用 CUDA 進行局部序列比對

Semi Global Sequence Alignment with CUDA

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1) 序列比對
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    2) Dynamic Programing
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    2) Alignment
3) 結果分析

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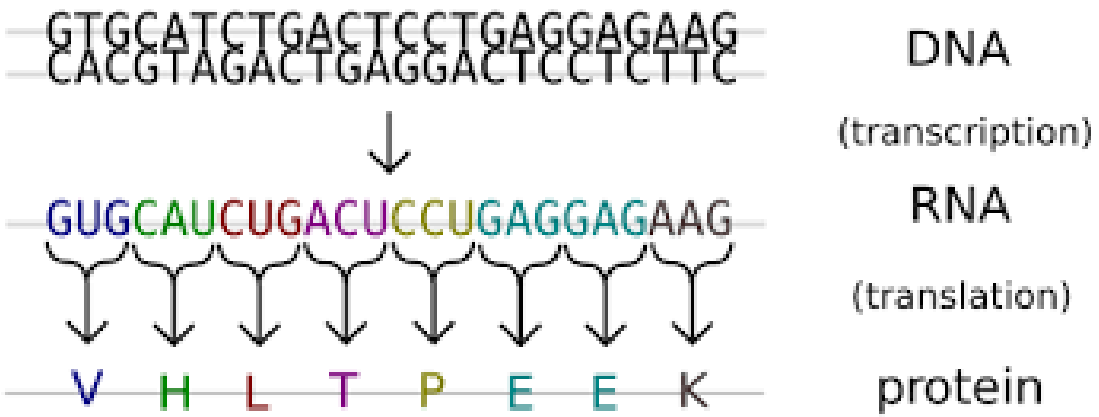
轉錄、轉譯




```
int main(int argc,char** argv){
    byte *gx_int,*gy_int;
    afg_unit *M,*M1,*M2,*GM,*GM1,*GM2;
    int xsize,ysize;
    int nthread,nblock;
```

突變

a.DNA → segment fault ☹

b.DNA → compile error ☹

c.DNA → segment fault ☹

d.DNA → overflow ☹

e.DNA → better program ☺

序列比對

ATGCCATTCGT

ATTCCCGT

Gap Open=-3

Gap Extension=-2

1 1-2 1 1-3-2-2 1 1 1

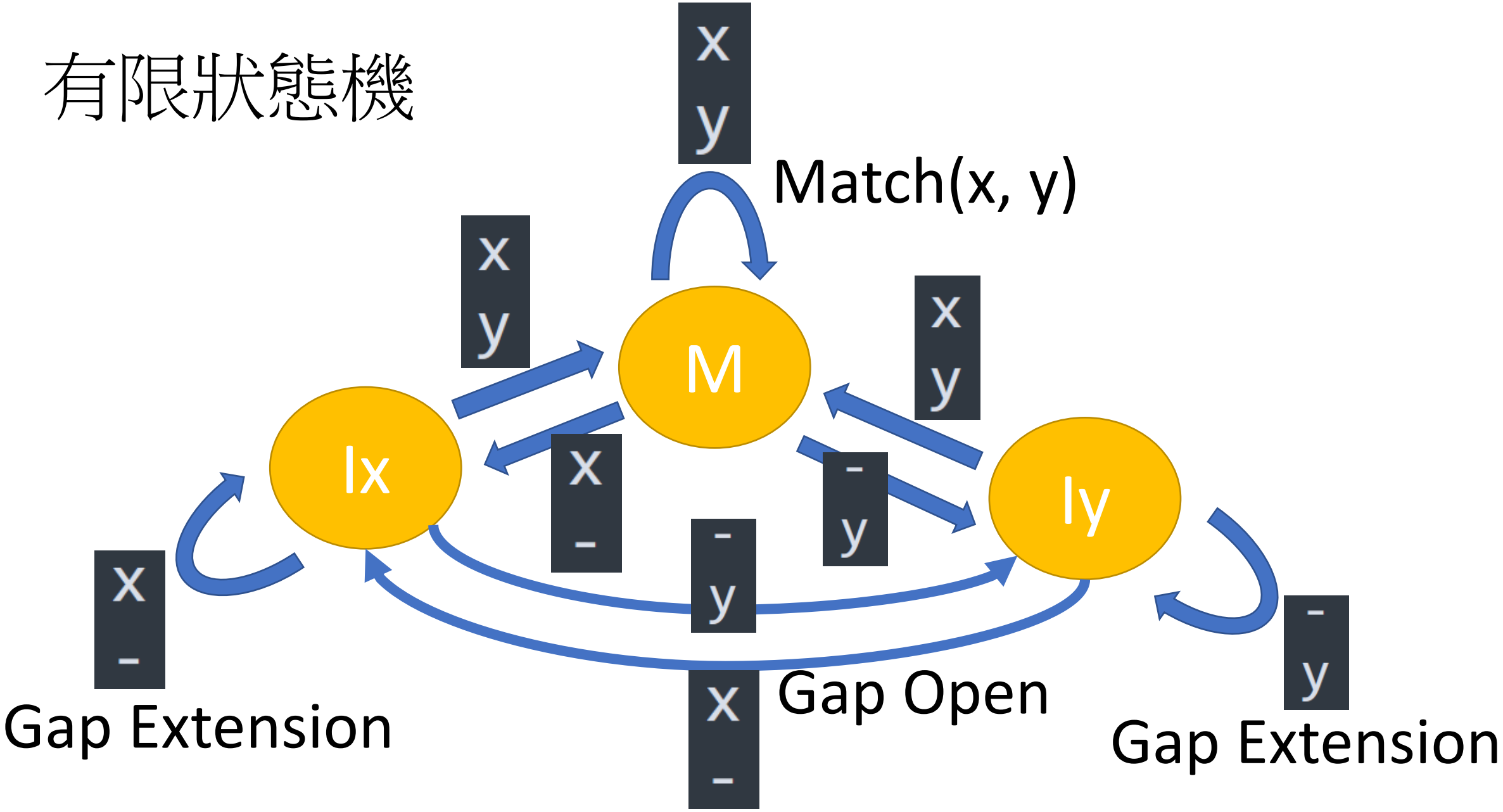
ATGCCATTCGT

ATTCC---CGT

=-2

	A	T	C	G
A	1	-2	-2	-1
T	-2	1	-1	-2
C	-2	-1	1	-2
G	-1	-2	-2	1

有限狀態機

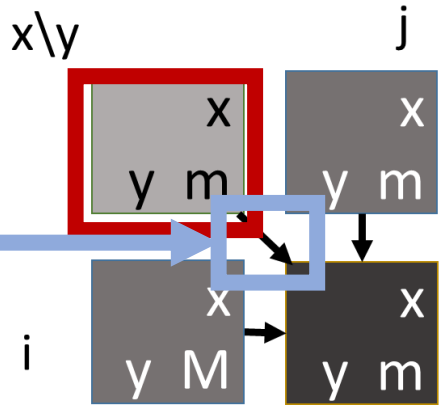

x
y
Match(x, y)
x
y
M
x
y
Ix
x
–
-
y
Iy
x
–
-
y
-
y
x
–
Gap Extension
Gap Open
Gap Extension

Dynamic Programming

$$\mathrm{M}(i,j) = match(Xi, Yj) + max \begin{cases} M(i-1,j-1) \\ Ix(i-1,j-1) \\ Iy(i-1,j-1) \end{cases}$$

