# Japan-Korea HPC Winter School Parallel Numerical Algorithm 2

Daisuke Takahashi
daisuke@cs.tsukuba.ac.jp
Center for Computational Sciences
University of Tsukuba

# Contents of Lecture

- Fast Fourier Transform (FFT)
- Cooley-Tukey FFT and parallelization
- Six-Step FFT and parallelization
- Nine-Step FFT and blocking, parallelization

# Fast Fourier Transform (FFT)

- The fast Fourier transform (FFT) is an algorithm for computing the discrete Fourier transform (DFT).
- Example applications in the scientific field
  - Solution of partial differential equations
  - Convolution, correlation calculations
  - Density function theory in first-principles calculations
- Example applications in the engineering field
  - Spectrum analyzers
  - CT scanners, MRI, and other image processing
  - With the OFDM (orthogonal frequency multiplex modulation) used in digital terrestrial television broadcasting and wireless LAN, FFTs are used in modulation/demodulation processing.

# Discrete Fourier Transform (DFT)

- Discrete Fourier transform (DFT) is given by

$$y(k) = \sum_{j=0}^{n-1} x(j)\omega_n^{jk}$$

$$0 \le k \le n-1,\ \omega_n = e^{-2\pi i/n}$$

# Matrix-based DFT Formulation (1/4)

- When $n = 4$, a DFT can be computed as follows:

$$y(0) = x(0)\omega^0 + x(1)\omega^0 + x(2)\omega^0 + x(3)\omega^0$$
$$y(1) = x(0)\omega^0 + x(1)\omega^1 + x(2)\omega^2 + x(3)\omega^3$$
$$y(2) = x(0)\omega^0 + x(1)\omega^2 + x(2)\omega^4 + x(3)\omega^6$$
$$y(3) = x(0)\omega^0 + x(1)\omega^3 + x(2)\omega^6 + x(3)\omega^9$$

# Matrix-based DFT Formulation (2/4)

- Can be expressed more simply when a matrix is used.

$$\begin{bmatrix} y(0) \\ y(1) \\ y(2) \\ y(3) \end{bmatrix} = \begin{bmatrix} \omega^0 & \omega^0 & \omega^0 & \omega^0 \\ \omega^0 & \omega^1 & \omega^2 & \omega^3 \\ \omega^0 & \omega^2 & \omega^4 & \omega^6 \\ \omega^0 & \omega^3 & \omega^6 & \omega^9 \end{bmatrix}$$

- Requires $n^2$ complex multiplications and $n(n-1)$ complex additions.

# Matrix-based DFT Formulation (3/4)

- Using the relation $\omega_n^{jk} = \omega_n^{jk \bmod n}$, can be written as follows:

$$\begin{bmatrix} y(0) \\ y(1) \\ y(2) \\ y(3) \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & \omega^1 & \omega^2 & \omega^3 \\ 1 & \omega^2 & \omega^0 & \omega^2 \\ 1 & \omega^3 & \omega^2 & \omega^1 \end{bmatrix}$$

# Matrix-based DFT Formulation (4/4)

- Decomposition of the matrix allows the number of multiplications to be reduced.

$$\begin{bmatrix} y(0) \\ y(2) \\ y(1) \\ y(3) \end{bmatrix} = \begin{bmatrix} 1 & \omega^0 & 0 & 0 \\ 1 & \omega^2 & 0 & 0 \\ 0 & 0 & 1 & \omega^1 \\ 0 & 0 & 1 & \omega^3 \end{bmatrix} \begin{bmatrix} 1 & 0 & \omega^0 & 0 \\ 0 & 1 & 0 & \omega^0 \\ 1 & 0 & \omega^2 & 0 \\ 0 & 1 & 0 & \omega^2 \end{bmatrix} \begin{bmatrix} x(0) \\ x(1) \\ x(2) \\ x(3) \end{bmatrix}$$

Performing this recursively, the amount of calculations can be reduced to $O(n \log n)$.
(The number of data must be a composite number.)

