Solving Linear Equations, FFT and Sorting on Distributed-Memory Architectures

SC3260/5260 High-Performance Computing

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Spring 2020

Solving System of Linear Equations

- Solving $Ax = b$ as a benchmark to rank world's top supercomputers (https://www.top500.org/).
- We will discuss the classical two-step approach:
  1) Gaussian Elimination;
  2) Back Substitution.
- We assume a 2D block data distribution on $\sqrt{P} \times \sqrt{P}$ procs.
  - Proc P_{ij} holds matrix block A_{ij}
  - Diagonal processor P_{ii} holds vector block b_i and computes x_i

P_{00} A_{00}, b_0 $\rightarrow x_0$	P_{01} A_{01}	P_{02} A_{02}
P_{10} A_{10}	P_{11} A_{11}, b_1 $\rightarrow x_1$	P_{12} A_{12}
P_{20} A_{20}	P_{21} A_{21}	P_{22} A_{22}, b_2 $\rightarrow x_2$

A Simple Example

- $$\begin{cases} 2x_0 + 4x_1 + 6x_2 = 8 \\ 3x_0 + 9x_1 + 15x_2 = 21 \\ 5x_0 + 12x_1 + 7x_2 = 2 \end{cases} \Rightarrow \begin{bmatrix} 2 & 4 & 6 \\ 3 & 9 & 15 \\ 5 & 12 & 7 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 8 \\ 21 \\ 2 \end{bmatrix}$$

System of linear equations *Matrix form* $Ax = b$

A Simple Example

- **Step 1:** Gaussian Elimination
  - Reduce $Ax = b$ to $Ux = y$ (*row echelon form*), where U is an upper triangular matrix (with 1 on diagonal).
  - Achieved by dividing a row by a non-zero number and subtracting a row by a multiple of another row.

$$\underbrace{\left[\begin{array}{ccc|c} 2 & 4 & 6 & 8 \\ 3 & 9 & 15 & 21 \\ 5 & 12 & 7 & 2 \end{array}\right]}_{A \qquad b} \rightarrow \underbrace{\left[\begin{array}{ccc|c} 1 & 2 & 3 & 4 \\ 0 & 1 & 2 & 3 \\ 0 & 0 & 1 & 2 \end{array}\right]}_{U \qquad y}$$

$$\searrow \underbrace{\begin{bmatrix} 2 & 0 & 0 \\ 3 & 3 & 0 \\ 5 & 2 & -12 \end{bmatrix}}_{L}$$

A lower triangular matrix L records intermediate steps of this process

A Simple Example

- **Step 2:** Back Substitution
  - Solve for x in $Ux = y$ in reverse order from x_{n-1} to x_0

$$\underbrace{\left[\begin{array}{ccc|c} 1 & 2 & 3 & 4 \\ 0 & 1 & 2 & 3 \\ 0 & 0 & 1 & 2 \end{array}\right]}_{U \quad\quad y} \Rightarrow \begin{cases} x_0 + 2x_1 + 3x_2 = 4 \\ x_1 + 2x_2 = 3 \\ x_2 = 2 \end{cases} \Rightarrow \begin{cases} x_0 = 0 \\ x_1 = -1 \\ x_2 = 2 \end{cases}$$

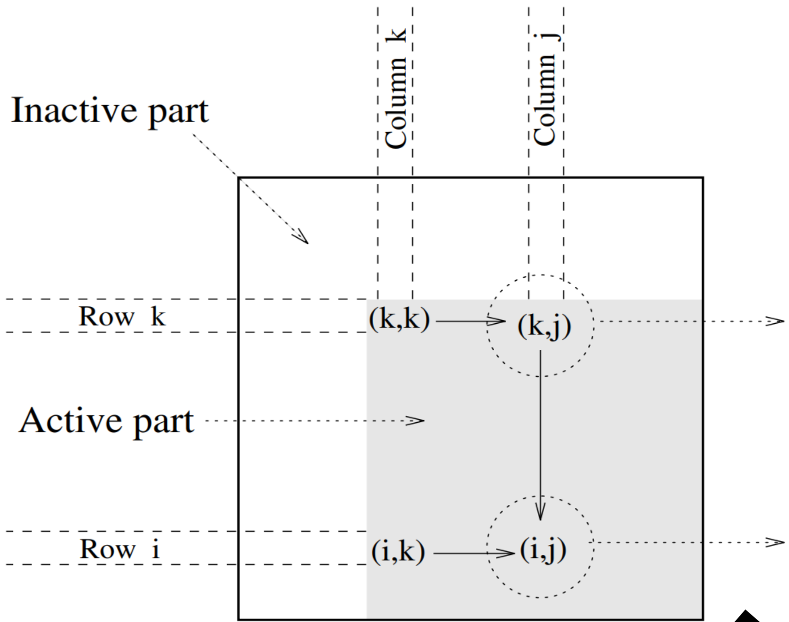
For an $n \times n$ matrix A, Step 1 (Gaussian Elimination) is more expensive taking $O(n^3)$ time, and Step 2 (Back Substitution) takes only $O(n^2)$ time.

Pseudocodes of Two Steps

```
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
```

```
1.   procedure BACK_SUBSTITUTION (U, x, y)
2.   begin
3.      for k := n − 1 downto 0 do   /* Main loop */
4.         begin
5.            x[k] := y[k];
6.            for i := k − 1 downto 0 do
7.               y[i] := y[i] − x[k] × U[i, k];
8.         endfor;
9.   end BACK_SUBSTITUTION
```

Illustration of Gaussian Elimination

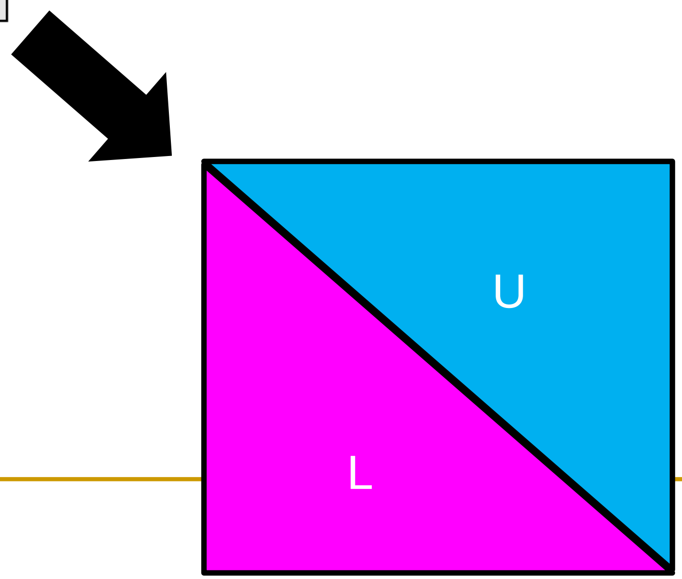


Division step

A[k,j] := A[k,j]/A[k,k]

Elimination step

A[i,j] := A[i,j] - A[i,k] x A[k,j]



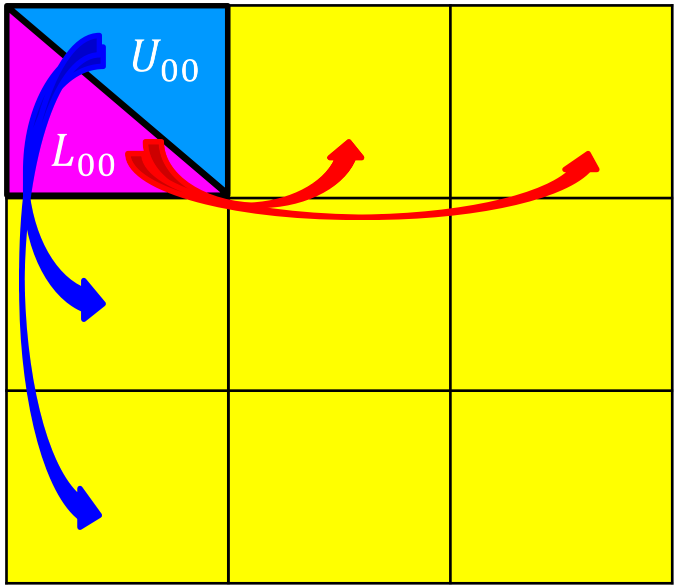
Gaussian Elimination in 2D Blocks

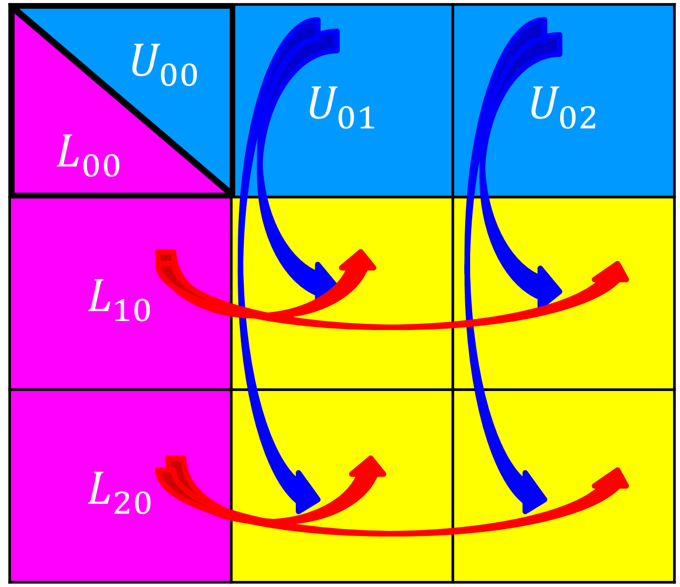
- For step $k = 0, 1, \ldots, \sqrt{P} - 1$:
  a) Processor P_{kk} performs local division and elimination on matrix block A_{kk} (resulting in L_{kk} and U_{kk});
  b) Processor P_{kk} broadcasts L_{kk} to all processors P_{kj} $(j > k)$, and U_{kk} to all processors P_{ik} $(i > k)$;
  c) Processors P_{kj} and P_{ik} $(i, j > k)$ perform local division and elimination (resulting in U_{kj} and L_{ik}, respectively);
  d) Processors P_{kj} broadcasts U_{kj} down to other processors in same column, and processors P_{ik} broadcasts L_{ik} to other processors to the right in same row;
  e) Processors P_{ij} $(i, j > k)$ perform local division and elimination (resulting in modified block $\widetilde{A_{ij}}$).

