

HPC Assignment 03: Serial Interpolation on Scattered Data

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Abstract

This report presents the implementation and performance analysis of a serial bilinear interpolation algorithm for mapping scattered 2D data points onto a structured mesh grid. The algorithm distributes particle values to four nearest grid points using area-based weighting. Performance is evaluated on both Lab PC and HPC cluster across five different problem configurations, with detailed analysis of time complexity, memory access patterns, and cache behavior.

1 Implementation Approach

1.1 Problem Overview

Given N scattered points $S = \{(x_i, y_i, f_i) | i = 1, 2, \dots, N\}$ where $f_i = 1$, we interpolate these values onto a structured $M \times M$ mesh grid $G = \{(X_i, Y_j)\}$ using bilinear interpolation.

1.2 Grid Structure and Cell Identification

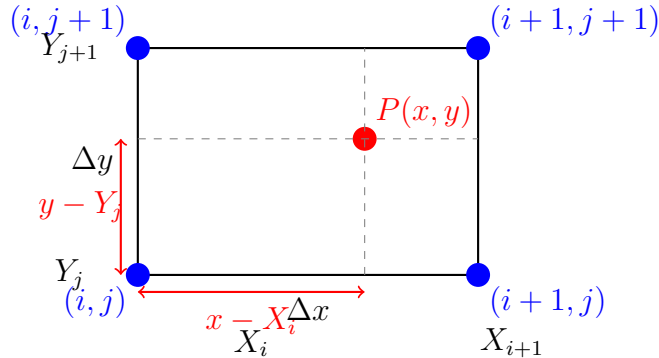


Figure 1: Grid cell structure showing a particle P at position (x, y) within cell (i, j)

For each scattered point (x, y) :

1. **Cell identification:** Calculate grid indices:

$$i = \left\lfloor \frac{x}{\Delta x} \right\rfloor, \quad j = \left\lfloor \frac{y}{\Delta y} \right\rfloor \quad (1)$$

where $\Delta x = \frac{1}{N_x}$, $\Delta y = \frac{1}{N_y}$

2. **Normalized distances:**

$$d_x = \frac{x - X_i}{\Delta x}, \quad d_y = \frac{y - Y_j}{\Delta y} \quad (2)$$

3. **Clamp to valid range:** If $i \geq N_x$, set $i = N_x - 1$ (same for j)

1.3 Weight Calculation (Area-Based)

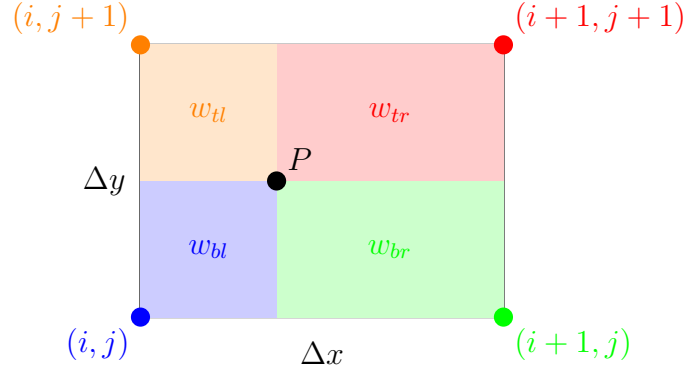


Figure 2: Area-based weight calculation. Each corner receives weight proportional to the area of the opposite sub-rectangle.

The weights are computed as:

$$w_{i,j} = (1 - d_x)(1 - d_y) \quad (\text{bottom-left}) \quad (3)$$

$$w_{i+1,j} = d_x(1 - d_y) \quad (\text{bottom-right}) \quad (4)$$

$$w_{i,j+1} = (1 - d_x)d_y \quad (\text{top-left}) \quad (5)$$

$$w_{i+1,j+1} = d_x d_y \quad (\text{top-right}) \quad (6)$$

Key insight: The weight for each corner equals the area of the sub-rectangle opposite to that corner. This ensures $\sum w = 1$, conserving the total value.

1.4 Memory Layout

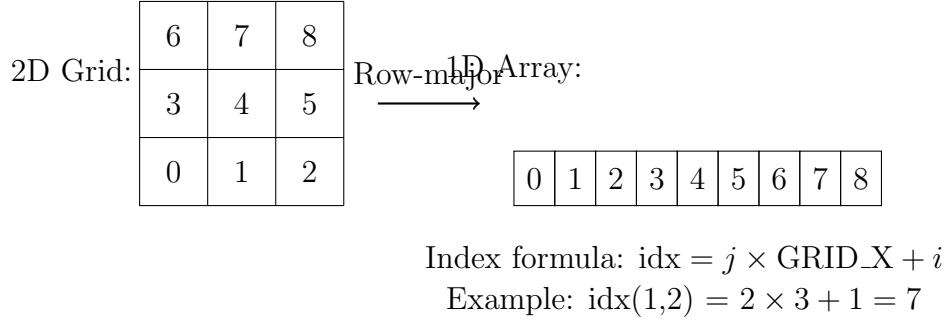


Figure 3: Row-major memory layout for 2D grid storage

The mesh is stored as a 1D array in **row-major order**:

$$\text{mesh_value}[j \times \text{GRID_X} + i] = F(X_i, Y_j) \quad (7)$$

This layout ensures spatial locality when accessing adjacent elements in the same row.

