.
  - k'th iteration does outer product of k'th column of A with k'th row of B.
  - Processors in k'th column broadcast their A block to their rows.
  - Processors in k'th row broadcast their B block to their columns.
  - Processor (i,j) computes $A_{i,k}$ $B_{k,j}$ and accumulates it into $C_{i,j}$.
- Matrices don't need to be square.
- Also allows more flexible mapping of processors to blocks.

3D matrix multiplication



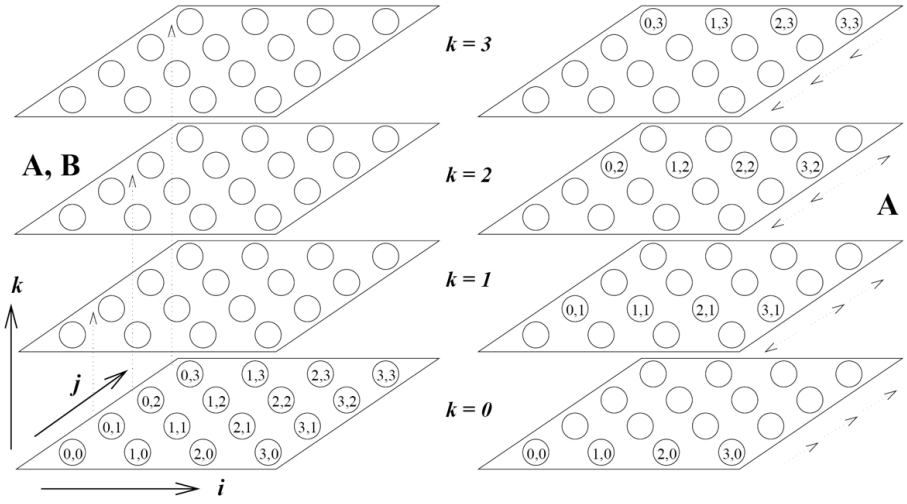
(a) Initial distribution of A and B (b) After moving $A[i,j]$ from $P_{i,j,0}$ to $P_{i,j,j}$



(c) After broadcasting $A[i,j]$ along j axis (d) Corresponding distribution of B

- The 2D algorithms up to now used at most n^2 processors. Since MM has $\Omega(n^3)$ operations, 2D algorithms have $\Omega(n)$ running time.
- We now show the DNS (Dekkel, Nassimi, Sahni) algorithm that can use n^3 processors.
- Arrange the n^3 processors in a n x n x n cube.
- For $0 \leq i, j, k \leq n$, processor $P_{i,j,k}$ computes $A_{i,k}$ $B_{k,j}$.
- Then processors in each column (i,j,:) does reduction to collect result onto processor $P_{i,j,0}$.