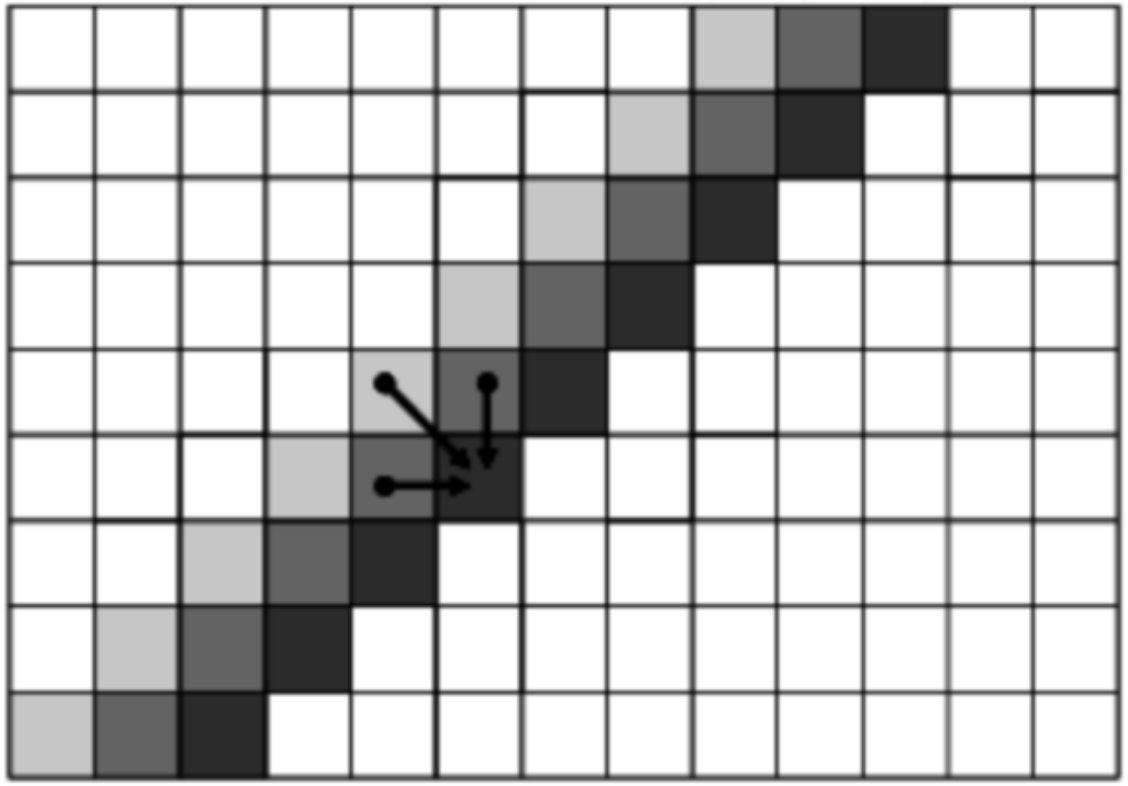
$$\mathrm{Ix}(i,j) = max \begin{cases} M(i-1,j) + gap \\ Ix(i-1,j) + ext \\ Iy(i-1,j) + gap \end{cases}$$

$$\mathrm{Iy}(i,j) = max \begin{cases} M(i,j-1) + gap \\ Ix(i,j-1) + gap \\ Iy(i,j-1) + ext \end{cases}$$



