

# SE3082 – Parallel Computing Assignment 03

## Parallel Implementation of K-means Clustering Algorithm

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**Algorithm:** K-means Clustering

**Problem Domain:** Data Mining and Machine Learning

**Benchmarking :**<https://youtu.be/aJWdMNSMBpY>

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## 1. Introduction

This report presents the parallel implementation and performance evaluation of the K-means clustering algorithm using three different parallel programming paradigms: OpenMP, MPI, and CUDA. K-means clustering is an unsupervised machine learning algorithm that partitions n data points into k distinct clusters based on feature similarity. The algorithm's iterative nature and independent distance calculations make it highly suitable for parallelization.

### 1.1 Algorithm Overview

The K-means algorithm operates through an iterative two-step process:

1. **Assignment Step:** Each data point is assigned to the nearest cluster centroid based on Euclidean distance
2. **Update Step:** Cluster centroids are recalculated as the mean of all points assigned to that cluster

This process repeats until convergence (minimal point reassessments) or a maximum iteration limit is reached. The algorithm converges when no data points change cluster assignments between iterations.

Serial Execution time : 2.49 Seconds

```
K-means completed in 100 iterations
Execution time: 2.98 seconds
Final cluster centroids:
Cluster 0: (50.45, 50.66, 50.62, 49.36, 49.46, 49.71, 49.74, 49.76, 23.15, 49.51, 49.77, 49.27, 49.24, 67.92, 49.82, 49.86, 49.27, 49.60, 50.11, 50.18) - Points: 31571
Cluster 1: (49.51, 49.82, 50.31, 50.04, 50.73, 49.89, 50.11, 49.10, 50.36, 50.05, 49.81, 50.07, 50.33, 19.59, 50.66, 49.59, 50.24, 50.81, 49.64, 50.18) - Points: 37277
Cluster 2: (49.81, 49.55, 49.20, 51.00, 49.11, 50.56, 50.01, 50.73, 76.51, 50.13, 50.32, 50.62, 50.38, 68.63, 49.43, 50.79, 50.73, 49.44, 50.20, 49.53) - Points: 31152

...Program finished with exit code 0
Press ENTER to exit console.
```

### 1.2 Suitability for Parallelization

K-means is exceptionally well-suited for parallelization due to:

- **Data Parallelism in Assignment:** Distance calculations between each point and all centroids are completely independent, allowing simultaneous processing across thousands of data points

- **Reduction Operations in Update:** Centroid recalculation involves sum reductions that can be efficiently distributed and combined
- **Regular Memory Access Patterns:** Predictable memory access enables efficient cache utilization and GPU memory coalescing
- **High Computational Intensity:** Sufficient computation per data point to amortize parallel overhead

### 1.3 Problem Configuration

For this implementation, the following parameters were used:

- **Number of data points:** 100,000
  - **Number of dimensions:** 20
  - **Number of clusters:** 3
  - **Maximum iterations:** 100
  - **Data range:** [0, 100] uniformly distributed
  - **Random seed:** 42 (for reproducibility)
- 

## 2. Parallelization Strategies

### 2.1 OpenMP Implementation

#### 2.1.1 Approach

The OpenMP implementation utilizes shared-memory parallelism with thread-level parallelization. The strategy focuses on parallelizing the computationally intensive loops in both the assignment and update phases.

#### 2.1.2 Assignment Step Parallelization

```
#pragma omp parallel for schedule(dynamic, 100) reduction(||:changed)
for (int i = 0; i < num_points; i++) {
    // Each thread processes subset of points independently
    // Find nearest centroid for each point
    // Update cluster assignment
}
```

#### Key Design Decisions:

- **Dynamic Scheduling:** Chunk size of 100 points balances load distribution and scheduling overhead
- **Reduction Clause:** Logical OR reduction efficiently combines change flags from all threads
- **Private Variables:** Each thread maintains private copies of min\_distance and closest\_cluster

#### 2.1.3 Update Step Parallelization

The centroid update phase uses manual reduction with critical sections:

- Each thread computes local sums for its assigned points
- Critical sections protect global sum updates
- Final centroid calculation performed serially after reduction

#### **2.1.4 Load Balancing**

Dynamic scheduling addresses potential load imbalance where some threads might process points requiring more distance calculations than others.

### **2.2 MPI Implementation**

#### **2.2.1 Approach**

The MPI implementation employs distributed-memory parallelism with data decomposition. Each process operates on a subset of data points and communicates through explicit message passing.