3D matrix multiplication



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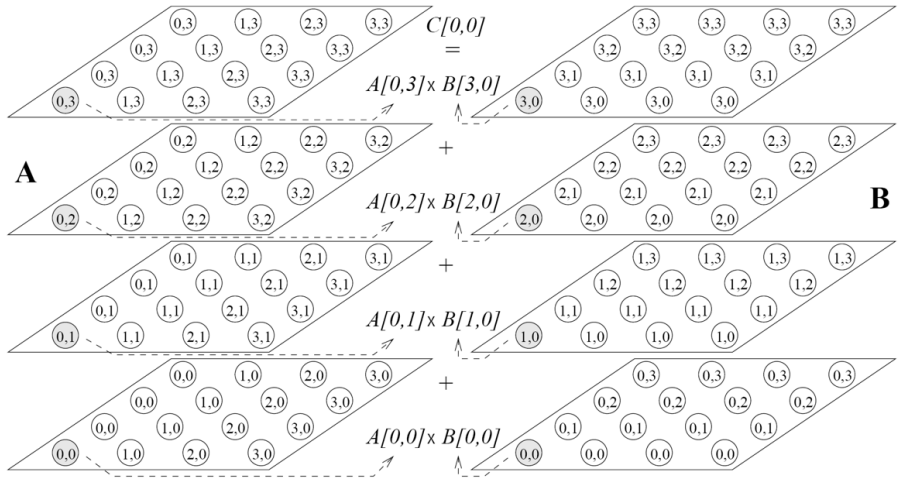
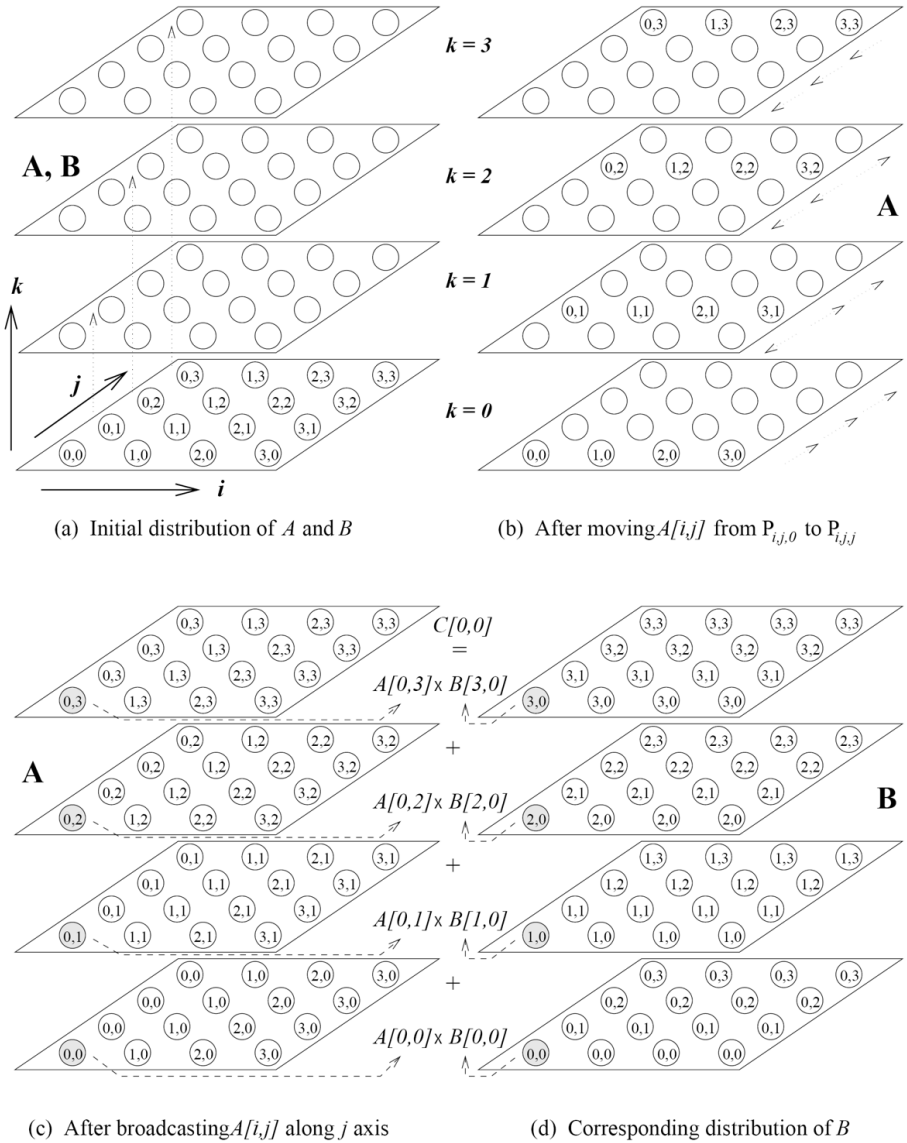


(c) After broadcasting $A[i,j]$ along j axis (d) Corresponding distribution of B

- Initially only processors $P_{i,j,0}$, for $0 \leq i,j \leq n-1$, hold the A and B matrices.
- (a) To distribute the data, the j'th group of processors along the i direction in 0'th (i,j)-plane send their data to corresponding processors in the j'th (i,j)-plane.
- (b) Then, in each (i,j)-plane, the processors along direction i broadcast in the j direction.
- Effect is that A is replicated in each (i,k)-plane.
- Do similar operations for B, so that B is replicated in each (k,j)-plane.
- Then do reduction in the k direction.
- The broadcast and reduction both take O(log n) time. So the total computation time is O(log n).