Next slide illustrates one step for $P = 9$ processors

Gaussian Elimination in 2D Blocks

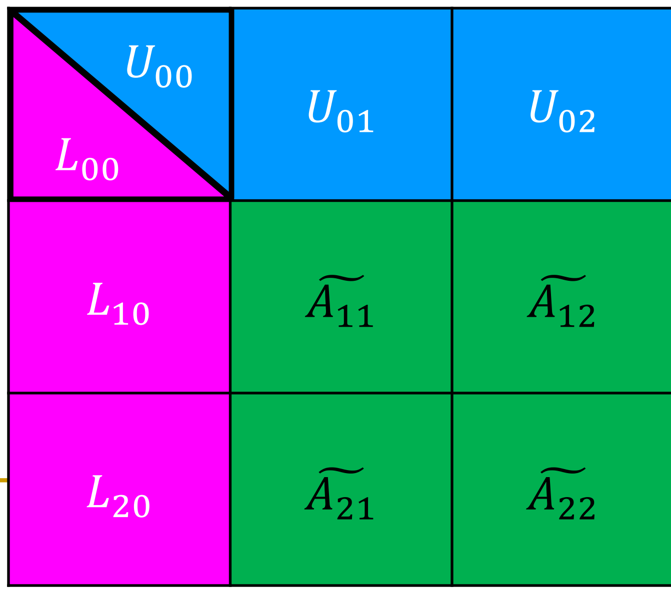
Step $k = 0$
(a)(b)

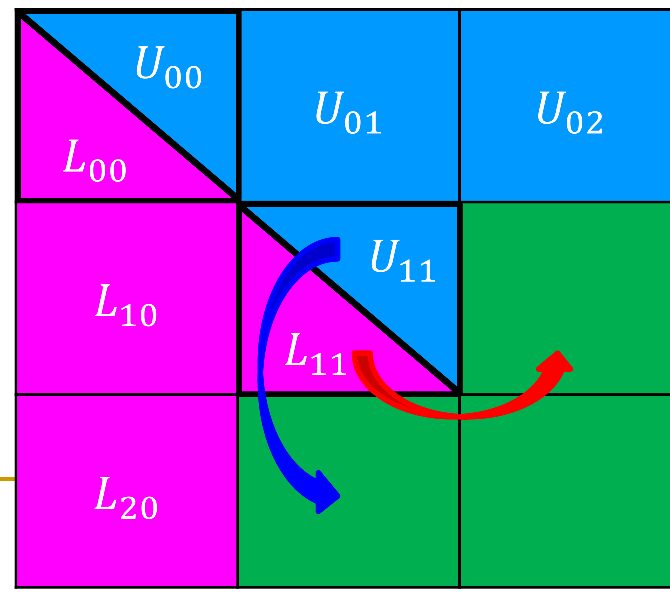




Step $k = 0$
(c)(d)

Step $k = 0$
(e)





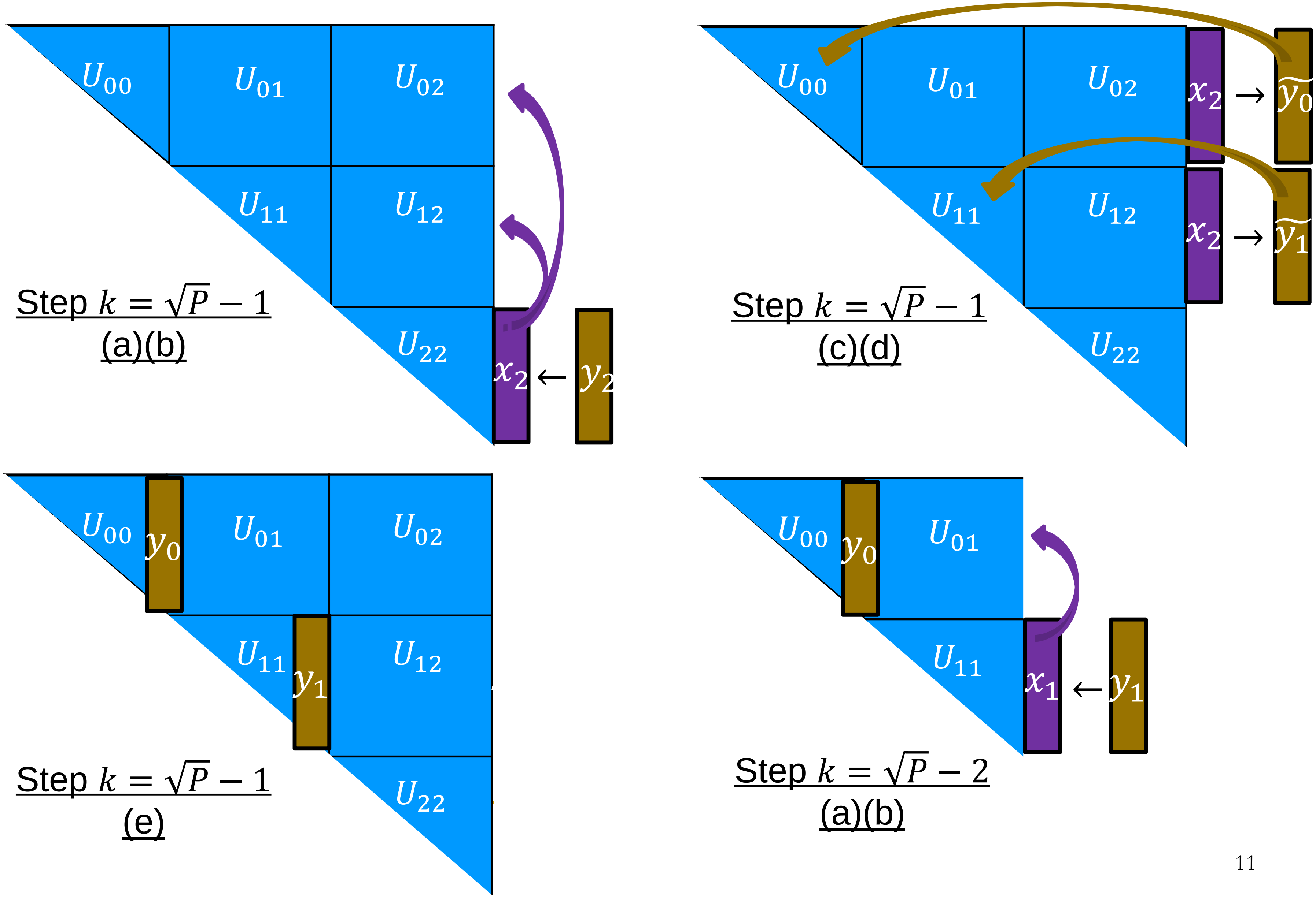
Step $k = 1$
(a)(b)

Back Substitution in 2D Blocks

- For step $k = \sqrt{P} - 1, \sqrt{P} - 2, \ldots, 0$:
  a) Processor P_{kk} performs local back substitution on matrix block U_{kk} and y_k (resulting in x_k);
  b) Processor P_{kk} broadcasts x_k to all processors P_{jk} $(j < k)$;
  c) Processors P_{jk} $(j < k)$ computes $\tilde{y}_j \leftarrow U_{jk} \times x_k$;
  d) Processors P_{jk} $(j < k)$ sends $\tilde{y}_j$ to processors $P_{j,j}$;
  e) Processors $P_{j,j}$ $(j < k)$ updates $y_j \leftarrow y_j - \tilde{y}_j$.

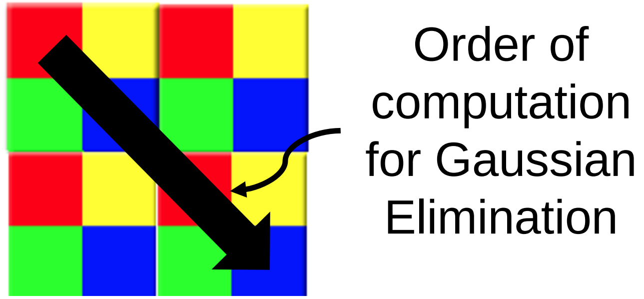
Next slide illustrates one step for $P = 9$ processors

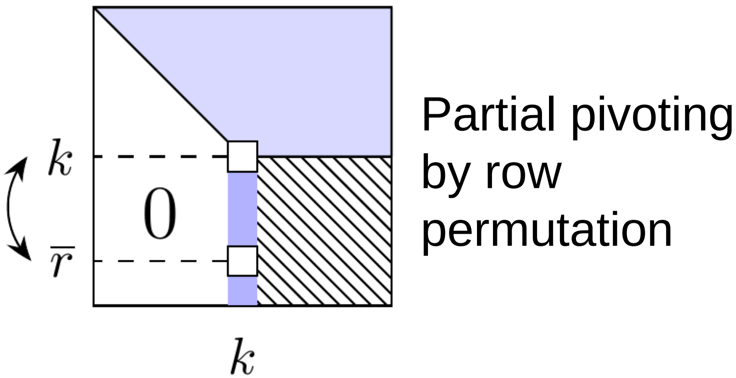
Back Substitution in 2D Blocks



Solving $Ax = b$ in Practice

- ***2D Block-cyclic*** distribution is used (for better load balance);
- ***Partial pivoting*** is used during Gaussian Elimination (for numerical stability);
- ***LU factorization*** of matrix A (for reusing left side).





These and other optimizations are implemented in the software package High-Performance Linpack (HPL) (http://www.netlib.org/benchmark/hpl/).

Fast Fourier Transform (FFT)

- **Discrete Fourier Transform (DFT):** converts a discrete signal of N samples from time domain $(x_0, x_1, \ldots, x_{N-1})$ to frequency domain $(y_0, y_1, \ldots, y_{N-1})$, or vice versa:

$$y_j = \sum_{k=0}^{N-1} w_N^{jk} \cdot x_k \,, \forall\, j = 0,1, \ldots N-1$$

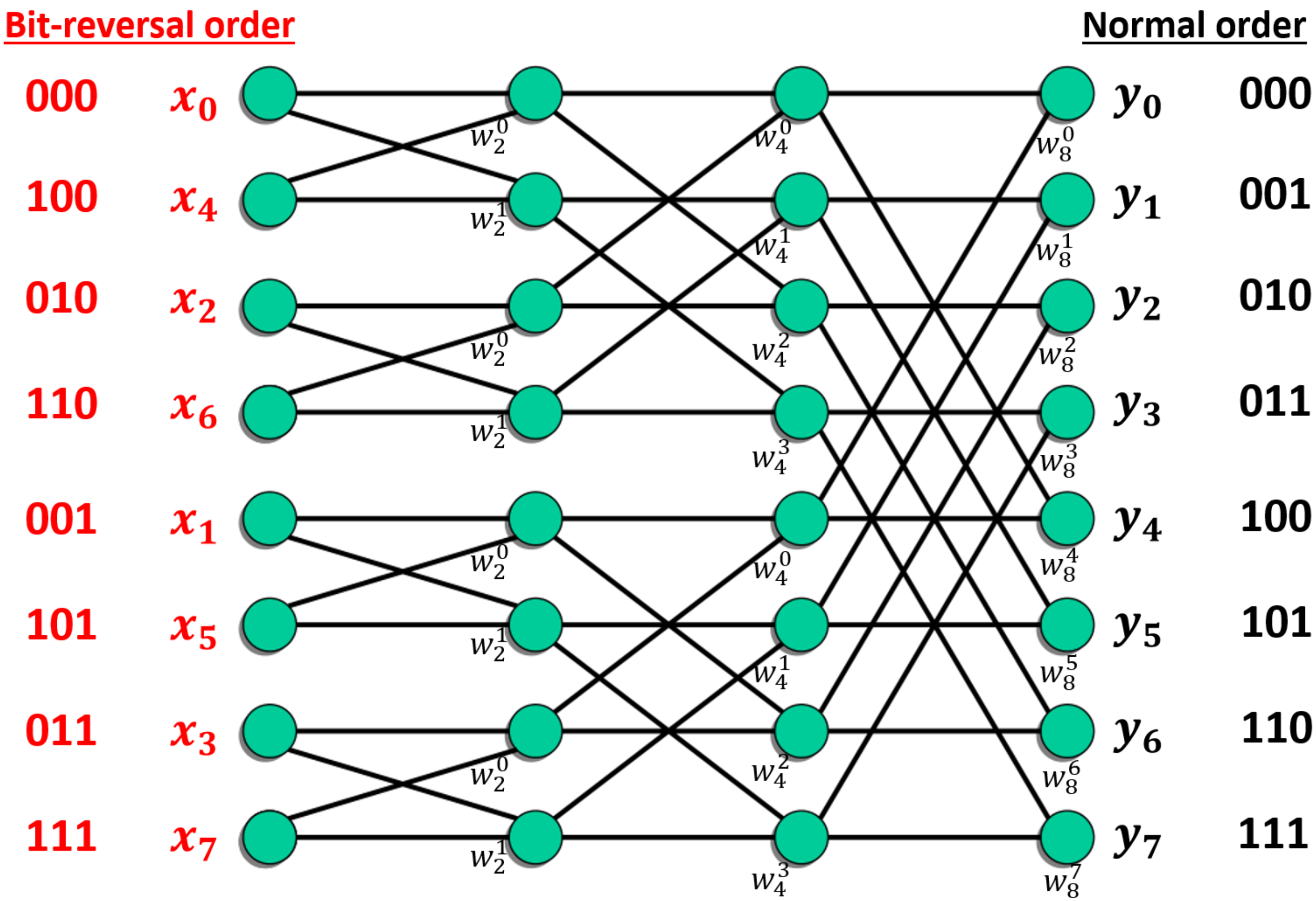
where $w_N = e^{-\frac{2\pi i}{N}}$ is the N-th root of unity, called the *twiddle factor*.

