HPC & Parallel Programming

Start from An Example

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An example of HPC & Parallel Programming: Matrix Multiplication

$$\begin{array}{cc} & \overrightarrow{b_1} \quad \overrightarrow{b_2} \\ & \downarrow \quad \downarrow \\ \begin{array}{c} \overrightarrow{a_1} \rightarrow \\ \overrightarrow{a_2} \rightarrow \end{array} \begin{bmatrix} 1 & 7 \\ 2 & 4 \end{bmatrix} \cdot \begin{bmatrix} 3 & 3 \\ 5 & 2 \end{bmatrix} = \begin{bmatrix} \overrightarrow{a_1} \cdot \overrightarrow{b_1} & \overrightarrow{a_1} \cdot \overrightarrow{b_2} \\ \overrightarrow{a_2} \cdot \overrightarrow{b_1} & \overrightarrow{a_2} \cdot \overrightarrow{b_2} \end{bmatrix} \end{array}$$

$$\quad\quad A \quad\quad\quad\quad B \quad\quad\quad\quad\quad\quad C$$

Matrix multiply

```c
int main()
{

    initMatrix();

    double time_spent = 0.0;
    clock_t begin = clock();

    matrixMultiply();

    clock_t end = clock();
    time_spent += (double)(end - begin) / CLOCKS_PER_SEC;
    printf("Time elpased is %f seconds", time_spent);

    return 0;

}
```

Matrix multiply

```c
#include <stdio.h>
#include <time.h>
#include <stdlib.h>
#define N 1000

double A[N][N], B[N][N], C[N][N];

void initMatrix()
{
    int i, j = 0;
    for (i = 0; i < N; i++) {
        for (j = 0; j < N; j++) {
            A[i][j] = rand() % 100 + 1;  //generate a number between [1, 100]
            B[i][j] = rand() % 100 + 1;  //generate a number between [1, 100]
        }
    }
}
```
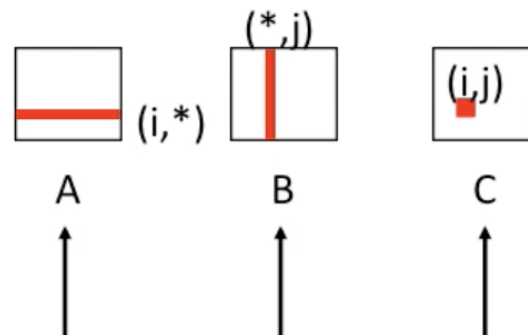
Matrix multiply

```c
void matrixMultiply() {
    int i, j, k = 0;
    for (i = 0; i < N; i++) {
        for (j = 0; j < N; j++) {
            for (k = 0; k < N; k++) {
                C[i][j] += A[i][k] * B[k][j];
            }
        }
    }
}
```
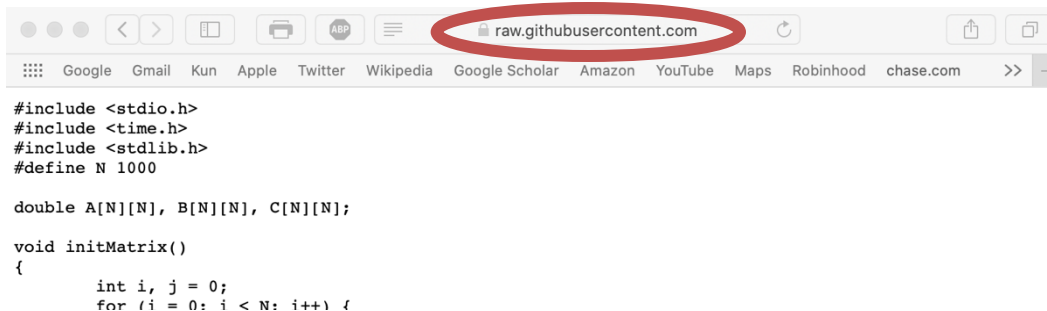
Inner loop:

(*,j)

(i,*)

(i,j)

A   B   C

$$\Theta\left(n^3\right)$$

Row-wise   Column-wise   Fixed

Matrix multiply

1. Raw

```c
#include <stdio.h>
#include <time.h>
#include <stdlib.h>
#define N 1000

double A[N][N], B[N][N], C[N][N];

void initMatrix()
{
        int i, j = 0;
        for (i = 0; i < N; i++) {
                for (j = 0; j < N; j++) {
                        A[i][j] = rand() % 100 + 1;  //generate a number between [1, 100]
                        B[i][j] = rand() % 100 + 1;  //generate a number between [1, 100]
                }
        }
}
```

2. Copy the URL

raw.githubusercontent.com

```c
#include <stdio.h>
#include <time.h>
#include <stdlib.h>
#define N 1000

double A[N][N], B[N][N], C[N][N];

void initMatrix()
{
        int i, j = 0;
        for (i = 0; i < N; i++) {
```
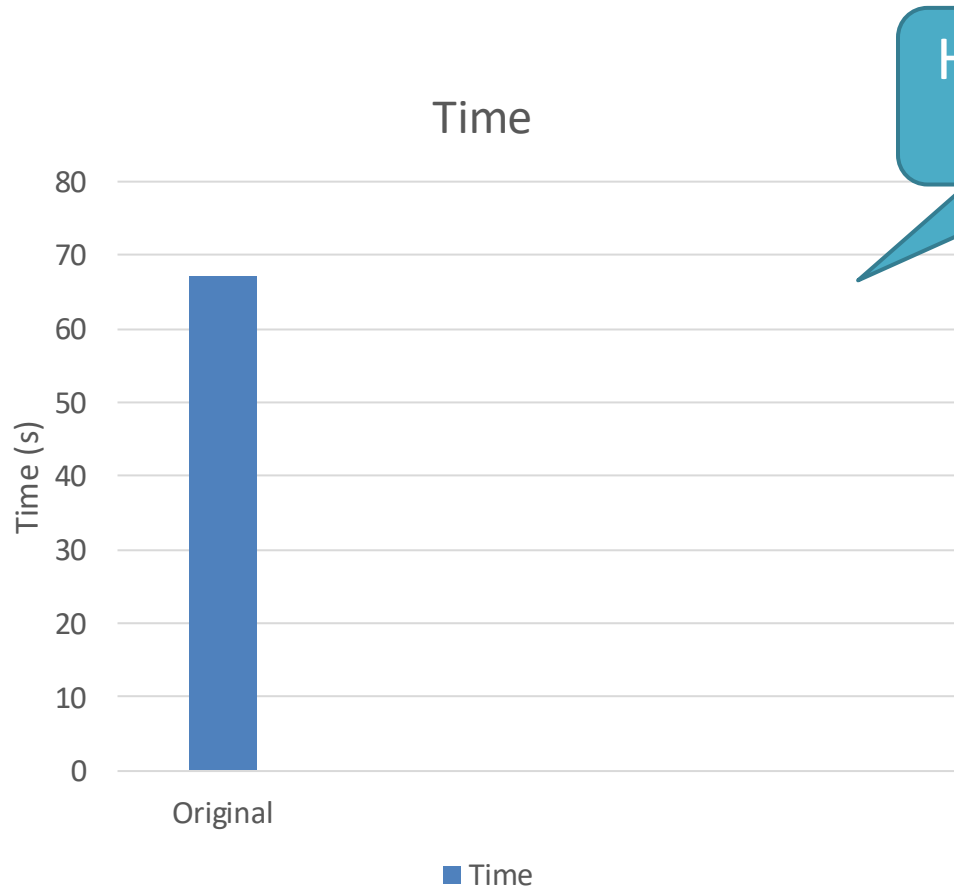
3.

$ wget URL

$ gcc filename.c –o filename.o

$ ./filename.o

(if no wget/gcc,
$ sudo apt install wget, gcc)

Matrix multiply

Time

How to run it faster?