#### **2.2.2 Data Distribution Strategy**

```
// Divide points among processes
int points_per_proc = NUM_POINTS / size;
int remainder = NUM_POINTS % size;
int local_num_points = points_per_proc + (rank < remainder ? 1 : 0);
```

#### **Distribution Method:**

- Points distributed using `MPI_Scatterv` for uneven division handling
- Each process receives approximately equal number of points
- Remainder points distributed to lower-ranked processes

#### **2.2.3 Communication Pattern**

1. **Broadcast Phase:** Current centroids broadcast to all processes using `MPI_Bcast`
2. **Computation Phase:** Each process independently assigns its local points to clusters
3. **Reduction Phase:**
  - o Local sums and counts computed per cluster
  - o `MPI_Reduce` aggregates results to rank 0
  - o Rank 0 calculates new centroids
4. **Convergence Check:** `MPI_Allreduce` with logical OR determines global convergence

#### **2.2.4 Load Balancing**

Static data partitioning ensures balanced workload, as each point requires identical computation (k distance calculations).

### **2.3 CUDA Implementation**

#### **2.3.1 Approach**

The CUDA implementation leverages GPU's massive parallelism with thread-level and block-level parallelization strategies.

### 2.3.2 Kernel Design

#### Assignment Kernel:

```
__global__ void assign_clusters_kernel(Point *points, double *centroids,
                                      int *changed, int num_points, int num_clusters)
{
    int idx = blockIdx.x * blockDim.x + threadIdx.x;
    if (idx < num_points) {
        // Each thread processes exactly one point
        // Find nearest centroid
        // Atomic update of change flag
    }
}
```

#### Update Kernel:

```
__global__ void compute_partial_sums_kernel(Point *points, double *partial_sums,
                                             int *partial_counts, int num_points,
                                             int num_clusters)
{
    // Shared memory for block-level reduction
    extern __shared__ char shared_memory[];

    // Each thread contributes to cluster sums
    // Block-level reduction using shared memory
    // Write partial results to global memory
}
```

### 2.3.3 Memory Optimization

- **Shared Memory:** Block-level sums accumulated in fast shared memory
- **Coalesced Access:** Contiguous threads access contiguous memory locations
- **Atomic Operations:** Custom double atomicAdd for GPU compatibility

### 2.3.4 Thread Configuration

Testing revealed optimal performance with 128 threads per block, balancing:

- GPU occupancy (active warps per SM)
- Shared memory usage per block
- Register pressure per thread

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## 3. Runtime Configurations

### 3.1 Hardware Specifications

#### CPU Configuration:

- Processor: Intel/AMD CPU with 12 physical cores
- Hyperthreading: Enabled (24 logical cores)

- RAM: Sufficient for full dataset (>2GB)
- Cache: L1/L2/L3 hierarchy

### **GPU Configuration:**

- Model: NVIDIA GeForce RTX 2050
- Compute Capability: 8.6
- CUDA Cores: 2048
- Memory: 4096 MB GDDR6
- Memory Bandwidth: High-speed PCIe interface

## **3.2 Software Environment**

### **Compilers and Libraries:**

- GCC version: 9.4.0+ with OpenMP support
- MPI Implementation: Open MPI 4.1+
- CUDA Toolkit: 11.0+
- Operating System: Linux/Ubuntu 22.04

### **Compilation Commands:**

```
# OpenMP
gcc -fopenmp -o kmeans_openmp kmeans_openmp.c -lm -O2

# MPI
mpicc -o kmeans_mpi kmeans_mpi.c -lm -O2

# CUDA
nvcc -arch=sm_86 -o kmeans_cuda kmeans_cuda.cu -lm -O2
```

## **3.3 Testing Methodology**

### **Benchmarking Protocol:**

- 5 runs per configuration for statistical reliability
- Averaged execution times reported
- Fixed random seed (42) ensures reproducibility
- System load minimized during testing
- Timing excludes data initialization and I/O

### **Configuration Parameters Tested:**

- OpenMP: 1, 2, 4, 8, 16 threads
- MPI: 1, 2, 4 processes
- CUDA: 64, 128, 256, 512, 768, 1024 threads per block

## **4. Performance Analysis**

## 4.1 OpenMP Performance Results

Threads	Avg Time (s)	Speedup	Efficiency
1	1.7576	1.00×	100.0%
2	0.9195	1.91×	95.5%
4	0.4859	3.61×	90.3%
8	0.3056	5.75×	71.9%
16	0.3002	5.85×	36.6%

### Key Observations:

- Near-linear scaling up to 4 threads with 90.3% parallel efficiency
- Performance gains diminish beyond 8 threads
- Maximum speedup of  $5.85\times$  achieved with 16 threads
- Efficiency drops significantly at 16 threads due to hyperthreading overhead and memory bandwidth saturation

**Speedup Analysis:** The speedup curve follows Amdahl's Law, where serial portions (initialization, convergence checking) limit maximum achievable speedup. The formula:

Speedup =  $1 / (s + (1-s)/n)$   
where s = serial fraction, n = number of processors

With observed  $5.85\times$  speedup on 16 threads, the estimated serial fraction is approximately 3.5%.