- **Fast Fourier Transform (FFT):** any algorithm that computes DFT in $O(n\log n)$ time instead of the naïve $O(n^2)$ complexity.

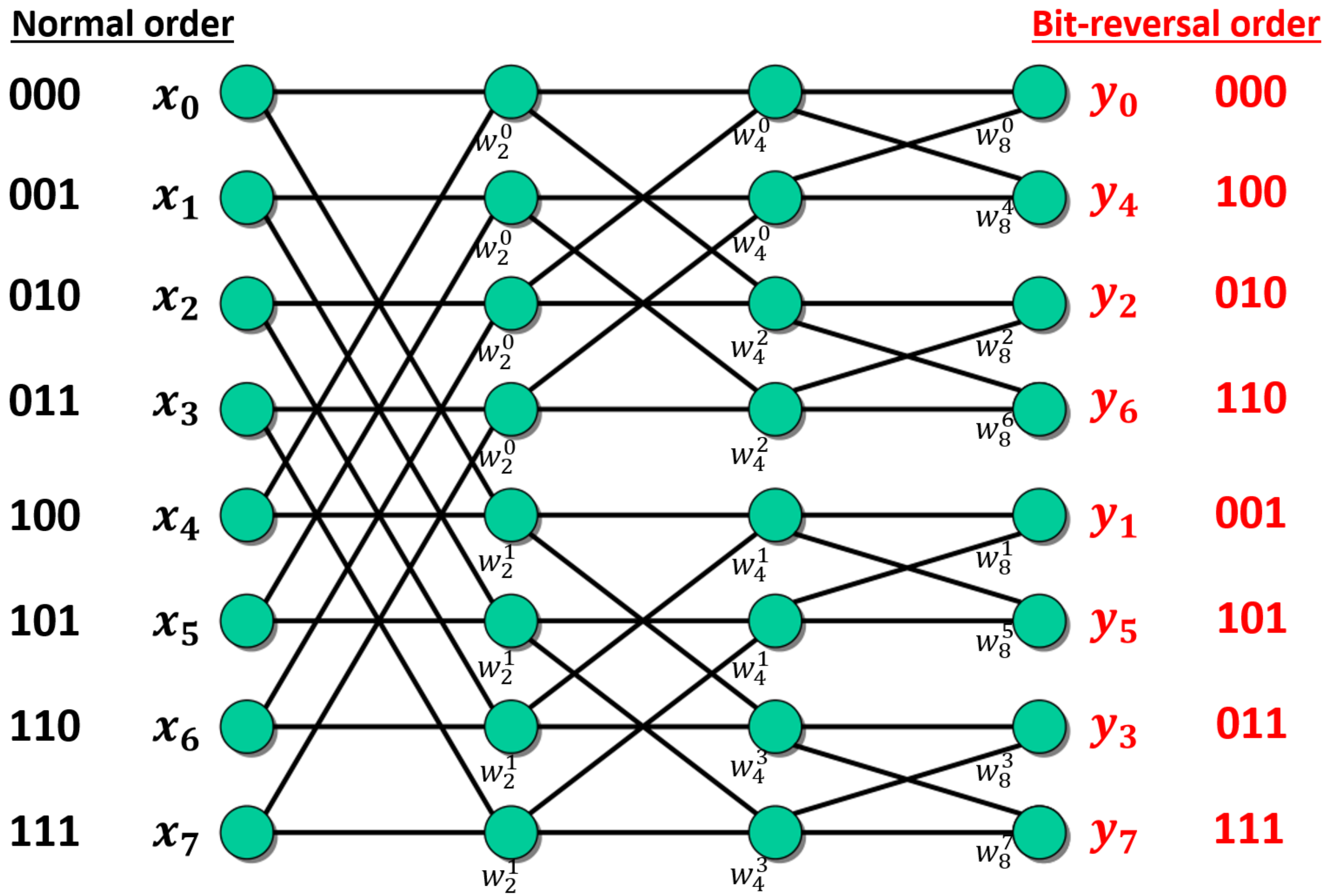
Fast Fourier Transform (FFT)

- FFT has numerous applications in science and engineering, and is considered to be one of the most important algorithms in the 20th century!
- We consider the classical *radix-2* algorithm and study two parallel implementations:
  1) Binary-Exchange Algorithm;
  2) Transpose Algorithm.
- For simplicity, we assume that both N and P (number of processors) are powers-of-2, i.e., $N = 2^r$, $P = 2^d$ and $d \leq r$.

Radix-2 FFT (Decimation in Time)



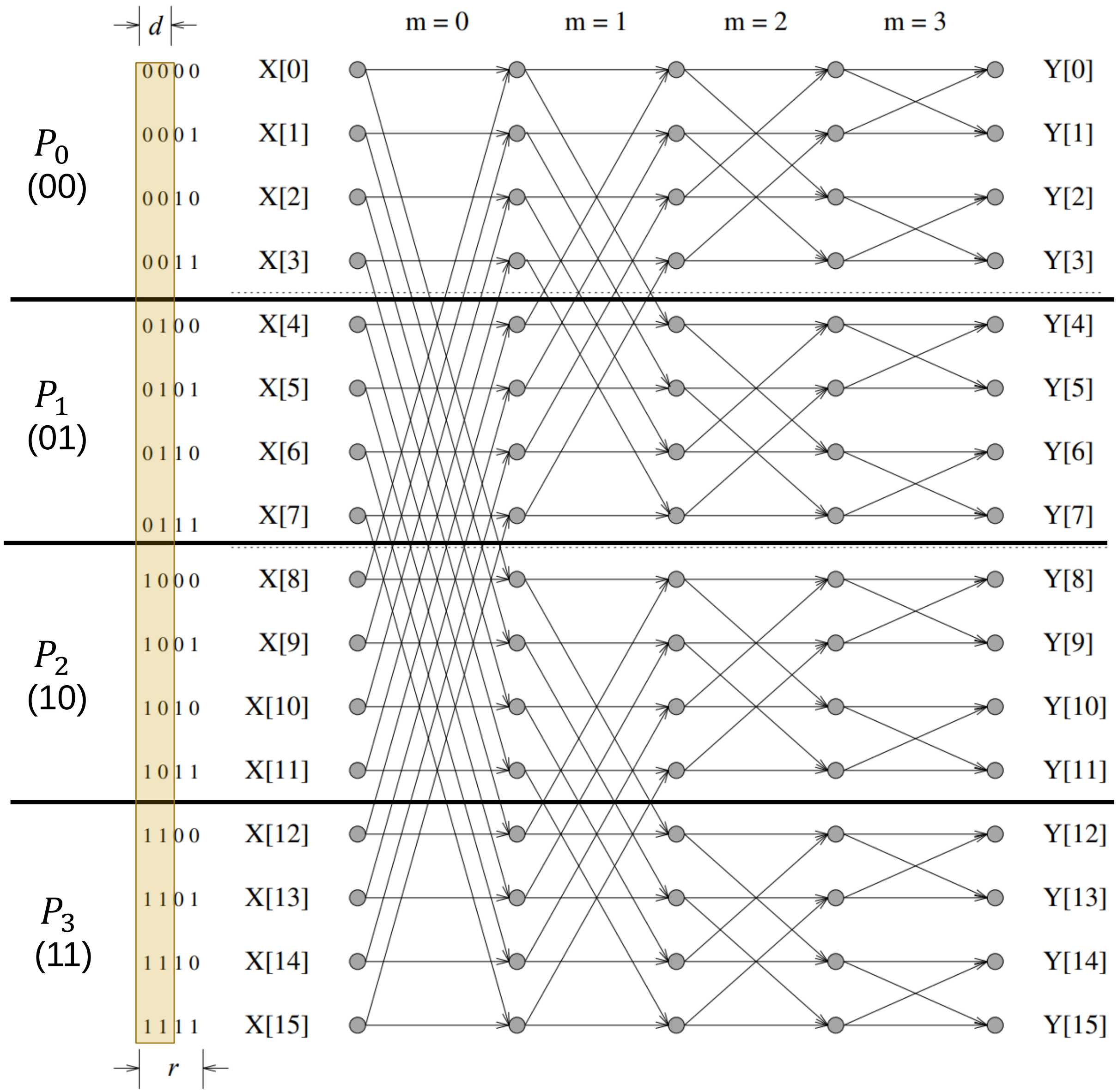
Radix-2 FFT (Decimation in Frequency)