# Comparison of the Amount of Operations Needed for Calculating DFTs and FFTs

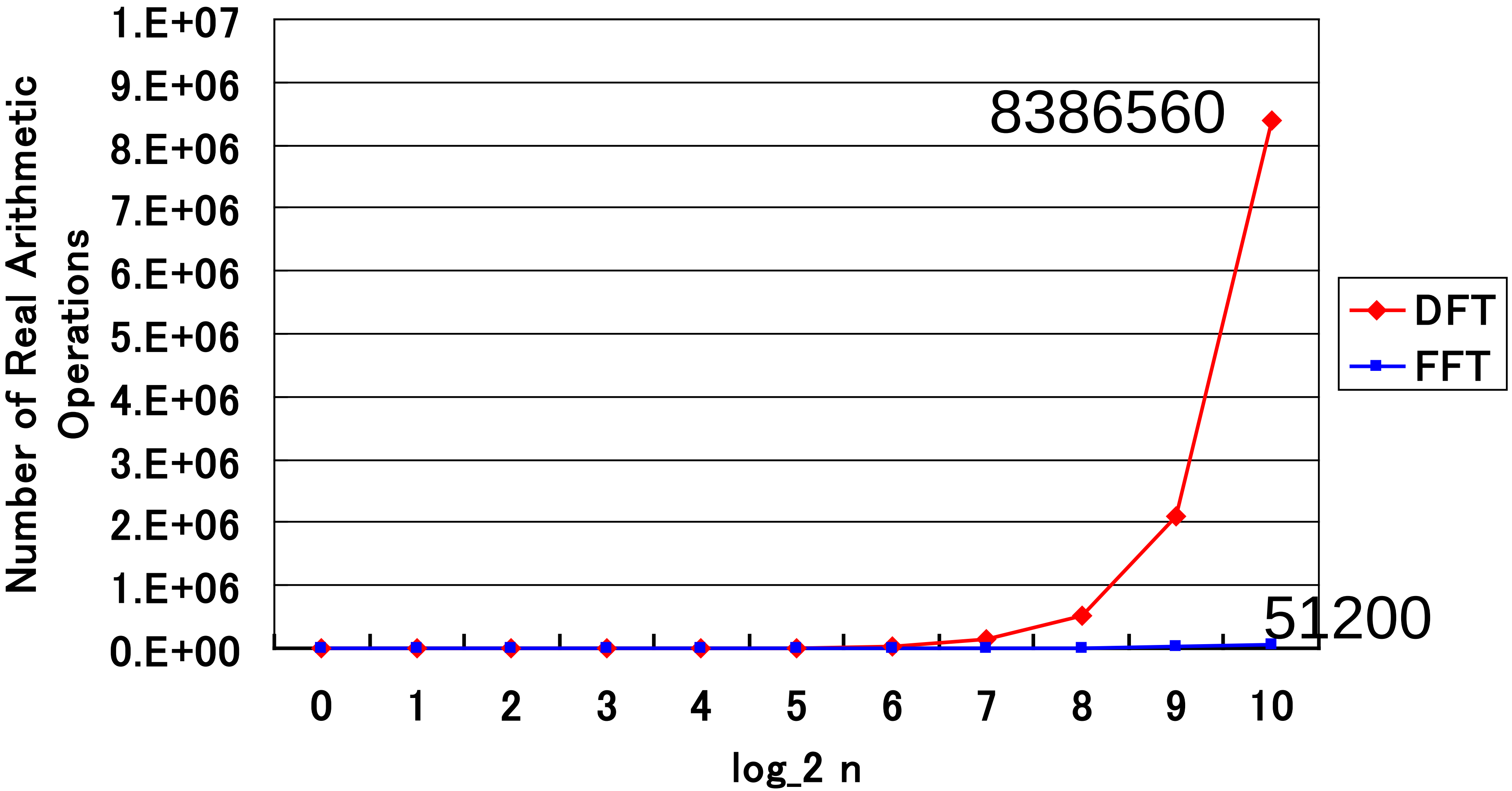
- Number of real operations for DFTs

$$T_{DFT} = 8n^2 - 2n$$

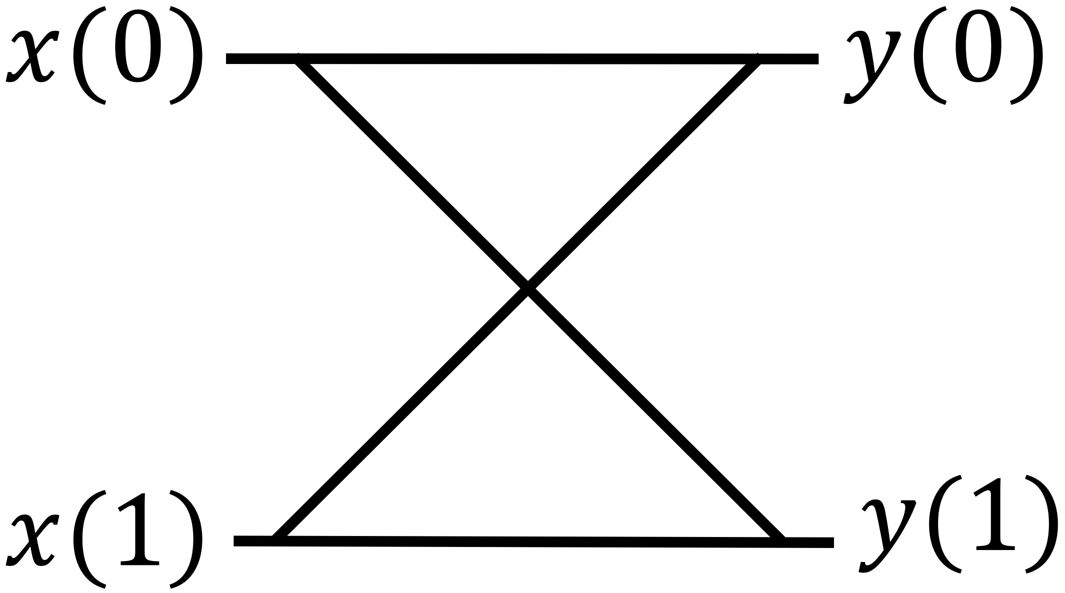
- Number of real operations for FFTs (When $n$ is a power of two)