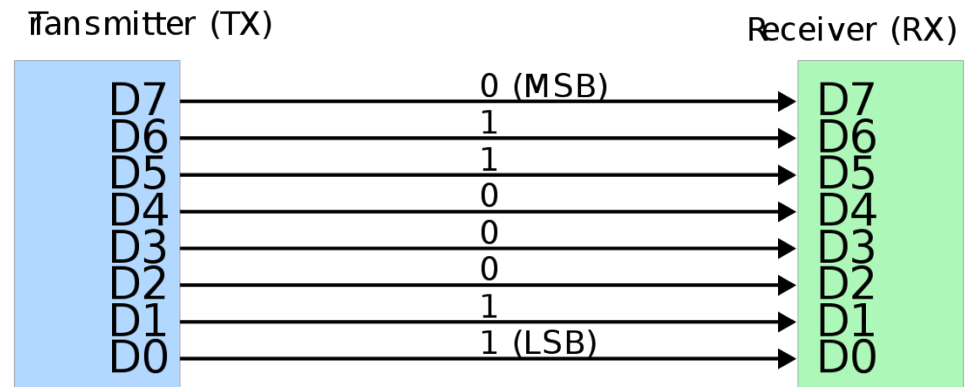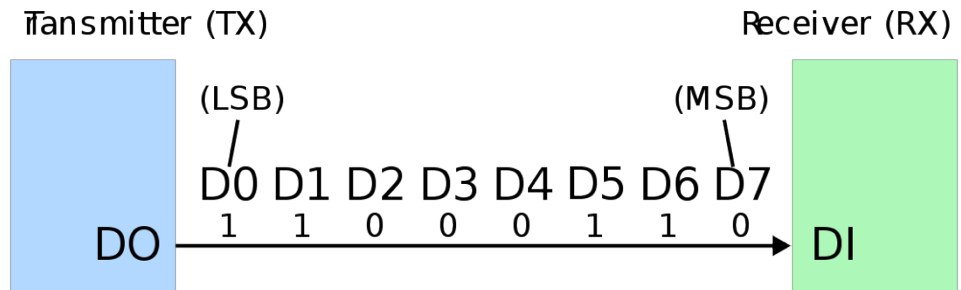1. Accelerate serial execution

2. Accelerate in parallel

How to run it faster?

Transmitter (TX)   Receiver (RX)

(LSB)   (MSB)

D0 D1 D2 D3 D4 D5 D6 D7
1   1   0   0   0   1   1   0

DO ──────────────────────────────► DI

1. Accelerate serial execution
Reduce unnecessary steps

2. Accelerate in parallel

Transmitter (TX)   Receiver (RX)

D7 ──────────── 0 (MSB) ──────────► D7
D6 ──────────── 1 ──────────────► D6
D5 ──────────── 1 ──────────────► D5
D4 ──────────── 0 ──────────────► D4
D3 ──────────── 0 ──────────────► D3
D2 ──────────── 0 ──────────────► D2
D1 ──────────── 1 ──────────────► D1
D0 ──────────── 1 (LSB) ──────────► D0

Option 1: Optimization using locality

```c
void matrixMultiply() {
        int i, j, k = 0;
        for (k = 0; k < N; k++) {
                for (i = 0; i < N; i++) {
                        for (j = 0; j < N; j++) {
                                C[i][j] += A[i][k] * B[k][j];
                        }
                }
        }
}
```
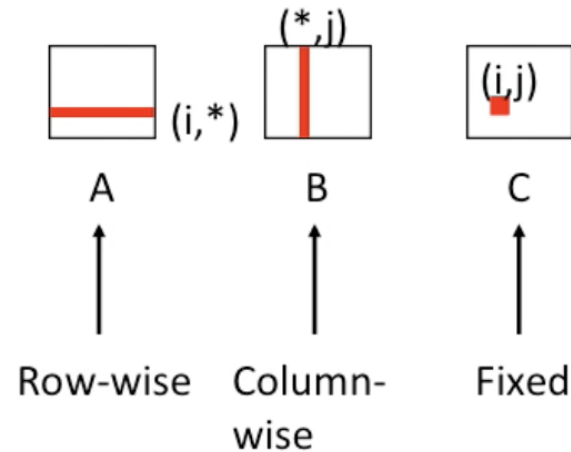
Inner loop:

A	B	C
(i,k)	(k,*)	(i,*)
Fixed	Row-wise	Row-wise

https://github.com/kevinsuo/CS7172/blob/master/matrix-opt.c
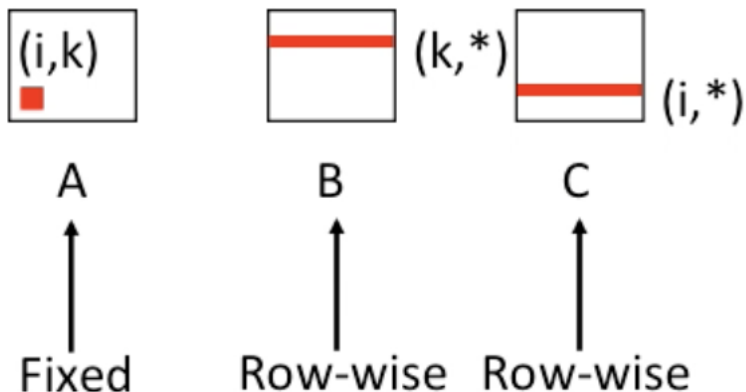
Option 1: Optimization using locality


```
ksuo@ksuo-VirtualBox ~/cs7172> ./a.o
Time elpased is 67.452589 seconds
ksuo@ksuo-VirtualBox ~/cs7172>
ksuo@ksuo-VirtualBox ~/cs7172>
ksuo@ksuo-VirtualBox ~/cs7172>
ksuo@ksuo-VirtualBox ~/cs7172>
ksuo@ksuo-VirtualBox ~/cs7172>
ksuo@ksuo-VirtualBox ~/cs7172>
ksuo@ksuo-VirtualBox ~/cs7172> ./a2.o
Time elpased is 18.149353 seconds
```

N=2000

3.7x

Inner loop:

(*,j)

(i,*)   A   B   C   (i,j)

Row-wise   Column-   Fixed
           wise

Inner loop:

(i,k)   A   (k,*)   B   (i,*)   C

Fixed   Row-wise   Row-wise
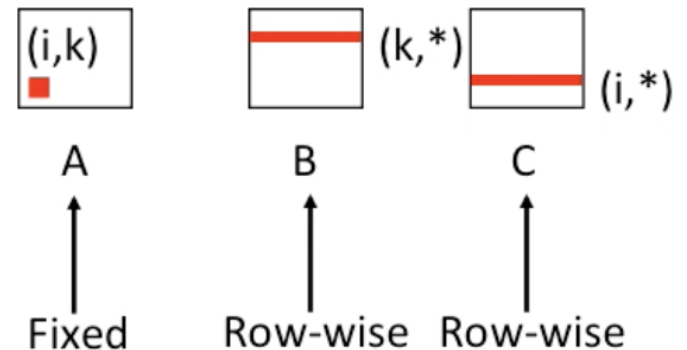
Option 1: Optimization using locality

- ## Temporal locality

  o Every inner loop reuse the value of A[i, k]

Inner loop:

(i,k) A Fixed

(k,*) B Row-wise

(i,*) C Row-wise

- ## Spatial locality

  o Divide the large matrix into smaller ones and put it inside the cache during calculation

n_x-Toeplitz Blocks

n_x-Toeplitz Blocks

$n_y \times n_y$

$N \times N$
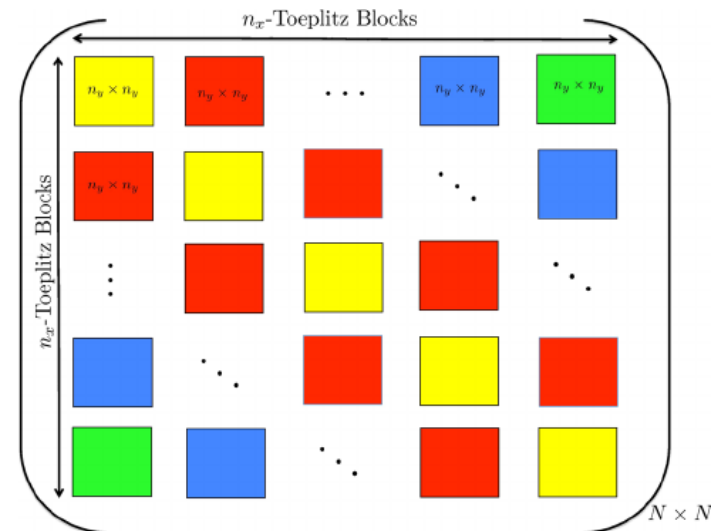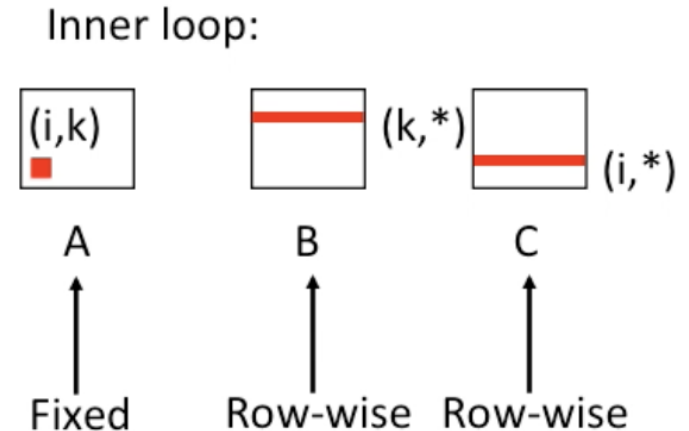
Option 1: Optimization using locality

```
void matrixMultiply() {
    int i, j, k = 0;
    int i2, j2, k2 = 0;

    for (k2 = 0; k2 < N; k2+=BLOCK_SIZE) {
        for (i2 = 0; i2 < N; i2+=BLOCK_SIZE) {
            for (j2 = 0; j2 < N; j2+=BLOCK_SIZE) {
                //inside each block
                for (k = k2; k < k2+BLOCK_SIZE; k++) {
                    for (i = i2; i < i2+BLOCK_SIZE; i++) {
                        for (j = j2; j < j2+BLOCK_SIZE; j++) {
                            C[i][j]+= A[i][k] * B[k][j];
                        }
                    }
                }
            }
        }
    }
}
```