3D matrix multiplication



(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

- The DNS algorithm isn't optimal using n^3 processors, since the total work is $O(n^3 \log n)$.
- For a cost optimal version, suppose $p=q^3$ for some $q \leq n$. Partition the matrix into q x q blocks, each of size (n/q) x (n/q).
- Then apply the same algorithm as before on the blocks.
- The broadcast and reduction both take $t_s \log q + t_w \left(\frac{n}{q}\right)^2 \log q$. The block multiplication takes $\left(\frac{n}{q}\right)^3$.
- Since $q = p^{\frac{1}{3}}$, the total time is $\frac{n^3}{p} + t_s \log p + \frac{t_w n^2}{p^{\frac{2}{3}}} \log p$.
- For isoefficiency, we need $n^3 = \Omega(n^2 p^{\frac{1}{3}} \log p)$, which implies $p = O\left(\left(\frac{n}{\log n}\right)^3\right)$.

Solving linear systems

$$\begin{aligned}
a_{0,0}x_0 &+ a_{0,1}x_1 &+ \cdots &+ a_{0,n-1}x_{n-1} &= b_0,\\
a_{1,0}x_0 &+ a_{1,1}x_1 &+ \cdots &+ a_{1,n-1}x_{n-1} &= b_1,\\
\vdots & \vdots & & \vdots & \vdots\\
a_{n-1,0}x_0 &+ a_{n-1,1}x_1 &+ \cdots &+ a_{n-1,n-1}x_{n-1} &= b_{n-1}.
\end{aligned}$$

$$\begin{aligned}
x_0 &+ u_{0,1}x_1 &+ u_{0,2}x_2 &+ \cdots &+ u_{0,n-1}x_{n-1} &= y_0,\\
& x_1 &+ u_{1,2}x_2 &+ \cdots &+ u_{1,n-1}x_{n-1} &= y_1,\\
& & & & \vdots & \vdots\\
& & & & x_{n-1} &= y_{n-1}.
\end{aligned}$$

$$1)\begin{cases} 5x+3y+2z=-2\\ x+y=2\\ 2x-y+z=3 \end{cases}\Rightarrow \left(\begin{array}{ccc|c} 5 & 3 & 2 & -2\\ 1 & 1 & 0 & 2\\ 2 & -1 & 1 & 3 \end{array}\right)\Rightarrow_{reorder}$$

$$\Rightarrow \left(\begin{array}{ccc|c} 1 & 1 & 0 & 2\\ 5 & 3 & 2 & -2\\ 2 & -1 & 1 & 3 \end{array}\right)\Rightarrow \begin{matrix} R_1\\ R_2-5R_1\\ R_3-2R_1 \end{matrix}\left(\begin{array}{ccc|c} 1 & 1 & 0 & 2\\ 0 & -2 & 2 & -12\\ 0 & -3 & 1 & -1 \end{array}\right)\Rightarrow$$