$$T_{FFT} = 5n \log_2 n$$

# Comparison of the Amount of Operations Needed for Calculating DFTs and FFTs



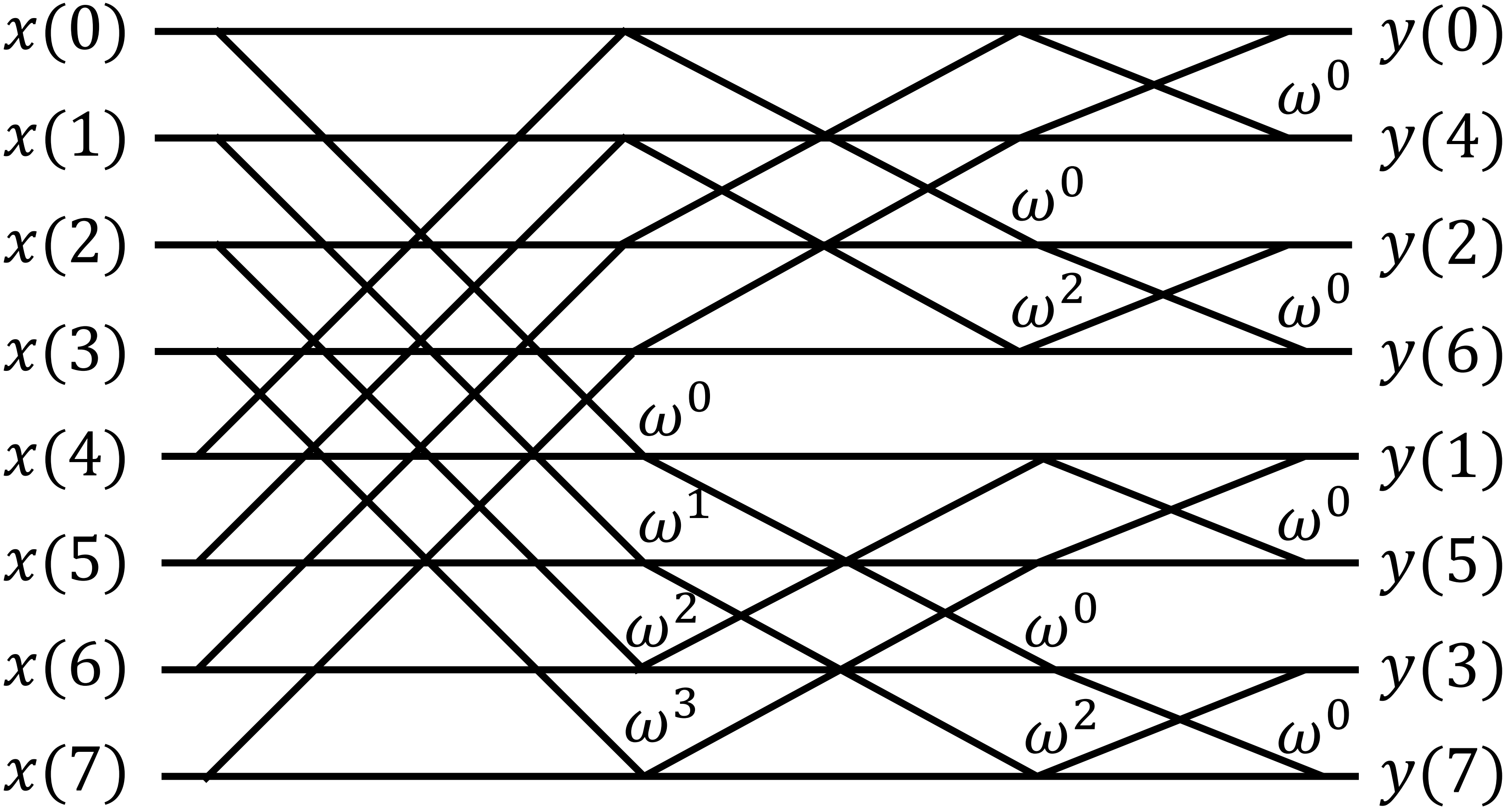
# Butterfly Operation




$$y(0) = x(0) + x(1)$$

$$y(1) = \omega\{x(0) + x(1)\}$$

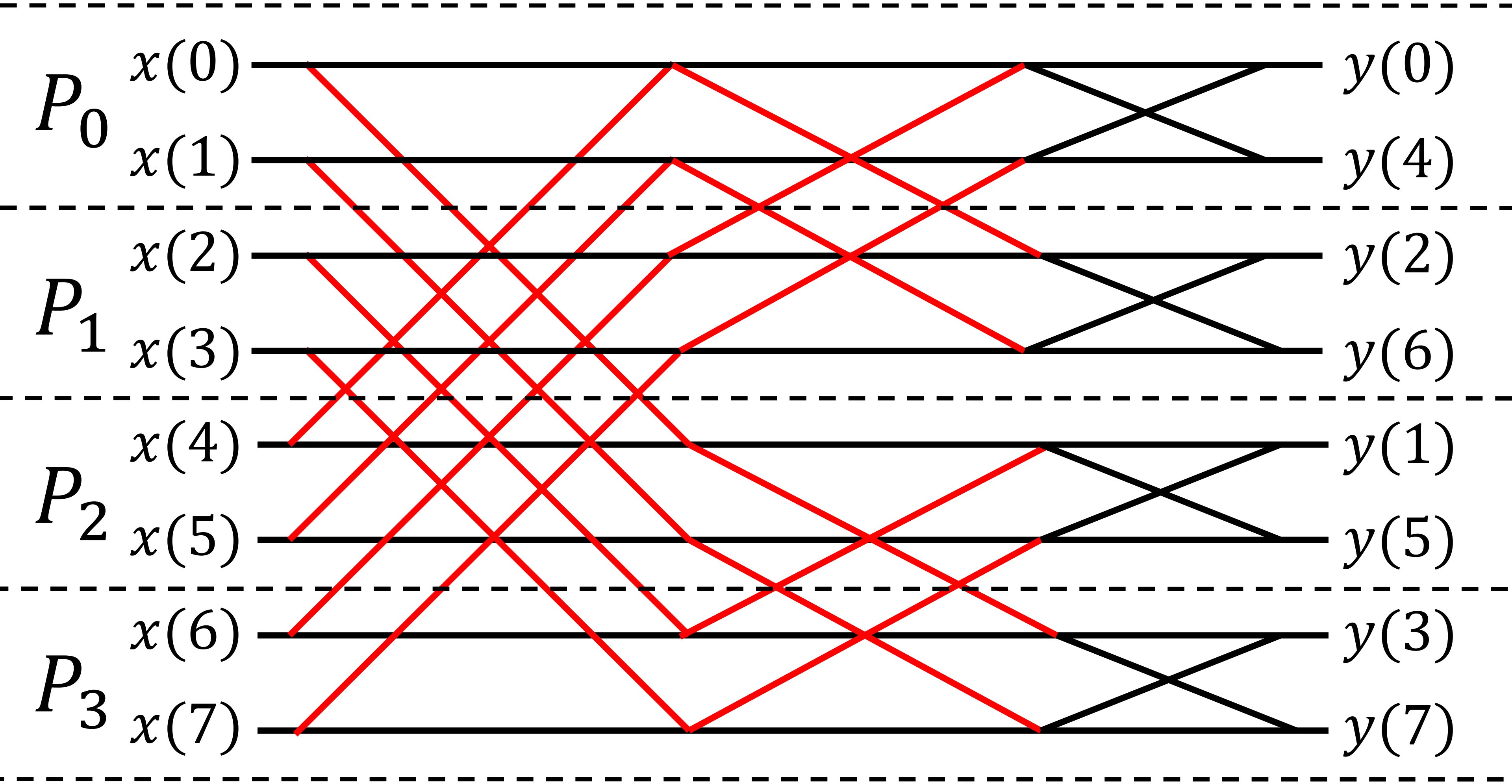
# Cooley-Tukey FFT Signal Flow Diagram



# Example of FFT Kernel

```
      SUBROUTINE FFT2(A,B,W,M,L)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION A(2,M,L,*),B(2,M,2,*),W(2,*)
C
      DO J=1,L
        WR=W(1,J)
        WI=W(2,J)
        DO I=1,M
          B(1,I,1,J)=A(1,I,J,1)+A(1,I,J,2)
          B(2,I,1,J)=A(2,I,J,1)+A(2,I,J,2)
          B(1,I,2,J)=WR*(A(1,I,J,1)-A(1,I,J,2))-WI*(A(2,I,J,1)-A(2,I,J,2))
          B(2,I,2,J)=WR*(A(2,I,J,1)-A(2,I,J,2))+WI*(A(1,I,J,1)-A(1,I,J,2))
        END DO
      END DO
      RETURN
      END
```