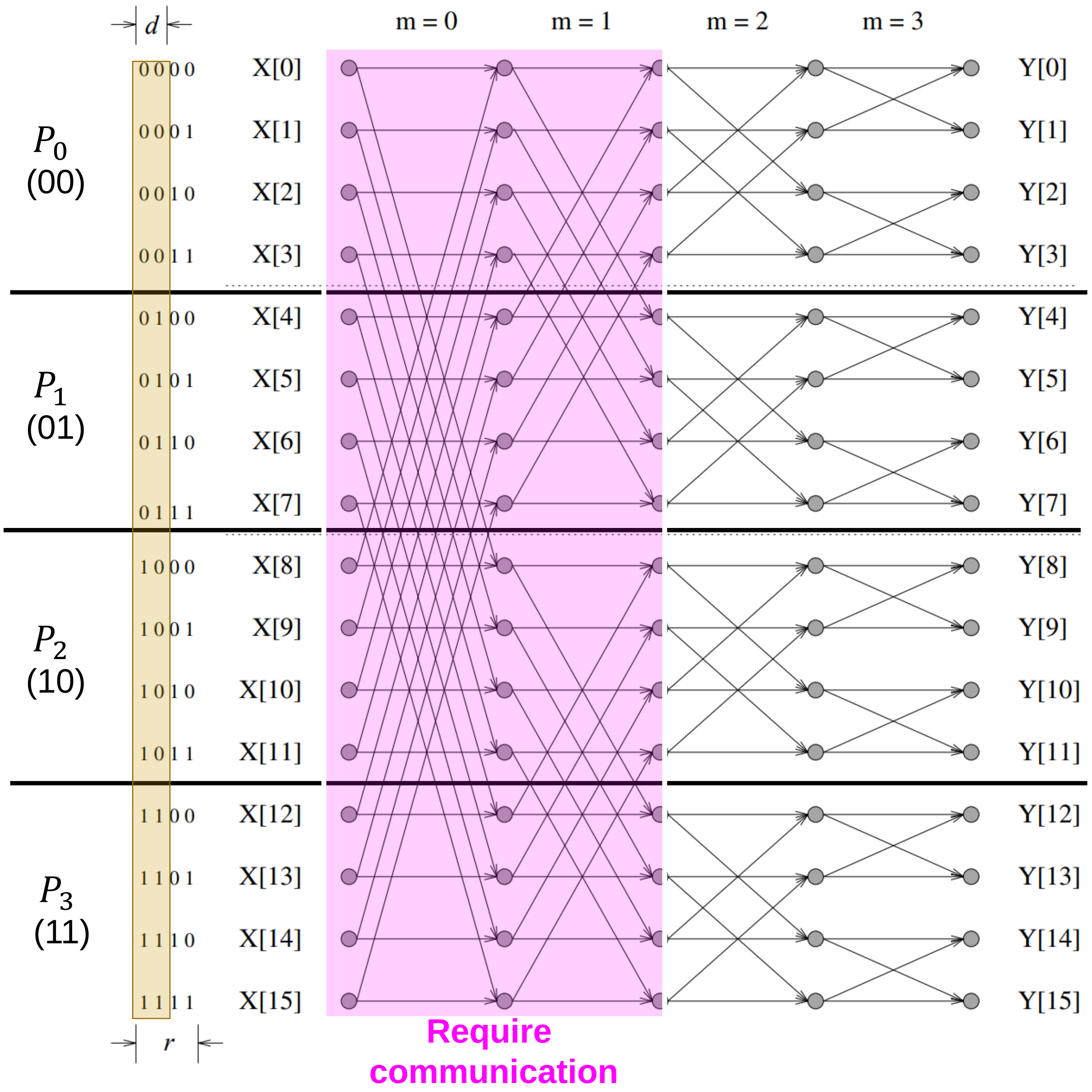
(1) Binary-Exchange Algorithm

- We assume **1D block** data distribution for the DIF implementation of the radix-2 algorithm:
  - Each processor holds N/P consecutive input values in x and responsible for computing the corresponding output values in y.
- The algorithm works in two phases:
  - Phase 1 (w/ communication): step $m = 0, 1, \dots, d-1$:
    a) Each processor P_i exchanges N/P numbers with processor $P_{i'}$, where P_i and $P_{i'}$ only differ in the m-th bit (from left);
    b) Each processor P_i does N/P local complex computations;
  - Phase 2 (local computation): step $m = d, \dots, r-1$:
    a) Each processor P_i does N/P local complex computations;