https://github.com/kevinsuo/CS7172/blob/master/matrix-opt2.c
N = 2000

$$\begin{pmatrix} & & 0 & 0 & 0 & 0 \\ J_1 & & 0 & 0 & 0 & 0 \\ 0 & 0 & & & 0 & 0 \\ 0 & 0 & J_2 & & 0 & 0 \\ 0 & 0 & 0 & 0 & & \\ 0 & 0 & 0 & 0 & & J_3 \end{pmatrix}$$

Option 1: Optimization using locality

Inner loop:

(i,k) A — Fixed

(k,*) B — Row-wise

(i,*) C — Row-wise

n_x-Toeplitz Blocks

n_x-Toeplitz Blocks

$n_y \times n_y$

$N \times N$

Option 1: Optimization using locality

Time

Optimal 2: Optimization using parallel

- The algorithm uses a divide-and-conquer approach. When the matrix order is very large, a recursive formula is used for calculation. The relevant recursive formula is described as follows:

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix} \rightarrow \begin{pmatrix} C_{1,1} & C_{1,2} \\ C_{2,1} & C_{2,2} \end{pmatrix}$$

Strassen algorithm

Task 1: $C_{1,1} = A_{1,1}B_{1,1} + A_{1,2}B_{2,1}$

Task 2: $C_{1,2} = A_{1,1}B_{1,2} + A_{1,2}B_{2,2}$

Task 3: $C_{2,1} = A_{2,1}B_{1,1} + A_{2,2}B_{2,1}$

Task 4: $C_{2,2} = A_{2,1}B_{1,2} + A_{2,2}B_{2,2}$

$$\Theta\left(n^{lg7}\right) \approx \Theta\left(n^{2.81}\right)$$

Optimal 2: Optimization using parallel

Thread 1:
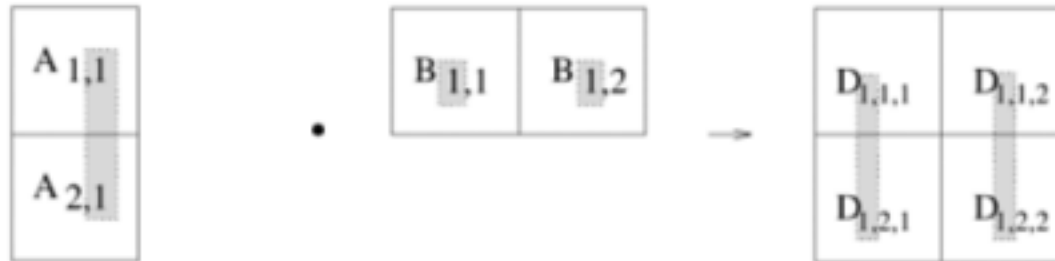
Thread 2:
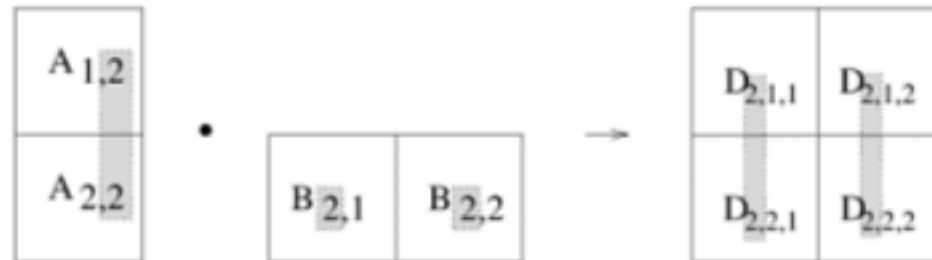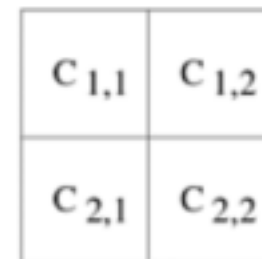
Optimization and Speedup
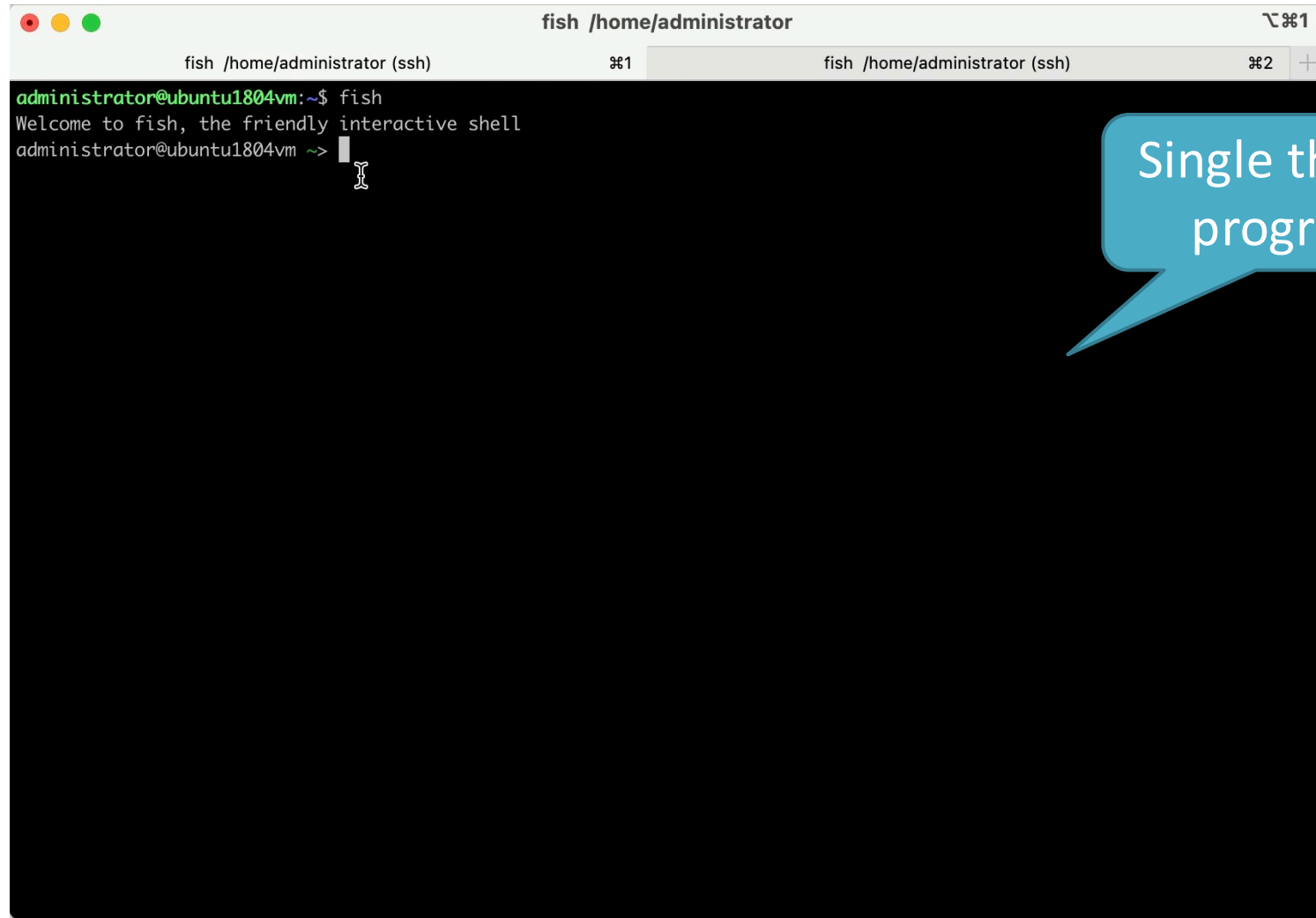
	N=200	N=400	N=800	N=1600
matrix				
matrix-opt1				
matrix-opt2				