# Parallelization of Cooley-Tukey FFT



# Amount of Communication with Parallel Cooley-Tukey FFT

- If $n$ is the number of nodes in a parallel Cooley-Tukey FFT, $\log_2 P$ stage communication is required.
- Because $(n/P)$ double-precision complex number data is communicated (MPI_Send, MPI_Recv) at each stage, the total amount of communication is as follows:

$$T_{Cooley-Tukey} = \frac{16n}{P} \log_2 P \ \text{(bytes)}$$

# FFT Algorithm for $n = n_1 n_2$

- Given by $n = n_1 n_2$

$$j = j_1 + j_2 n_1,\ \ j_1 = 0, 1, \dots, n_1 - 1,\ j_2 = 0, 1, \dots, n_2 - 1$$
$$k = k_2 + k_1 n_2,\ k_1 = 0, 1, \dots, n_1 - 1,\ k_2 = 0, 1, \dots, n_2 - 1$$

- Using the above expression, the DFT formulation can be rewritten as follows:

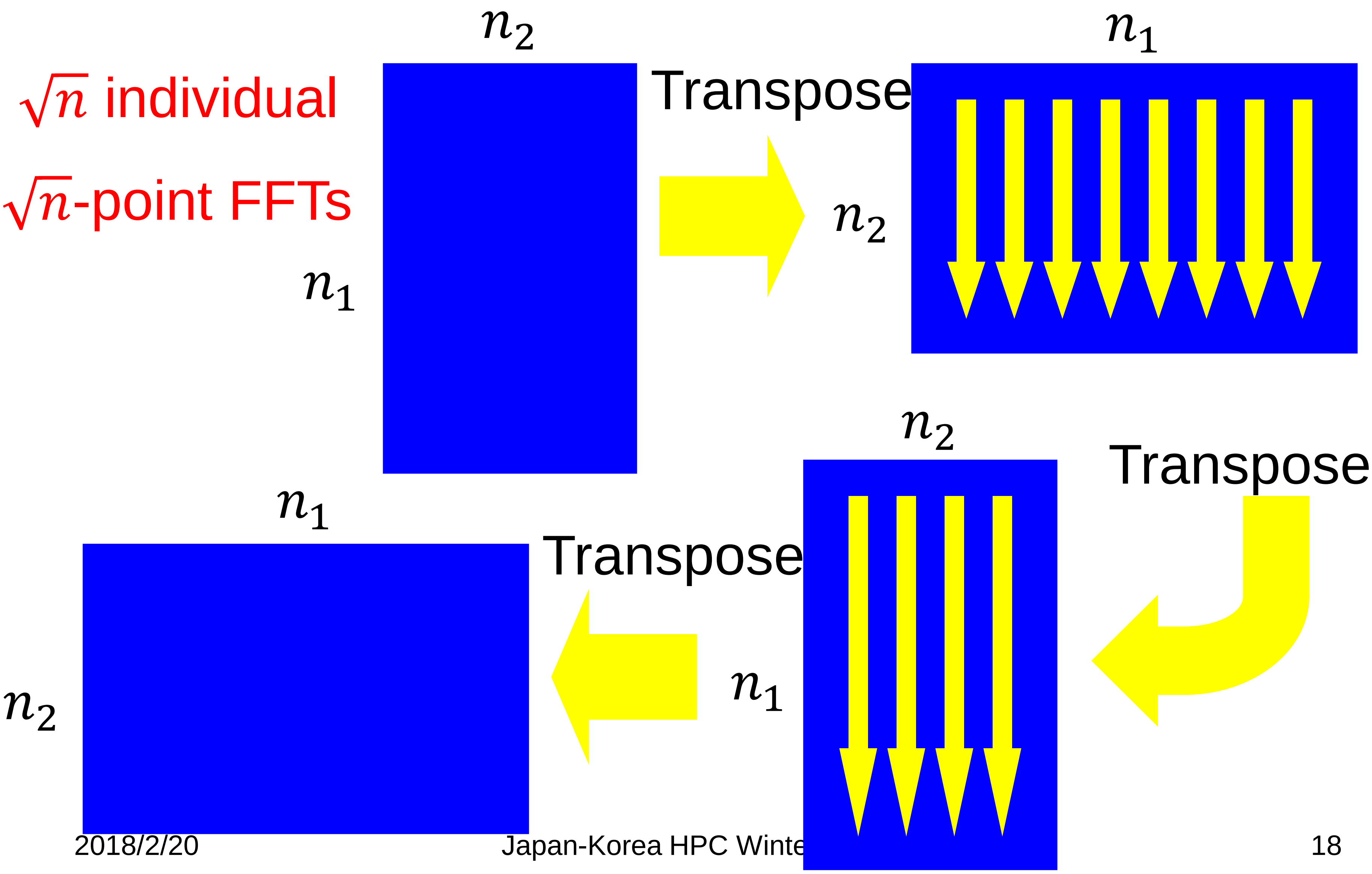
$$y(k_2, k_1) = \sum_{j_1=0}^{n_1-1} \left[ \sum_{j_2=0}^{n_2-1} x(j_1, j_2) \omega_{n_2}^{j_2 k_2}\, \omega_{n_1 n_2}^{j_1 k_2} \right] \omega_{n_1}^{j_1 k_1}$$

- An $n$-point FFT decomposes into an $n_1$-point FFT and an $n_2$-point FFT.

