

### **University of Pisa**

# **Computer Architecture 2023-24**

### **KMeans parallel implementation**

Students
Carlo Pio Pace
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#### Input:

- Dataset of points
- Number of clusters K
- Max # of iterations

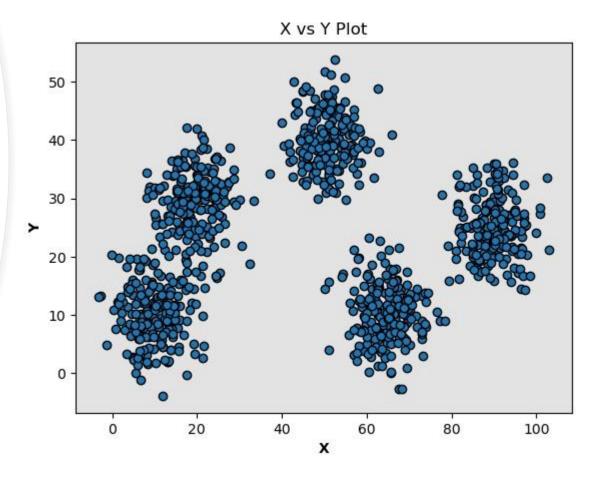
#### Output:

- A set of K points called Centroids
- The membership of each point in the dataset to one of the K clusters

#### Parameters:

- K=5
- Max # of iterations = 10

#### 1) Start Execution



#### Input:

- Dataset of points
- Number of clusters K
- Max # of iterations

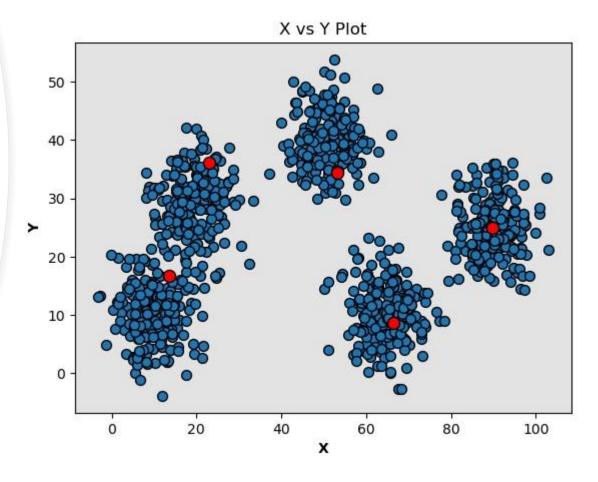
#### Output:

- A set of K points called Centroids
- The membership of each point in the dataset to one of the K clusters

#### Parameters:

- K=5
- Max # of iterations = 10

#### 2) Initialization of K random Centroids



#### Input:

- Dataset of points
- Number of clusters K
- Max # of iterations

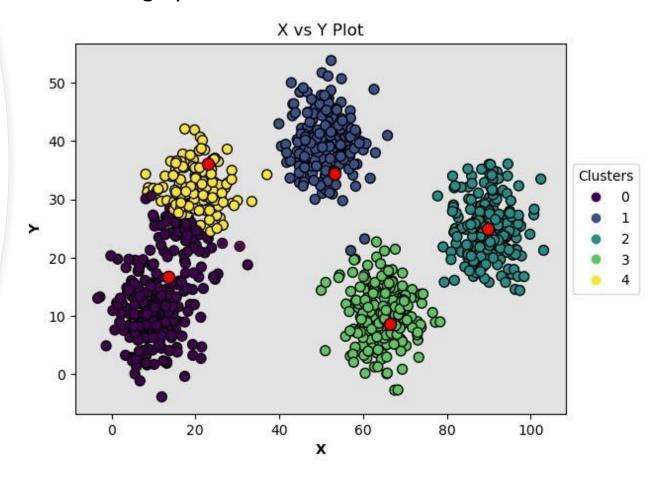
#### Output:

- A set of K points called Centroids
- The membership of each point in the dataset to one of the K clusters

#### Parameters:

- K=5
- Max # of iterations = 10

#### 3) Assign points to clusters



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#### Input:

- Dataset of points
- Number of clusters K
- Max # of iterations

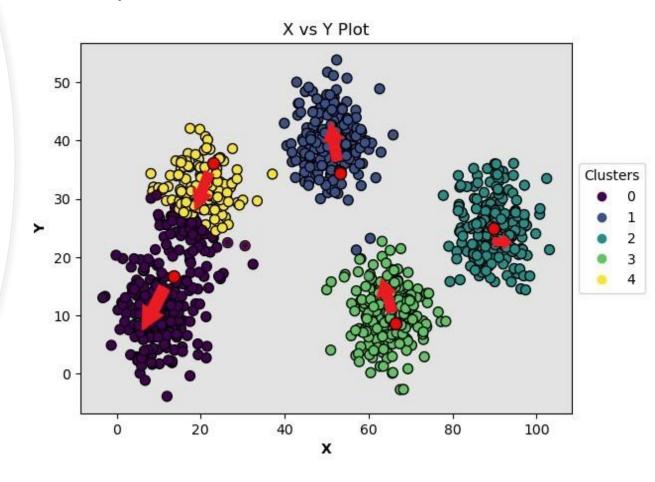
#### Output:

- A set of K points called Centroids
- The membership of each point in the dataset to one of the K clusters

#### Parameters:

- K=5
- Max # of iterations = 10

#### 4) Update Centroids



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#### Input:

- Dataset of points
- Number of clusters K
- Max # of iterations

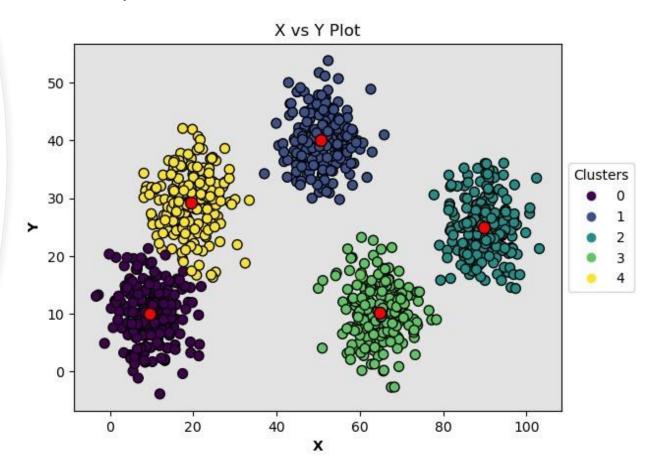
#### Output:

- A set of K points called Centroids
- The membership of each point in the dataset to one of the K clusters

#### Parameters:

- K=5
- Max # of iterations = 10

#### 5) Repeat from 3 until Max # of iterations

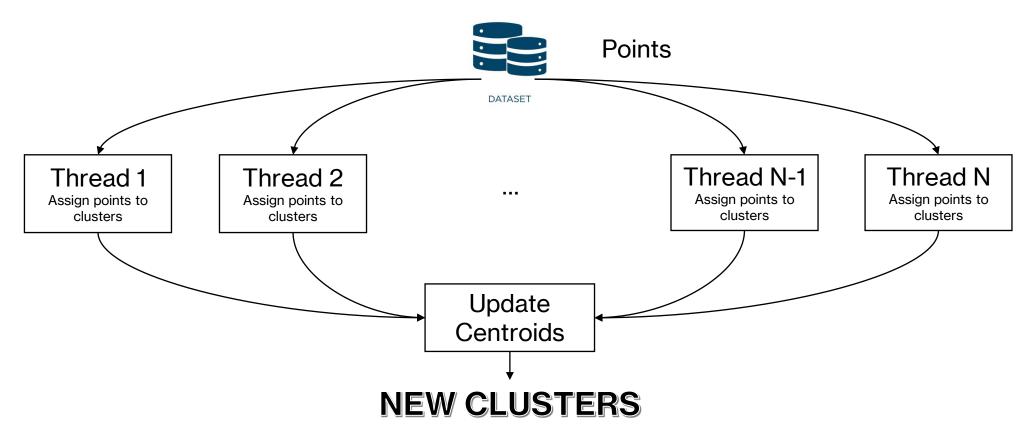


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# The Goal

To obtain a solution that has an execution time of maximum 5 seconds on 10M dataset points.