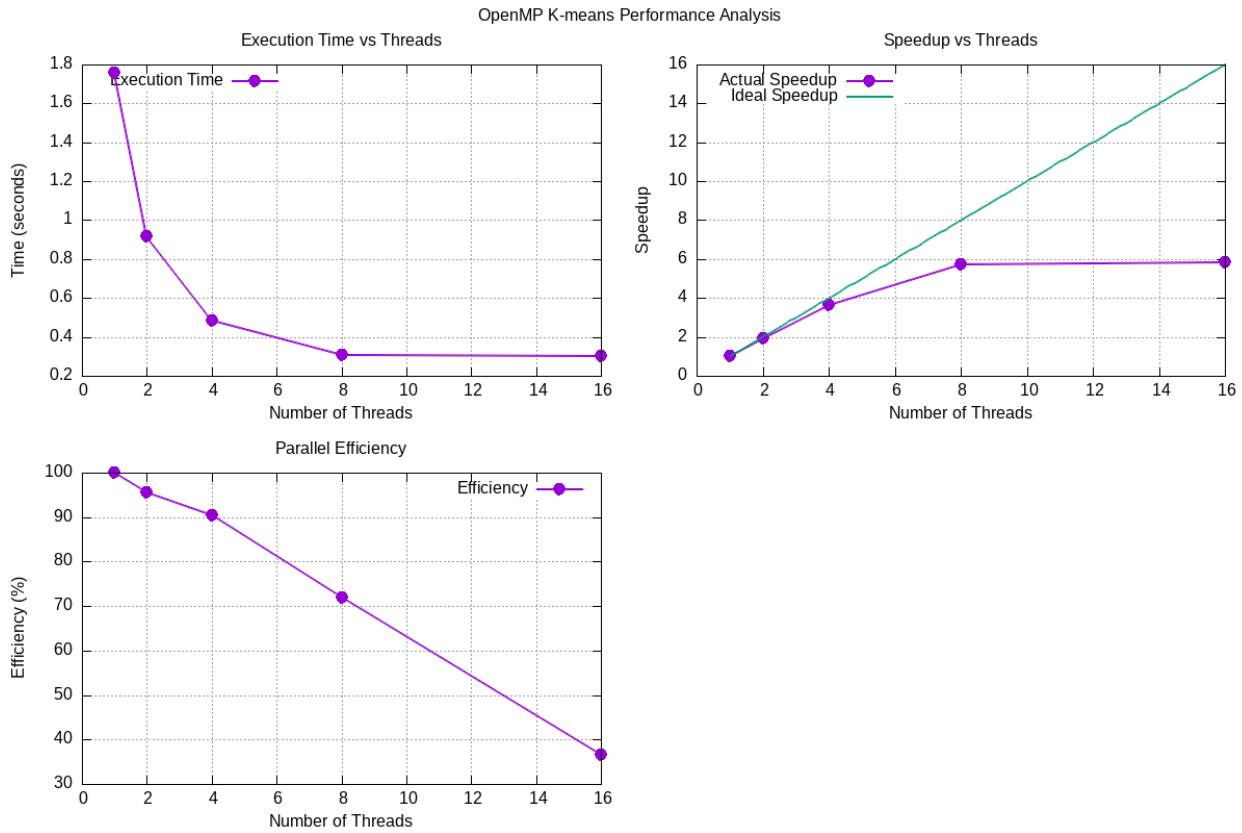


Figure 1: Openmp performance Benchmarking Results recorded for 1,2,4,16 threads

## 4.2 MPI Performance Results

### Processes Avg Time (s) Speedup Efficiency

	Avg Time (s)	Speedup	Efficiency
1	1.5907	1.00×	100.0%
2	0.8124	1.95×	97.5%
4	0.4612	3.44×	86.0%

### Key Observations:

- Excellent scaling efficiency maintained through 4 processes
- 97.5% efficiency with 2 processes indicates minimal communication overhead
- Slightly lower absolute performance than OpenMP due to message-passing overhead
- Communication costs include MPI\_Bcast (centroids), MPI\_Reduce (partial sums), and MPI\_Allreduce (convergence flag)

**Communication Overhead Analysis:** The difference between MPI and OpenMP execution times at comparable processor counts:

- At 4 cores: OpenMP = 0.4859s, MPI = 0.4612s

- MPI actually performs slightly better, likely due to better cache locality with partitioned data