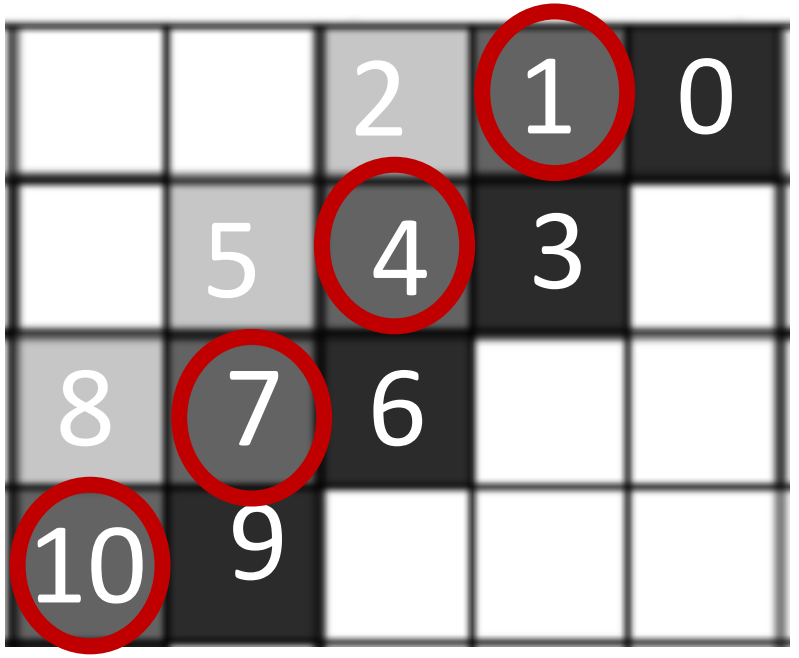
Data Dependency

x\y M2 M1 M



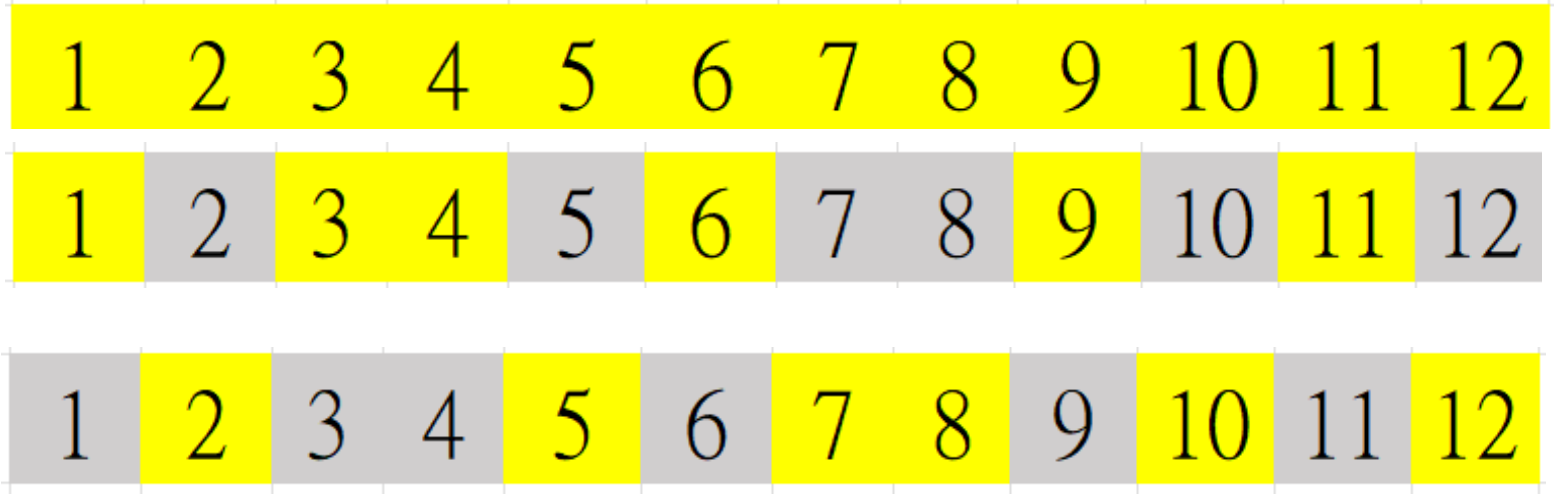
- 平行運算
- 線性空間複雜度

Coalescing

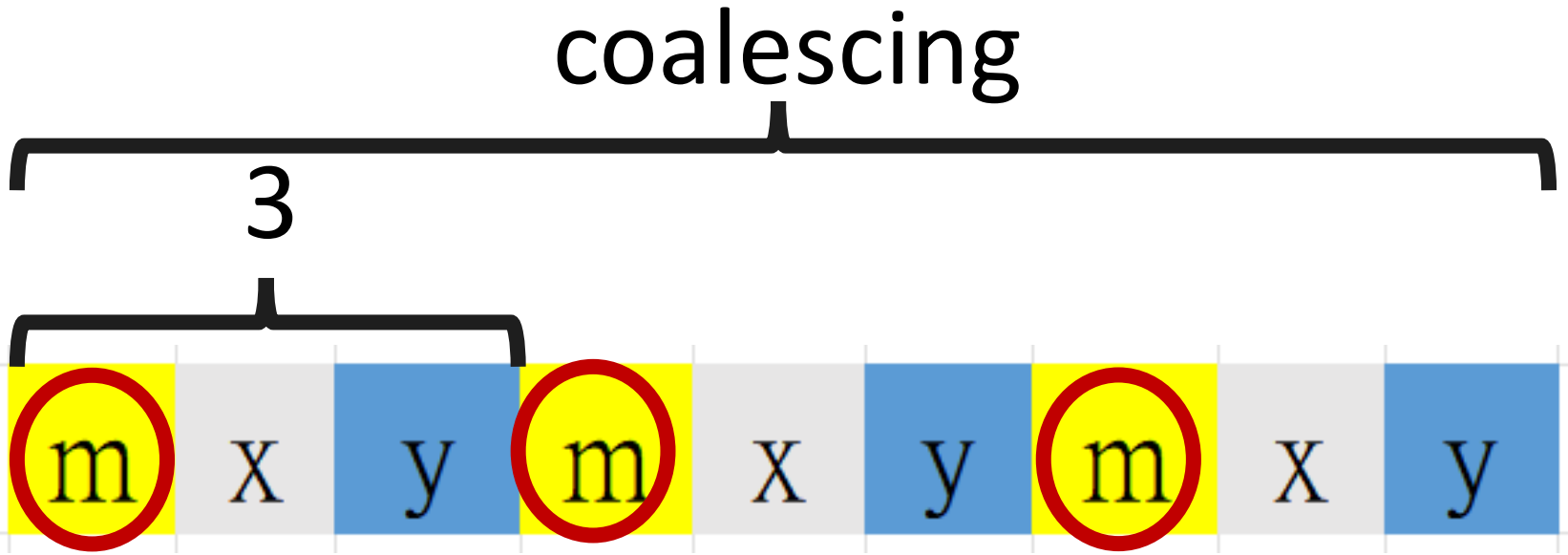


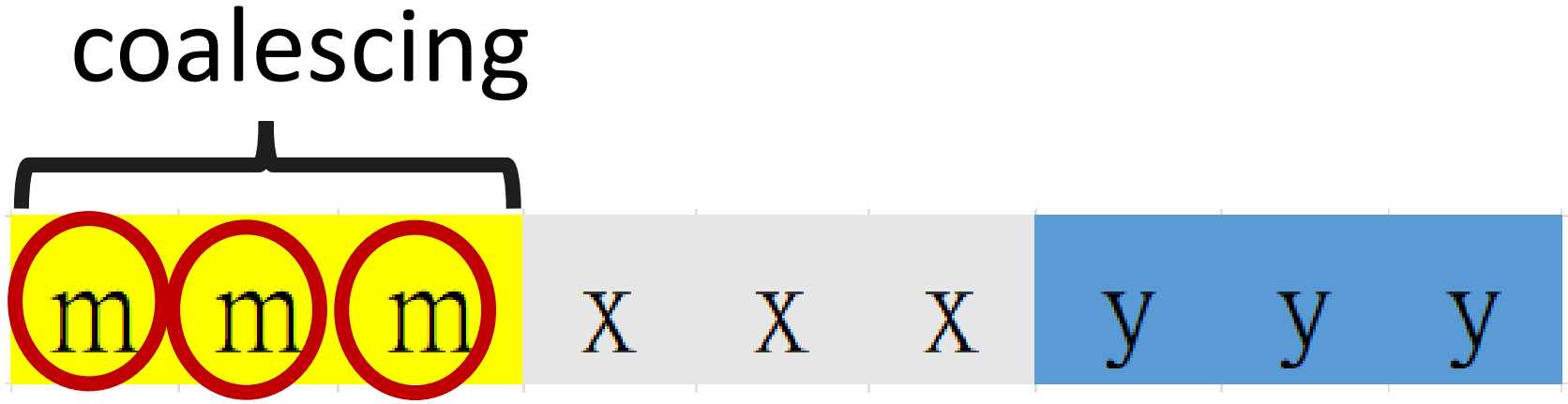
Global Memory: GPU 可存取的記憶體的其中一種，
因為 CUDA Thread 只要有指標皆可存取，故命名之。
SIMD: single instruction multiple data

```
if(a[tid]>5){
    c=a[tid];
}else{
    c=b[tid];
}
```



Warp: 在一個 Block 中連續的 threads，通常是 32 條。
Block: GPU 會把多條連續的 threads 分成多個 Blocks，每個 Block 具有一個 Multiprocessor
Multiprocessor: 平行運算單位，他會挑選一個 Warp 的 threads 進行 SIMD 平行運算