	N=200	N=400	N=800	N=1600
matrix				
matrix-opt1				
matrix-opt2				

Single thread app demo

Multi-thread app demo

Multi-thread program

Optimal 2: Optimization using parallel
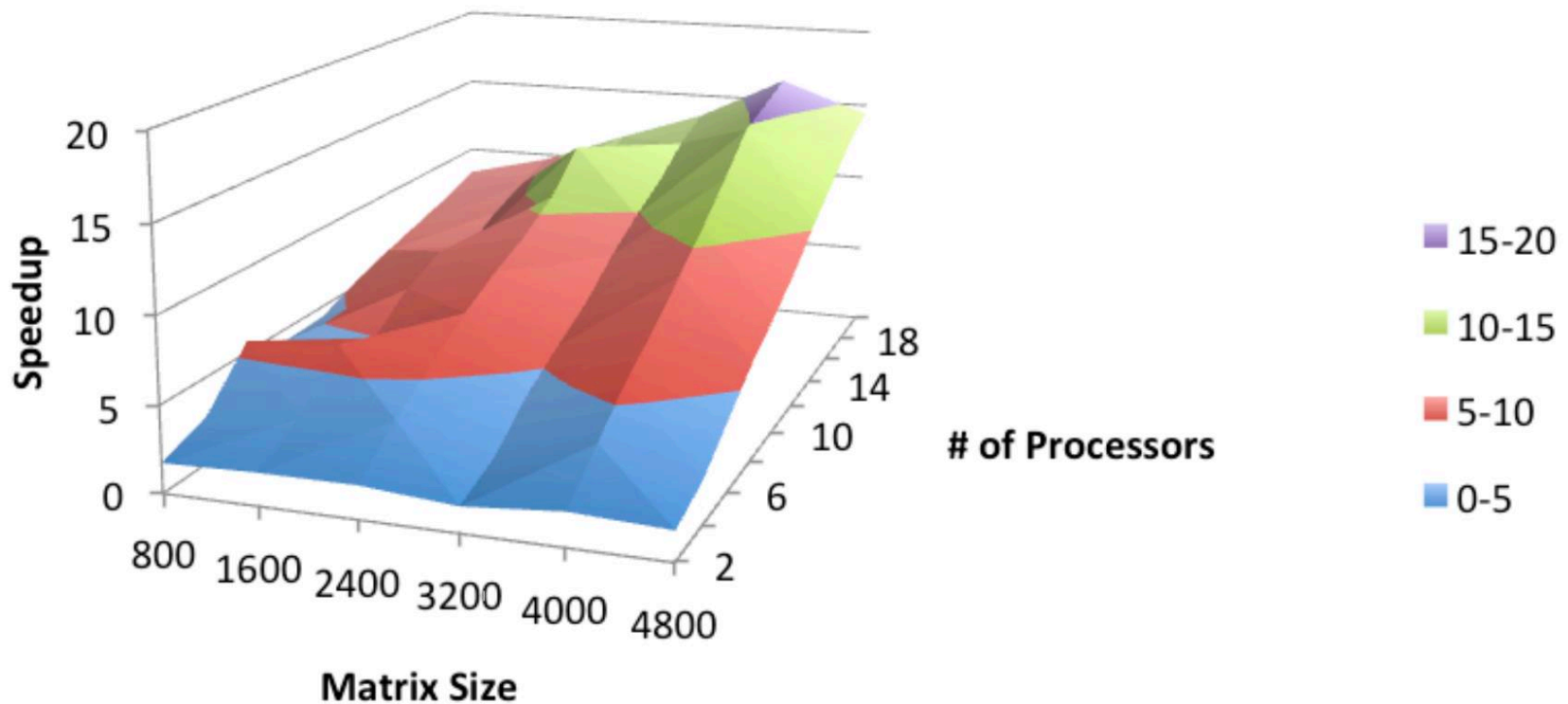
https://www.cse.unr.edu/~fredh/class/415/Nolan/matrix_multiplication/writeup.pdf

Reading Materials

- ## Strassen algorithm

    o In 1969, Volker Strassen proposed a matrix multiplication algorithm with a complexity of $O(n^{2.807})$: [Link](#). This was the first time in history that computational complexity of matrix multiplication was reduced below $O(n^3)$.

- ## Coppersmith–Winograd algorithm

    o In 1990, Don Coppersmith and Shmuel Winograd made a groundbreaking achievement by reducing the complexity to $O(n^{2.3727})$. Paper: [Link](#)

Without Strassen algorithm

$$\begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix}$$

8 submatrix multiplication

$$C_{11} = A_{11} B_{11} + A_{12} B_{21}$$
$$C_{12} = A_{11} B_{12} + A_{12} B_{22}$$
$$C_{21} = A_{21} B_{11} + A_{22} B_{21}$$
$$C_{22} = A_{21} B_{12} + A_{22} B_{22}$$

4 matrix additions

Each equation requires two matrix multiplications and one matrix addition. Using T(n) to represent the multiplication between two matrices, the above equation can be expressed as the following recursive formula:
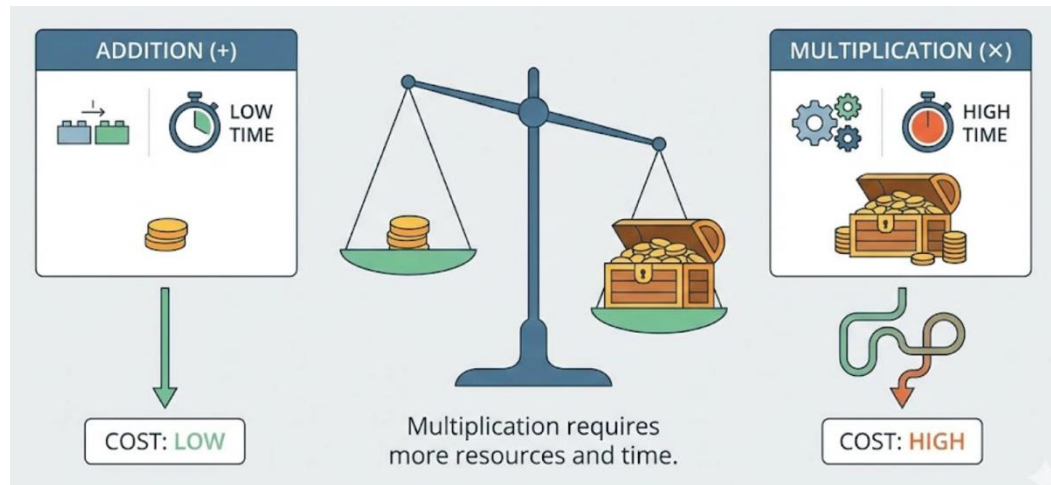
$$T(n) = 8T(n/2) + \Theta(n^2) \quad \Longrightarrow \quad T(n) = \Theta(n^3)$$

8 submatrix multiplication

4 matrix additions, with submatrices of size n/2 x n/2.