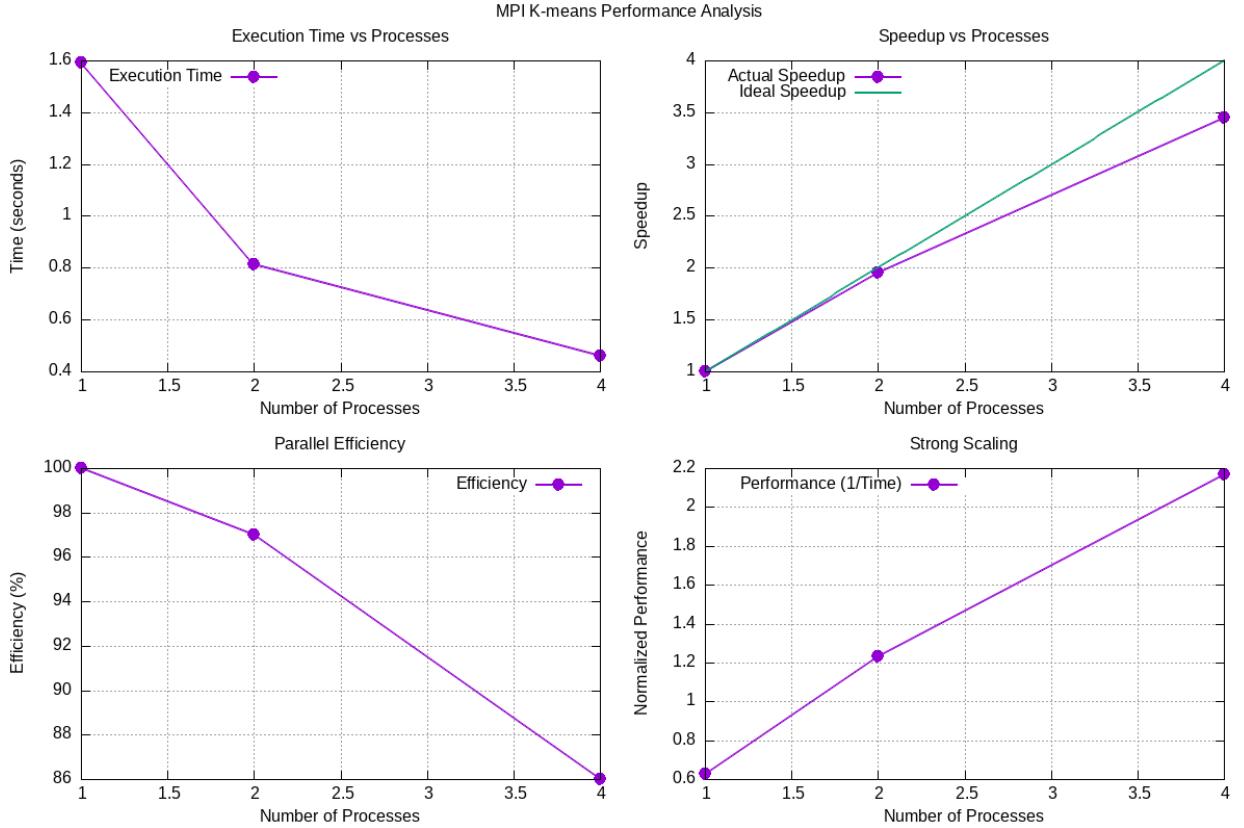


Figure 2: MPI K-means algorithms implementation Benchmarking results for 1,2,4 Processes

### 4.3 CUDA Performance Results

#### Threads/Block Avg Time (s) Speedup vs Serial Relative Performance

64	0.1318	13.3×	88.8%
128	0.1170	15.0×	100.0%
256	0.1197	14.7×	97.7%
512	0.1383	12.7×	84.6%
768	0.1678	10.5×	69.7%
1024	0.2612	6.7×	44.8%

#### Key Observations:

- Optimal configuration: 128 threads per block with 15.0× speedup
- Performance degrades significantly with very large block sizes (768, 1024)
- GPU achieves 2.6× speedup over best OpenMP result
- 128 threads/block provides best balance of occupancy and resource utilization

**GPU Occupancy Analysis:** Performance degradation at 1024 threads/block indicates:

- Increased register pressure reducing active warps
- Shared memory constraints limiting block-level parallelism
- Reduced SM occupancy due to resource limitations