coalescing
3
m
x
y
m
x
y
m
x
y


coalescing
m
m
m
x
x
x
y
y
y

Above CUDA 3.0

Normal code 😐 ⟶ good performance ☺

excellent code 😎 ⟶ excellent performance 😎

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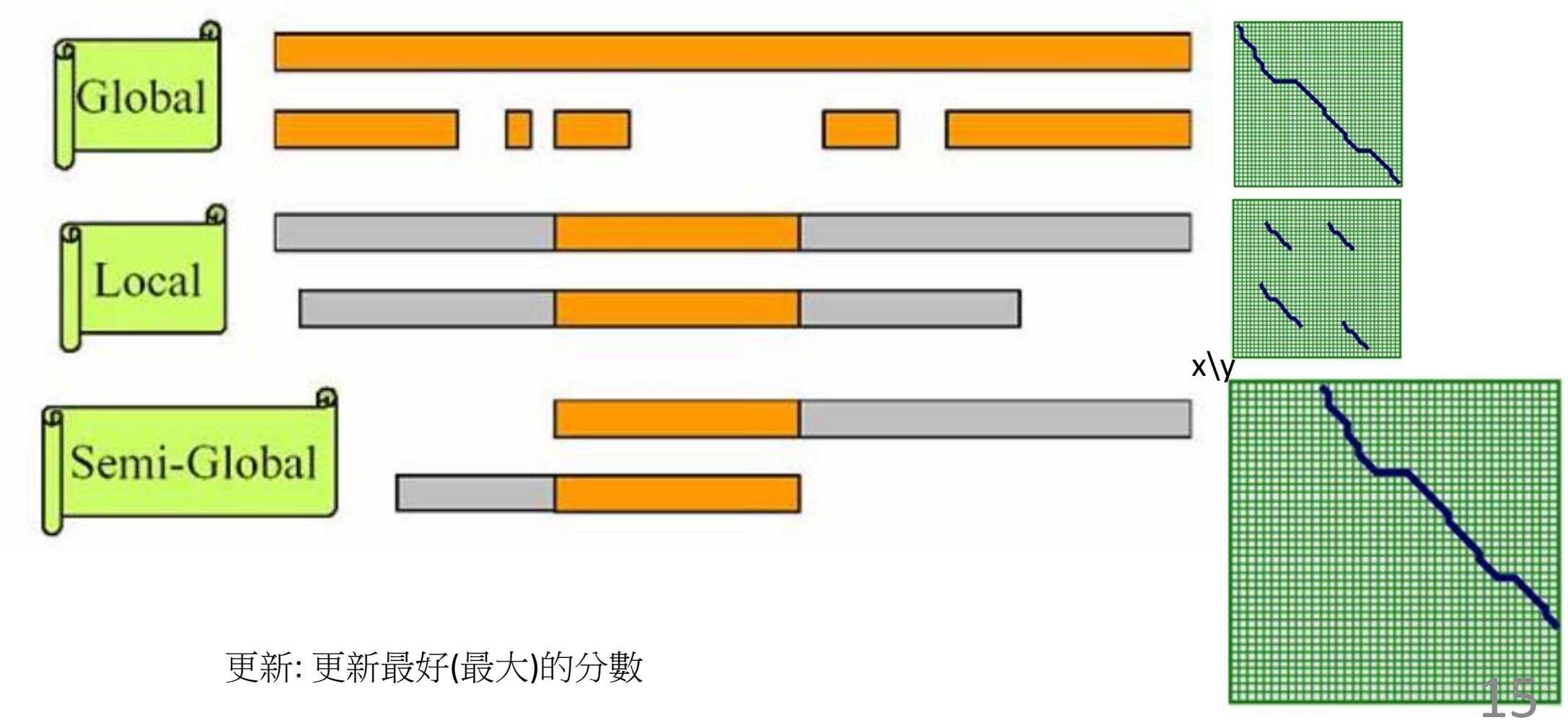
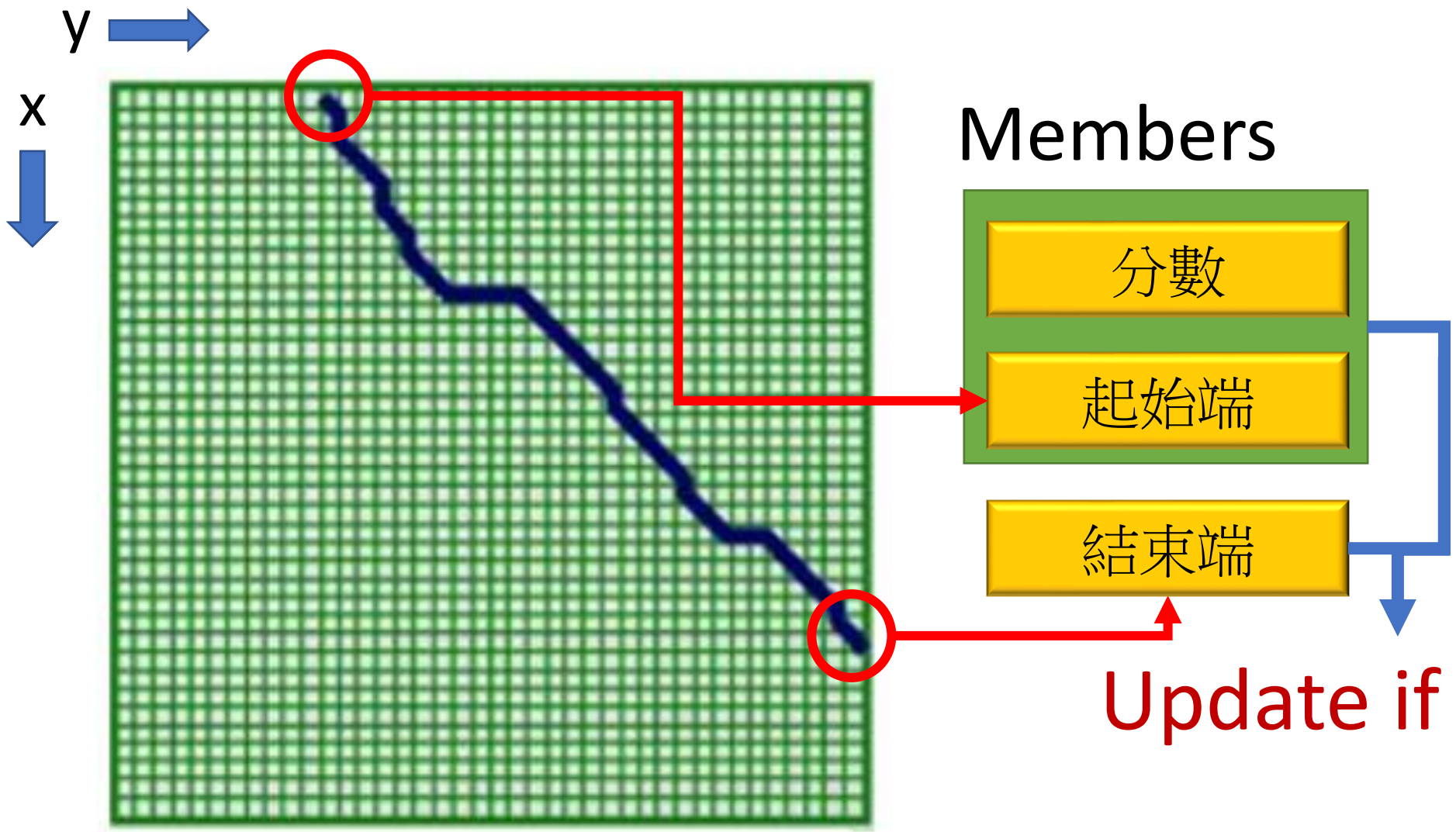
Semi Global