# How to make it work in parallel



# How to make it work in parallel

# Visual Studio

```
for (int indexOfPoint = arguments->startIndex; indexOfPoint < arguments->endIndex; indexOfPoint++) {
    30 (0,07%)
                 123
                                  Point *point=accessByIndex(arguments->points, indexOfPoint);
                 124
                 125
    28 (0,07%)
                                  for (int clusterIndex = 0; clusterIndex < arguments->K; clusterIndex++) {
    63 (0,16%)
                 126
                 127
                 128
                                      float sumPartial = 0:
                                      for (int dim = 0; dim < arguments->DIM; dim++) {
   120 (0,30%)
                 129
                                          Point* centroidPoint = accessByIndex(arguments->centroids, clusterIndex);
    94 (0,23%)
                 130
                                          sumPartial += pow(centroidPoint->coordinate[dim] - point->coordinate[dim], 2);
28145 (70,22%)
                 131
                 132
                                      // Compute distance from a point to all centroids
                 133
                                      dists[clusterIndex] = sqrt(sumPartial);
 3473 (8,66%)
                 134
                                                                                        x \in R^{DIM}, y \in R^{DIM} d(x,y) = \sqrt{\sum_{i=1}^{DIM} (x_i - y_i)^2}
                 135
```

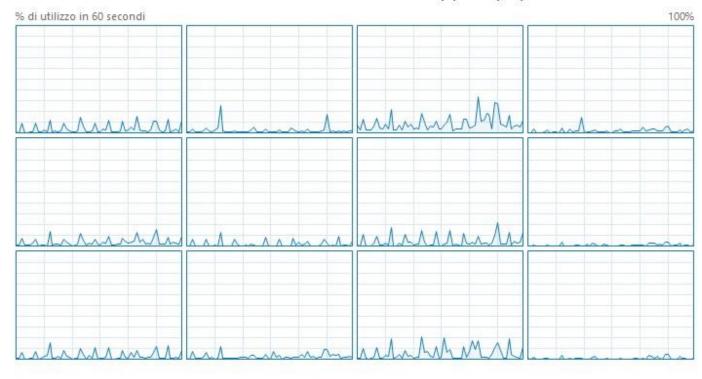
Idea: exploit thread parallelism to work independently on different chunks of equal size of the dataset and then merge the results to update the centroids as in the sequential version.

#### **Architecture used**

- CPU: Intel<sup>®</sup> Core<sup>™</sup> i7-8700 Processor
  - 6 Cores, 12 Threads
  - Clock: Up to 3.20 Ghz
  - Max Turbo Frequency:
     4.60 GHz
  - Cache:
    - ➤ Level 1: 384 KB
    - ➤ Level 2: 1.5 MB
    - ➤ Level 3: 12 MB
- RAM: 16 GB DDR4 2133 MHz

#### CPU

Intel(R) Core(TM) i7-8700 CPU @ 3.20GHz



Utilizzo	Velocità		Velocità di base:	3,19 GHz	
7%	3,16 GHz		Processori fisici:	1	
1 70	3,100	1 12	Cores:	6	
Processi	Thread	Handle	Processori logici:	12	
263	3828	143324	Virtualizzazione:	Abilitato	
			Cache L1:	384 KB	
Tempo di attività			Cache L2:	1,5 MB	
1:12:10:18			Cache L3: 12,01		

#### **Architecture used**

- CPU: Intel<sup>®</sup> Core<sup>™</sup> i7-8700 Processor
  - 6 Cores, 12 Threads
  - Clock: Up to 3.20 Ghz
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     4.60 GHz
  - Cache:
    - ➤ Level 1: 384 KB
    - > Level 2: 1.5 MB
    - ➤ Level 3: 12 MB
- RAM: 16 GB DDR4 2133 MHz

#### **Cache details**

- Level 1:
  - Data: 32 Kbytes 8-way set associative;
  - Instructions: 32 Kbytes 8way set associative;
- Level 2 : 256 Kbytes 4-way set associative;
- Level 3: 12 Mbytes 16-way set associative;

# **Measuring method**

#### Function clock() in time.h C library

#### Why:

- It calculates CPU time and not Wall-clock time (with small errors)
- On modern machines, precision of ms
- C is a standard
- C is the language in which we developed the algorithm

#### How it works:

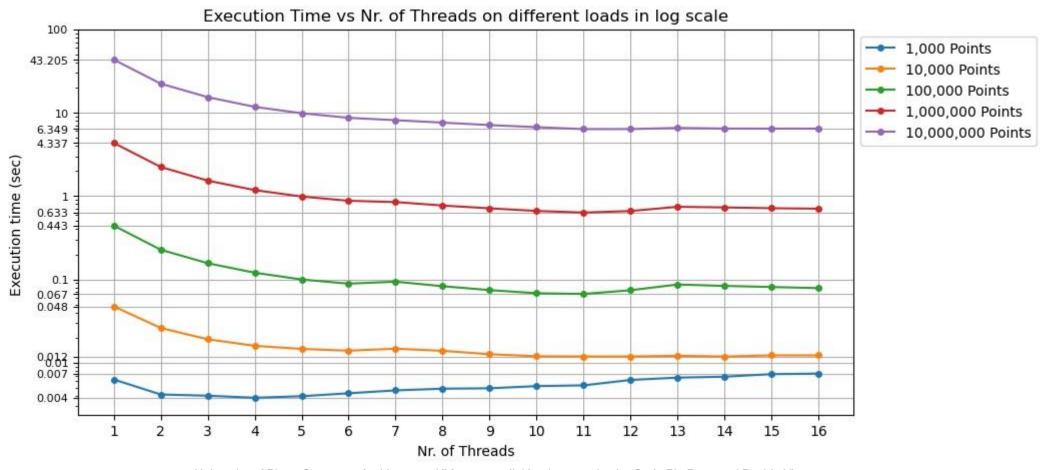
The function clock() defined in this library returns the corresponding cpu time at the instant when it's called.

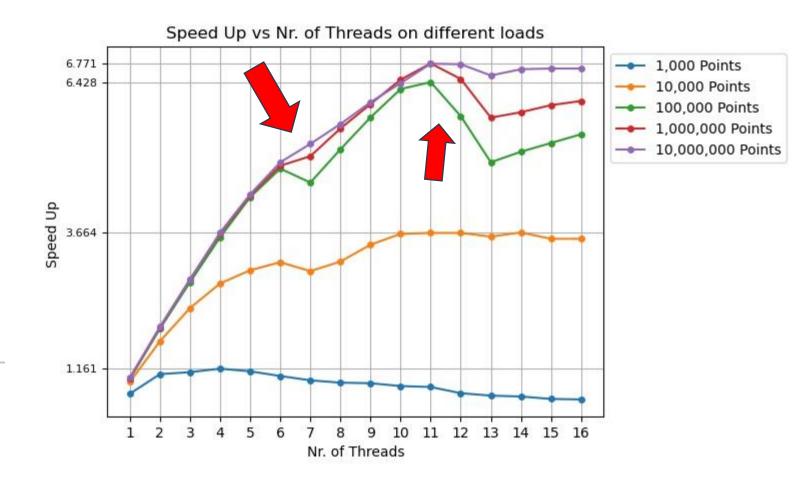
# Measuring method

```
@echo off
REM parameter 1 Number of algorithm execution
REM parameter 2 Dataset size
REM parameter 3 Maximum number of thread to reach
REM Check if all three parameters are provided
if "%~3"=="" (
    echo Please provide three input parameters.
    exit /b 1
set "exe path=filepath"
set "result file=results.txt"
for /l %%i in (1, 1, %3) do (
        echo datasetPath=clustering dataset %2.csv
        echo csvCharSplit=,
        echo numberOfClusters K=5
        echo maxIterations=10
        echo nrThreads=%%i
    ) > config.properties
  for /L %%c in (1,1,%1) do (
    echo Running .exe program for thread %%i
    %exe path%
    echo Program executed for thread %%i.
  REM Rename the file to the desired format
  rename %result file% KmeansMeasure %2 %%i
pause
```

```
start_alg = clock();
for (int nrIteration = 0; nrIteration < MAX_ITERATIONS; nrIteration++) {
    // Wake up all the sospended threads.
    for (int i = 0; i < NR_THREADS; i++) {
       ResumeThread(handles[i]);
    // Wait until all the threads has produced their results and then come to sleep.
    WaitForMultipleObjects(NR_THREADS, suspendEvents, TRUE, INFINITE);
    // Aggregate partial results
    for (int j = 0; j < K; j++) {
       Point* totSum = accessByIndex(&sums, j);
       for (int i = 0; i < NR_THREADS; i++) {
           Point* partialSum = accessByIndex(results[i].sums, j);
           for (int dim = 0; dim < DIM; dim++) {
                totSum->coordinate[dim] += partialSum->coordinate[dim];
            counts[j] += results[i].counts[j];
    updateCentroids(K, DIM, &centroids, &sums, counts);
    // Reset the variables to track sospension next iterations.
    for (int i = 0; i < NR_THREADS; i++) {
       ResetEvent(suspendEvents[i]);
end_alg = clock();
```

# **CPU time comparison**





# Speed Up – What's Up?



CORE 0	CPU 0	CPU 1		
CORE 1	CPU 2	CPU 3		
CORE 2	CPU 4	CPU 5		
CORE 3	CPU 6	CPU 7		
CORE 4	CPU 8	CPU 9		
CORE 5	CPU 10	CPU 11		

How the software threads are assigned to our logical core units?