# Six-Step FFT Algorithm

1. Matrix transposition
2. $n_1$ individual $n_2$-point multicolumn FFT
3. Twiddle factor ($\omega_{n_1 n_2}^{j_1 k_2}$) multiplication
4. Matrix transposition
5. $n_2$ individual $n_1$-point multicolumn FFT
6. Matrix transposition

# Six-Step FFT Algorithm

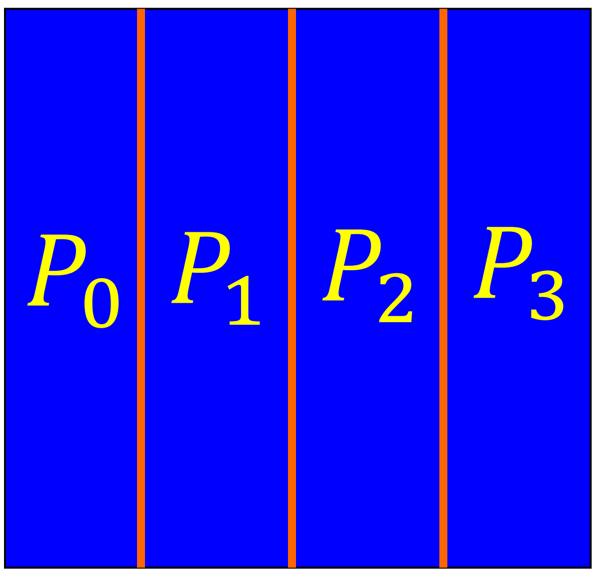


# Six-Step FFT Program Example

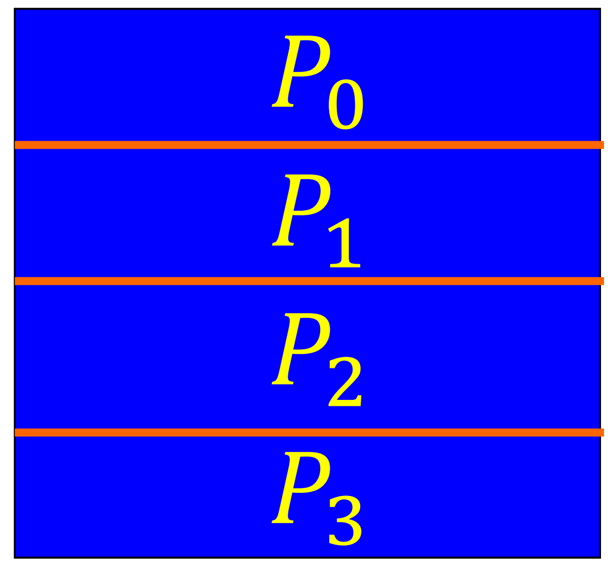
```
      SUBROUTINE FFT(A,B,W,N1,N2)
      COMPLEX*16 A(*),B(*),W(*)
C
      CALL TRANS(A,B,N1,N2)                    Matrix transposition
      DO J=1,N1
        CALL FFT2(B((J-1)*N2+1),N2)            N1 individual N2-point multicolumn FFT
      END DO
      DO I=1,N1*N2
        B(I)=B(I)*W(I)                         Twiddle factor (W) multiplication
      END DO
      CALL TRANS(B,A,N2,N1)                    Matrix transposition
      DO J=1,N2
        CALL FFT2(A((J-1)*N1+1),N1)            N2 individual N1-point multicolumn FFT
      END DO
      CALL TRANS(A,B,N1,N2)                    Matrix transposition
      RETURN
      END
```

# Method for Distribution an Array

- When using MPI for parallelization, memory can be conserved if the array is divided at each node.
- Block distribution
  - Contiguous areas are divided by the number of nodes.




Block distribution divided at each column




Block distribution divided at each row

# Matrix Transposition Using All-to-All Communication (MPI_Alltoall)

| P0 | P1 | P2 | P3 |
|---|---|---|---|
| 0 | 8 | 16 | 24 |
| 1 | 9 | 17 | 25 |
| 2 | 10 | 18 | 26 |
| 3 | 11 | 19 | 27 |
| 4 | 12 | 20 | 28 |
| 5 | 13 | 21 | 29 |
| 6 | 14 | 22 | 30 |
| 7 | 15 | 23 | 31 |

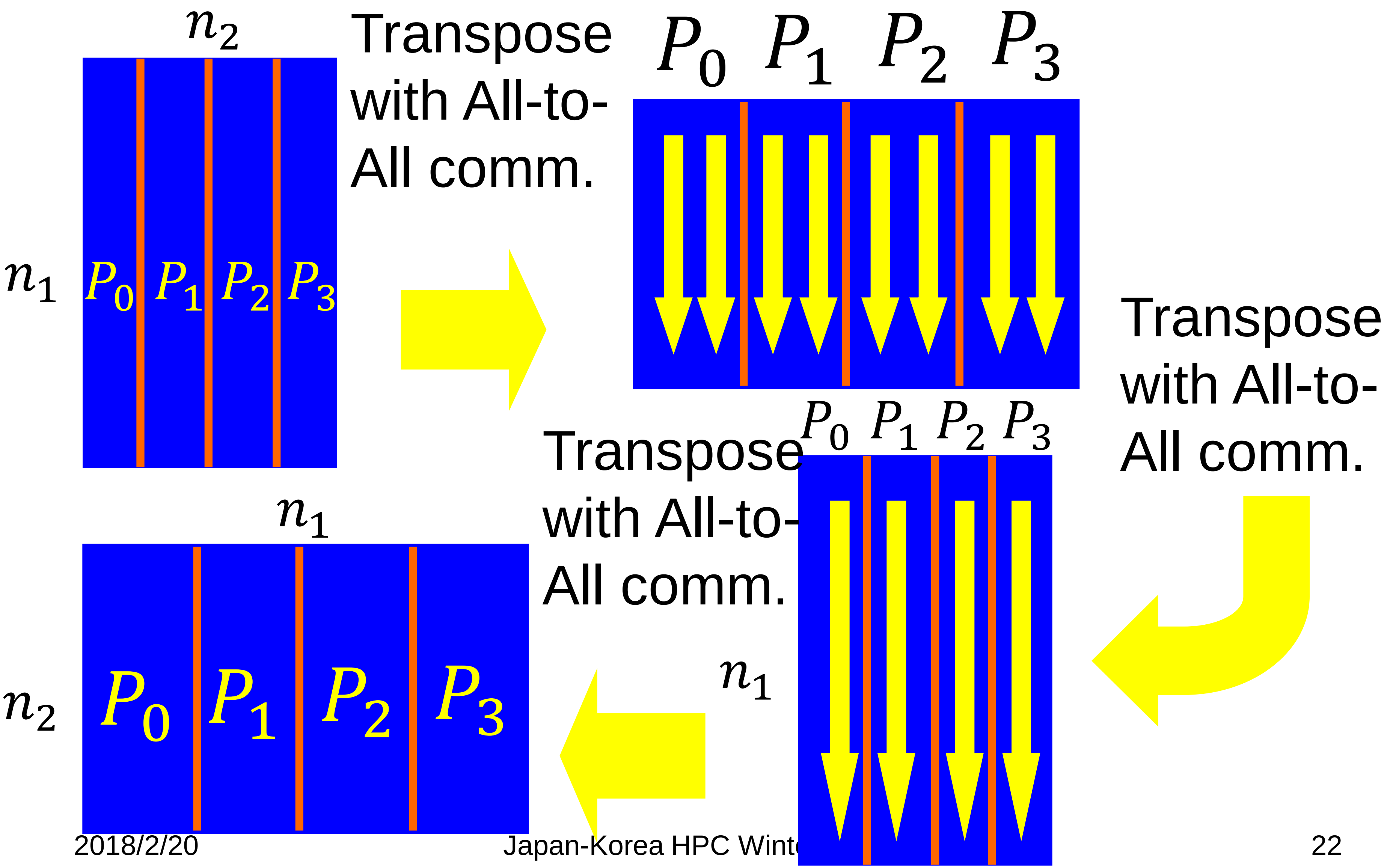
All-to-All Comm.