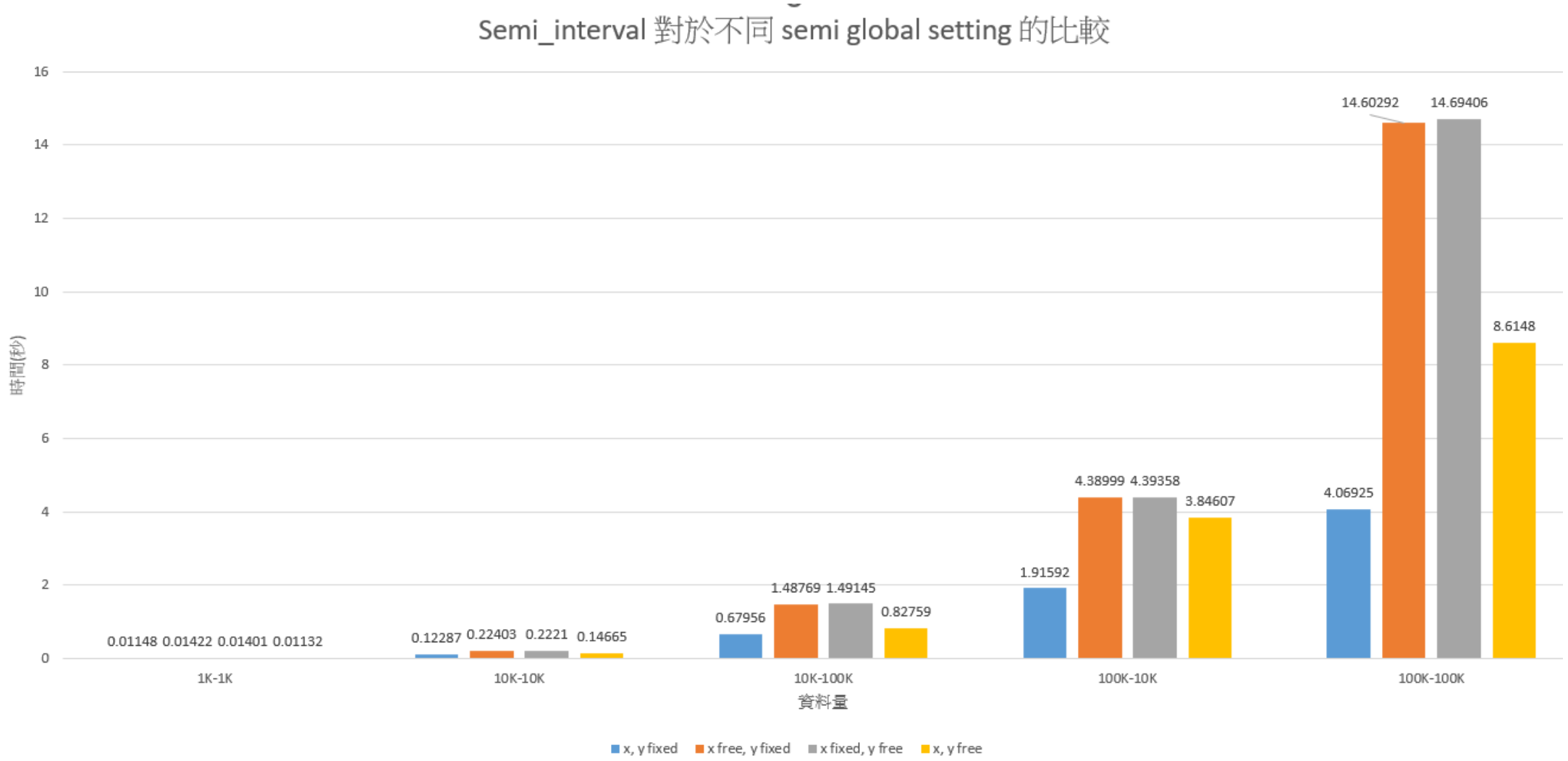


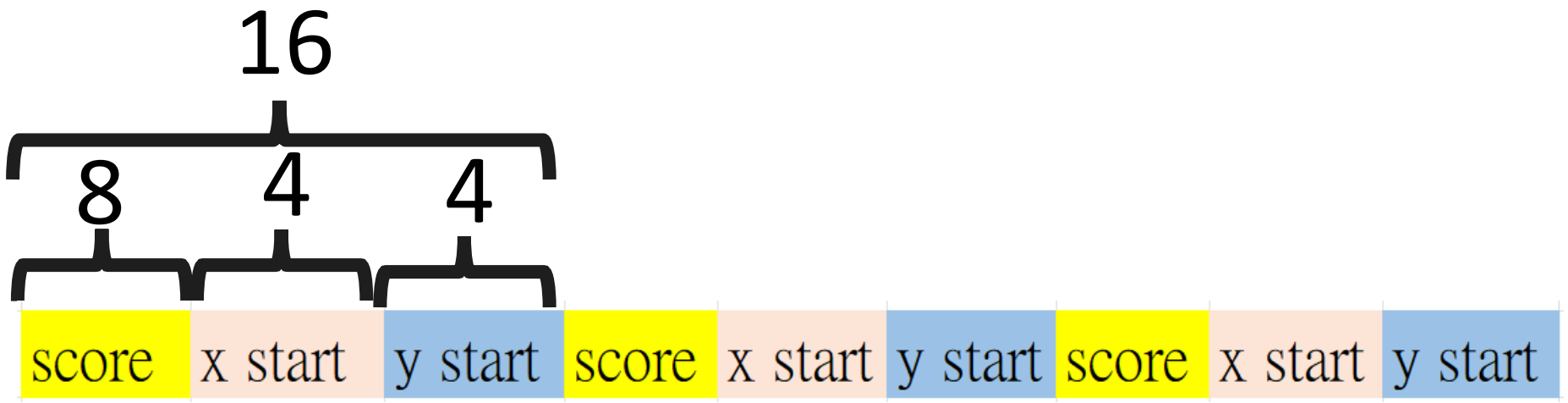
更新: 更新最好(最大)的分數

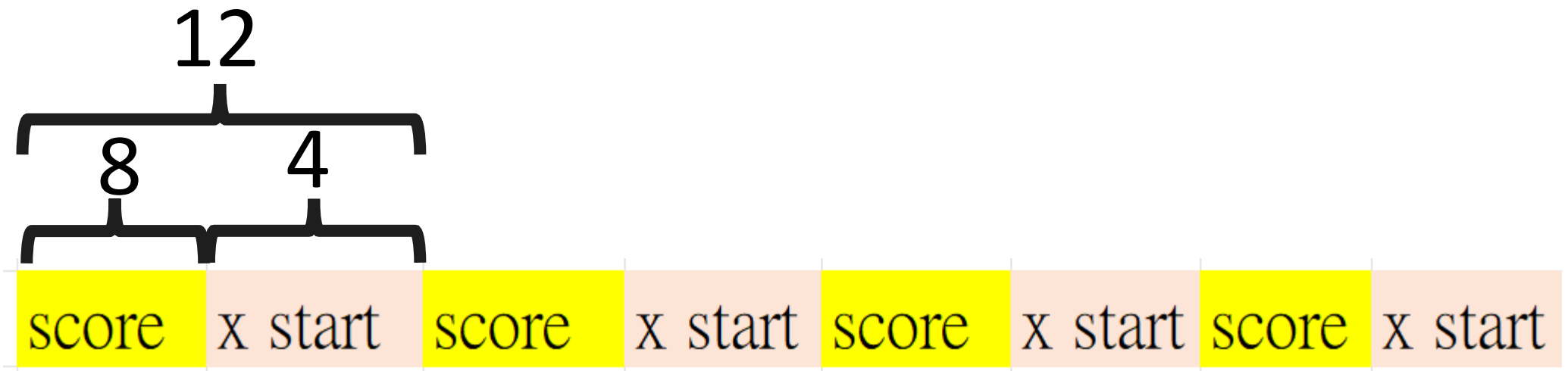
取得比對區間



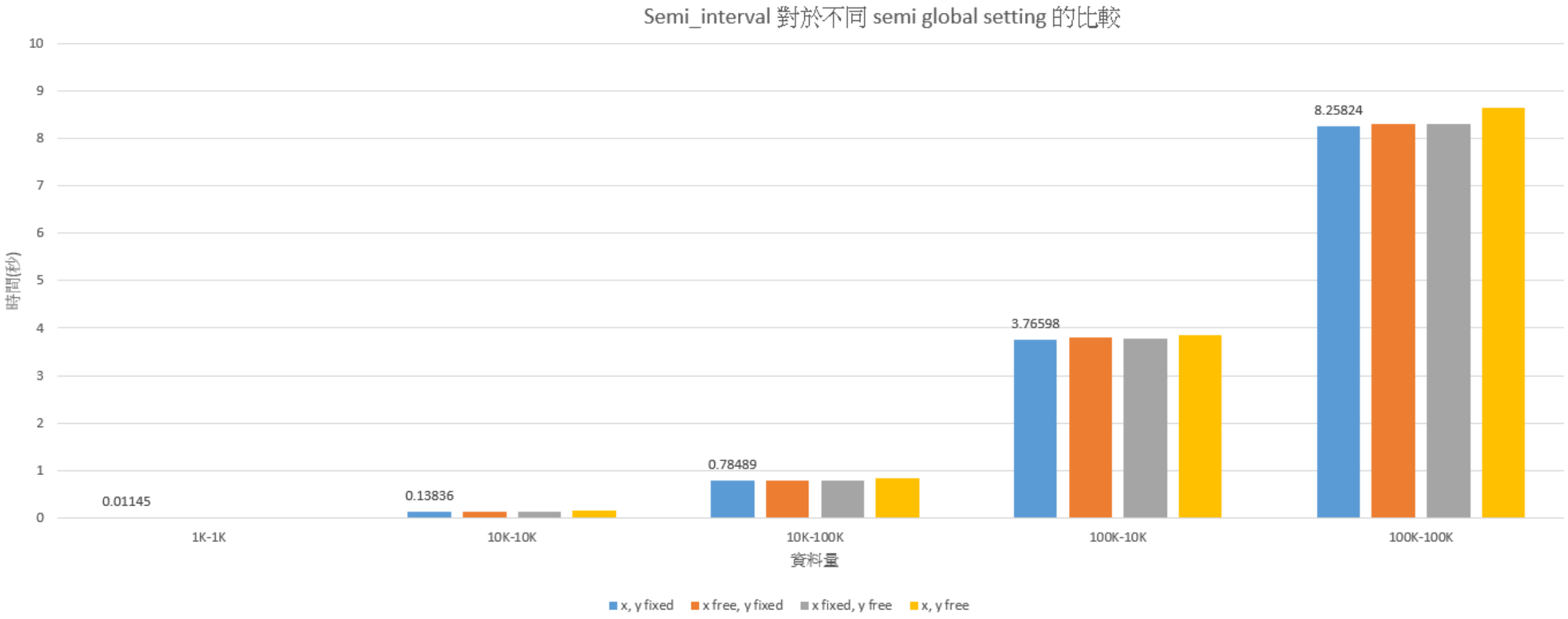
Semi Global Setting




16
8
4
4
score
x start
y start
score
x start
y start
score
x start
y start


12
8
4
score
x start
score
x start
score
x start
score
x start

Semi Global Setting (記憶體對齊後)