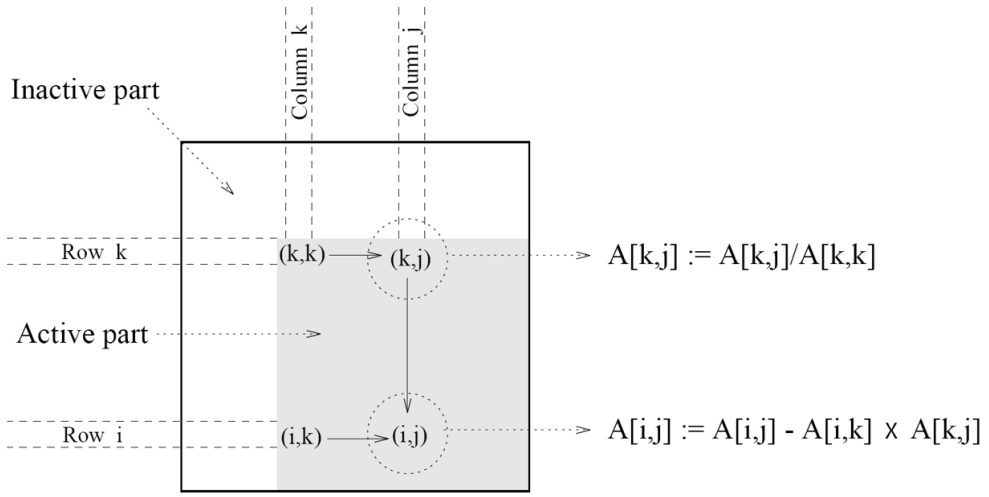
$$\Rightarrow_{simplify\ R_2} \begin{matrix} R_1\\ -\frac{1}{2}R_2\\ R_3 \end{matrix}\left(\begin{array}{ccc|c} 1 & 1 & 0 & 2\\ 0 & 1 & -1 & 6\\ 0 & -3 & 1 & -1 \end{array}\right)\Rightarrow \begin{matrix} R_1\\ R_2\\ R_3+3R_2 \end{matrix}\left(\begin{array}{ccc|c} 1 & 1 & 0 & 2\\ 0 & 1 & -1 & 6\\ 0 & 0 & -2 & 17 \end{array}\right)\Rightarrow$$

$$\begin{matrix} r=r'=n\\ \Rightarrow\\ independent\ system \end{matrix}\begin{cases} x+y=2\\ y-z=6\\ -2z=17 \end{cases}\Rightarrow\begin{cases} x=\frac{9}{2}\\ y=-\frac{5}{2}\\ z=-\frac{17}{2} \end{cases}$$

- Given a system of n linear equations, we can reduce it to triangular form using Gaussian Elimination.
- Then the triangular equations can be solved by back substitution.
- As we'll see, Gaussian Elimination takes $O(n^3)$ operations, and back substitution takes $O(n^2)$ operations. So linear systems can be solved in $O(n^3)$ operations.
- Given a matrix A, if Ax = b needs to be solved for multiple b vectors, can also use Gaussian Elimination to compute the LU factorization of A, i.e. A = LU, where L is a lower triangular and U is an upper triangular matrix.
  - Then LUx = b can be solved by first solving Ly = b using backwards substitution, then solving Ux = y using backwards substitution.
  - Both steps take $O(n^2)$ time. So solving Ax = b for each b takes $O(n^2)$ instead of $O(n^3)$ time.
  - The initial LU decomposition takes $O(n^3)$ time.

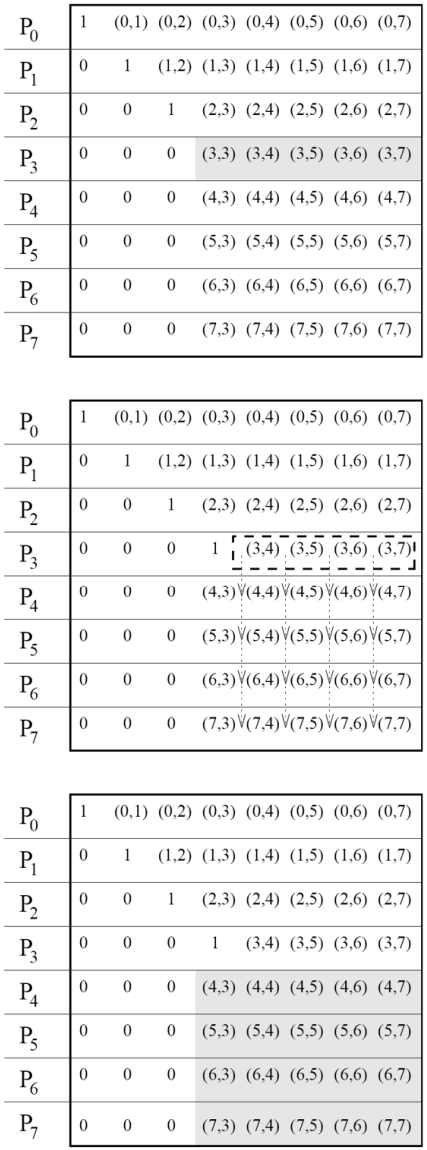
Gaussian Elimination

```
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
```