| P0 | P1 | P2 | P3 |
|---|---|---|---|
| 0 | 2 | 4 | 6 |
| 1 | 3 | 5 | 7 |
| 8 | 10 | 12 | 14 |
| 9 | 11 | 13 | 15 |
| 16 | 18 | 20 | 22 |
| 17 | 19 | 21 | 23 |
| 24 | 26 | 28 | 30 |
| 25 | 27 | 29 | 31 |

Local Transposition

| P0 | P1 | P2 | P3 |
|---|---|---|---|
| 0 1 | 2 3 | 4 5 | 6 7 |
| 8 9 | 10 11 | 12 13 | 14 15 |
| 16 17 | 18 19 | 20 21 | 22 23 |
| 24 25 | 26 27 | 28 29 | 30 31 |

# Parallel Six-Step FFT Algorithm



# Parallel Six-Step FFT Program Example

```
      SUBROUTINE PARAFFT(A,B,W,N1,N2,NPU)
      COMPLEX*16 A(*),B(*),W(*)
C
      CALL PTRANS(A,B,N1,N2,NPU)           Global matrix transposition using MPI_ALLTOALL
      DO J=1,N1/NPU
         CALL FFT2(B((J-1)*N2+1),N2)       (N1/NPU) individual N2-point multicolumn FFT
      END DO
      DO I=1,(N1*N2)/NPU
         B(I)=B(I)*W(I)                    Twiddle factor (W) multiplication
      END DO
      CALL PTRANS(B,A,N2,N1,NPU)           Global matrix transposition using MPI_ALLTOALL
      DO J=1,N2/NPU
        CALL FFT2(A((J-1)*N1+1),N1)        (N2/NPU) individual N1-point multicolumn FFT
      END DO
      CALL PTRANS(A,B,N1,N2,NPU)           Global matrix transposition using MPI_ALLTOALL
      RETURN
      END
```

# Amount of Communication of Parallel Six-Step FFT

- If $P$ is the number of nodes in a parallel six-step FFT, all-to-all communication is required three times.
- With all-to-all communication, because each node sends an $(n/P^2)$ double-precision complex data to $P-1$ nodes, the total amount of communication is as follows:

$$T_{Six-Step} = 3 \cdot (P-1) \cdot \frac{16n}{P^2} \text{ (Bytes)}$$

# Comparison of Amount of Communication with Parallel Cooley-Tukey FFT and Parallel Six-Step FFT

- Amount of communication with parallel Cooley-Tukey FFT

$$T_{Cooley-Tukey} = \frac{16n}{P} \log_2 P$$

- Amount of communication with parallel six-step FFT

$$T_{Six-Step} = 3 \cdot (P - 1) \cdot \frac{16n}{P^2}$$

- Of these two methods, when $P > 8$, the parallel six-step FFT will have the lower amount of communication.

# Problems with the Six-Step FFT

- In a multicolumn FFT, when $\sqrt{n}$-point each column FFT exceeds the cache size, the performance will decrease significantly.
- A distributed-memory parallel computer, when processing a large-size FFT ($2^{24}$ points or more, for example), will be unable to achieve high performance.

# 3-D Formulation

- For very large FFTs, we should switch a 3-D formulation.
- If $n$ has factors $n_1$, $n_2$ and $n_3$ then

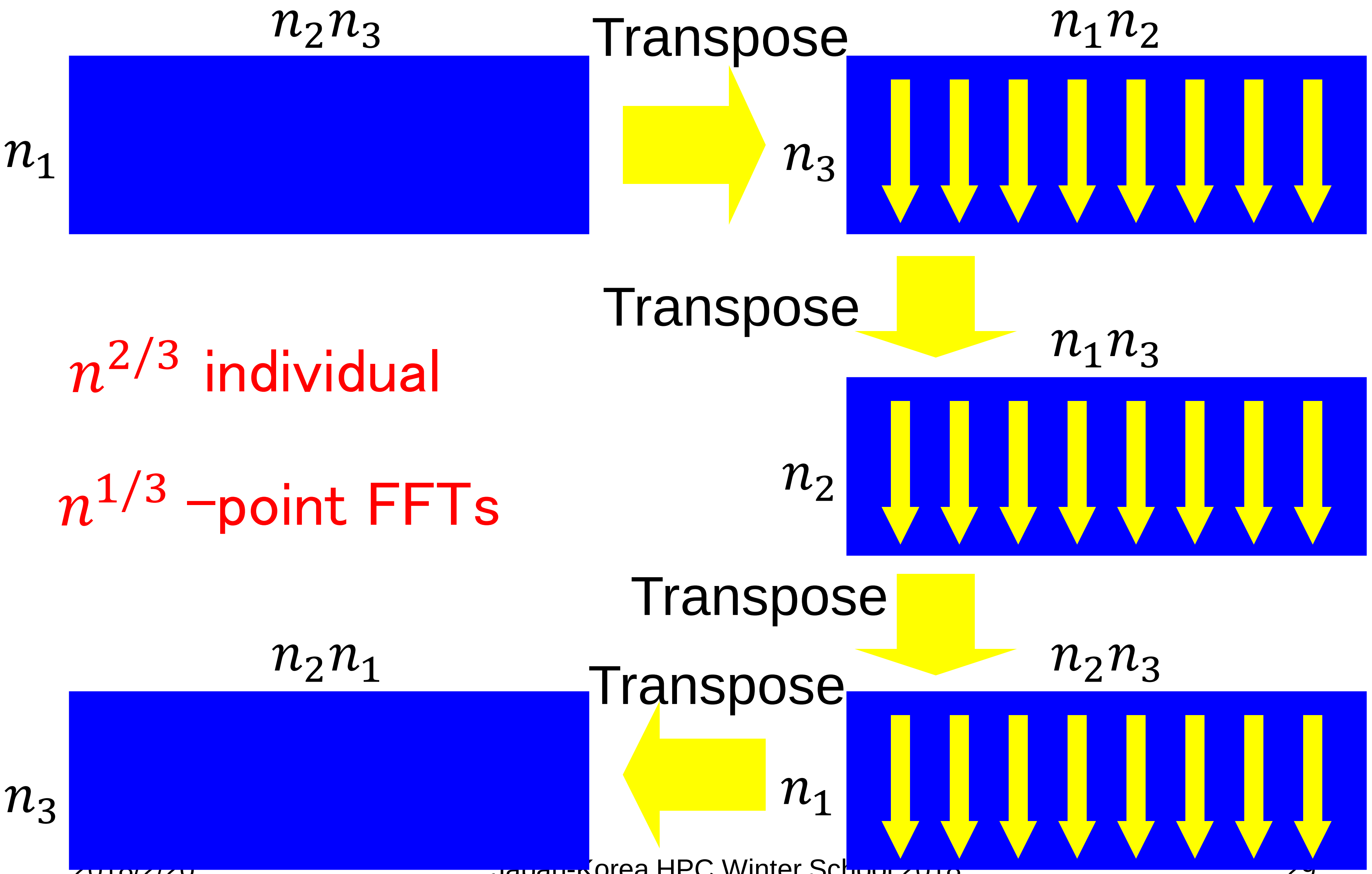
$$y(k_3,k_2,k_1)=\sum_{j_1=0}^{n_1-1}\sum_{j_2=0}^{n_2-1}\sum_{j_3=0}^{n_3-1}x(j_1,j_2,j_3)$$

$$\omega_{n_3}^{j_3k_3}\omega_{n_2n_3}^{j_2k_3}\omega_{n_2}^{j_2k_2}\omega_{n}^{j_1k_3}\omega_{n_1n_2}^{j_1k_2}\omega_{n_1}^{j_1k_1}$$