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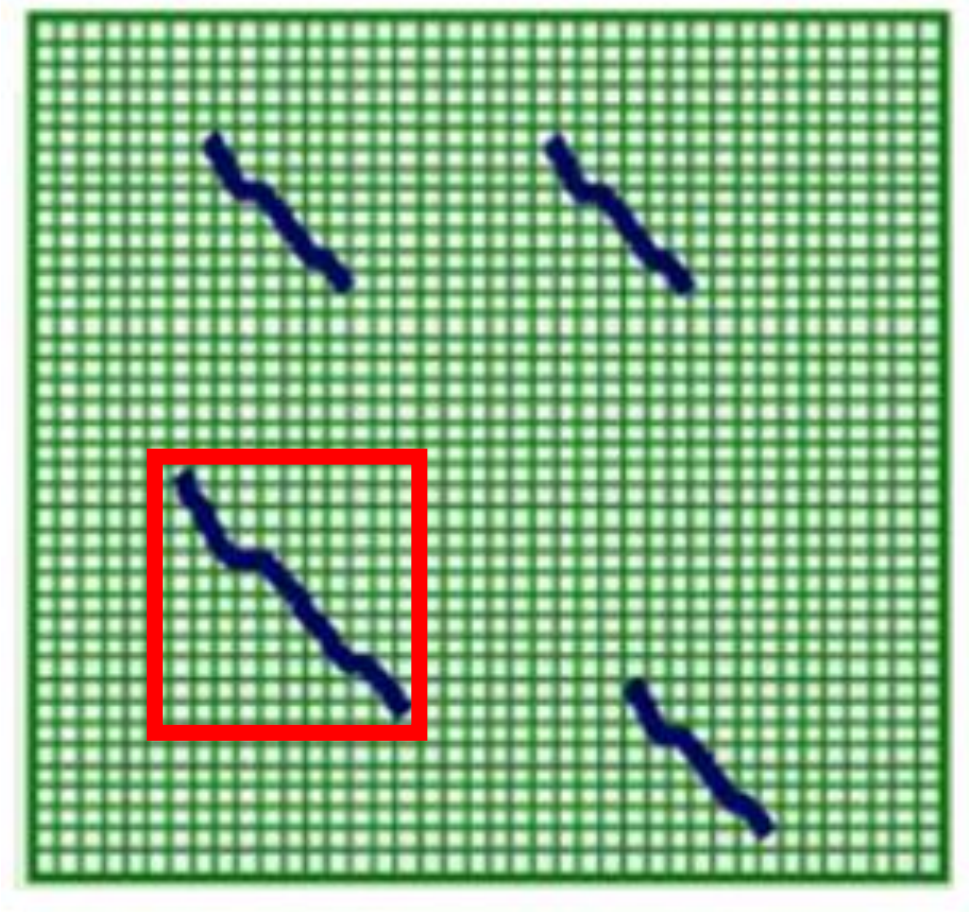
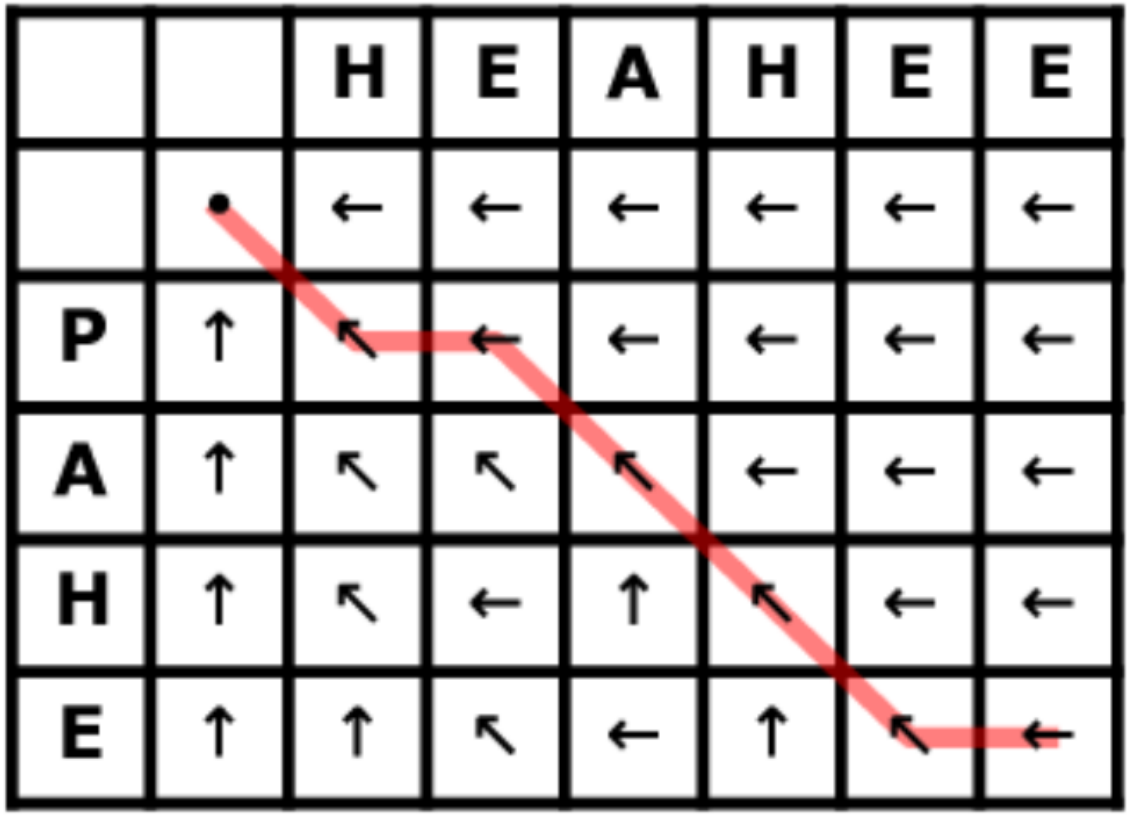
如何得到序列比對