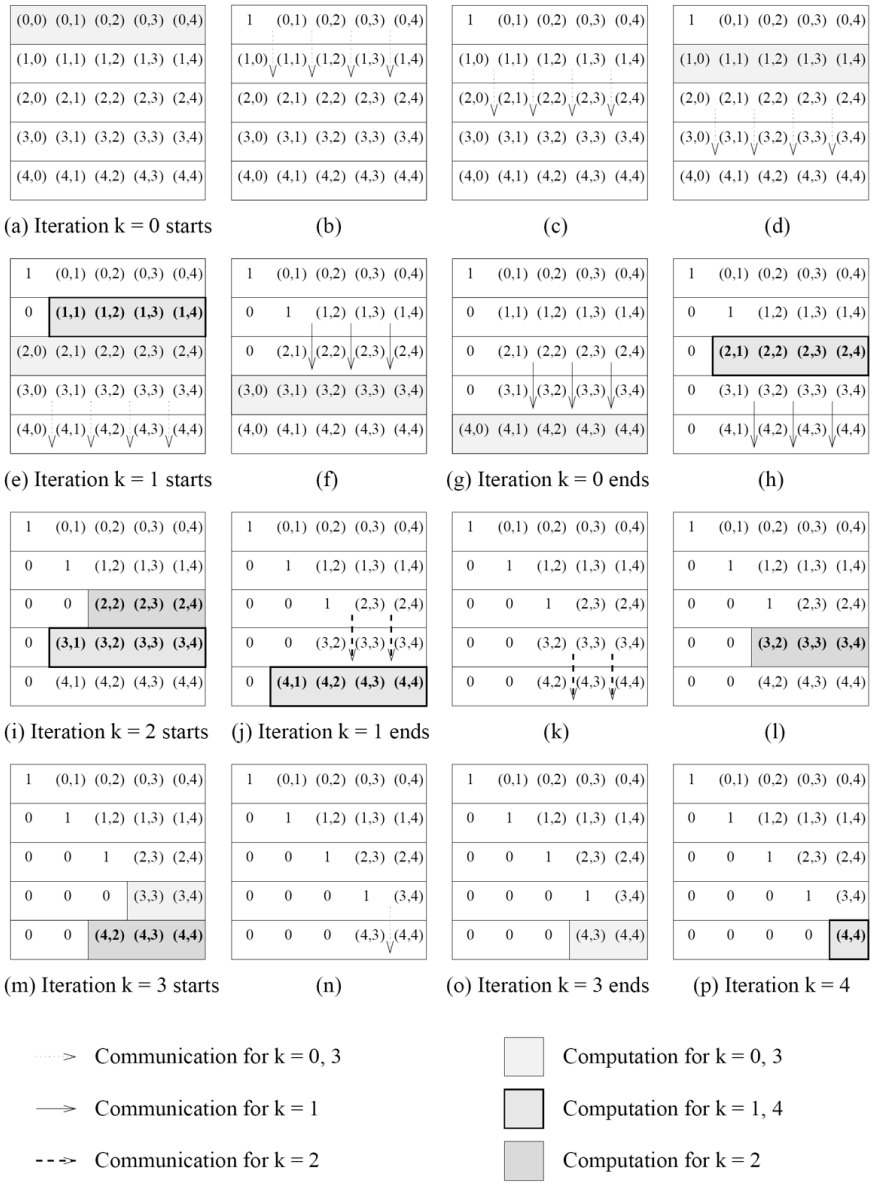
- Three nested loops of size n, so $O(n^3)$ time.
- Here we assume for simplicity that A[k,k], which we divide by on line 6, is never 0.
  - We also ignore numerical accuracy issues.
  - These are addressed using pivoting.
- Iteration k of the algorithm uses A[k,k] to eliminate all nonzeros in column k.
- If we don't perform lines 7, 8, 13 and 14, the algorithm produces the LU decomposition of A, with L and U stored in the lower and upper triangular parts of A.