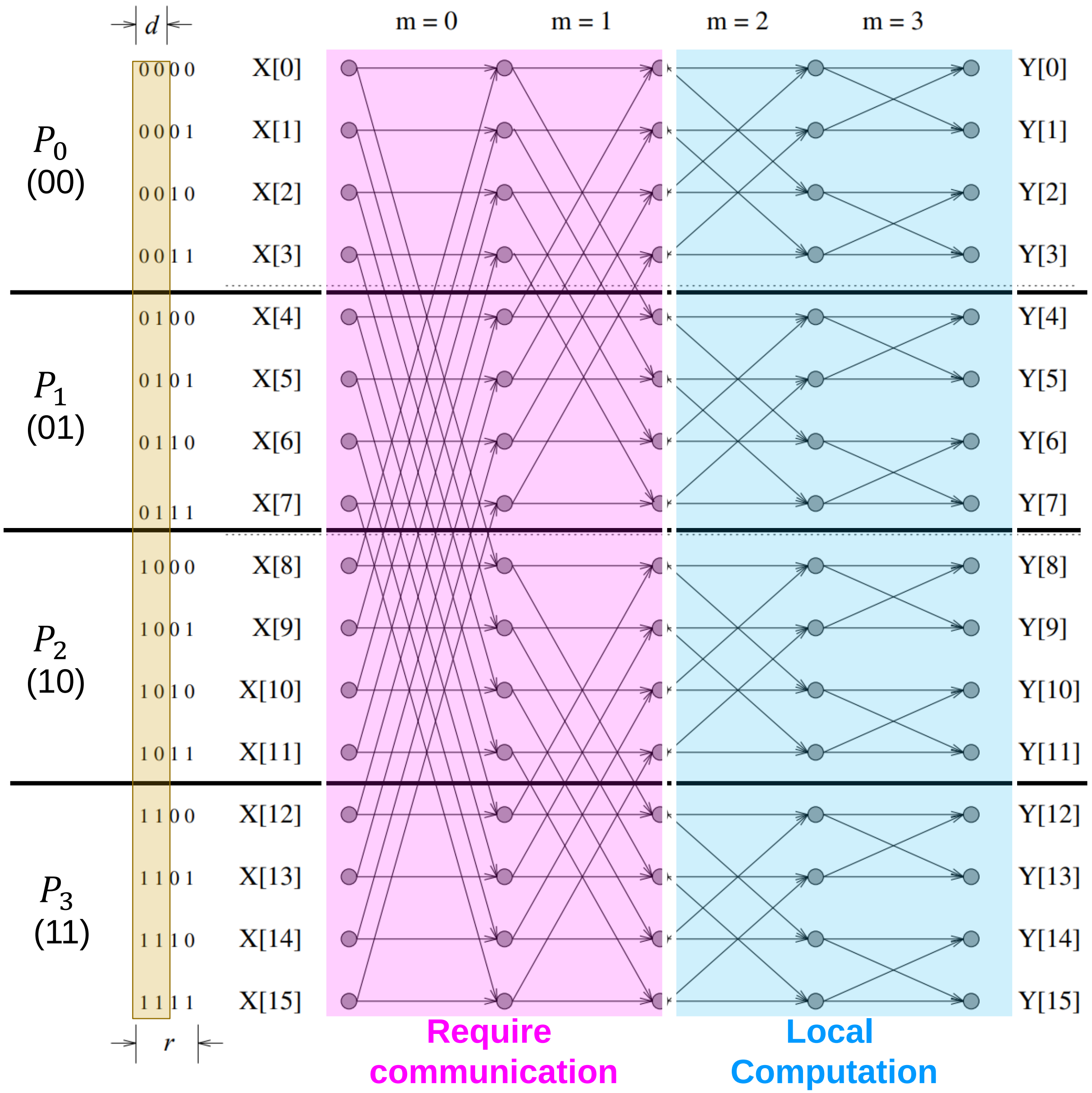
(1) Binary-Exchange Algorithm



(1) Binary-Exchange Algorithm



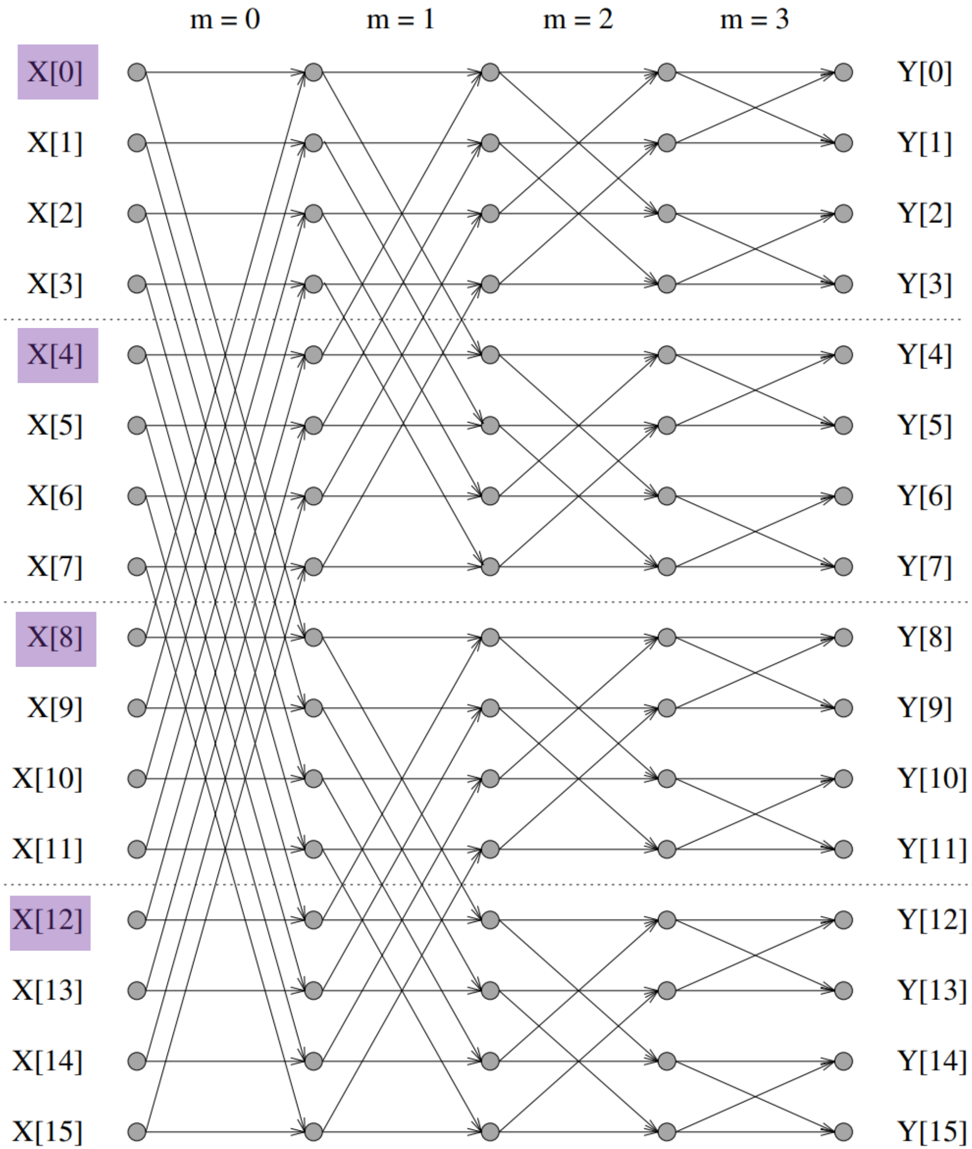
(1) Binary-Exchange Algorithm

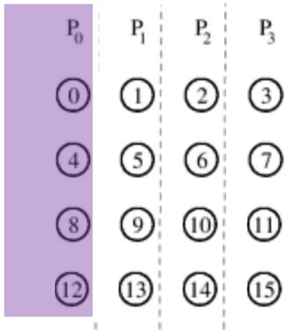


(2) Transpose Algorithm

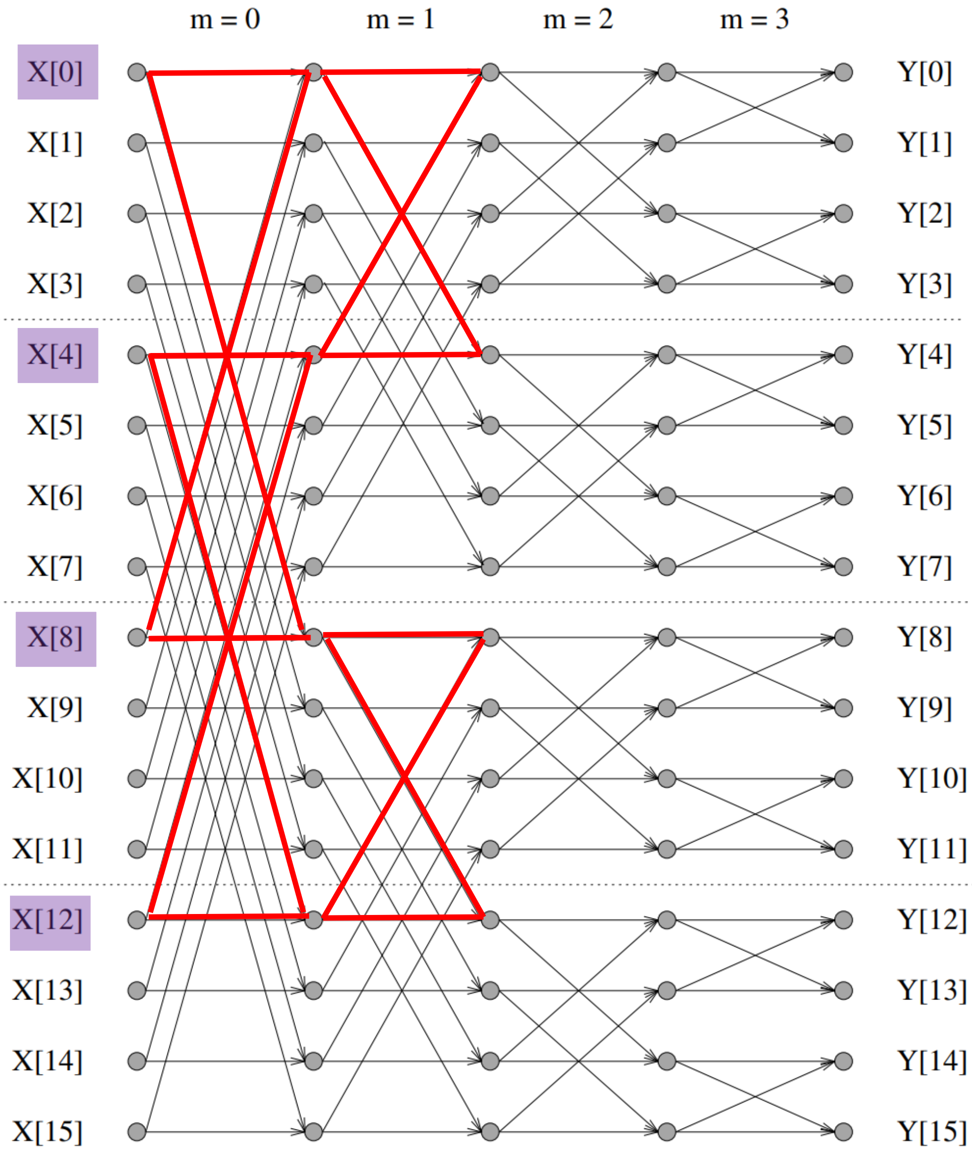
- We assume:
  - The input data (vector x) is arranged in a $\sqrt{N} \times \sqrt{N}$ matrix (in row-major order);
  - The matrix is distributed in **1D block-cyclic (column)** manner to the processors;
- The algorithm works in three steps:
  1) Each processor does $\sqrt{N}/P$ local FFTs for each column of the matrix it holds;
  2) Perform a global matrix transpose through an all-to-all personalized communication (MPI_Alltoall);
  3) Each processor again does $\sqrt{N}/P$ local FFTs for each column of the new matrix it holds;