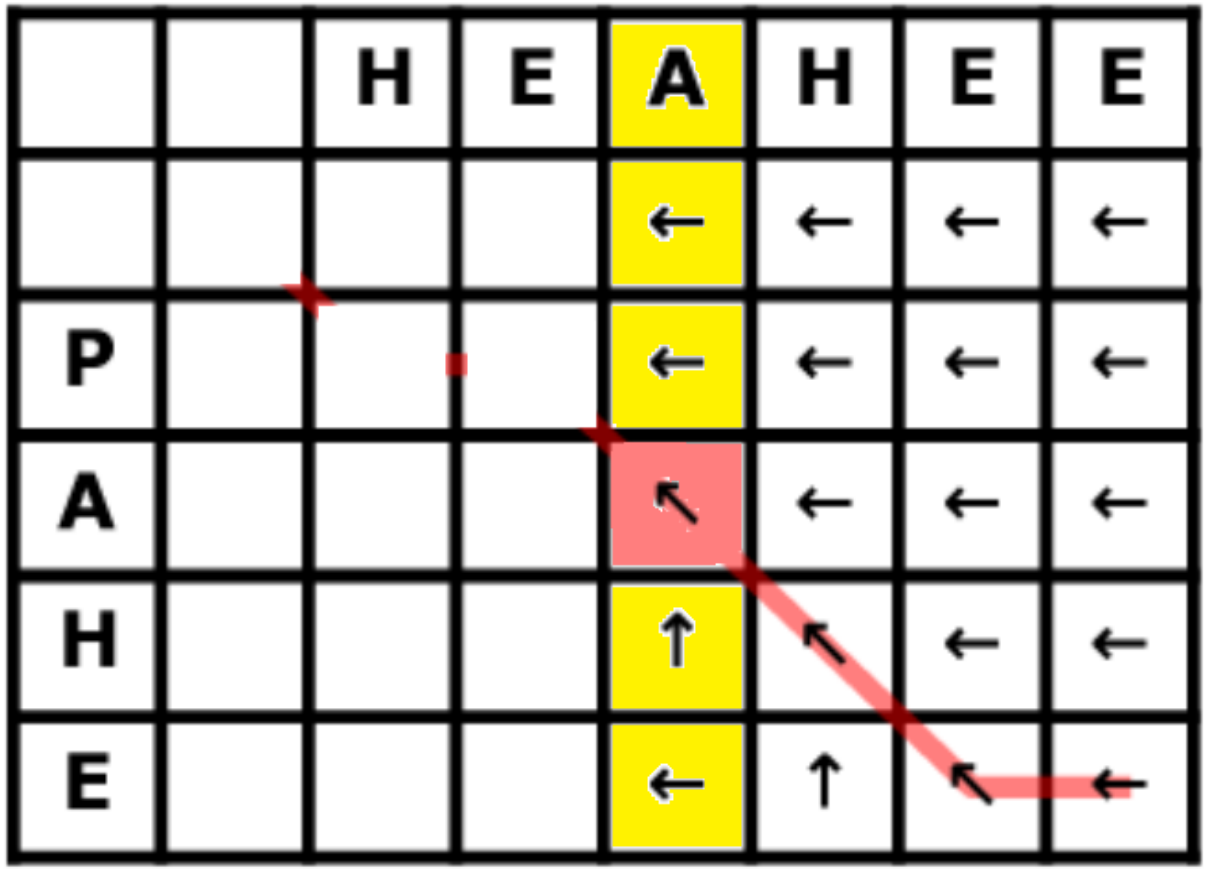


產生比對

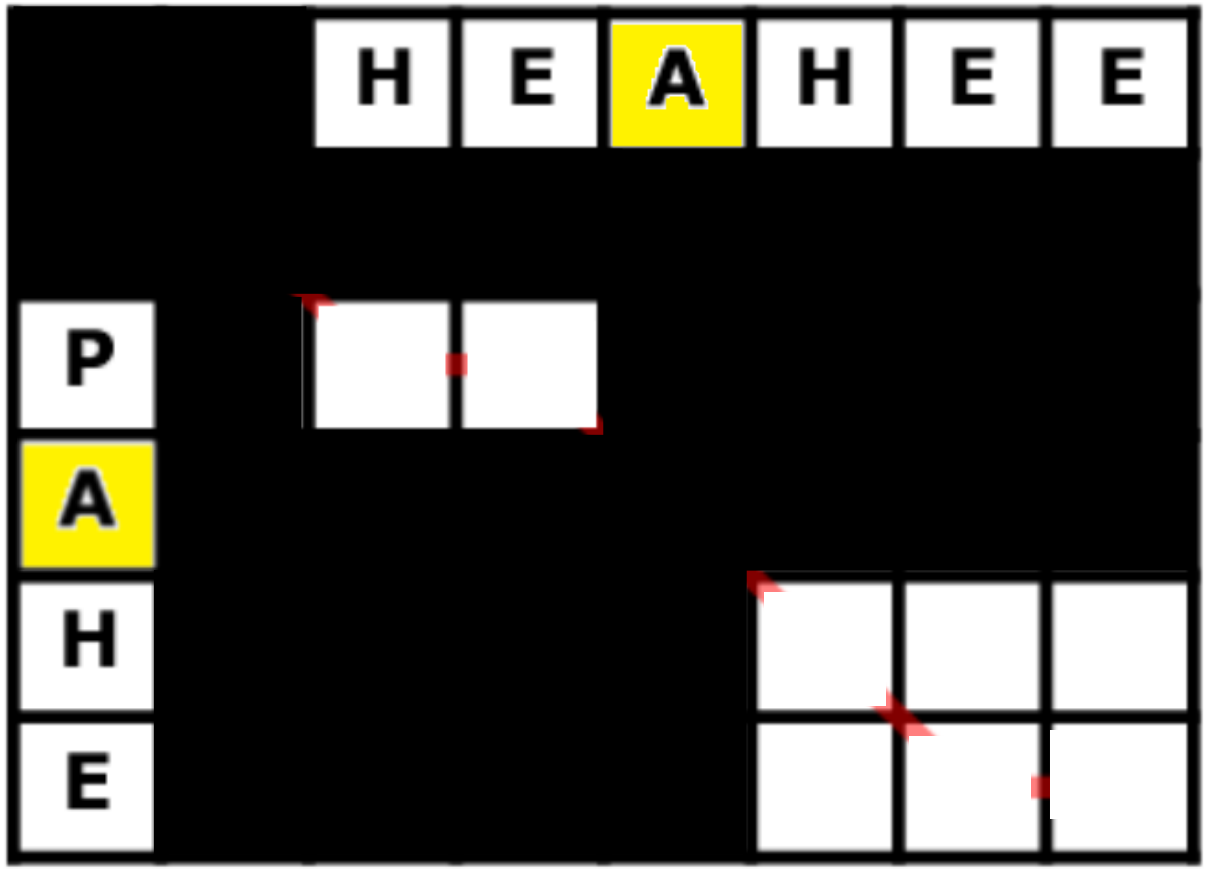


空間複雜度
=O(n^2)

找中間點



切割

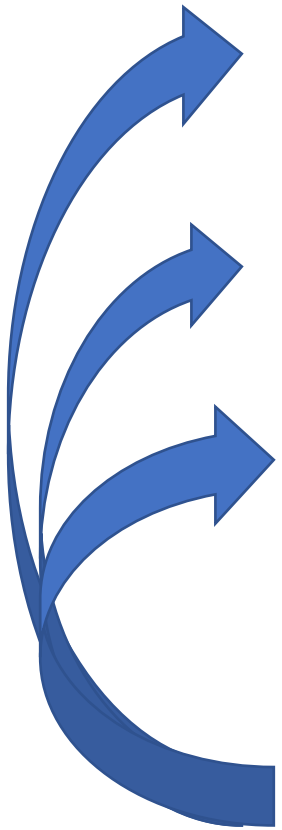


T(n,m)

=nm+nm/2+nm/4+...

=O(nm)

Conquer and Divide



1. 遞迴中斷點可使用O(n^2)演算法 (60000*60000) (印出比對結果)。
2. 找到切割點，將題目分成兩個子問題，(0,0) 初始化在函式外。
3. 解決左邊的子問題
4. 印出切割點比對，若 x 是一個 gap，右邊子問題 (0,0) 位置初始為 (m,x,y):=(-inf,-inf,0)，否則為 (0,-inf,-inf)
5. 解決右邊的子問題

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      - Dynamic Programing with CUDA
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時間複雜度

n>>t, n, m 是 X, Y 序列的長度，t 為 GPU 可平行化數量的最大值

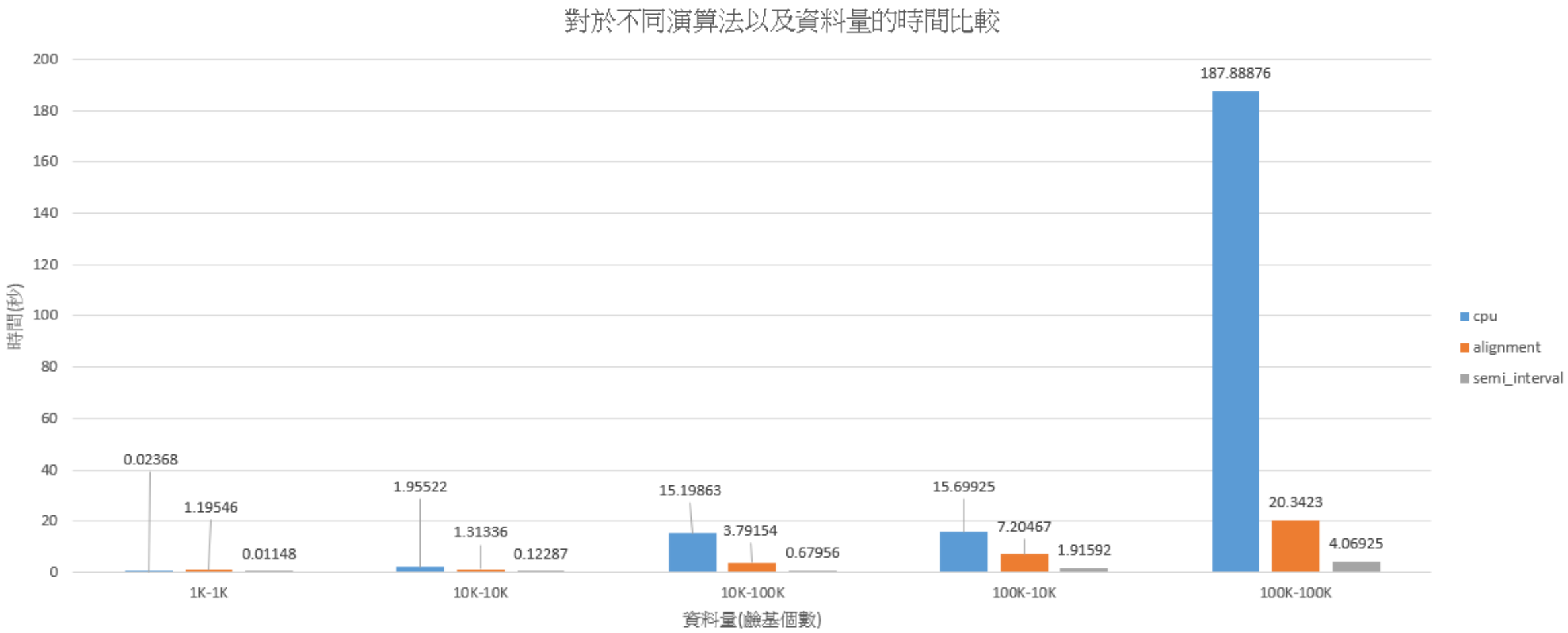
Semi Global Interval

- CPU: T(n,m)=O(nm)
- GPU: T(n,m)=O((n/t)m)