Parallel Gaussian Elimination



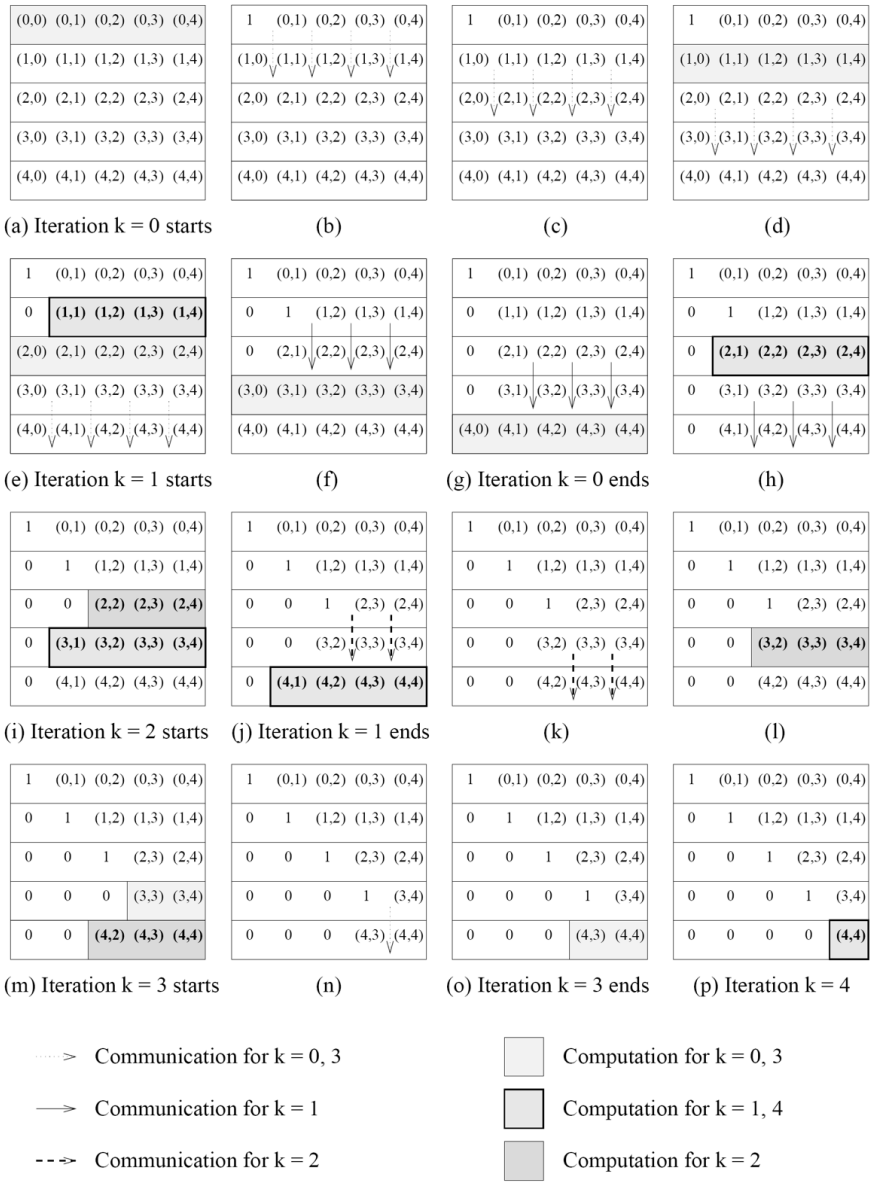
- Consider the k'th iteration.
  - In step (a), divide the k'th row by A[k,k].
  - In (b), broadcast the k'th row to the higher rows.
  - In (c), each row subtracts the proper multiple of row k from itself.
- Total time over all iterations k for steps (a) and (c) take $\sum_{k=0}^{n-1}(n-k-1) = O(n^2)$.
- For each k, step (b) takes $\left(t_s + t_w(n-k-1)\right)\log n$. Thus, over all n iterations, it takes $O(n^2 \log n)$.
- Total work is $O(n^3 \log n)$, so this isn't cost optimal.