Strassen algorithm basic idea

- Multiplication is expensive than additions

- Reduce the number of matrix multiplications by adding the cost of more matrix additions

Strassen algorithm basic idea

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \cdot \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix} \rightarrow \begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix}$$

$$S_1 = B_{12} - B_{22}$$
$$S_2 = A_{11} + A_{12}$$
$$S_3 = A_{21} + A_{22}$$
$$S_4 = B_{21} - B_{11}$$
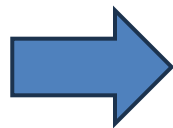$$S_5 = A_{11} + A_{22}$$
$$S_6 = B_{11} + B_{22}$$
$$S_7 = A_{12} - A_{22}$$
$$S_8 = B_{21} + B_{22}$$
$$S_9 = A_{11} - A_{21}$$
$$S_{10} = B_{11} + B_{12}$$

$$P_1 = A_{11} \times S_1$$
$$P_2 = S_2 \times B_{22}$$
$$P_3 = S_3 \times B_{11}$$
$$P_4 = A_{22} \times S_4$$
$$P_5 = S_5 \times S_6$$
$$P_6 = S_7 \times S_8$$
$$P_7 = S_9 \times S_{10}$$

$$C_{11} = P_5 + P_4 - P_2 + P_6$$
$$C_{12} = P_1 + P_2$$
$$C_{21} = P_3 + P_4$$
$$C_{22} = P_5 + P_1 - P_3 - P_7$$

18 matrix additions

7 submatrix multiplication

10 intermediate matrices

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Strassen algorithm time complexity

$$P_1 = A_{11} \times S_1$$
$$P_2 = S_2 \times B_{22}$$
$$P_3 = S_3 \times B_{11}$$
$$P_4 = A_{22} \times S_4$$
$$P_5 = S_5 \times S_6$$
$$P_6 = S_7 \times S_8$$
$$P_7 = S_9 \times S_{10}$$

7 submatrix multiplication

$$C_{11} = P_5 + P_4 - P_2 + P_6$$
$$C_{12} = P_1 + P_2$$
$$C_{21} = P_3 + P_4$$
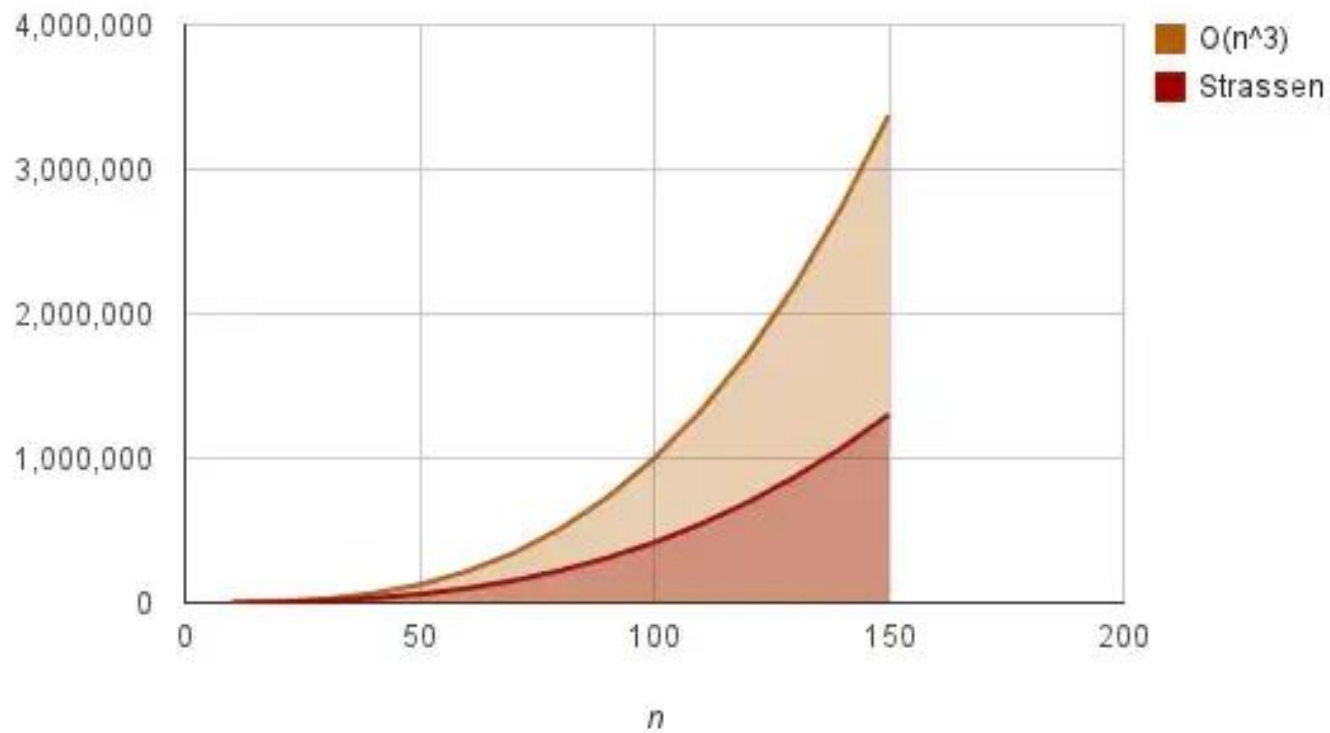$$C_{22} = P_5 + P_1 - P_3 - P_7$$

18 matrix additions

$$T(n) = 7T(n/2) + \Theta(n^2) = \Theta(n^{lg7}) \approx \Theta(n^{2.81})$$

7 submatrix multiplication

18 matrix additions, with submatrices of size n/2 x n/2.
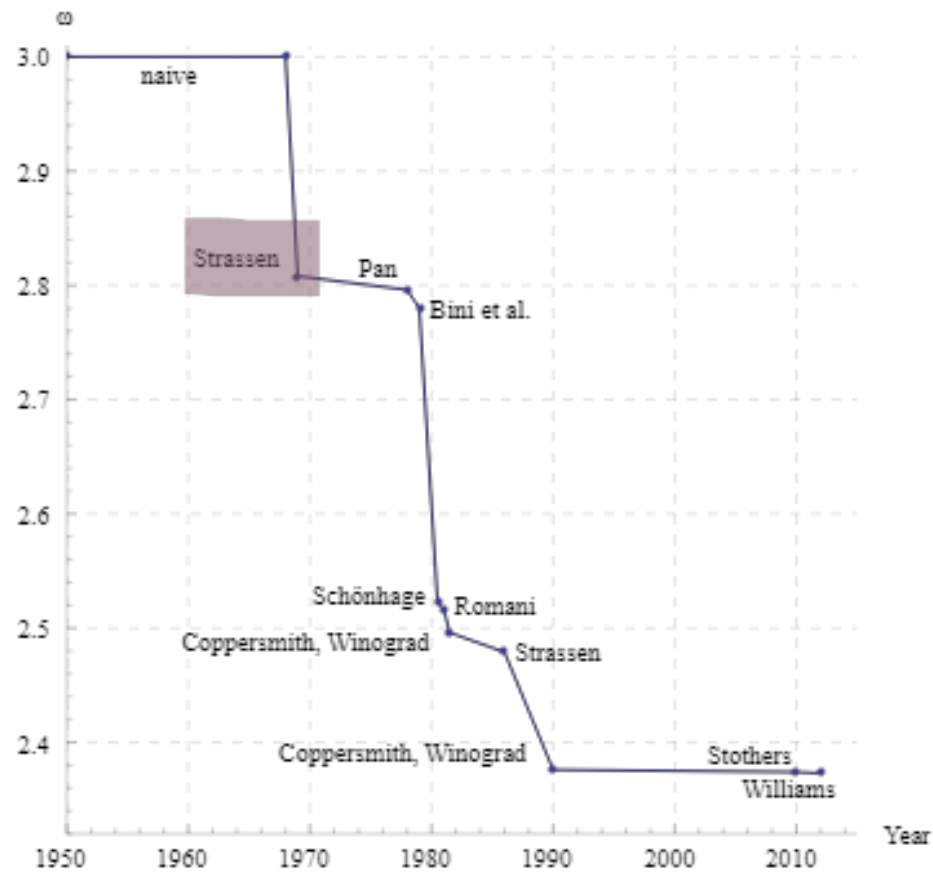
Strassen algorithm time complexity

The larger the value of n, the more time the Strassen algorithm saves.