The O.S. schedule them according his own policy

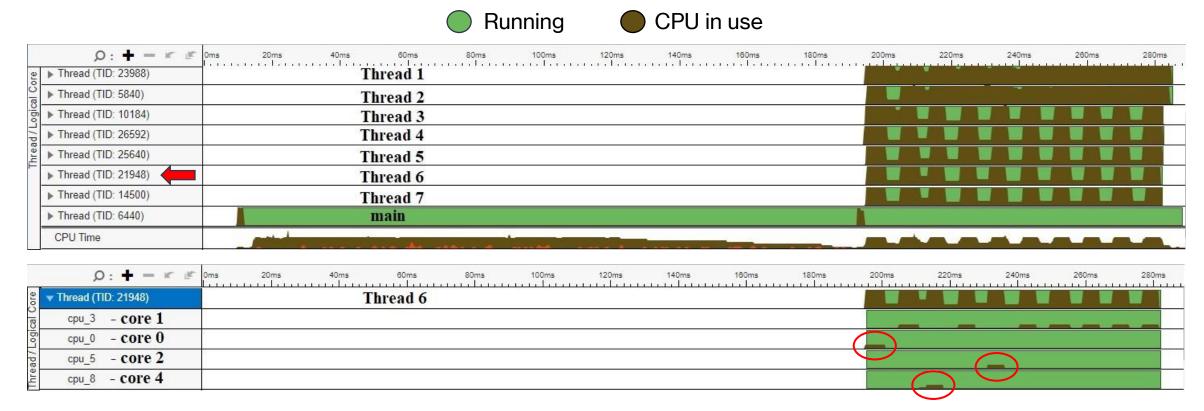
# Speed Up – What's Up?



- 100 000 Points dataset

- 7 Threads

- Clusters=5 & Max # of iterations = 10

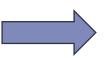


# Speed Up – What's Up?

### **Affinity:**

The explicit request to O.S. to assign a process or thread to a specific logical core inside a specific physical core.

# **Using affinity**



# Following logical cores order

CORE 0	CPU 0	CPU 1 T2
CORE 1	CPU 2 T3	CPU 3 T4
CORE 2	CPU 4 T5	CPU 5
CORE 3	CPU 6	CPU 7
CORE 4	CPU 8	CPU 9
CORE 5	CPU 10	CPU 11

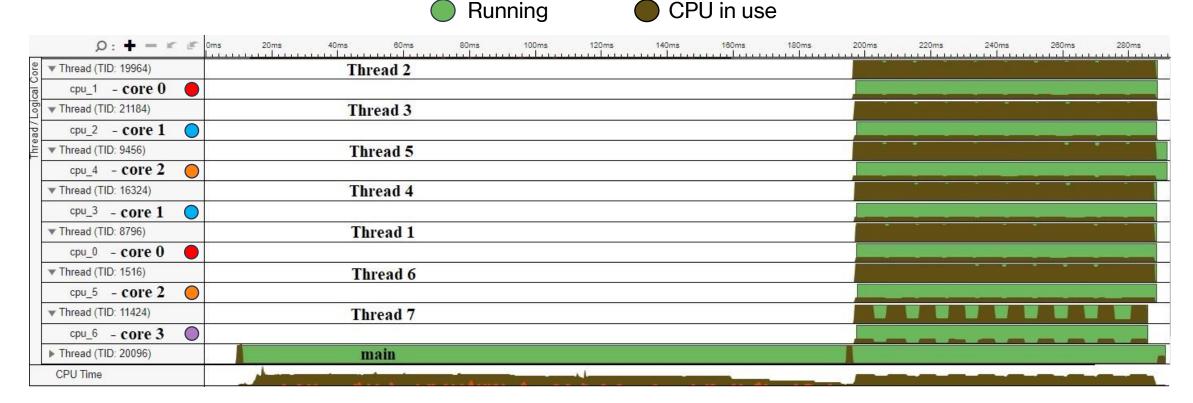
# Following logical cores order



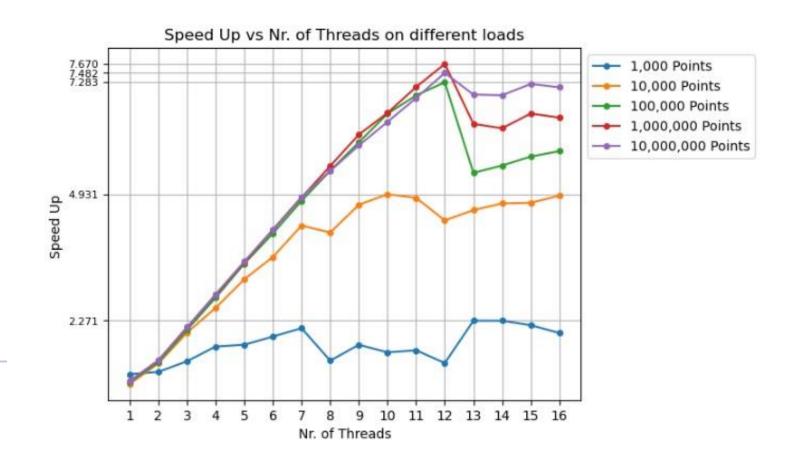
- 100 000 Points dataset

- 7 Threads

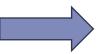
- Clusters=5 & Max # of iterations = 10



# affinity set to follow logical cores order



## **Using affinity**



# Following physical cores order

CORE 0	CPU 0	CPU 1 T7
CORE 1	CPU 2 T2	CPU 3
CORE 2	CPU 4 T3	CPU 5
CORE 3	CPU 6 T4	CPU 7
CORE 4	CPU 8 T5	CPU 9
CORE 5	CPU 10 T6	CPU 11

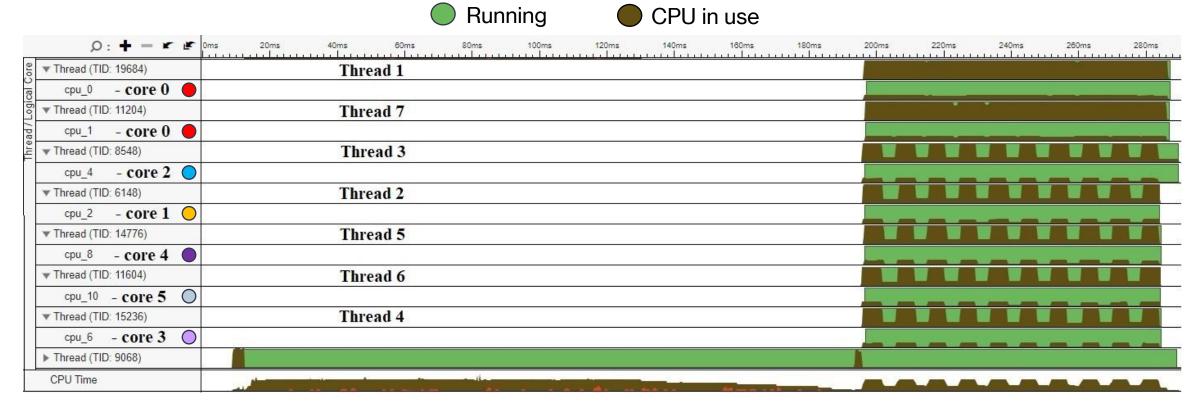
# Following physical cores order



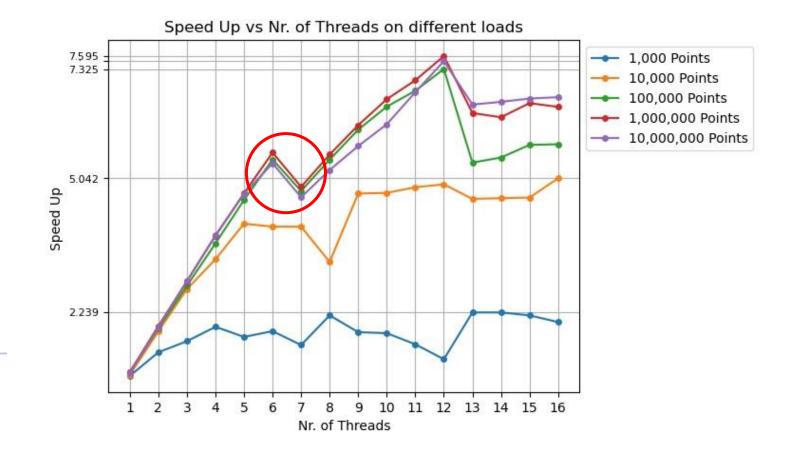
- 100 000 Points dataset

- 7 Threads

- Clusters=5 & Max # of iterations = 10



affinity set to follow physical cores order



# What's the cause of this effect?

**Memory bound**: issues on the memory subsystem (cache) that causes the introduction of stalls inside pipeline slots due miss.