# Nine-Step FFT Algorithm

1. Matrix transposition
2. $n_1 n_2$ individual $n_3$-point multicolumn FFT
3. Twiddle factor ($\omega_{n_2 n_3}^{j_2 k_3}$) multiplication
4. Matrix transposition
5. $n_1 n_3$ individual $n_2$-point multicolumn FFT
6. Twiddle factor ($\omega_{n}^{j_1 k_3} \omega_{n_1 n_2}^{j_1 k_2}$) multiplication
7. Matrix transposition
8. $n_2 n_3$ individual $n_1$-point multicolumn FFT
9. Matrix transposition

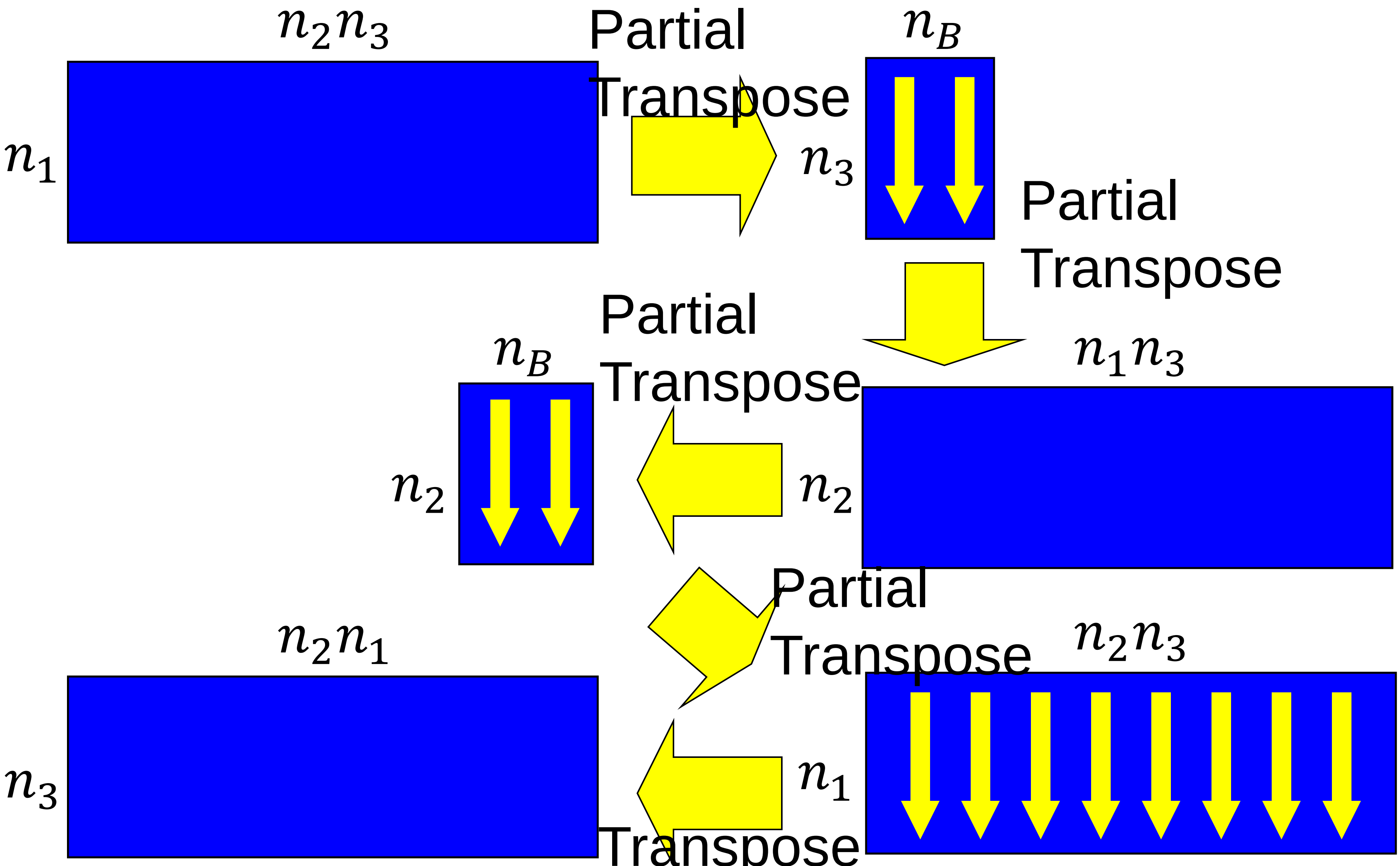
# Nine-Step FFT Algorithm




$n^{2/3}$ individual

$n^{1/3}$ -point FFTs

# Block Nine-Step FFT Algorithm



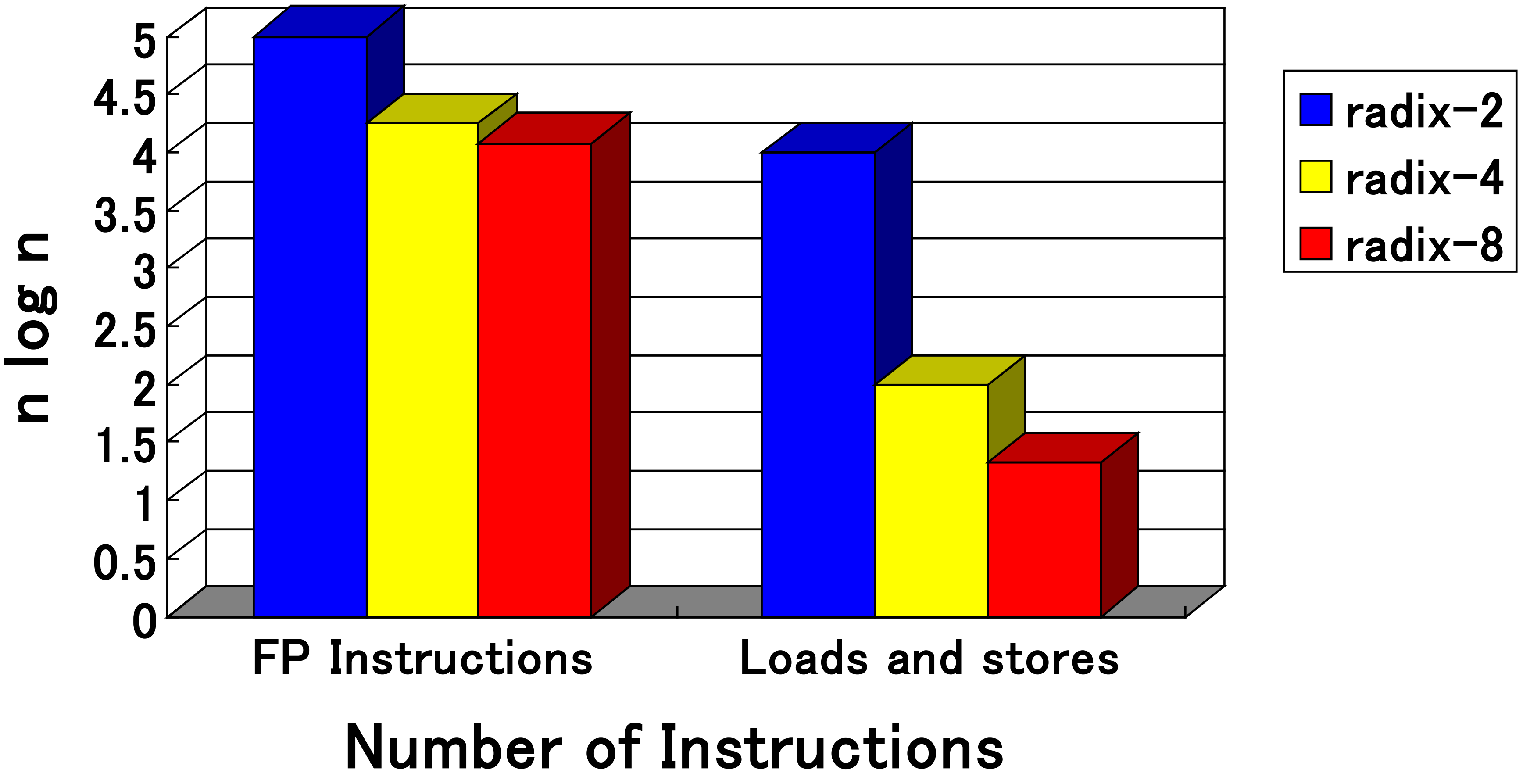
# In-Cache FFT Algorithm

- In a multicolumn FFT, the following can be conceived of as in-cache FFTs, whereby each column FFT is placed in the cache.
  - Cooley-Tukey algorithm (bit-reversal permutation is needed)
  - Stockham algorithm (bit-reversal permutation is unnecessary)
- The higher radices are more efficient in terms of both memory and floating-point operations.
- In view of the high ratio of floating-point instructions to memory operations, the radix-8 FFT is more advantageous than the radix-4 FFT.

# Real Inner-Loop Operations for Radix-2, 4 and 8 FFT Kernels

| | Radix-2 | Radix-4 | Radix-8 |
|---|---|---|---|
| Loads and Stores | 8 | 16 | 32 |
| Multiplications | 4 | 12 | 32 |
| Additions | 6 | 22 | 66 |
| Total floating-point operations ($n \log_2 n$) | 5 | 4.25 | 4.083 |
| Floating-point instructions | 10 | 34 | 98 |
| Floating-point / memory ratio | 1.25 | 2.125 | 3.063 |