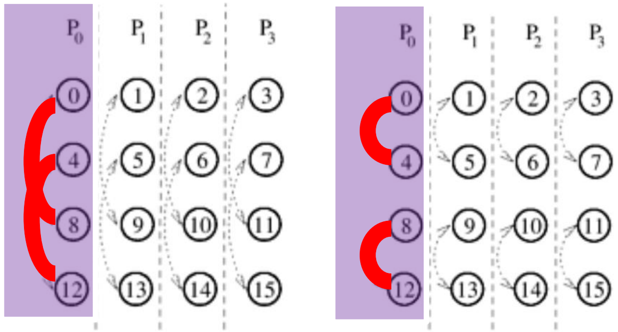
(2) Transpose Algorithm





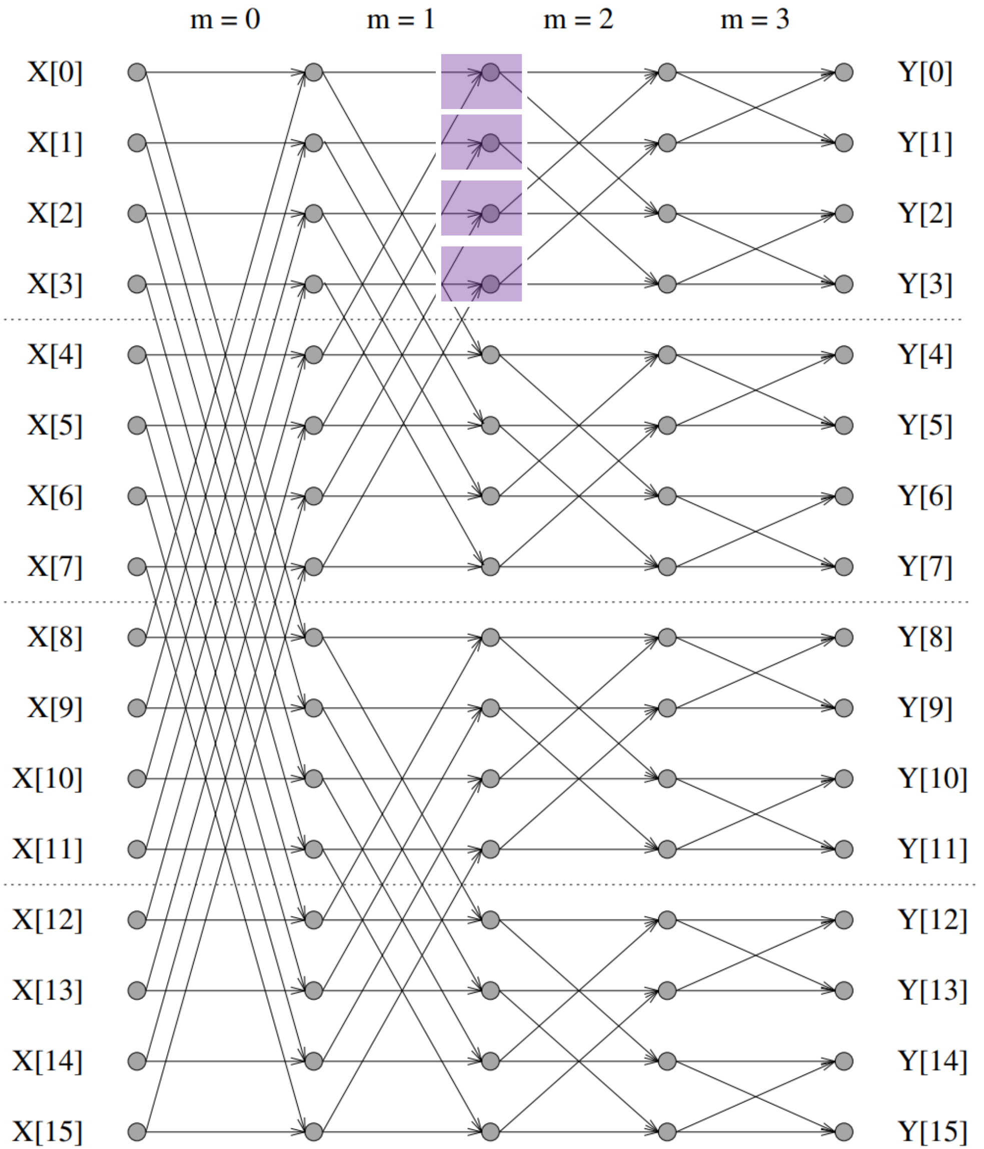
(2) Transpose Algorithm

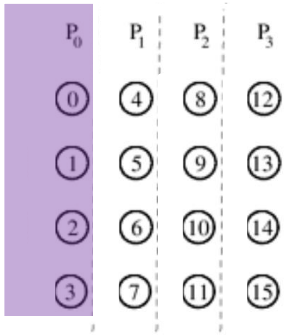




__Step 1__: Local FFT for each column (on same processor)

(2) Transpose Algorithm

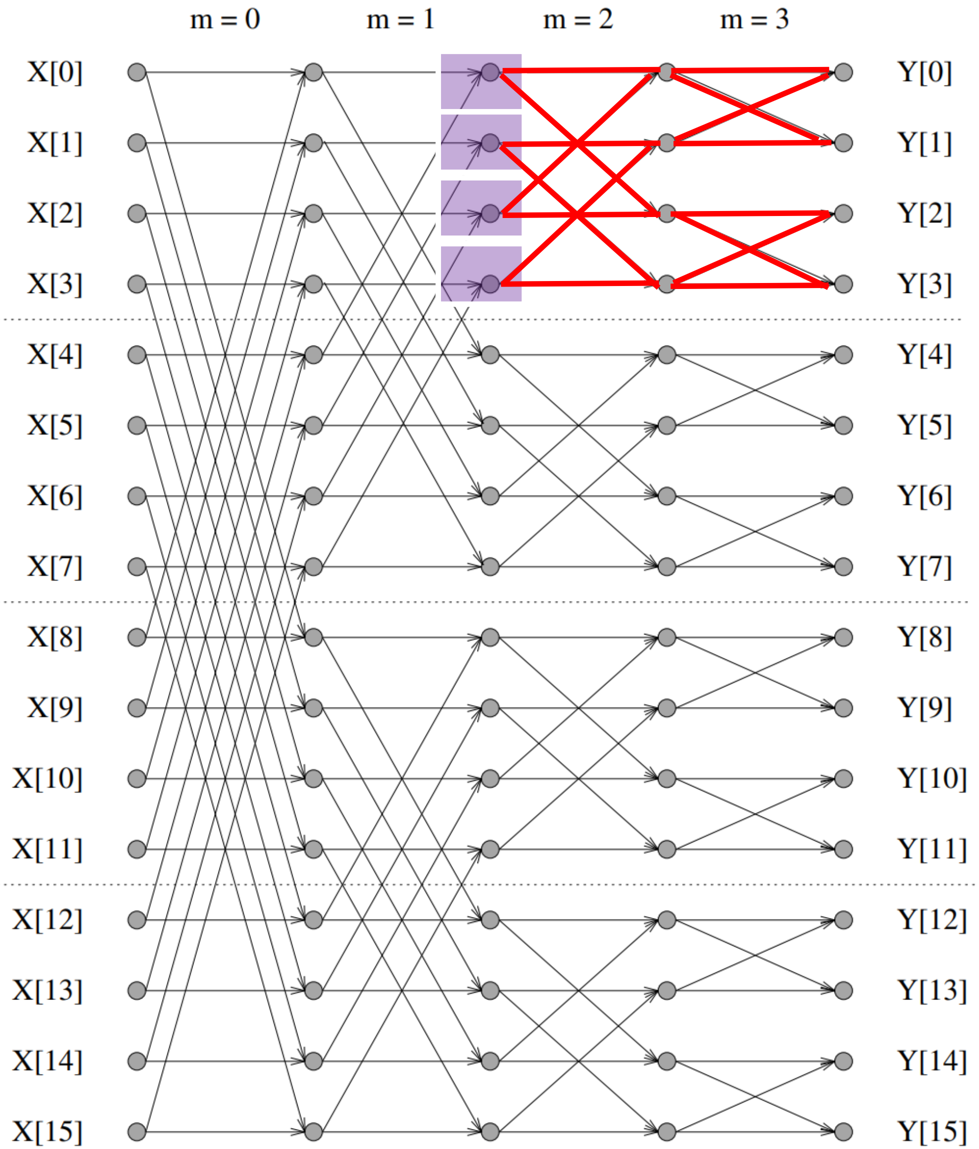


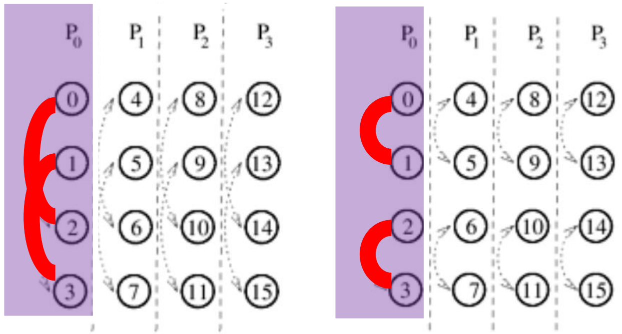


Step 1: Local FFT for each column (on same processor)

Step 2: Transpose matrix (all-to-all personalized comm)

(2) Transpose Algorithm





__Step 1__: Local FFT for each column (on same processor)

__Step 2__: Transpose matrix (all-to-all personalized comm)

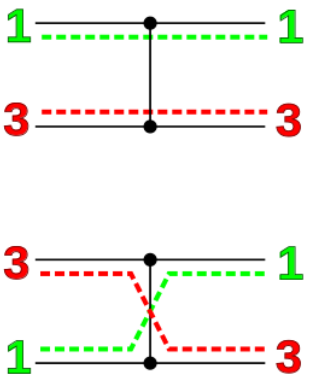
__Step 3__: Local FFT for each column (on same processor)

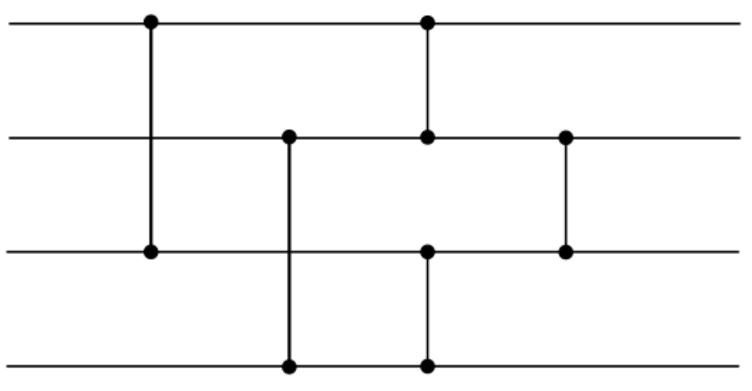
Sorting Algorithms

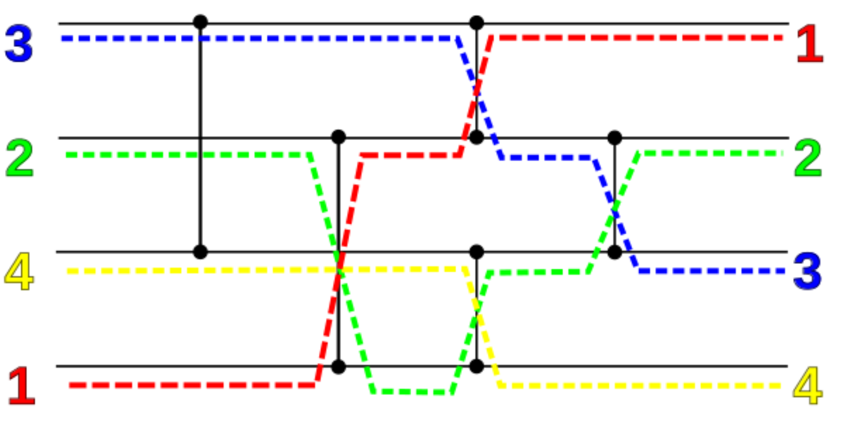
- A sorting algorithm arranges a list of n numbers or items in ascending or descending order --- a very important procedure in scientific computing.
- We have seen previously quicksort and mergesort in shared-memory architectures.
- In this class, we discuss three other sorting algorithms and their parallel implementations:
  1) Bitonic Sort;
  2) Brick Sort;
  3) Shear Sort.

Sorting Networks

- A sorting network sorts a fixed number of input values using a network of comparators connected by wires.





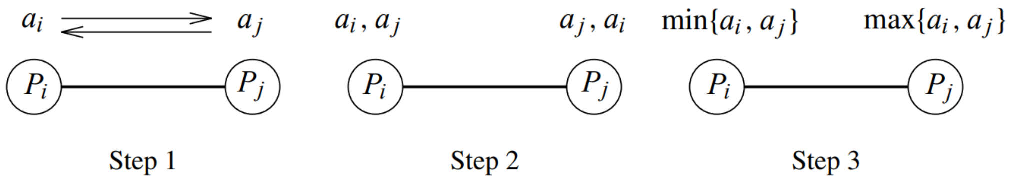


Why is this sorting network able to sort any four input values in ascending order?

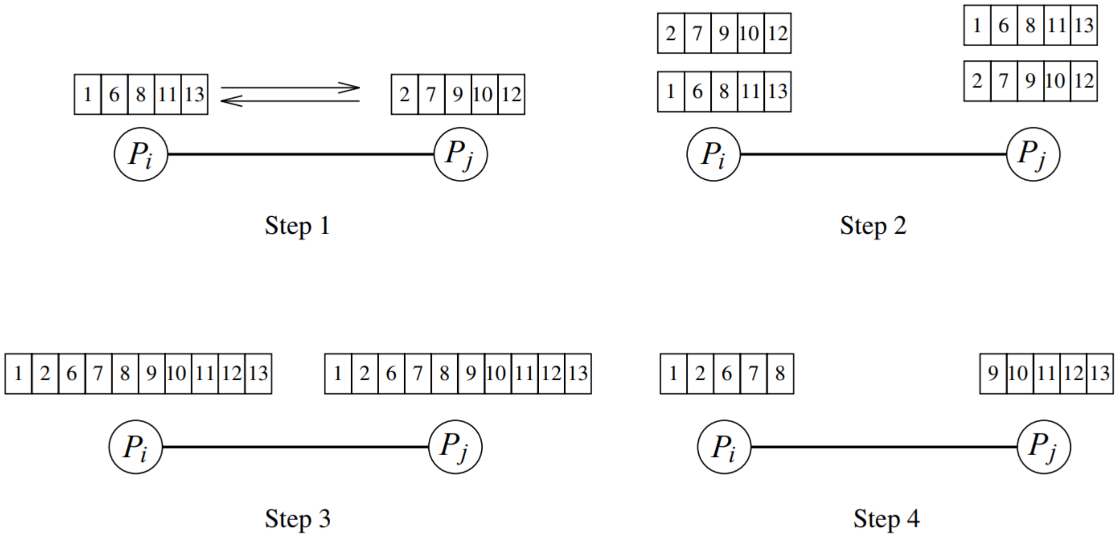
Figure source: https://en.wikipedia.org/wiki/Sorting_network

Basic Comparison Operations in Parallel

- **Compare-Exchange** (one element per process)

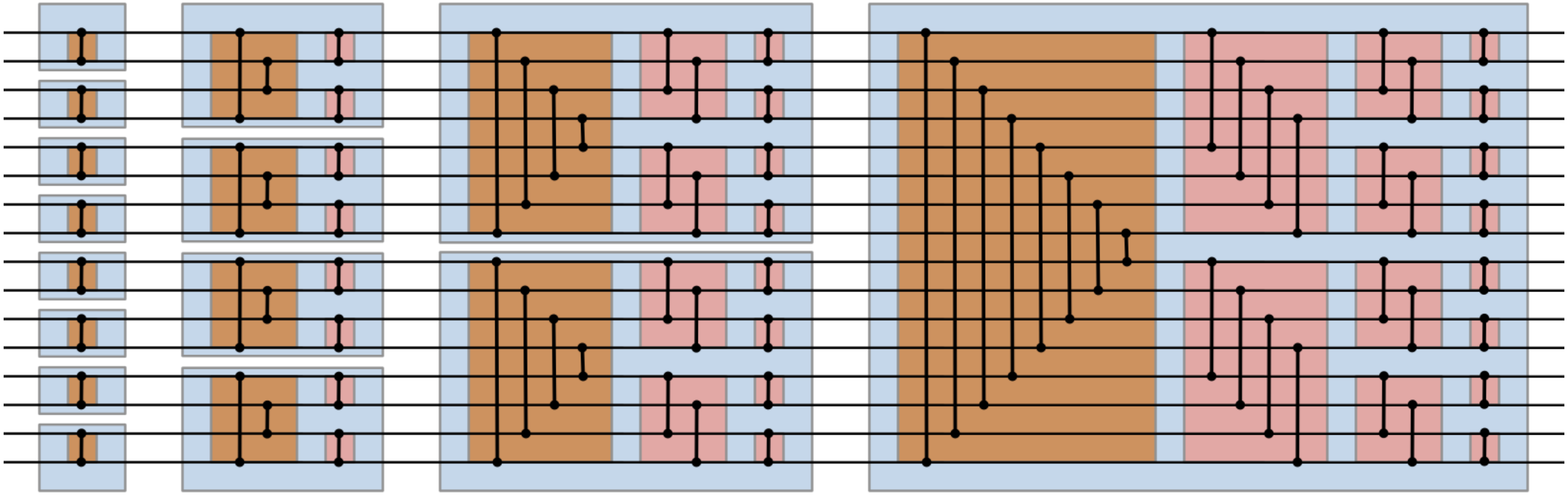


- **Compare-Split** (multiple elements per process)



(1) Bitonic Sort

- **Bitonic Sorting Network**
  - Constructed recursively using divide-and-conquer for any number of inputs n that is a power of 2 (*read the reference materials on details of its construction*).