# How to interpret the values



Physical Core / Thread / Function / Call Stack	CPU Time ▼	Memory Bound				LLC Miss	Landa	Ctores	
		L1 Bound	L2 Bound	L3 Bound	DRAM Bound	Store Bound	Count	Loads	Stores
core_3	134.242ms	22.1%	0.9%	0.5%	0.5%	0.1%	26,000	93,847,000	31,655,000
▶ core_0	101.974ms	20.0%	0.4%	2.0%	0.0%	0.1%	0	68,471,000	23,465,000
core_5	95.614ms	20.5%	0.6%	1.3%	0.0%	0.0%	0	68,627,000	23,218,000
▶ core_1	95.175ms	19.1%	0.7%	1.1%	0.0%	0.0%	0	75,413,000	25,441,000
⊳ core_4	83.709ms	19.8%	0.7%	0.7%	0.4%	0.1%	0	62,803,000	21,190,000
core_2	74.812ms	17.9%	0.6%	0.5%	0.4%	0.2%	0	57,551,000	19,422,000

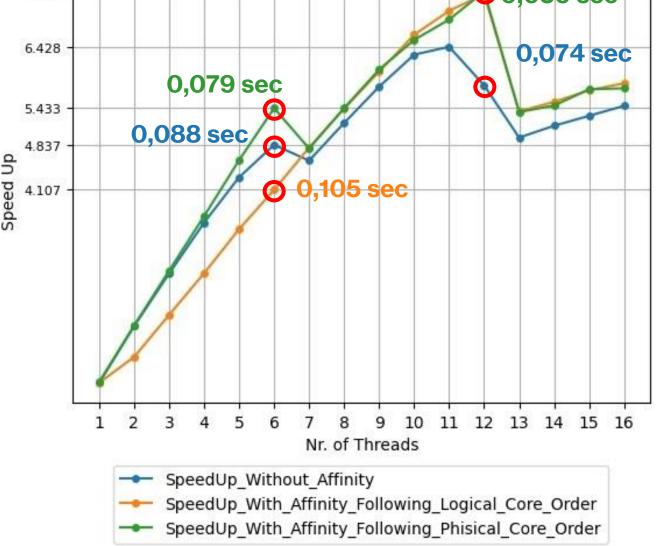
- 100 000 Points dataset

- 6 Threads

- Without Affinity

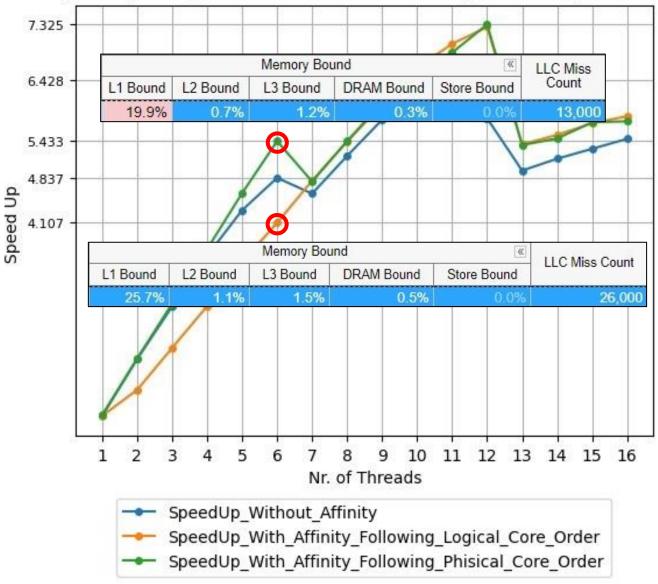
**Comparison on** 100.000 points with different affinity methodologies

## Speed Up comparison between methodologies on 100,000 Points **0**0,059 sec 7.325 0,074 sec 0,079 sec 0,088 sec



Comparison on 100.000 points with different affinity methodologies

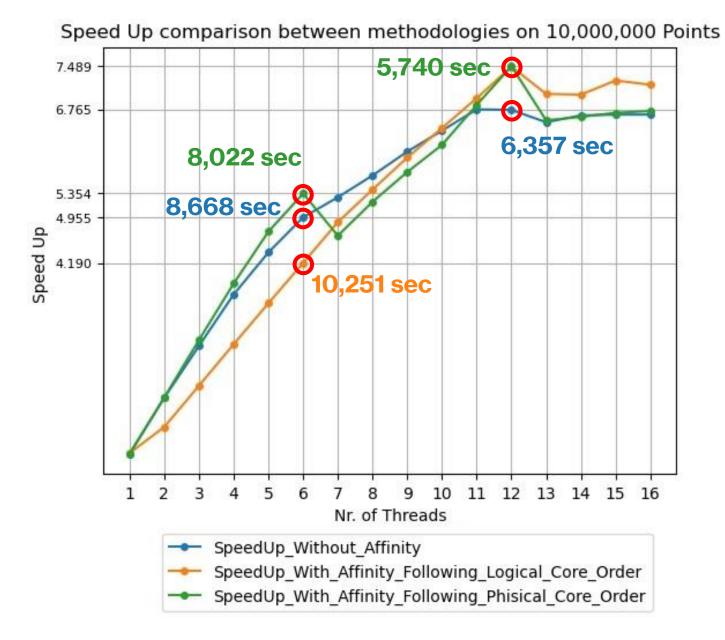
#### Speed Up comparison between methodologies on 100,000 Points



Comparison on 100.000 points with different affinity methodologies

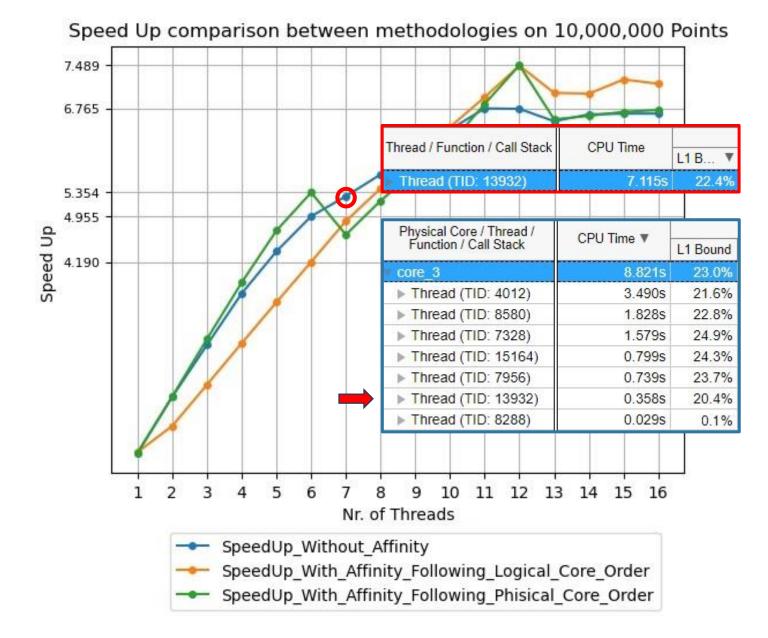
#### Speed Up comparison between methodologies on 100,000 Points 7.325 6.428 Memory Bound LLC Miss CPU Time ▼ Count L2 Bound L3 Bound DRAM Bound Store Bound L1 Bound 5.433 224 530ms 0.9% 1.2% 26,000 0.4% 4.837 Speed Up Memory Bound LLC Miss CPU Time ▼ 4.107 Count L1 Bound L2 Bound L3 Bound DRAM Bound Store Bound 226.410ms 25.5% 1.2% 0.5% 26,000 Nr. of Threads SpeedUp Without Affinity SpeedUp\_With\_Affinity\_Following\_Logical\_Core\_Order SpeedUp With Affinity Following Phisical Core Order

Comparison on 10.000.000 points with different affinity methodologies



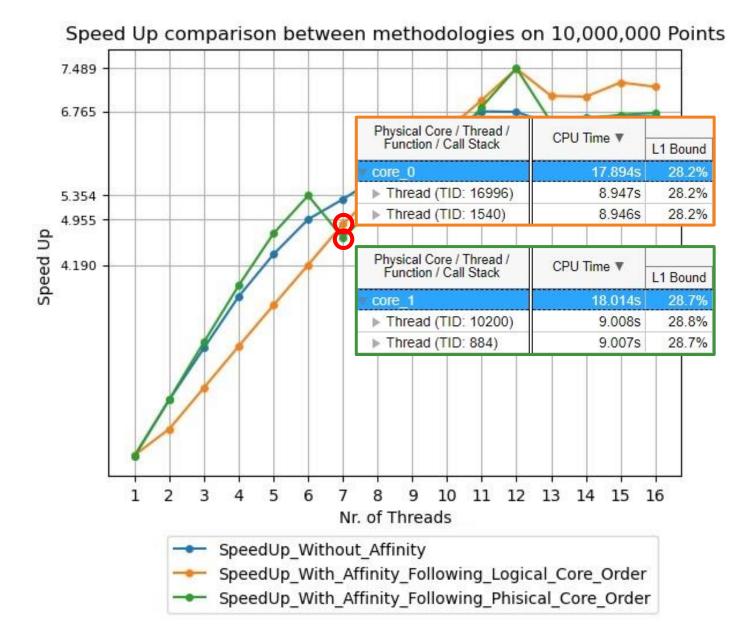
# Comparison on 10.000.000 points with different affinity methodologies

The O.S obtains a smoother curve increasing the load and in some cases better than with fixed affinity management.