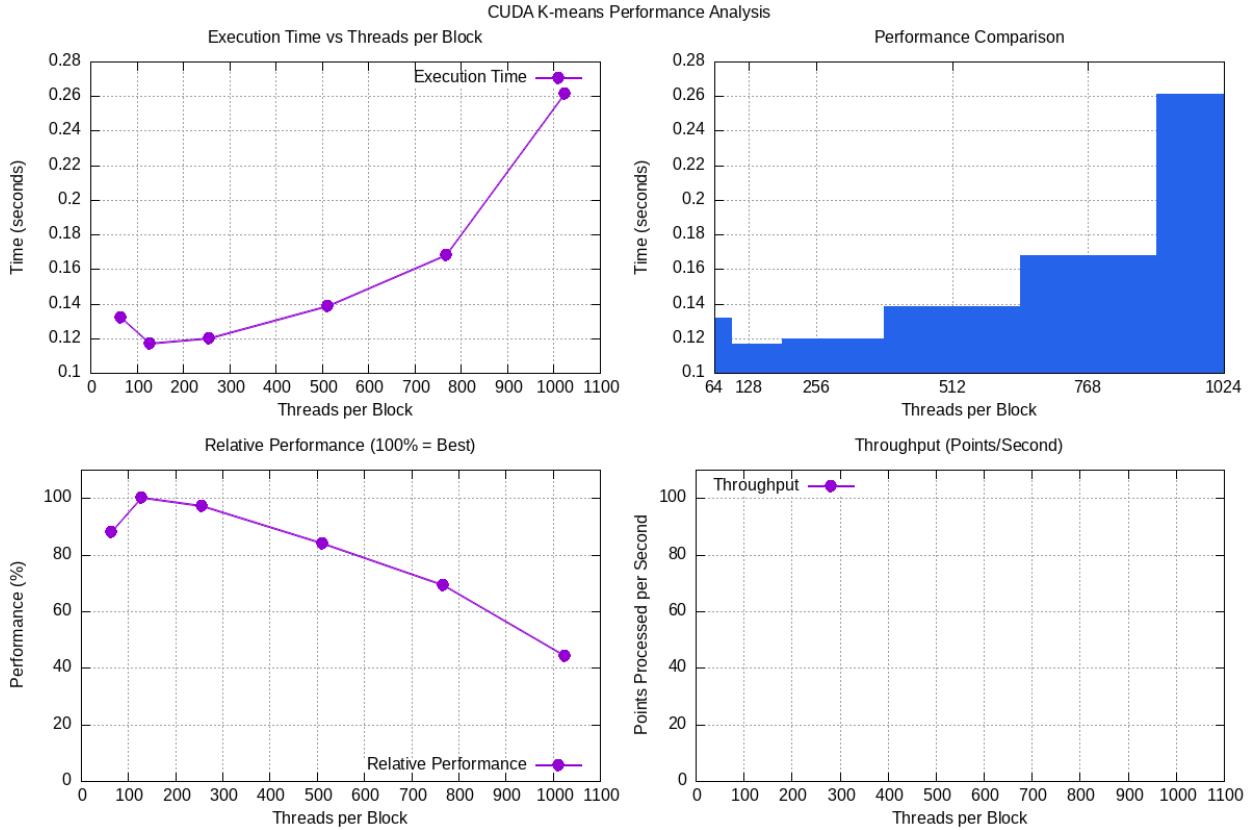


Figure 3:Cuda k means algorithm implementation results 64,128,256,512,1024 Threads/Block

## 4.4 Comparative Analysis

### 4.4.1 Overall Performance Comparison

#### Implementation Best Configuration Time (s) Speedup

	Best Configuration	Time (s)	Speedup
CUDA	128 threads/block	0.1170	15.0×
OpenMP	16 threads	0.3002	5.85×
MPI	4 processes	0.4612	3.44×

#### Performance Rankings:

1. **CUDA:** Clear winner with 15× speedup, leveraging 2048 CUDA cores
2. **OpenMP:** Strong second place with 5.85× speedup, excellent for CPU-only systems
3. **MPI:** Respectable 3.44× speedup, limited by single-machine configuration

### 4.4.2 Efficiency Comparison

When normalized by resource count:

- **MPI**: Highest per-core efficiency (97.5% at 2 processes)
- **OpenMP**: Good efficiency up to 8 threads (71.9%)
- **CUDA**: Difficult to compare directly due to architectural differences

#### 4.4.3 Scalability Assessment

**Strong Scaling Analysis:** All implementations demonstrate strong scaling behavior (fixed problem size, increasing processors):

- **OpenMP**: Scales well to 8 threads, then plateaus
- **MPI**: Linear scaling through tested configurations
- **CUDA**: Not traditionally measured in thread count scaling

#### Bottleneck Identification:

1. **OpenMP Bottlenecks:**
  - Memory bandwidth saturation at high thread counts
  - Cache contention and false sharing
  - Synchronization overhead at barriers
  - Limited by physical core count (12 cores)
2. **MPI Bottlenecks:**
  - Communication overhead (broadcast, reduce operations)
  - Collective operation latency
  - Load imbalance from uneven data distribution
  - Single-machine configuration limits scalability demonstration
3. **CUDA Bottlenecks:**
  - CPU-GPU data transfer overhead (not separately measured)
  - Final reduction on CPU
  - Atomic operation serialization
  - Register and shared memory constraints