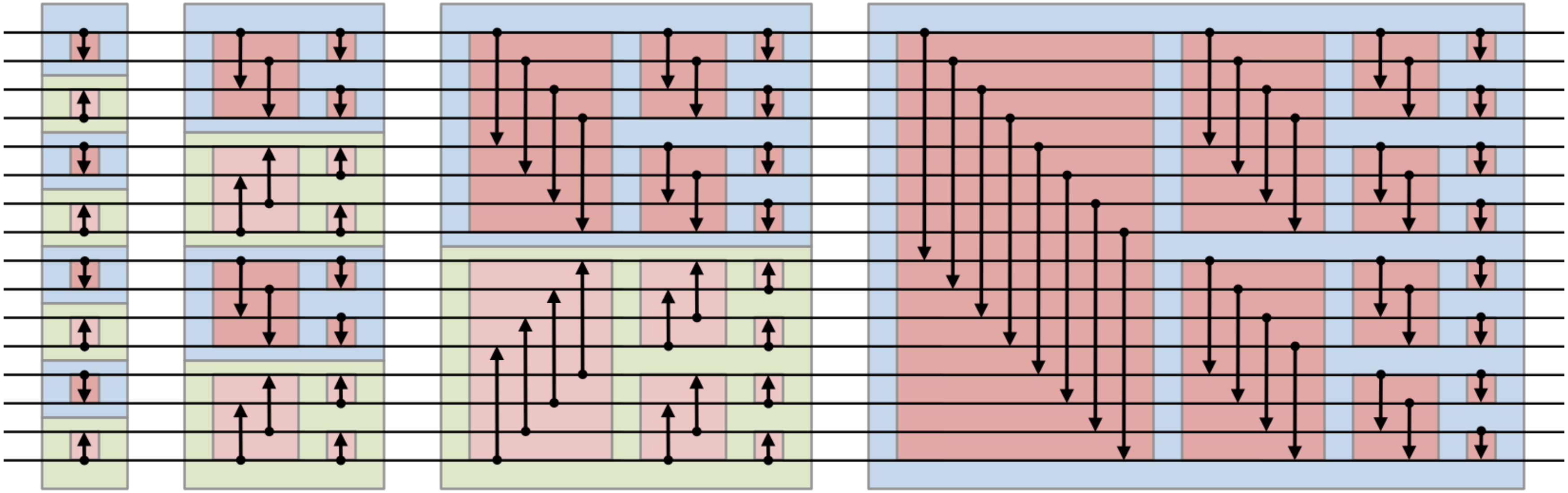


Standard form: *the larger number of a comparator always goes down.*

Figure source: https://en.wikipedia.org/wiki/Bitonic_sorter

(1) Bitonic Sort

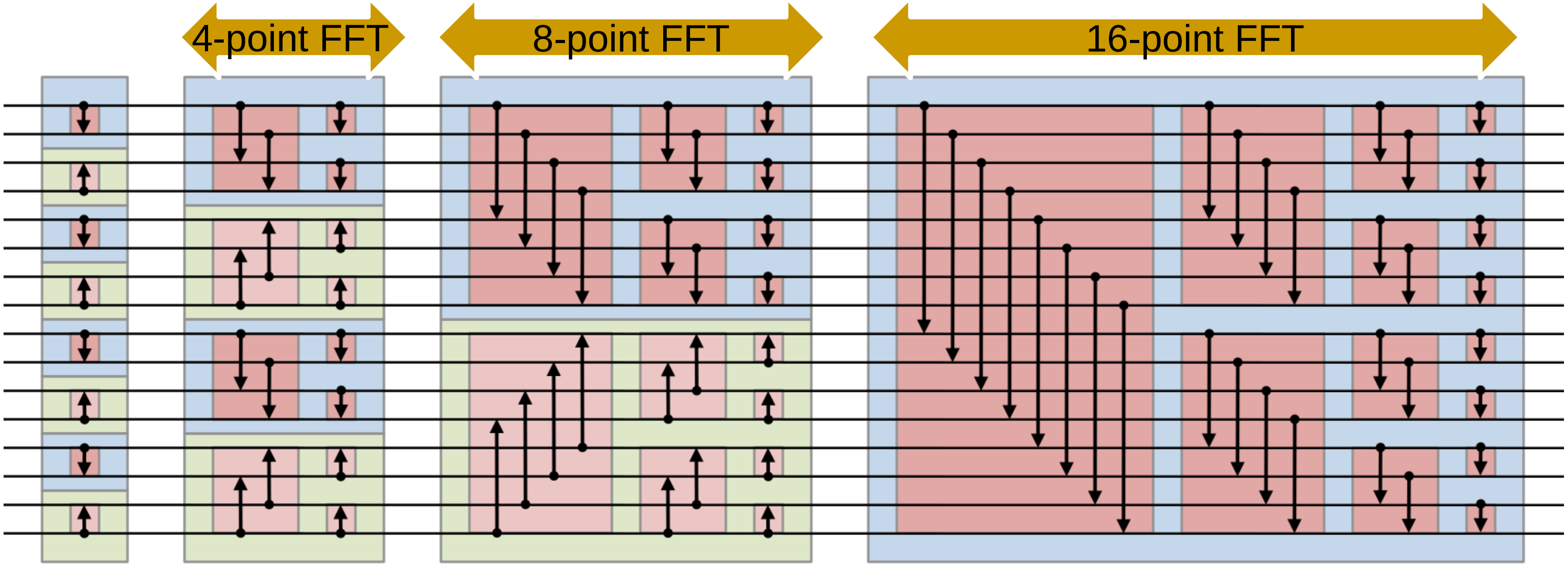
- **Bitonic Sorting Network**
  - Constructed recursively using divide-and-conquer for any number of inputs n that is a power of 2 (*read the reference materials on details of its construction*).



Non-standard form: *the larger number of a comparator goes to point of arrow.*

(1) Bitonic Sort in Parallel

Observe that a bitonic sorting network (non-standard) has multiple stages of computations with FFT-like structures.



(1) Bitonic Sort in Parallel

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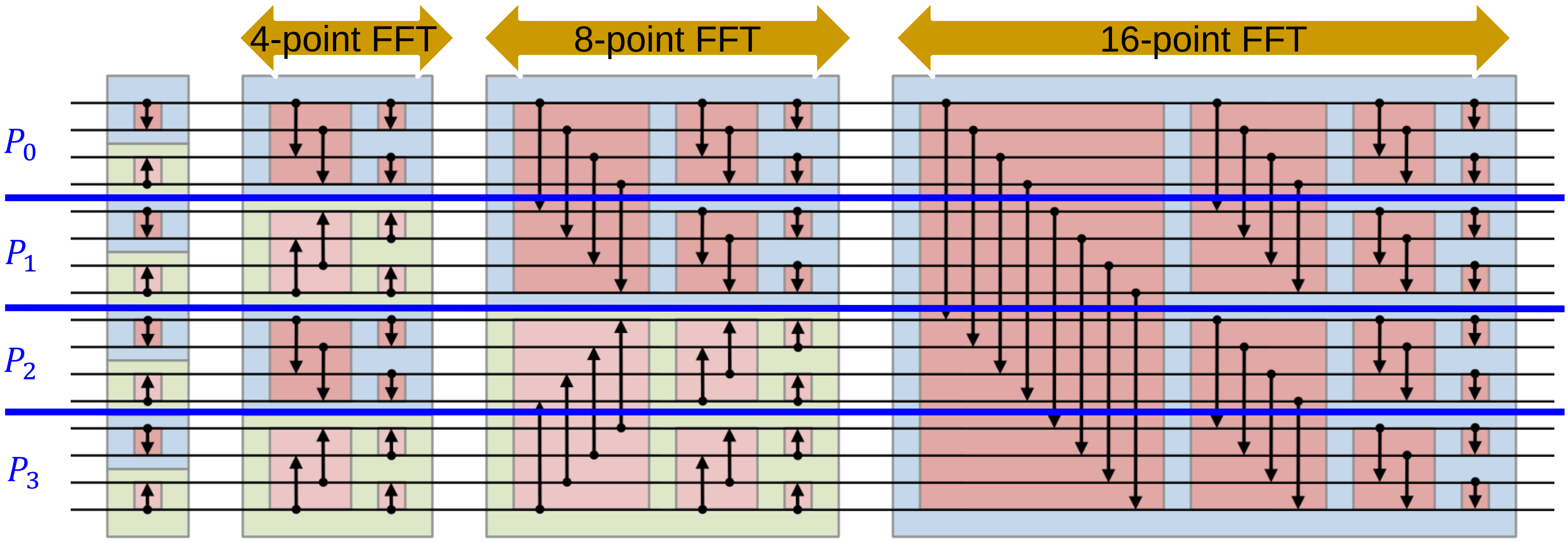
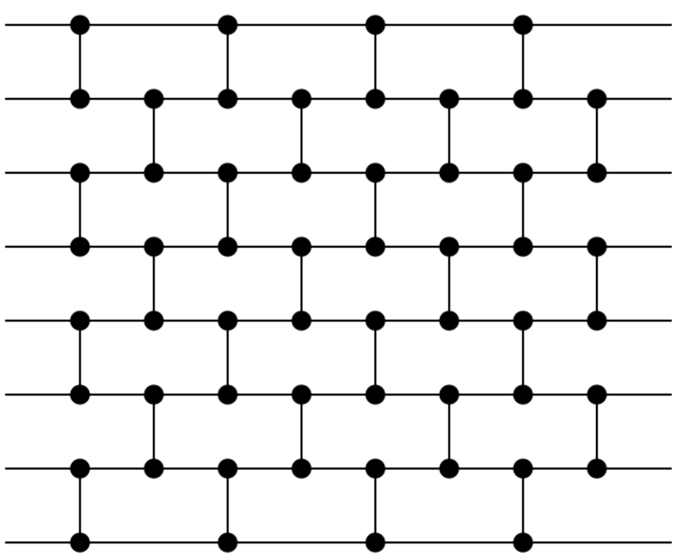


Parallel algorithms similar to Binary-Exchange for FFT can be implemented for Bitonic Sort.

- *1D Block distribution* of data, and comparisons across two processors can be done via *compare-exchange* operations.

(2) Brick Sort

- **Odd-Even Sorting Network**
  - Constructed by n levels of comparators connected in a "brick-like" pattern, with alternating odd and even sorting steps (it's also called *Odd-Even Transposition Sort*).