# Comparison on 10.000.000 points with different affinity methodologies

The O.S obtains a smoother curve increasing the load and in some cases better than with fixed affinity management.



# **Optimizations**

#### **OPT.1: Data structures**

```
// Define the structure for a Point
vtypedef struct {
    double coordinate[3];
} Point;
```

```
DynamicList points;
DynamicList centroids;
DynamicList sums;
```



```
Point* points = (Point*)malloc(DATASET_SIZE * sizeof(Point));
Point* centroids = (Point*)malloc(K * sizeof(Point));
Point* sums = (Point*)malloc(K * sizeof(Point));
```

# **Optimizations**

#### **OPT.2: Math.h**

```
for (int clusterIndex = 0; clusterIndex < arguments->K; clusterIndex++) {
   float sumPartial = 0;
   for (int dim = 0; dim < arguments->DIM; dim++) {
       sumPartial += pow(arguments->centroids[clusterIndex].coordinate[dim] - point.coordinate[dim], 2);
   // Compute distance from a point to all centroids
   dists[clusterIndex] = sqrt(sumPartial);
for (int clusterIndex = 0; clusterIndex < arguments->K; clusterIndex++) {
   float sumPartial = 0;
   for (int dim = 0; dim < arguments->DIM; dim++) {
       double partialDiff = arguments->centroids[clusterIndex].coordinate[dim] - point.coordinate[dim];
       sumPartial += partialDiff * partialDiff;
   // Compute distance from a point to all centroids
   dists[clusterIndex] = sqrt(sumPartial);
```

# **Optimizations**

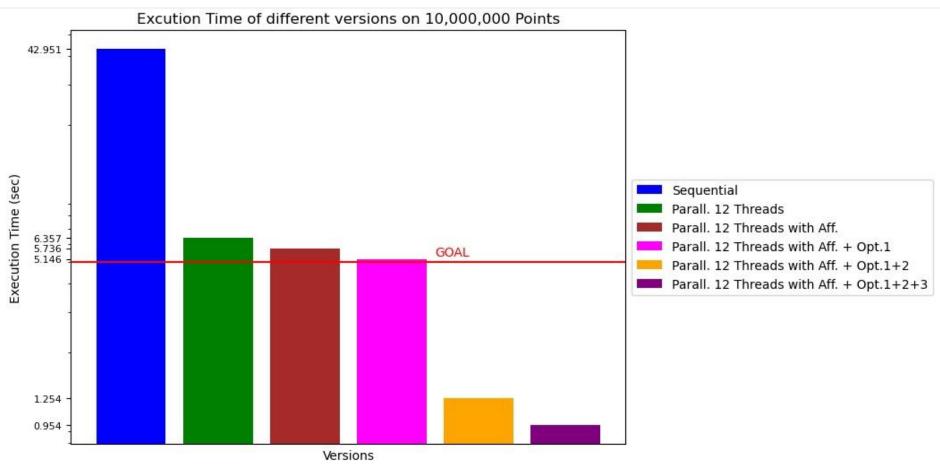
#### **OPT.3: To act on the algorithm** ... a little

We are not actually interested in obtaining the exact distance, but only to discover the minimum among all the centroids.

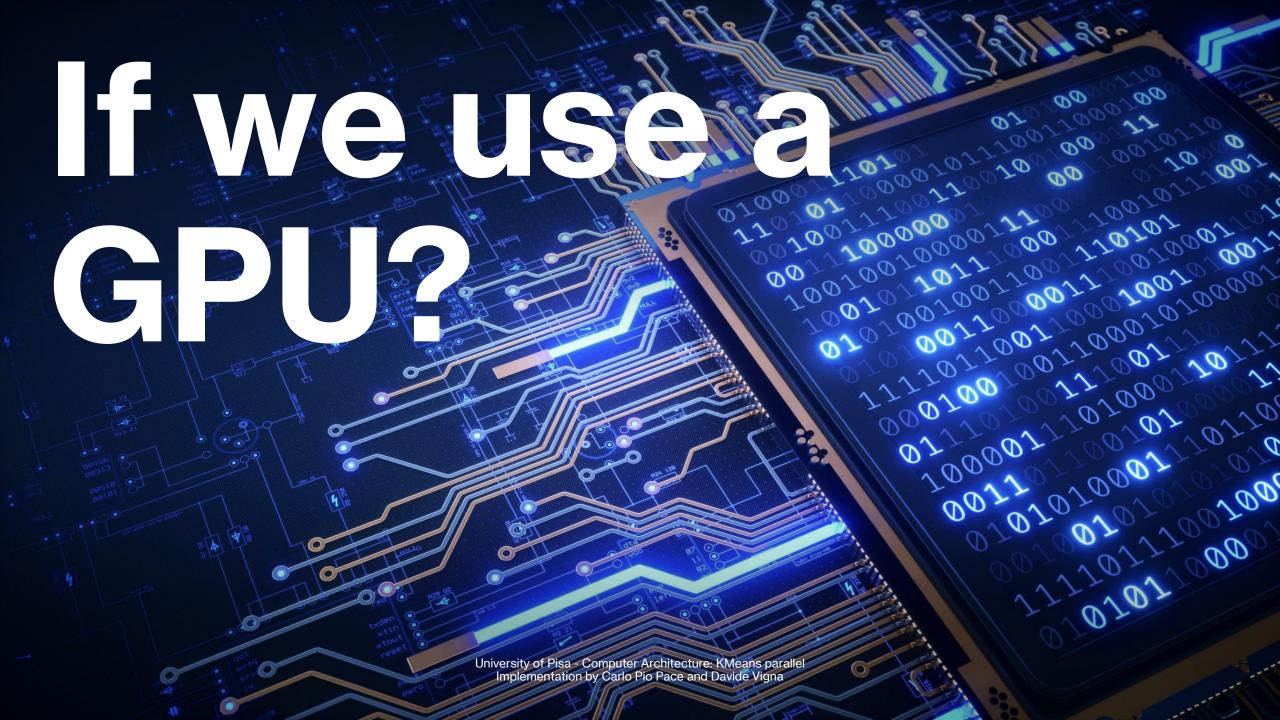
We can avoid to compute the square root.

```
for (int clusterIndex = 0; clusterIndex < arguments->K; clusterIndex++) {
    float sumPartial = 0;
    for (int dim = 0; dim < arguments->DIM; dim++) {
        double partialDiff = arguments->centroids[clusterIndex].coordinate[dim] - point.coordinate[dim];
        sumPartial += partialDiff * partialDiff;
    }
    // Compute distance from a point to all centroids
    //*dists[clusterIndex] = sqrt(sumPartial);*/
    dists[clusterIndex] = sumPartial;
}
```

# **Optimizations results**



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# **GPU Nvidia GeForce GTX 1060**