Strassen algorithm time complexity
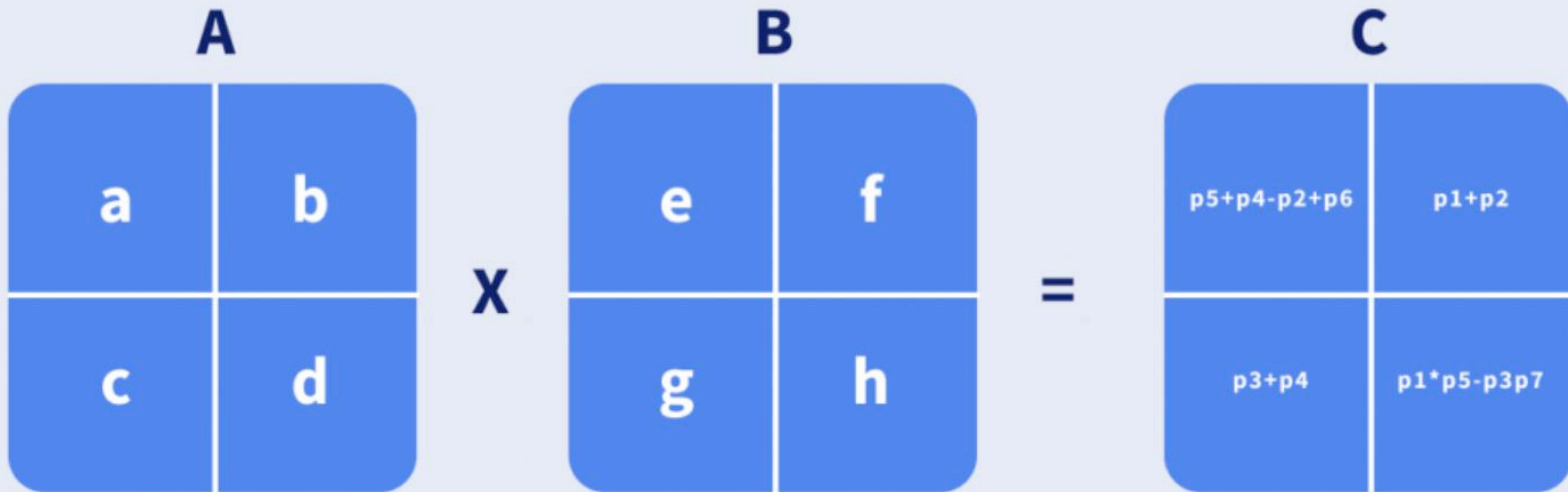
Strassen algorithm

$p1 = a(f-h)$ $p2 = (a+b)h$
$p3 = (c+d)e$ $p4 = d(g-e)$
$p5 = (a+d)(e+h)$ $p6 = (b-d)(g+h)$
$p7 = (a-c)(e+f)$

A

a	b
c	d

X

B

e	f
g	h

=

C

p5+p4-p2+p6	p1+p2
p3+p4	p1*p5-p3p7

Coppersmith–Winograd algorithm basic idea

The mathematician Carl Friedrich Gauss (1777–1855) once noticed that although the product of two complex numbers

$$(a + bi)(c + di) = ac - bd + (bc + ad)i$$

seems to involve *four* real-number multiplications, it can in fact be done with just *three*: ac, bd, and $(a + b)(c + d)$, since

$$bc + ad = (a + b)(c + d) - ac - bd.$$

- Winograd extended this principle to matrix multiplication.
- By decomposing matrix multiplication into smaller-scale computations, the number of multiplications is further reduced by increasing the number of additions
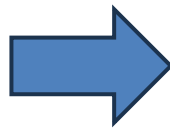
Coppersmith–Winograd algorithm basic idea

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \cdot \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix} \rightarrow \begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix}$$
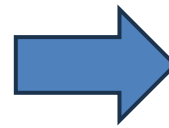
$S1 = A21 + A22$
$S2 = S1 - A11$
$S3 = A11 - A21$
$S4 = A12 - S2$

$T1 = B21 - B11$
$T2 = B22 - T1$
$T3 = B22 - B12$
$T4 = T2 - B21$

$M1 = A11 * B11$
$M2 = A12 * B21$
$M3 = S4 * B22$
$M4 = A22 * T4$
$M5 = S1 * T1$
$M6 = S2 * T2$
$M7 = S3 * T3$

7 smaller size multiplication

$U1 = M1 + M2$
$U2 = M1 + M6$
$U3 = U2 + M7$
$U4 = U2 + M5$
$U5 = U4 + M3$
$U6 = U3 - M4$
$U7 = U3 + M5$

more matrix additions

$C11 = U1$
$C12 = U5$
$C21 = U6$
$C22 = U7$

$$O\left(n^{2.376}\right)$$

Strassen algorithm time complexity
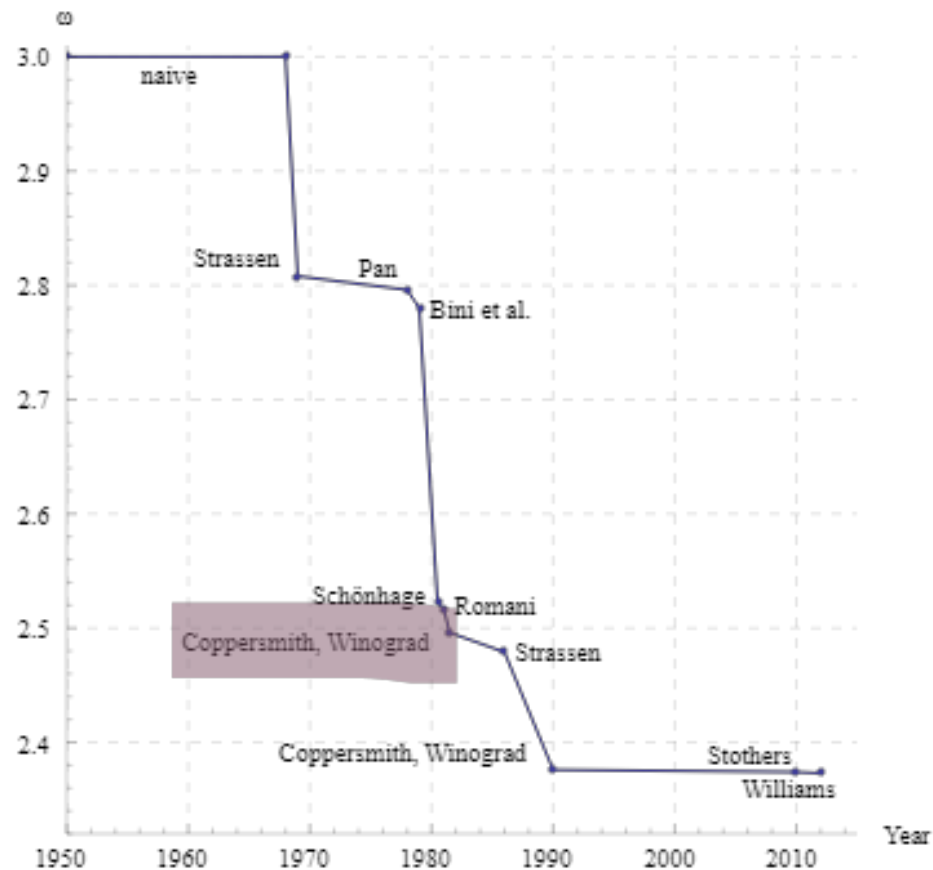
Summary Comparison Table

Feature	Strassen Algorithm	Coppersmith–Winograd (CW) Algorithm
Theoretical Complexity	$\approx O(n^{2.81})$	$\approx O(n^{2.37})$
Practicality	Widely used for large-scale matrices	Extremely low (Mainly used for theoretical research)
Constant Factors	Relatively small	Enormously large
Hardware Optimization	Easier to adapt for GPU/Parallel computing	Extremely difficult
Main Contribution	Proved matrix multiplication can be $< O(n^3)$	Pushed the theoretical lower bound of complexity

Example of distributed system: sorting

- Sorting on a single machine, e.g., Database

select field_a from table_b order by field_a limit 100, 10;

```
db.collection_b
.find()
.sort({"field_a":1})
.skip(100)
.limit(10);
```