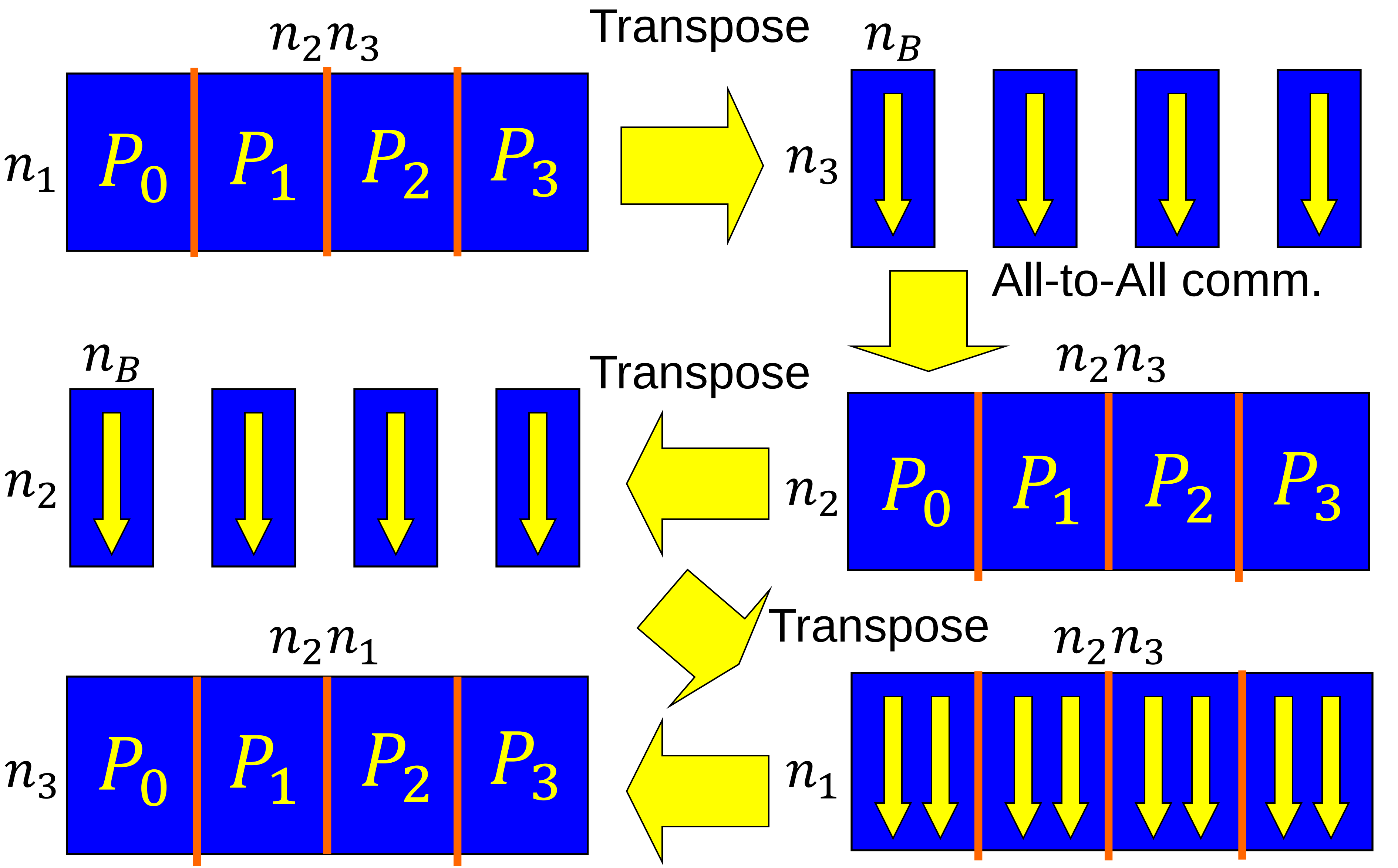
# Number of Instructions for FFTs



# Blocking of a Nine-Step FFT

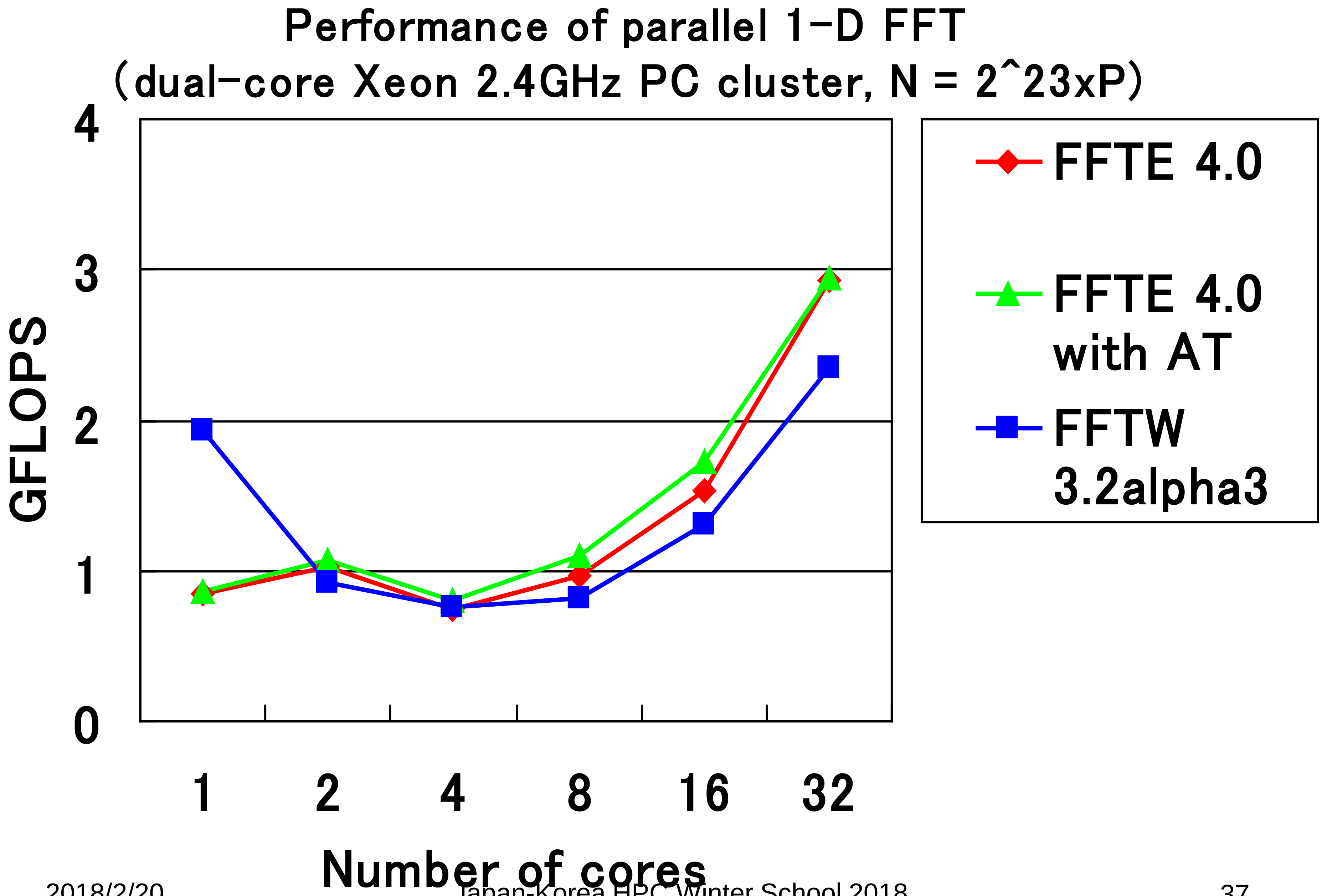
- Data in the cache, having been used for matrix transposition, can also be used with the multicolumn FFTs, thereby increasing the reusability of data in the cache.
- Once data from the main memory has been loaded into the cache, have it remain in cache as much as possible.
- Reuse data in the cache as much as possible, and when that data is truly no longer needed, write it back to the main memory.

# Parallel Nine-Step FFT Algorithm

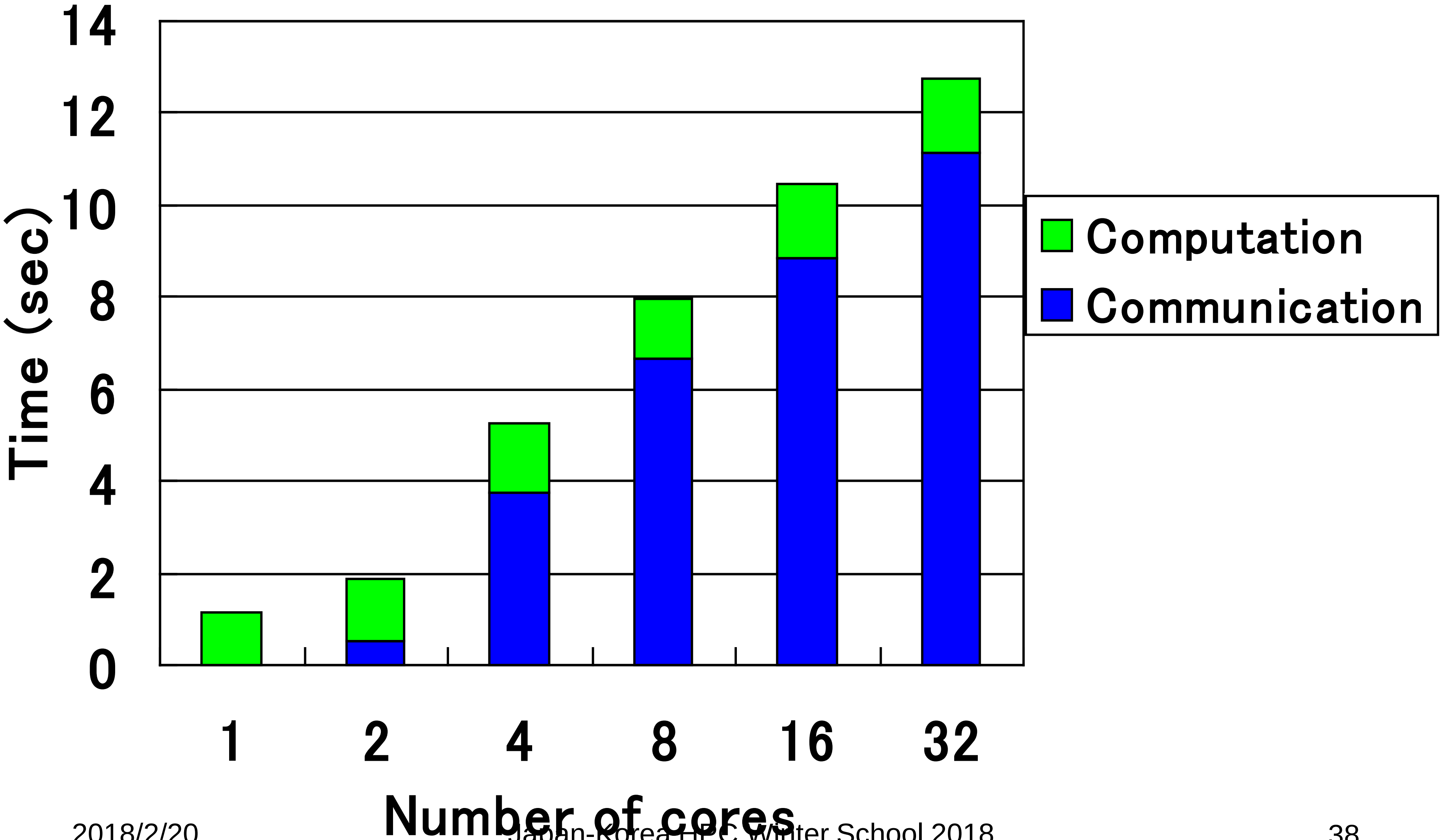


# Advantages of a Block Nine-Step FFT

- With an ordinary FFT algorithm such as the Stockham FFT
  - Number of operations: $5n \log_2 n$
  - Number of main memory accesses: $4n \log_2 n$
- With a block nine-step FFT
  - Number of operations: $5n \log_2 n$
  - Number of main memory accesses: Ideally $12n$
- Because a portion of the nine-step FFT performs $n^{1/3}$-point FFT blocking, the proposed block nine-step FFT can be called a “double blocking” algorithm.


Performance of parallel 1-D FFT
(dual-core Xeon 2.4GHz PC cluster, N = 2^23xP)
GFLOPS
4
3
2
1
0
1
2
4
8
16
32
Number of cores
FFTE 4.0
FFTE 4.0 with AT
FFTW 3.2alpha3

# Breakdown of parallel 1-D FFT (dual-core Xeon 2.4GHz PC cluster, N=2^23xP)



# Examples of Parallel FFT Libraries

- Commercial parallel numeric computation libraries
  - Intel Cluster MKL (Math Kernel Library)
    - OpenMP version and MPI version can be used.
  - AMD ACML (AMD Core Math Library)
    - OpenMP version can be used.
- Open source parallel FFT libraries
  - FFTW (http://www.fftw.org/)
    - OpenMP version and MPI version can be used.
  - FFTE (http://www.ffte.jp/)
    - OpenMP version, MPI version, and OpenMP+MPI version can be used.

# Summary

- The FFT (fast Fourier transform) has been introduced as a parallel numeric computing algorithm.
- The key is how to distribute the problem area.
  - Block distribution, cyclic distribution, block-cyclic distribution
- With a parallel FFT, because the communication part is mainly all-to-all communication, parallelization is relatively easy.
- Not only it is important to reduce the amount of communication, but the use of blocking, etc., is also important to localize the memory accesses.