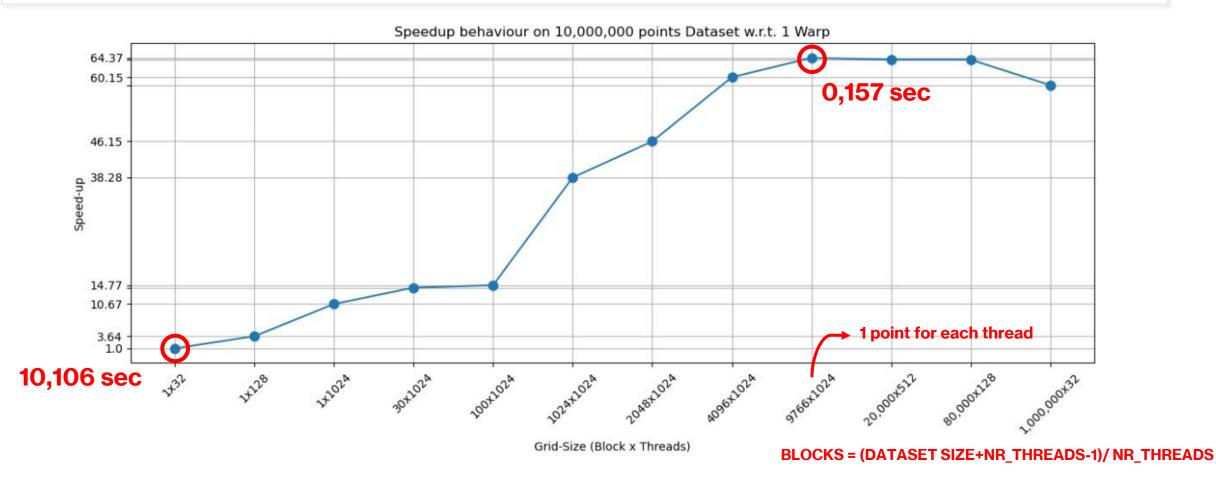


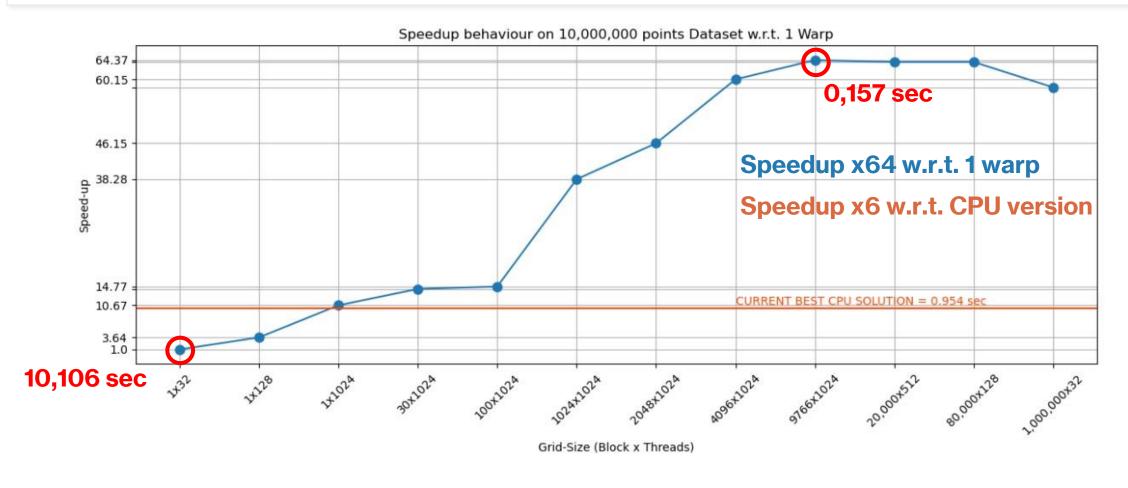
```
Device 0: "NVIDIA GeForce GTX 1060 6GB"
 CUDA Driver Version / Runtime Version
                                                12.4 / 12.4
 CUDA Capability Major/Minor version number:
                                                6.1
 Total amount of global memory:
                                                6144 MBytes (6442188800 bytes)
 (010) Multiprocessors, (128) CUDA Cores/MP: 1280 CUDA Cores
                                                1759 MHz (1.76 GHz)
 GPU Max Clock rate:
 Memory Clock rate:
                                                4004 Mhz
 Memory Bus Width:
                                                192-bit
 L2 Cache Size:
                                                1572864 bytes
 Maximum Texture Dimension Size (x,y,z)
                                                1D=(131072), 2D=(131072, 65536), 3D=(16384, 16384, 16384)
 Maximum Layered 1D Texture Size, (num) layers 1D=(32768), 2048 layers
 Maximum Layered 2D Texture Size, (num) layers 2D=(32768, 32768), 2048 layers
 Total amount of constant memory:
                                                65536 bytes
 Total amount of shared memory per block:
                                                49152 bytes
 Total shared memory per multiprocessor:
                                                98304 bytes
 Total number of registers available per block: 65536
 Maximum number of threads per multiprocessor: 2048
 Maximum number of threads per block:
                                                1024
 Max dimension size of a thread block (x,y,z): (1024, 1024, 64)
 Max dimension size of a grid size (x,y,z): (2147483647, 65535, 65535)
 Maximum memory pitch:
                                                2147483647 bytes
 Texture alignment:
                                                512 bytes
```

We mantain the same exact structure of the parallel CPU version

- 2 kernel functions
  - 1) assignPointsToClusterKernel<< <blooks, threads >> > (d\_points, d\_centroids, d\_membership, d\_sums, d\_counts, SIZE);
  - 2) updateCentroidsKernel << <1, K >> > (d\_centroids, d\_sums, d\_counts);
- Same measurement methods: function clock() in time.h C library
  - Focus on pure execution time
- What is its behavior? How do we select the # of blocks and threads?

```
printf("\nStart of the algorithm :");
start_alg = clock();
// Main loop of KMeans algorithm
for (int iter = 0; iter < MAX_ITERATIONS; ++iter) {
   // Launch kernel to assign points to clusters
    assignPointsToClusterKernel << <blocks, threads >> > (d_points, d_centroids, d_membership, d_sums, d_counts, SIZE);
    cudaDeviceSynchronize();
   // Launch kernel to update centroids
    updateCentroidsKernel << <1, K >> > (d_centroids, d_sums, d_counts);
    cudaDeviceSynchronize();
end_alg = clock();
printf("End of the algorithm: \n");
```





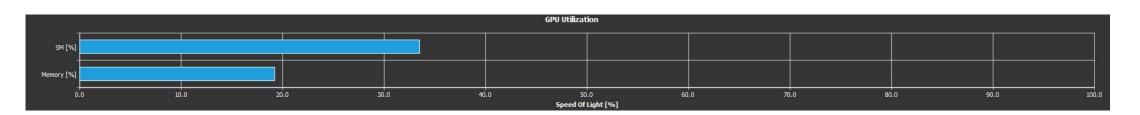
### **GPU – Profiler**



Recommendations

[Warning] This kernel exhibits low compute throughput and memory bandwidth utilization relative to the peak performance of this device. Achieved compute throughput and/or memory bandwidth below 60.0% of peak typically indicate latency issues. Look at `Scheduler Statistics` and `Warp State Statistics` for potential reasons.





### **GPU – Profiler**

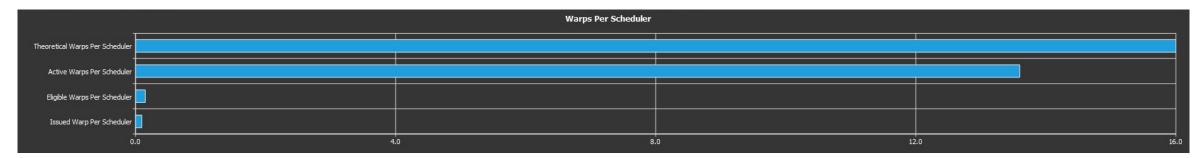


#### Recommendations

Issue Slot Utilization

[Warning] Every scheduler is capable of issuing two instructions per cycle, but for this kernel each scheduler only issues an instruction every 10.4 cycles. This might leave hardware resources underutilized and may lead to less optimal performance. Out of the maximum of 16 warps per scheduler, this kernel allocates an average of 13.60 active warps per scheduler, but only an average of 0.15 warps were eligible per cycle. Eligible warps are the subset of active warps that are ready to issue their next instruction. Every cycle with no eligible warp results in no instruction being issued and the issue slot remains unused. To increase the number of eligible warps either increase the number of active warps or reduce the time the active warps are stalled.





Atomic operations on double generate errors at compilation time!!

We used this one!

Two options:

How to solve?