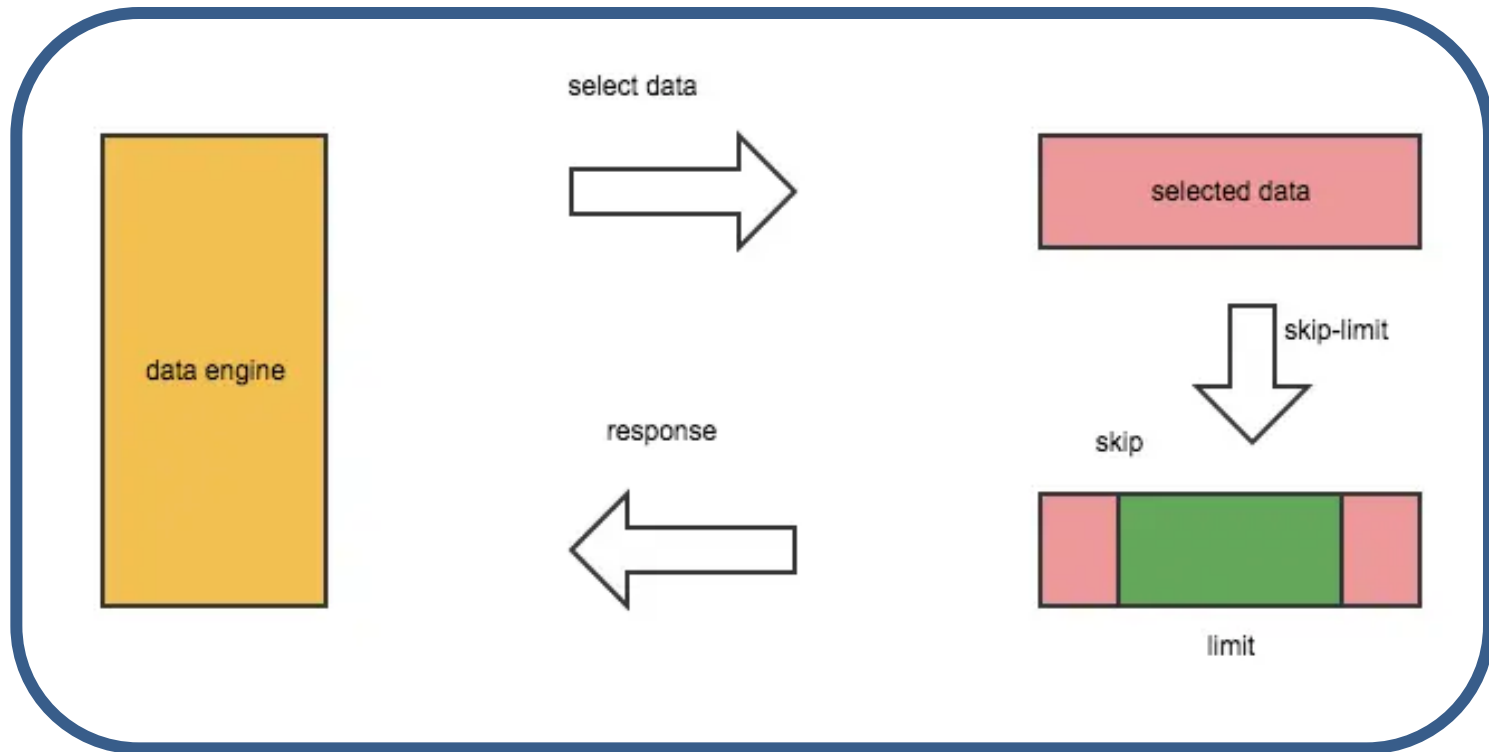|	field_a	field_b	field_c
100			
...			
...			
110			

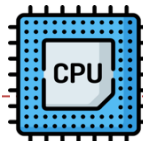From line 100 to the next 10 lines of data

Example of distributed system: sorting
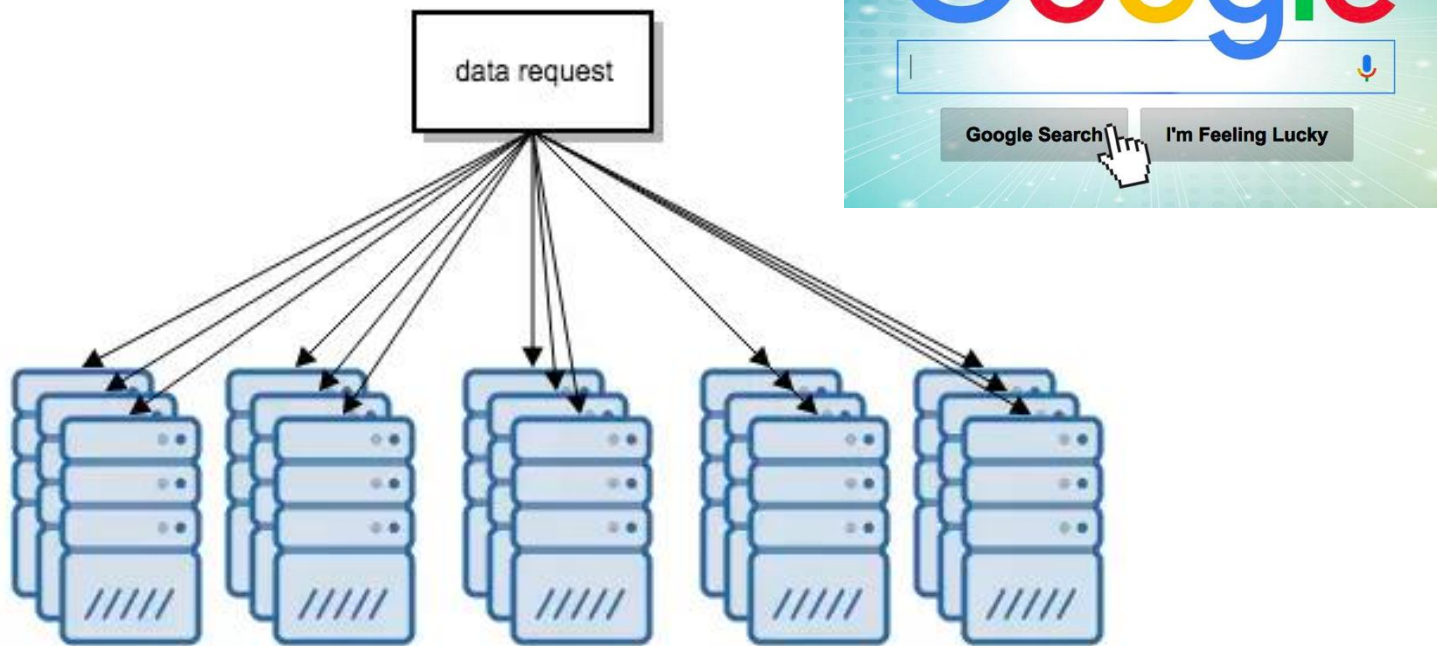
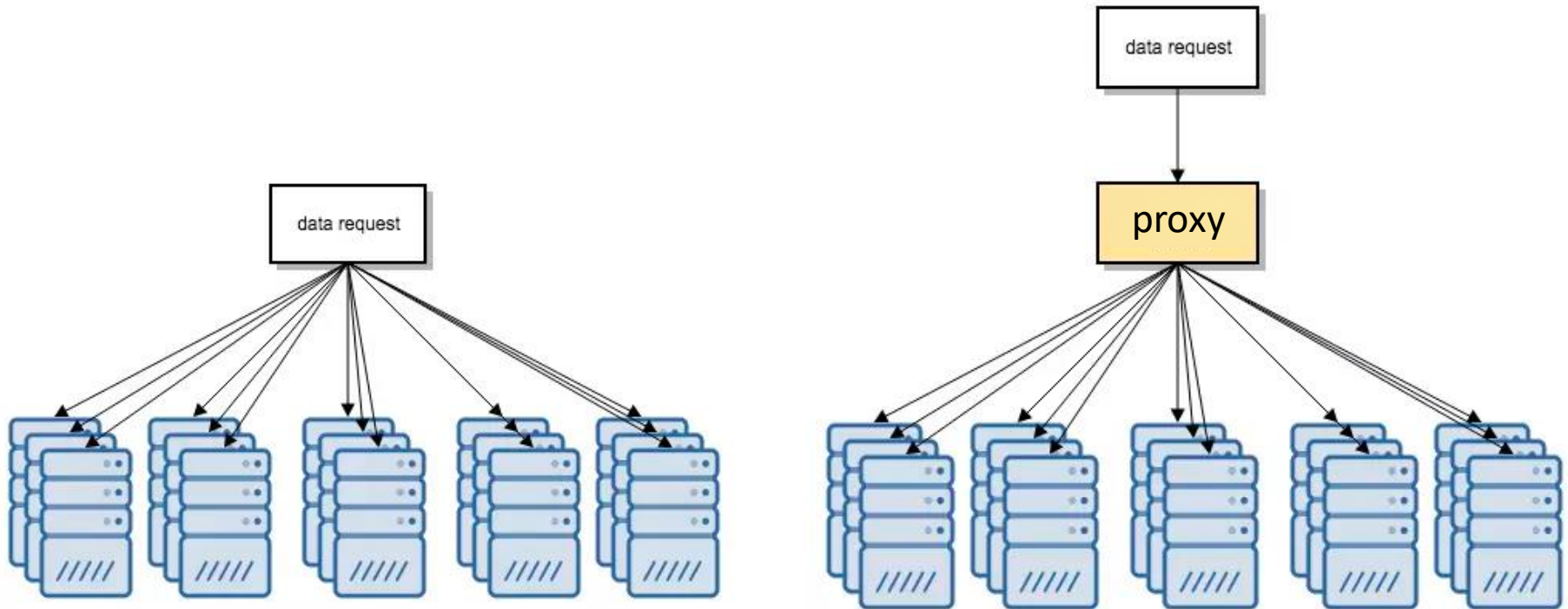- Workflow on a single node