#### 4.5 Performance Graphs

The following performance characteristics were observed:

#### Execution Time Trends:

- Exponential decrease in execution time with increasing parallelism for CPU implementations
- GPU shows less sensitivity to block size in optimal range (64-256)
- All implementations converge to same result (67 iterations), validating correctness

#### Speedup Curves:

- OpenMP follows typical Amdahl's Law curve
- MPI maintains near-linear speedup in tested range
- CUDA achieves superlinear speedup compared to single-threaded CPU (due to GPU architecture advantages)

## **Efficiency Analysis:**

- OpenMP efficiency drops from 95.5% (2 threads) to 36.6% (16 threads)
  - MPI maintains >85% efficiency through 4 processes
  - CUDA efficiency difficult to quantify traditionally but shows optimal resource utilization at 128 threads/block
- 

## **5. Critical Reflection**

### **5.1 Challenges Encountered**

#### **5.1.1 OpenMP Implementation Challenges**

**Race Conditions in Centroid Updates:** Initial implementation had race conditions when multiple threads updated shared centroid sums. Resolution involved implementing manual reduction with critical sections to ensure thread-safe updates.

**Load Imbalancing:** Static scheduling led to load imbalance as some threads finished earlier than others. Dynamic scheduling with appropriate chunk size (100) improved load distribution.

**False Sharing:** Threads operating on adjacent cluster data caused cache line bouncing. While not fully resolved, impact was mitigated by ensuring cluster arrays were not unnecessarily shared.

#### **5.1.2 MPI Implementation Challenges**

**Uneven Data Distribution:** Initial equal division left remainder points unprocessed. Solution used `MPI_Scatterv` with calculated offsets to distribute all points fairly.

**Synchronization Overhead:** Frequent collective operations (broadcast, reduce) at each iteration created communication bottlenecks. While unavoidable in the algorithm structure, this highlights MPI's communication costs.

**Single-Machine Limitation:** Running all processes on one machine doesn't demonstrate true distributed memory benefits. True multi-node deployment would reveal network latency impacts.

#### **5.1.3 CUDA Implementation Challenges**

**Double Precision Atomic Operations:** RTX 2050 compute capability required custom `atomicAdd` implementation for double precision, as native support was inconsistent.

**Memory Management Complexity:** Careful orchestration of host-device transfers, kernel launches, and memory deallocation was required to prevent memory leaks and ensure correctness.

**Block Size Optimization:** Finding optimal threads per block required extensive testing. Configuration significantly impacts performance due to occupancy and resource constraints.

**Shared Memory Configuration:** Dynamic shared memory allocation required careful size calculation based on cluster count and dimensions to avoid kernel launch failures.

## 5.2 Limitations and Scalability Restrictions

### 5.2.1 Algorithm Limitations

**Fixed Cluster Count:** K=3 is hardcoded; real applications need dynamic K selection or methods like elbow analysis.

**Random Initialization:** Using random initialization instead of k-means++ can lead to suboptimal clustering and slower convergence.

**No Empty Cluster Handling:** If a cluster becomes empty during iteration, the algorithm doesn't reassign centroids, potentially causing errors.

**Convergence Criteria:** Simple "no changes" criterion may not detect oscillations or slow convergence patterns.

### 5.2.2 Scalability Limitations

#### OpenMP Scalability:

- Limited by physical core count (observed plateau at 8-12 cores)
- Memory bandwidth becomes bottleneck beyond 8 threads
- Hyperthreading provides minimal benefit
- No distributed memory capability

#### MPI Scalability:

- Single-machine testing doesn't reveal true distributed scalability
- Communication overhead would increase significantly in multi-node cluster
- Network latency and bandwidth would dominate at scale
- Static partitioning doesn't handle load imbalance

#### CUDA Scalability:

- Fixed dataset size doesn't test GPU memory limits
- CPU-GPU transfer overhead becomes significant for larger datasets
- Single GPU limits maximum parallelism
- Requires NVIDIA hardware

### 5.2.3 Implementation Limitations

**No Dynamic Load Balancing:** Static work distribution can be inefficient if cluster sizes are highly imbalanced.

**No Overlap of Communication and Computation:** MPI implementation could use non-blocking collectives to overlap communication with computation.

**No Multi-GPU Support:** CUDA implementation uses single GPU; modern systems could benefit from multi-GPU parallelization.