- 1. Harware option: nvcc kernel.cu -o KMeansCuda -arch=sm\_61 (Faster)
- 2. Software (Slower)

https://docs.nvidia.com/cuda/cuda-compiler-driver-nvcc/index.html#gpu-feature-list

### Memory usage

Constant memory

Shared Memory

```
// Algorithm parameters used inside the device.
__constant__ int K;
__constant__ int DIM;
__constant__ int DATASET_SIZE;

// Set constant values
cudaMemcpyToSymbol(K, &K_HOST, sizeof(int));
cudaMemcpyToSymbol(DIM, &DIM_HOST, sizeof(int));
cudaMemcpyToSymbol(DATASET_SIZE, &DATASET_SIZE_HOST, sizeof(int));
```

```
// Inside main function
// Launch kernel to assign points to clusters
assignPointsToClusterKernel << <blooks, threads , K_HOST *sizeof(Point) >> >
cudaDeviceSynchronize();

// Inside kernel function
// Dynamic shared memory for centroids among blocks
extern __shared__ Point sharedCentroids[];

// Load centroids into shared memory for the first k and wait the others
if (threadIdx.x < K) {
    sharedCentroids[threadIdx.x] = centroids[threadIdx.x];
}
__syncthreads();</pre>
```

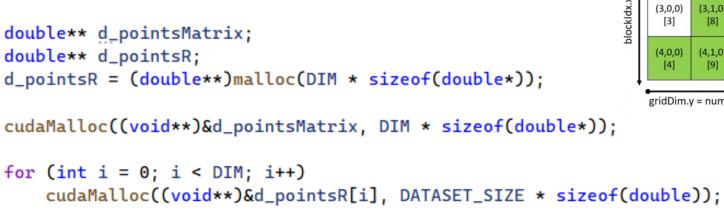
To maximaze the usage of the architecure, considering that we are operating with bi-dimensional points, let's exploit gpu features, and use a 2D grid, in order to do so, we need to change the data structure previuosly used, to a 2D matrix.

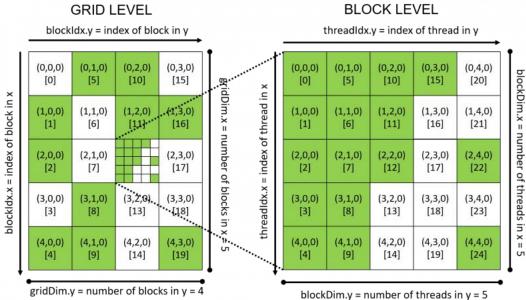
# 2D Matrix of doubles



```
double** pointsMatrix;
pointsMatrix = (double**)malloc(sizeof(double**) * DIM);
for (int i = 0; i < DIM; i++)
    pointsMatrix[i] = (double*)malloc((sizeof(double*) * DATASET_SIZE));</pre>
```

### 2D-GRID

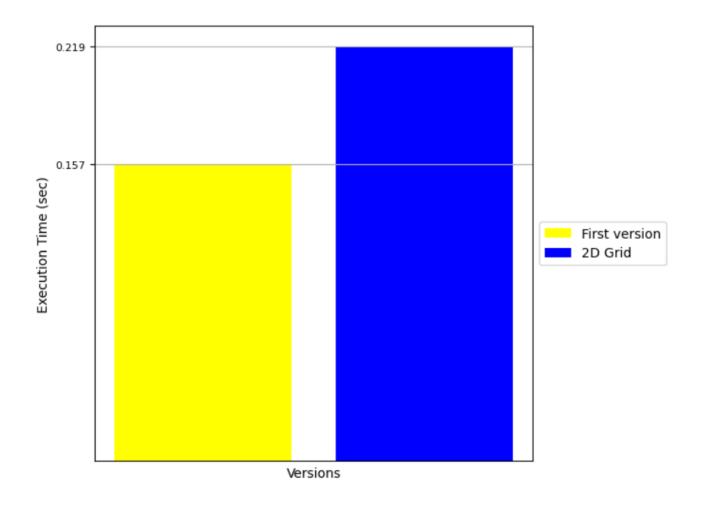




We used block size large enough to cover the entire dataset, and in order to provide enough warps to schedule, using the architecture at it's maximum.

```
//with this values it's possible to modify blocks size
int dimBlockX = 32;
int dimBlockY = 32;
// this values are calculated in order to use the minimum number of threads to cover the entire dataset
// and to use matrix of N X N
dim3 blockSize(dimBlockX, dimBlockY);
int dimGrid = ceil(sqrt(((DATASET_SIZE - (dimBlockX * dimBlockY) - 1)) / (dimBlockX * dimBlockY)));
int dimGridX = dimGrid;
int dimGridY = dimGrid;
dim3 gridSize(dimGridX,dimGridY);
assignPointsToClusterKernel << < gridSize, blockSize >> >
```

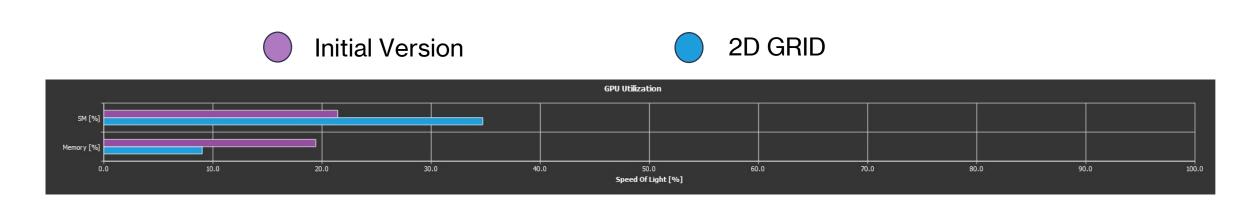
# Execution time comparison between Initial version and using a 2D Grid



### **GPU – Profiler**



We reached the goal of increasing the usage of the Multiprocessors (+60% SM utilization) but the exploiting of the memory subsystem of the cache is worse with the new version (-53%)



# Why?

# Flattening!

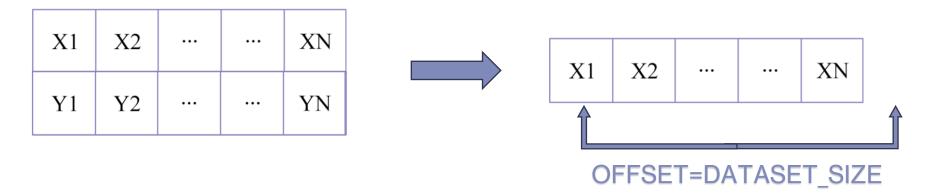
On gpu, if we are operating on bi-dimensional data, if is possible, is highly reccomended to perform a flattening and operate on one dimension data structure.

Our first implementation alredy used a data structure that exploited a sort of flattening.

```
typedef struct {
    double coordinate[3];
} Point;
Point* points = (Point*)malloc(DATASET_SIZE_HOST * sizeof(Point));
Point* d_points;
cudaMalloc((void**)&d_points, DATASET_SIZE_HOST * sizeof(Point));
```

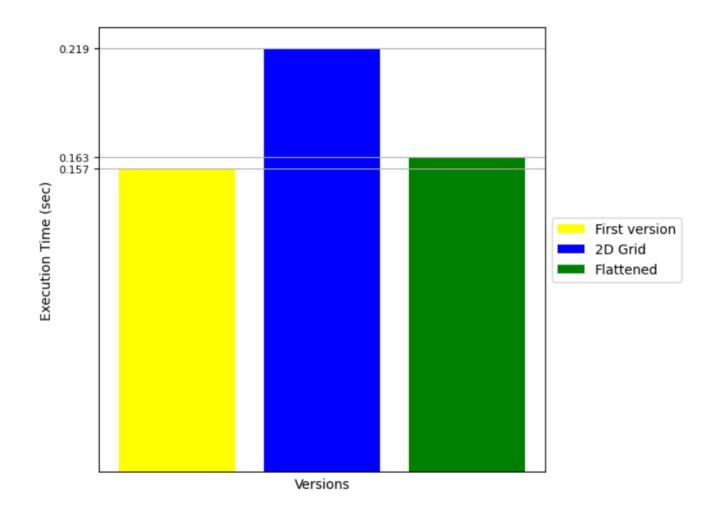
## Flattening!

To prove this supposition we used another data structure, a 2D matrix flattened to an array.



```
double* d_pointsArray;
cudaMalloc((void**)&d_pointsArray, DIM * DATASET_SIZE * sizeof(double));
```

Comparison of execution time on 10 millions points between initial version, 2D Grid and Flattened version



Reducing the number of calls on atomic operations: is there any way?

assignPointsToClusterKernel

```
// Update sums and counts
for (int dim = 0; dim < DIM; dim++) {
    atomicAdd(&sums[minIndex].coordinate[dim], points[idx].coordinate[dim]);
}
atomicAdd(&counts[minIndex], 1);</pre>
```

How many times? DATASET\_SIZE x (DIM +1)



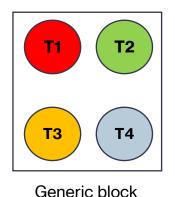
In our case: DIM=2 and DATASET\_SIZE = 10 000 000

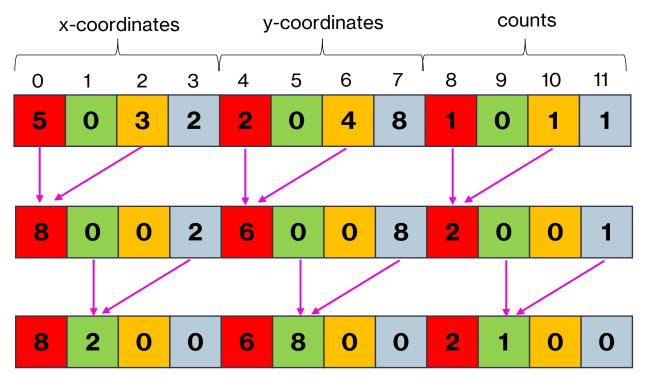
30 000 000 calls per iteration

Can we do better exploiting our GPU architecture?