One server CPU

Example of distributed system: sorting

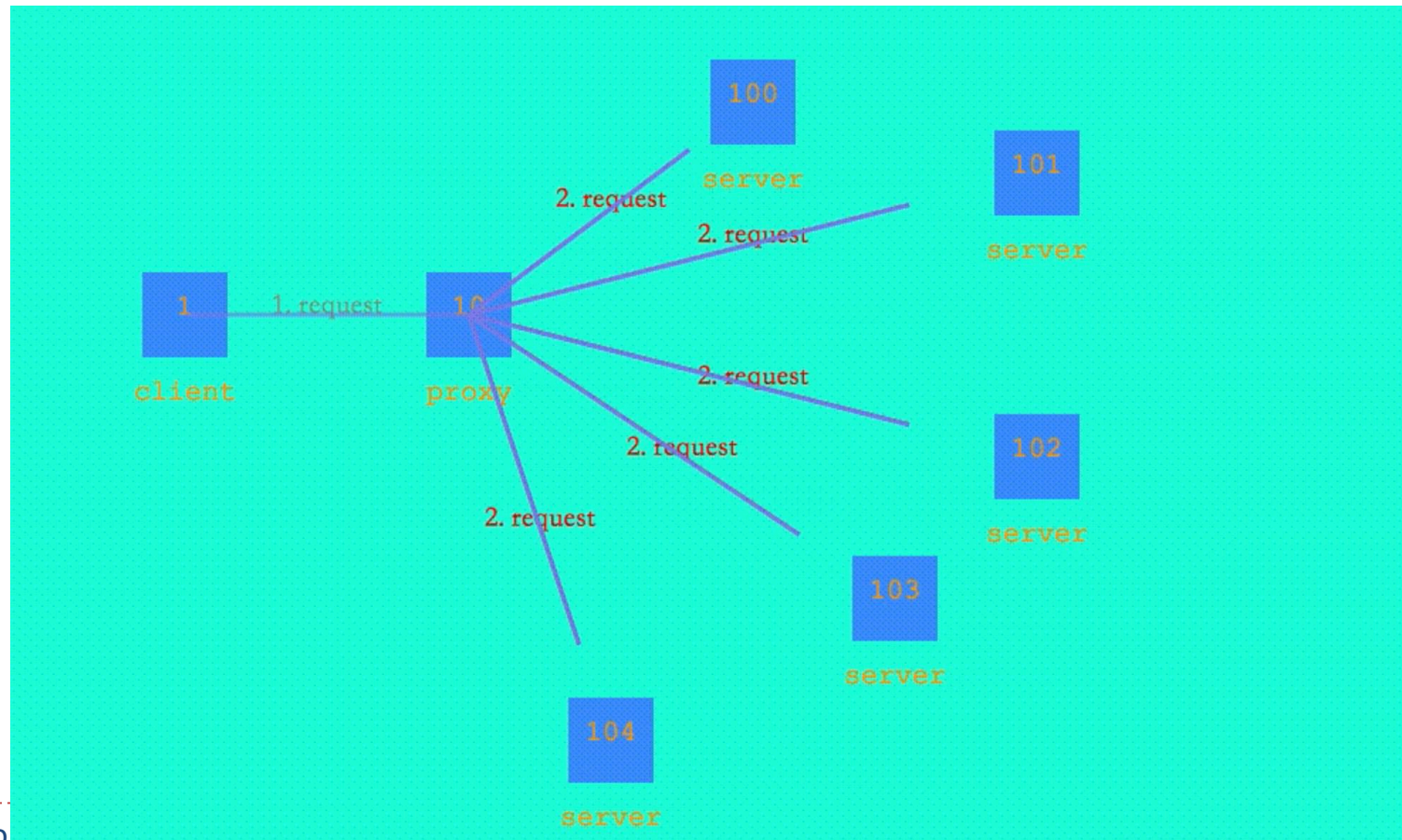- If the data is too much and single node cannot hold

Example of distributed system: sorting
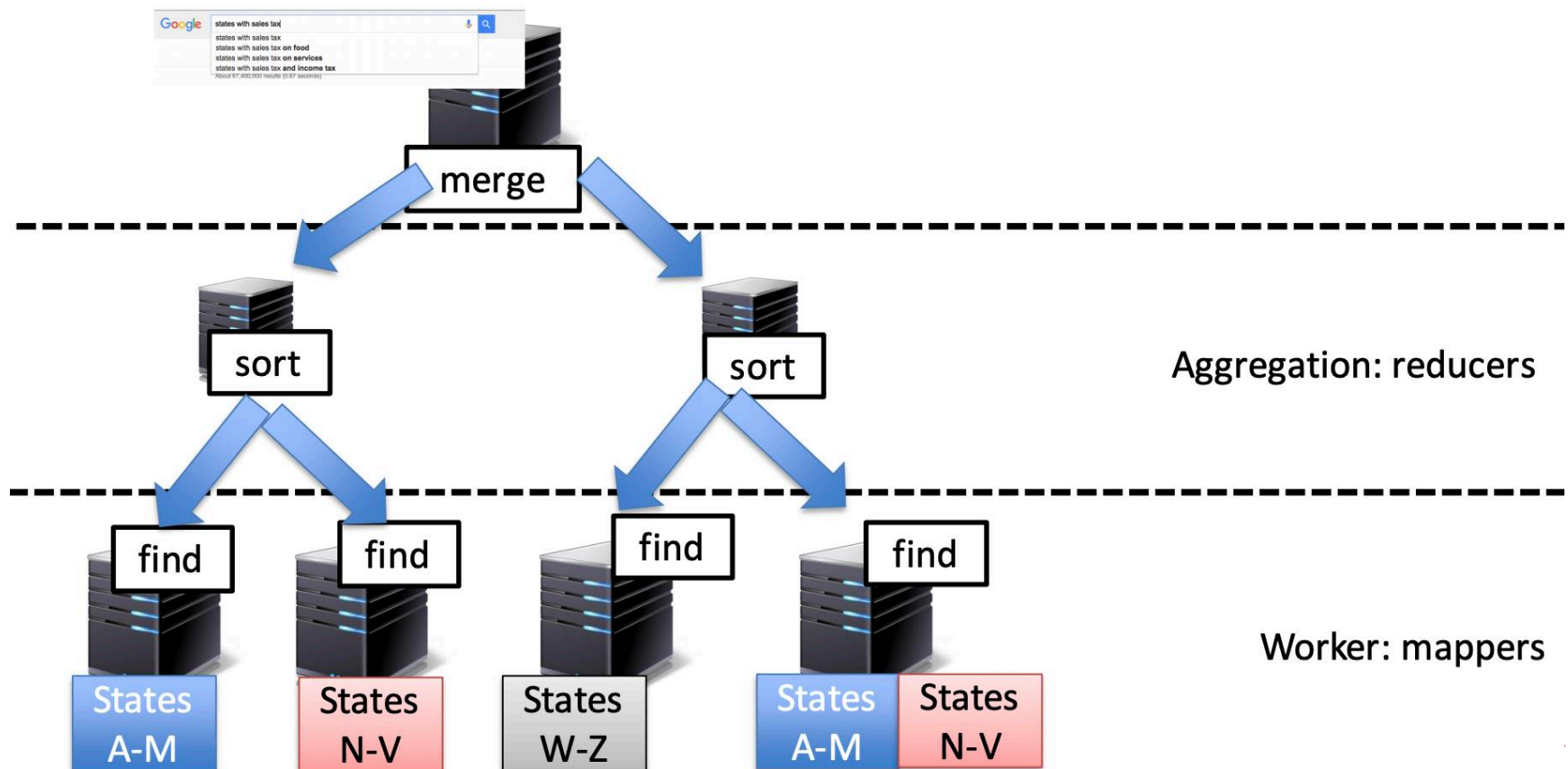
- Choose a node for merge processing

Example of distributed system: sorting

- Workflow

Example of distributed system: sorting

- How Do Request Get Processed in a Data Center

Example of distributed system: sorting

- How Google Search Works

- https://www.youtube.com/watch?v=0eKVizvYSUQ

Conclusion

- Why study HPC & parallel programming?

- What to learn?

- Course structure

- Course policy

- An example of HPC & parallel programming