Unsorted array: 2, 1, 4, 9, 5, 3, 6, 10

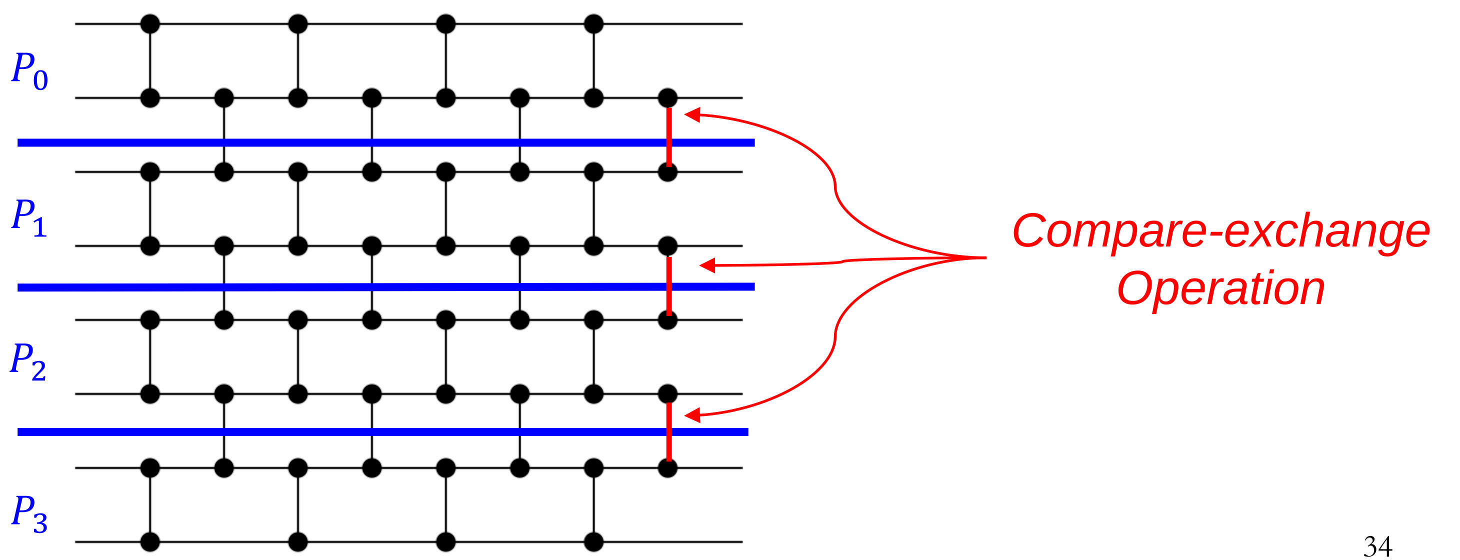
Step 1(odd):	2	1	4	9	5	3	6	10
Step 2(even):	1	2	4	9	3	5	6	10
Step 3(odd):	1	2	4	3	9	5	6	10
Step 4(even):	1	2	3	4	5	9	6	10
Step 5(odd):	1	2	3	4	5	6	9	10
Step 6(even):	1	2	3	4	5	6	9	10
Step 7(odd):	1	2	3	4	5	6	9	10
Step 8(even):	1	2	3	4	5	6	9	10

Sorted array: 1, 2, 3, 4, 5, 6, 9, 10

Figure source: https://www.geeksforgeeks.org/odd-even-transposition-sort-brick-sort-using-pthreads/

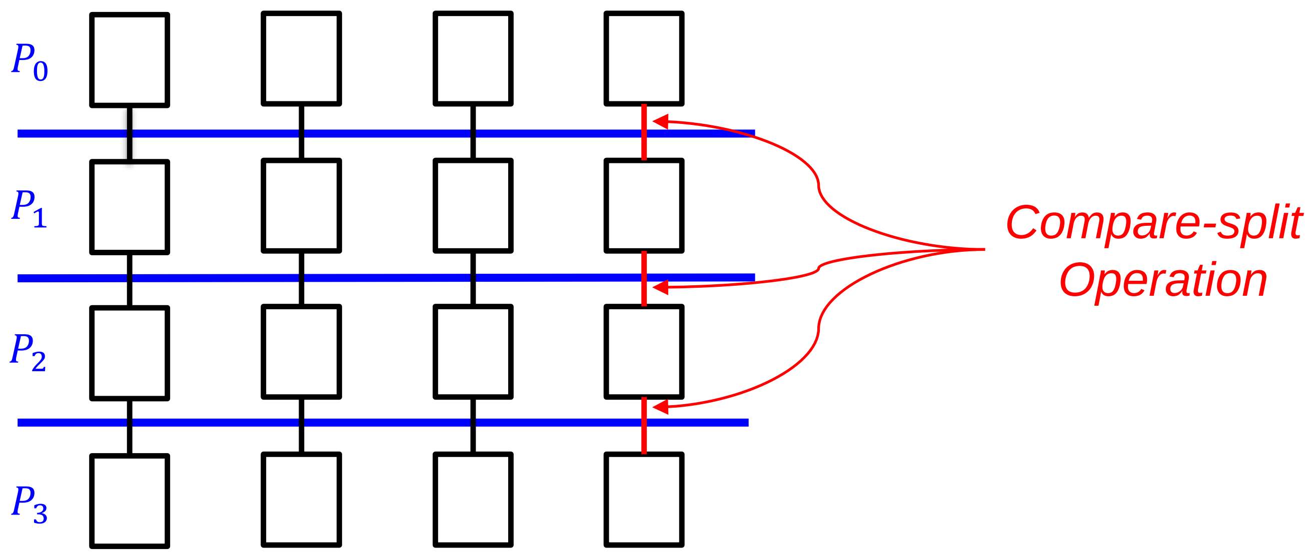
(2) Brick Sort in Parallel

- **Parallel Implementation 1**:
  - 1D Block distribution;
  - Follow exactly the same pattern of an n-step odd-even sorting network;
  - Only boundary elements of a processor need communication (done via *compare-exchange*).



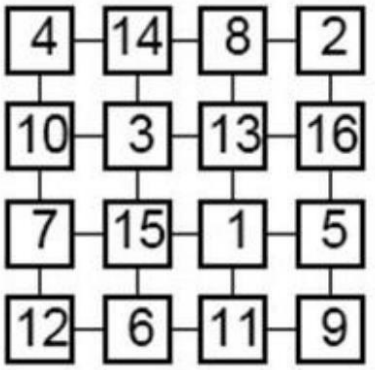
(2) Brick Sort in Parallel

- **Parallel Implementation 2**:
  - 1D Block distribution;
  - Follow the same pattern again, but treating blocks of elements together ➔ P steps instead of n;
  - Entire block of elements of a processor need to be communicated and compared (done via *compare-split*).



(3) Shear Sort

- Algorithm works in 2D:
  - A list of n numbers initially arranged in a $\sqrt{n} \times \sqrt{n}$ matrix;
  - For step $k = 1, 2, \ldots, \lg n + 1$:
    - If k is odd, sort odd rows in *ascending* order and sort even rows in *descending* order;
    - If k is even, sort all columns in *ascending* order;
  - The final list will be sorted in 2D snake-like order.



Original placement of numbers

Shear Sort

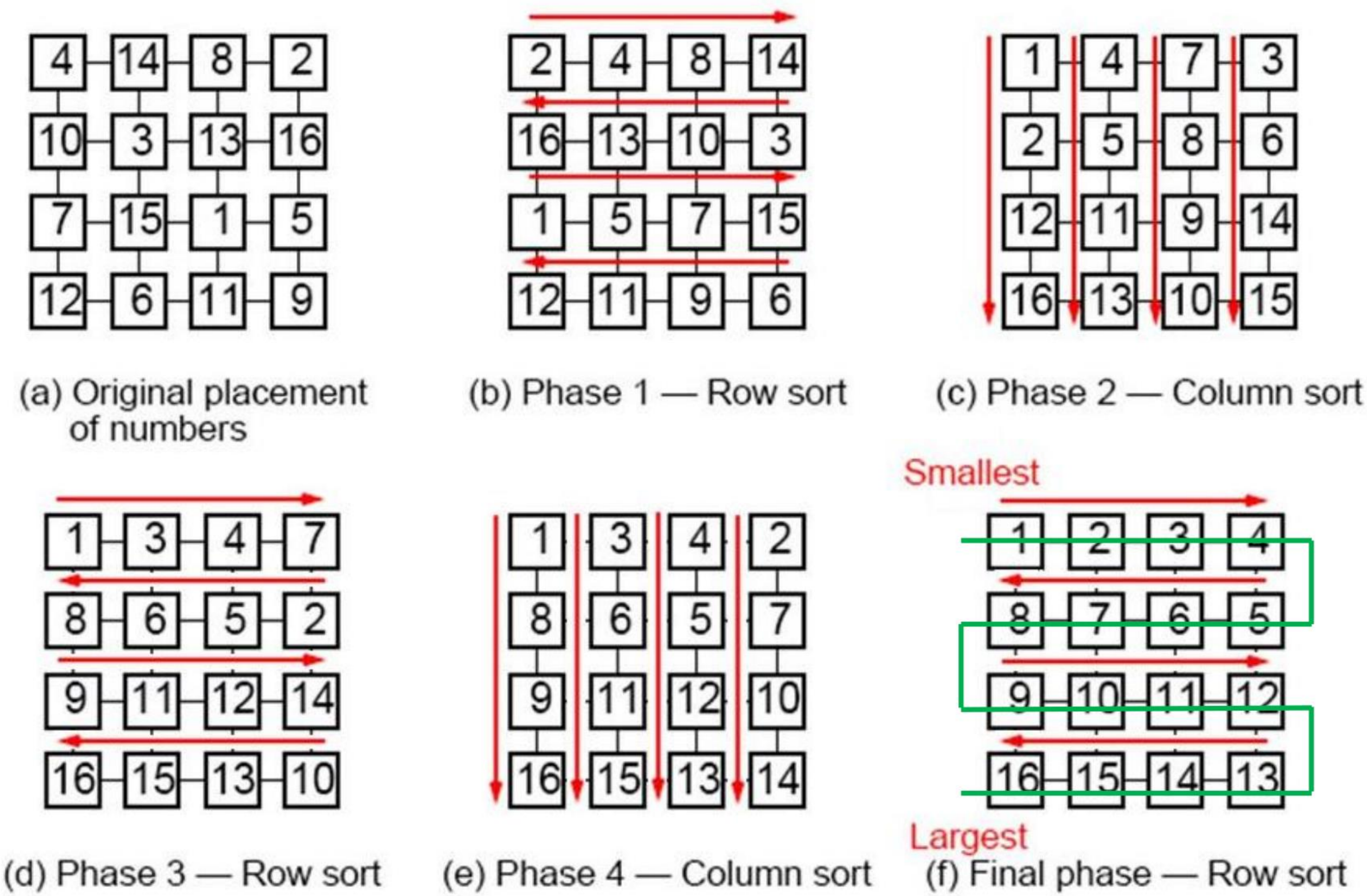
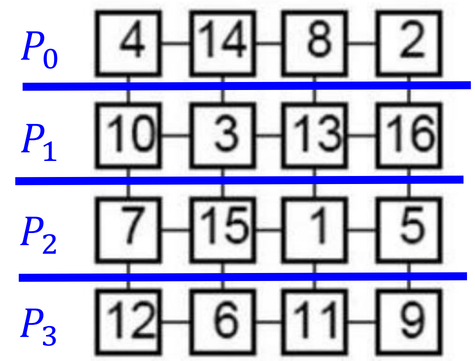


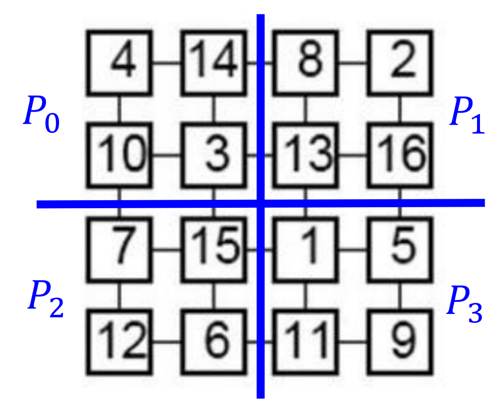
Figure source: https://slideplayer.com/

Shear Sort in Parallel

- **1D Block Implementation:**
  - Row-sorting can be done *locally* on each processor;
  - Column-sorting can be done across processors with *Brick Sort* for each column.



- **2D Block Implementation:**
  - Both row-sorting and column-sorting can be done with *Brick Sort* across multiple processor groups (rows and columns).



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