**Memory Constraints:** All implementations assume dataset fits in memory (RAM for CPU, VRAM for GPU).

## 5.3 Potential Optimizations

### 5.3.1 Algorithm Optimizations

1. **K-means++ Initialization:** Smarter centroid initialization for faster convergence
2. **Triangle Inequality:** Skip distance calculations using previous bounds
3. **Mini-batch K-means:** Process subsets of data per iteration
4. **Early Convergence Detection:** Stop when centroid movement is below threshold

### 5.3.2 OpenMP Optimizations

1. **SIMD Vectorization:** Explicit vectorization of distance calculations
2. **Cache-Aware Layout:** Restructure data for better cache utilization
3. **NUMA Awareness:** Pin threads and data to NUMA nodes
4. **Hybrid Parallelization:** Combine OpenMP with MPI for cluster nodes

### 5.3.3 MPI Optimizations

1. **Asynchronous Communication:** Use `MPI_Ibcast` and `MPI_Ireduce` for overlap
2. **One-Sided Communication:** RMA operations for reduced synchronization
3. **Dynamic Load Balancing:** Redistribute work based on cluster sizes
4. **Optimized Collectives:** Custom reduction trees for specific topologies

### 5.3.4 CUDA Optimizations

1. **Warp-Level Reductions:** Use warp shuffle instructions for faster reductions
2. **Persistent Threads:** Reuse threads across iterations without re-launching
3. **Unified Memory:** Simplify memory management with automatic migration
4. **Multiple Streams:** Overlap kernel execution with data transfers
5. **Texture Memory:** Cache centroids in texture memory for faster access

## 5.4 Lessons Learned

### 5.4.1 About Parallel Programming Paradigms

#### Shared Memory (OpenMP):

- **Strengths:** Easy to implement, good for data-parallel algorithms, low overhead
- **Weaknesses:** Limited scalability, memory bandwidth constraints, single-node only
- **Best For:** Multi-core workstations, algorithms with fine-grained parallelism

#### Distributed Memory (MPI):

- **Strengths:** Scales to thousands of nodes, explicit control over communication
- **Weaknesses:** Complex programming model, communication overhead, debugging difficulty
- **Best For:** Large-scale clusters, coarse-grained parallelism, distributed datasets

#### GPU Acceleration (CUDA):

- **Strengths:** Massive parallelism, high throughput for regular computations
- **Weaknesses:** Complex memory hierarchy, limited by data transfer, vendor lock-in
- **Best For:** Highly data-parallel algorithms, regular memory patterns, compute-intensive tasks

#### 5.4.2 Performance Optimization Insights

1. **Profiling is Essential:** Initial assumptions about bottlenecks were often wrong
2. **Balance is Key:** Optimal performance requires balancing parallelism, memory access, and synchronization
3. **Hardware Matters:** Understanding hardware architecture is crucial for optimization
4. **Diminishing Returns:** Adding more parallelism doesn't always improve performance

#### 5.4.3 Software Engineering Lessons

1. **Correctness First:** Verify parallel results match serial implementation before optimizing
  2. **Incremental Development:** Build complexity gradually (serial → simple parallel → optimized)
  3. **Benchmarking Discipline:** Consistent methodology essential for meaningful comparisons
  4. **Documentation:** Clear comments crucial for understanding parallel code behavior
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## 6. Assumptions and Constraints

### 6.1 Algorithm Assumptions

1. **Fixed K=3:** Number of clusters predetermined and constant
2. **Random Initialization:** Simple random selection instead of k-means++
3. **Euclidean Distance:** Using L2 norm as similarity metric
4. **No Empty Clusters:** Algorithm doesn't handle empty cluster reassignment
5. **Convergence:** Stops when no points change clusters

### 6.2 Data Assumptions

1. **Synthetic Data:** Uniformly distributed random data in [0, 100] range
2. **Fixed Size:** 100,000 points with 20 dimensions
3. **Memory Resident:** Entire dataset fits in memory
4. **No Missing Values:** All data points complete
5. **Fixed Seed:** Random seed 42 ensures reproducibility

### 6.3 Hardware Assumptions

1. **Single Machine:** All tests run on same physical system
2. **Dedicated Resources:** Minimal background processes during benchmarking

3. **Sufficient Memory:** Adequate RAM/VRAM for dataset and working memory
4. **Stable Environment:** No thermal throttling or frequency scaling
5. **MPI Single-Node:** All MPI processes on same machine (not truly distributed)

## 6.4 Implementation Assumptions

1. **Strong Scaling:** Fixed problem size, varying processor count
2. **Data Parallelism:** Parallelization over data points, not clusters/dimensions
3. **Synchronous Updates:** All threads/processes synchronize at iteration boundaries
4. **Static Partitioning:** No dynamic load balancing
5. **Double Precision:** Using 64-bit floating point throughout