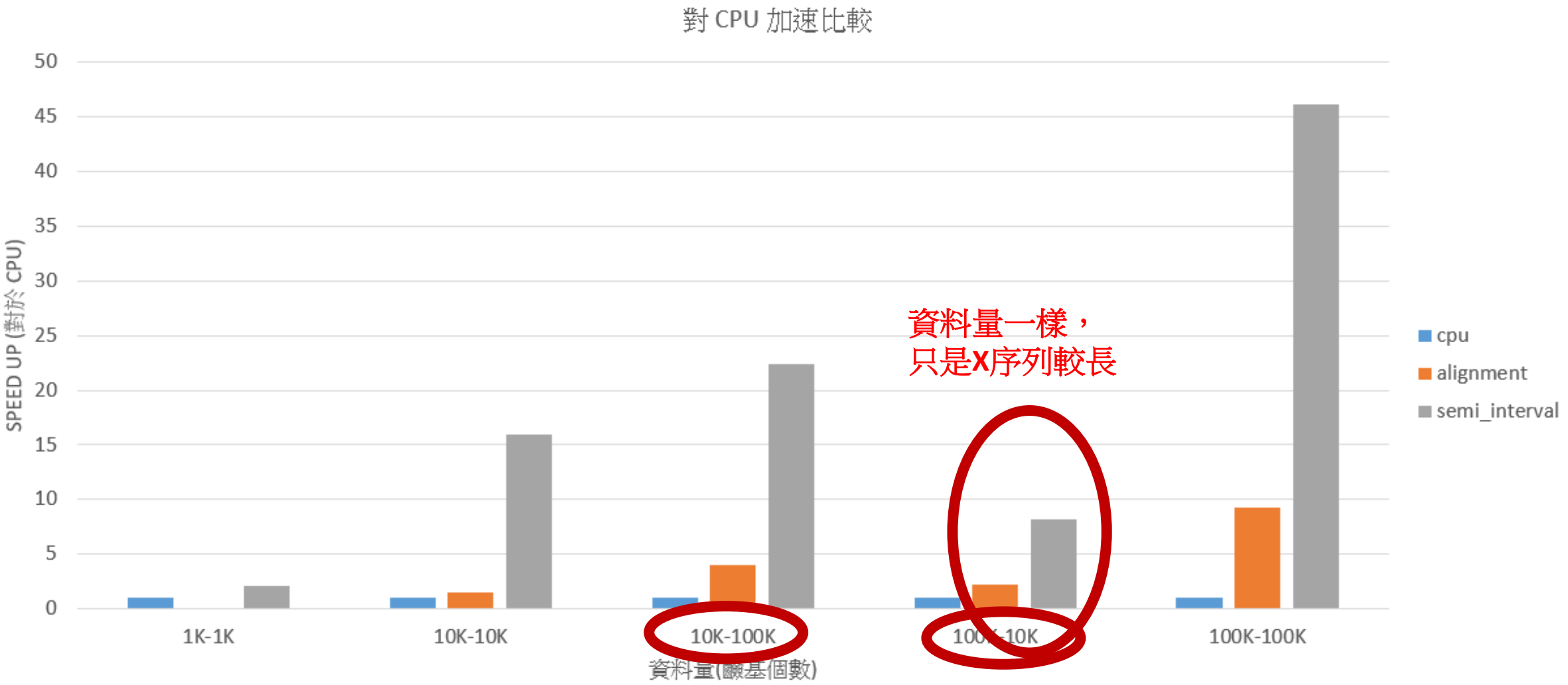
Alignment

- CPU: T(n,m)=O(nm)
- GPU: T(n,m)=O((n/t)m)　　;if t==n (O(mlgn))

Global alignment

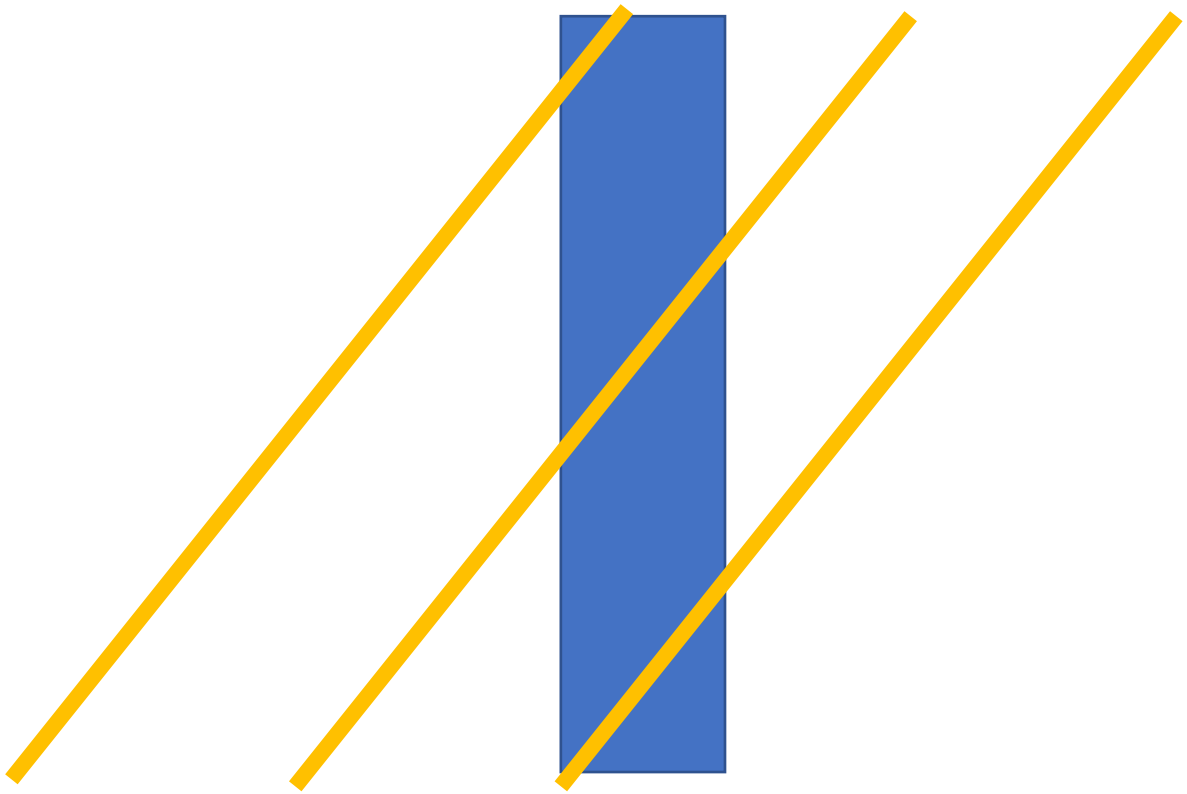


Global alignment



Cache Miss

10K-100K



100K-10K

我的原始碼

- https://github.com/paul90317/Semi-Sequence-Alignment-with-Cuda

致謝

賀保羅 教授(指導教授)

盧宥霖 學長(實驗室裡做 CUDA 研究的學長)

圖片 連結

- Data Dependency
- Semi Global
- Semi Global Matrix