Rewrite assignPointsToClusterKernel in order to perform for each cluster a PARALLEL - TREE – REDUCTION exploiting the shared memory in each block

Status of shared memory inside a block for i-cluster



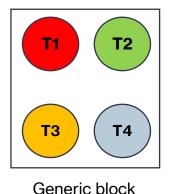


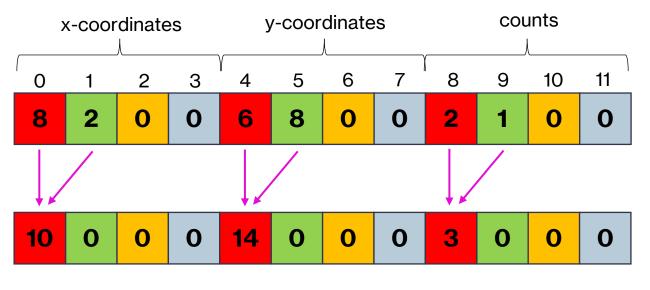
stride = blockDim.x/2

stride = stride /2

Rewrite assignPointsToClusterKernel in order to perform for each cluster a PARALLEL - TREE – REDUCTION exploiting the shared memory of each block

Status of shared memory inside a block for i-cluster





A BLOCK NEVER HANDLES ONLY 4 THREADS!!

Now only T1 performs atomic opertations !!

This is just an example: let see the impact on real data

Reducing the number of calls on atomic operations

- Initial version: DATASET\_SIZE x (DIM +1) → 30 000 000 calls per iteration
- Opt. version: NR\_BLOCKS x (DIM +1) x K → ~ 150 000 calls per iteration

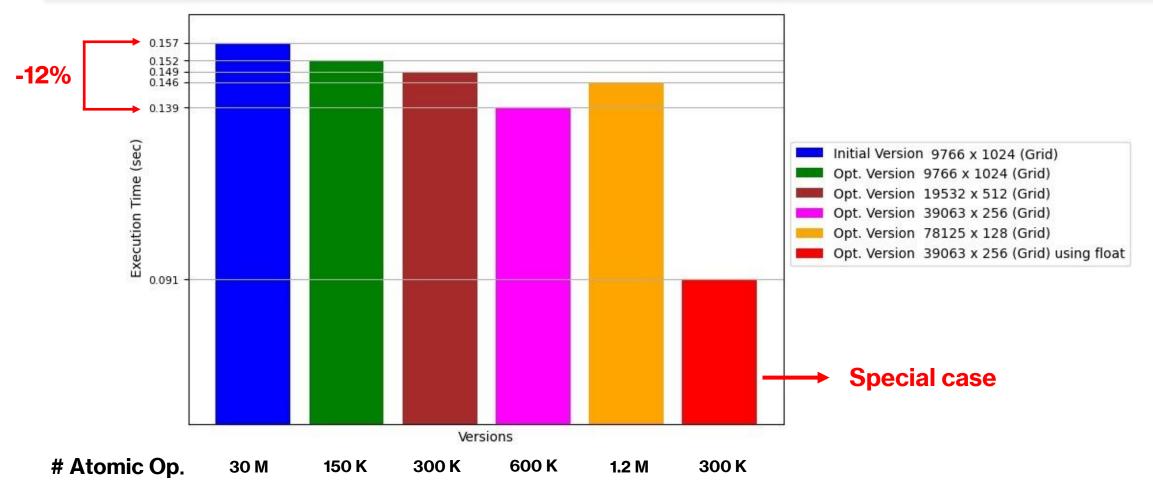
DIM=2 DATASET\_SIZE = 10 000 000

NR\_BLOCKS=9766 THREADS=1024 K(# of clusters)=5

PAY ATTENTION: the opt. version introduces additional synchronizations among threads in the same block

\_\_syncthreads();

We have to find a trade-off between # of blocks and # of threads

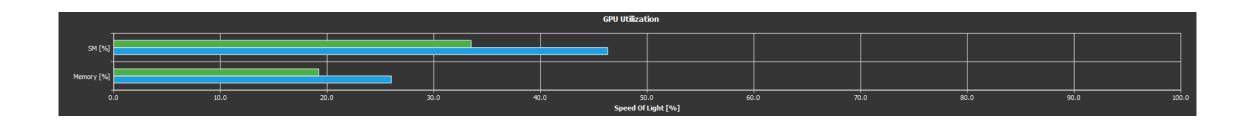




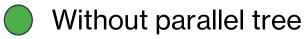
Without parallel tree

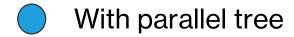
With parallel tree



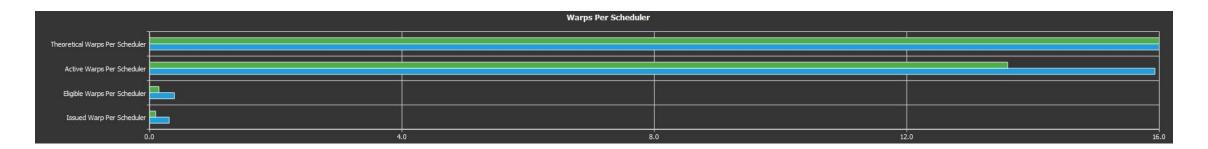










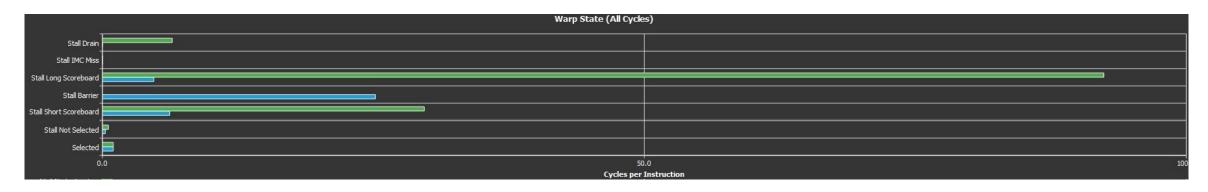




\_\_syncthreads();

Without parallel tree

With parallel tree



### **Optimizations summary**

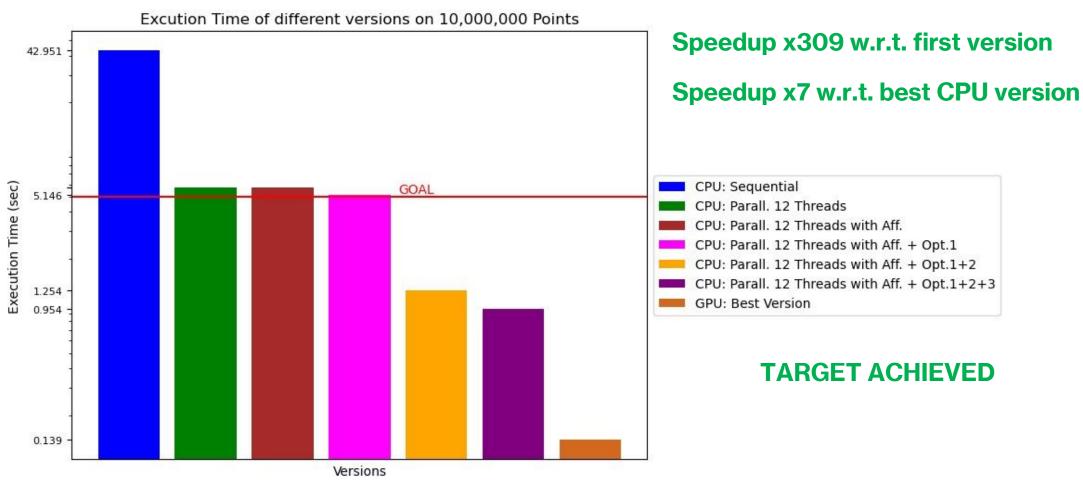
### For CPU Parallel version:

- 1. From a dynamic list of points, to an array of points [Opt.1];
- 2. Switching from usage of pow() function, to executing directly the square of the number (N<sup>2</sup>=N X N) [Opt.2];
- 3. Find the minimum distance between to points, without using the square root [Opt.3];

#### For GPU version:

1. Usage of parallel tree reduction technique;

### **Conclusions**



University of Pisa - Computer Architecture: KMeans parallel Implementation by Carlo Pio Pace and Davide Vigna

# Thank you