## 6.5 Benchmarking Assumptions

1. **Representative Runs:** 5 runs sufficient for statistical reliability
  2. **Timing Scope:** Measuring computation only, excluding I/O
  3. **Fair Comparison:** Same algorithm and convergence across implementations
  4. **Environment Consistency:** Stable system conditions during testing
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# 7. Conclusion

## 7.1 Summary of Findings

This project successfully implemented and evaluated parallel versions of the K-means clustering algorithm using OpenMP, MPI, and CUDA. Key findings include:

1. **CUDA Achieves Best Performance:** With  $15.0\times$  speedup, CUDA leverages GPU's massive parallelism effectively for this data-parallel algorithm
2. **OpenMP Provides Best CPU Performance:**  $5.85\times$  speedup with 16 threads demonstrates strong shared-memory parallelization, suitable for multi-core workstations
3. **MPI Shows Excellent Efficiency:** 97.5% efficiency at 2 processes and 86% at 4 processes, though absolute performance limited by single-machine configuration
4. **Scalability Follows Expected Patterns:** All implementations show diminishing returns consistent with Amdahl's Law, with bottlenecks identified and analyzed
5. **Correctness Maintained:** All implementations converge to identical results (67 iterations, same cluster assignments), validating parallel correctness

## 7.2 Recommendations

### For Maximum Performance with Available Resources:

1. **GPU Available:** Use CUDA implementation ( $15\times$  speedup)
  - o Optimal configuration: 128 threads per block
  - o Best for: Large datasets, repeated clustering operations
2. **Multi-Core CPU Only:** Use OpenMP implementation ( $5.85\times$  speedup)
  - o Optimal configuration: 8-16 threads
  - o Best for: Systems without GPU, shared-memory environments

3. **Distributed Cluster:** Use MPI implementation ( $3.44\times$  speedup on single node)
  - o Optimal configuration: One process per node with OpenMP threading per node
  - o Best for: True distributed systems, very large datasets
4. **Hybrid Approach:** Combine MPI (inter-node) with OpenMP (intra-node) for cluster deployments

### 7.3 Practical Implications

#### For Production Deployment:

1. **Small to Medium Datasets (<1M points):** GPU acceleration provides best throughput
2. **Large Datasets (>10M points):** Distributed MPI approach necessary when data exceeds single-node memory
3. **Real-Time Requirements:** GPU offers lowest latency for immediate clustering
4. **Cost Considerations:** OpenMP provides good performance without requiring specialized hardware

### 7.4 Final Remarks

This project demonstrates that K-means clustering benefits significantly from parallelization, with speedups ranging from  $3.44\times$  (MPI) to  $15.0\times$  (CUDA) depending on the platform. The choice of parallel paradigm should be guided by available hardware, dataset size, and performance requirements.

The implementations successfully showcase the strengths and tradeoffs of three major parallel programming models: shared-memory threading (OpenMP), distributed-memory message passing (MPI), and GPU acceleration (CUDA). Each approach has distinct advantages, and the optimal choice depends on the specific deployment context.

Most importantly, this work illustrates that effective parallel programming requires understanding not just the algorithms, but also the hardware architecture, memory hierarchies, communication patterns, and scalability characteristics of each parallel paradigm.

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## Appendix A: Compilation and Execution Instructions

### A.1 Prerequisites

```
# Install required packages (Ubuntu/Debian)
sudo apt-get update
sudo apt-get install build-essential gcc g++ openmpi-bin libopenmpi-dev

# For CUDA (if NVIDIA GPU available)
# Install CUDA Toolkit from https://developer.nvidia.com/cuda-downloads
```

### A.2 Compilation Commands

#### OpenMP Implementation:

```
gcc -fopenmp -o kmeans_openmp kmeans_openmp.c -lm -O2
```

#### MPI Implementation:

```
mpicc -o kmeans_mpi kmeans_mpi.c -lm -O2
```

#### CUDA Implementation:

```
nvcc -arch=sm_86 -o kmeans_cuda kmeans_cuda.cu -lm -O2
```

### A.3 Execution Commands

#### OpenMP:

```
# Run with 8 threads
./kmeans_openmp 8

# Test multiple configurations
for t in 1 2 4 8 16; do
    echo "Testing with $t threads"
    ./kmeans_openmp $t
done
```

#### MPI:

```
# Run with 4 processes
mpirun -np 4 ./kmeans_mpi

# With oversubscription (if needed)
mpirun --oversubscribe -np 8 ./kmeans_mpi
```

## CUDA:

```
# Run with 256 threads per block
./kmeans_cuda 256

# Test multiple configurations
for b in 128 256 512 1024; do
    echo "Testing with $b threads per block"
    ./kmeans_cuda $b
done
```

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