Pipelined Gaussian Elimination



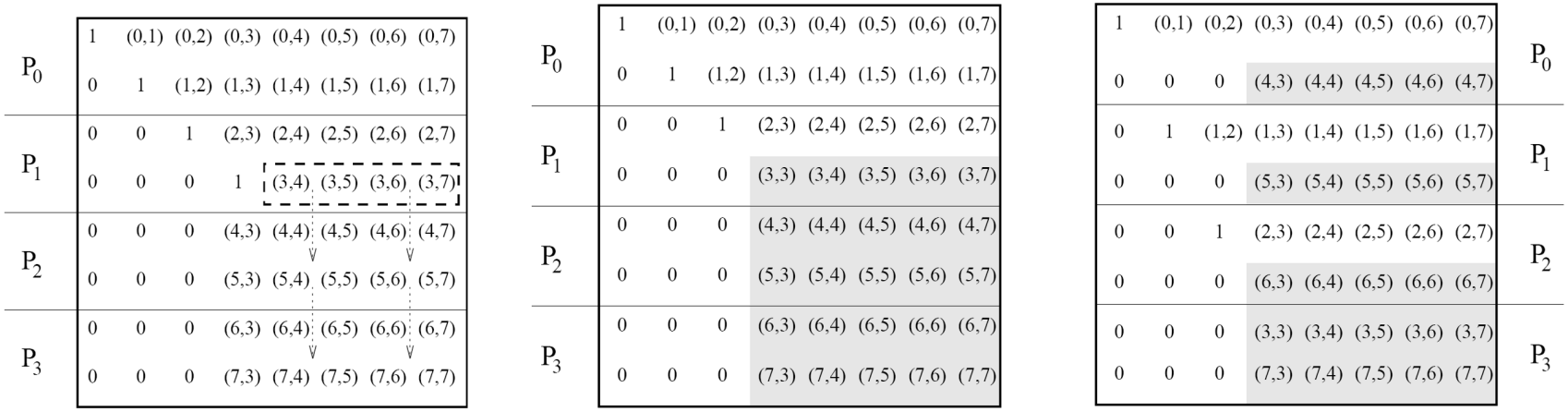
- One problem with previous algorithm is that it waited till iteration k was finished (i.e., the entire k'th column has been eliminated using the k'th row) before starting iteration k+1.
- We can use a more efficient pipelined algorithm, where each row uses and sends data as quickly as possible.
  - When a row receives data from the previous row, it sends the data to the next row.
  - The row eliminates a variable.
  - Then the row waits for new data from the previous row.
  - When the first nonzero in the row is the diagonal element, it divides out by this row and sends this to the next row.
  - Then the row stops.

Pipelined Gaussian Elimination



- For each row, call the 3 steps (recv, send, eliminate) a cycle.
  - A row eliminates a variable every cycle.
- The last row receives its last piece of data after n cycles.
  - So the entire algorithm finishes after O(n) cycles.
- Each cycle involves dividing, subtracting or sending O(n) items, so takes O(n) time.
- So algorithm takes total $O(n^2)$ time.
- So total work is $O(n^3)$, and the algorithm is work optimal.

Fewer processors, load balancing



(a) Block 1-D mapping

(b) Cyclic 1-D mapping

- If we have < n processors, we can assign n/p consecutive rows per processor.
  - Each processor does $O(\frac{n}{p}\sum_i(n-i)) = O(n^3/p)$ work.
- However, this leads to the initial processors finishing earlier than the later processors.
  - Total idle work (i.e. idle time x number of idle processors) = $\Theta(n^3)$.
- To prevent idling and achieve better load balancing, can assign the rows in cyclic (round robin) order to the processors.
  - Load difference between different processors in any iteration is then at most one row.
  - Each row contains O(n) work and algorithm runs O(n) iterations, so each process has $O(n^2)$ idle work, and total idle work $O(pn^2)$.