2 Theoretical Analysis

2.1 Time Complexity

Table 1: Algorithm Complexity Analysis

Aspect	Analysis
Outer loop	Maxiter iterations
Inner loop	N_{points} particles per iteration
Work per particle	$O(1)$ (constant operations)
Total Time Complexity	$O(\text{Maxiter} \times N_{\text{points}})$

The algorithm scales linearly with both the number of iterations and particles.

2.2 Arithmetic Operations Per Particle

Table 2: Operation Count Per Particle

Operation Type	Count	Details
Divisions (/)	2	$d_x = (x - X_i)/\Delta x$, $d_y = (y - Y_j)/\Delta y$
Multiplications (\times)	6	4 weights \times 1-2 products each
Additions/Subtractions ($+/-$)	4	$1 - d_x$, $1 - d_y$, index calculations
Total FLOPs	$\approx 12-15$	

2.3 Memory Access Analysis

Table 3: Memory Access Per Particle

Access Type	Size	Pattern	Cache Behavior
Read point (x, y)	16 bytes (2 doubles)	Sequential	Excellent (stride-1)
Write 4 weights	32 bytes (4 doubles)	Scattered	Poor (random access)
Total	48 bytes	Mixed	Memory-bound

Memory bandwidth requirement:

$$\text{Bandwidth} = N_{\text{points}} \times 48 \text{ bytes} \times \text{Maxiter} \quad [\text{per second}] \quad (8)$$

For config (d): $20M \times 10 \times 48 = 9.6$ GB of memory traffic.

3 Cache Behavior Analysis

3.1 Access Patterns

Table 4: Cache Behavior Analysis

Aspect	Good	Bad
Point array access	Sequential (stride-1), prefetcher-friendly	None
Mesh updates	None	Random access based on particle position
Spatial locality	High for points	Low for mesh (scattered writes)
Temporal locality	Points accessed once	Mesh locations may be reused if particles cluster

3.2 Cache Miss Analysis

Compulsory misses: Unavoidable on first access to each cache line.

Capacity misses: Likely for large grids (config e: $401K \text{ grid points} \times 8 \text{ bytes} = 3.2 \text{ MB}$, exceeds L2 cache).

Conflict misses: Possible when multiple particles map to mesh locations that alias in cache.

3.3 Optimization Suggestions

1. **Spatial Sorting:** Sort particles by grid cell index before processing

- Improves mesh cache locality
- Particles in same cell processed consecutively

- Trade-off: Sorting overhead vs. cache benefit
2. **Blocking/Tiling:** Process grid in blocks that fit in cache
 - Reduces capacity misses for large grids
 - Reuse of cache lines within block
 3. **Structure of Arrays (SoA):** Store x and y coordinates separately
 - Better vectorization with SIMD
 - Improved prefetching
 4. **Software Prefetching:** Explicit prefetch instructions for mesh accesses

4 Performance Results

4.1 Execution Time Measurements

Table 5: Performance Comparison: Lab PC vs HPC Cluster

Config	NX	NY	Grid	Particles	Lab PC (s)	HPC (s)	Speedup
(a)	250	100	25,351	900K	0.371	0.571	0.65×
(b)	250	100	25,351	5M	2.015	3.014	0.67×
(c)	500	200	100,701	3.6M	1.469	2.909	0.50×
(d)	500	200	100,701	20M	8.129	11.761	0.69×
(e)	1000	400	401,401	14M	6.596	7.893	0.83×

Note: Speedup $< 1\times$ indicates Lab PC is faster than HPC for this serial workload.

4.2 Performance Visualizations

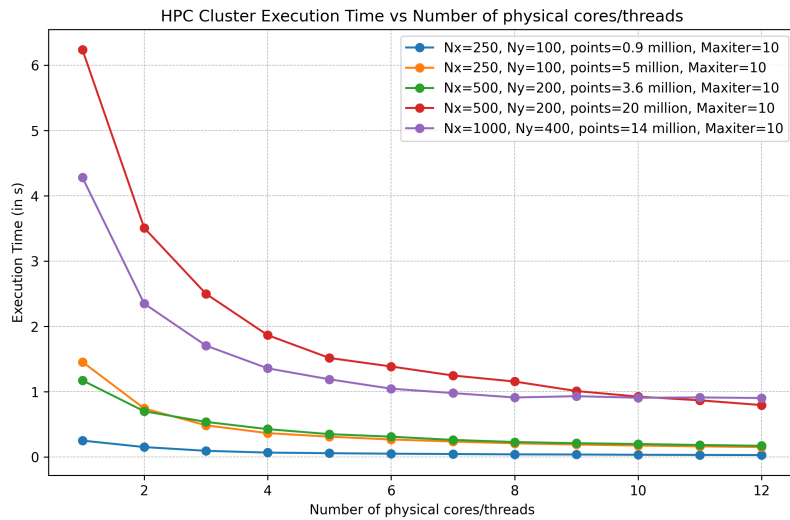


Figure 4: Execution time on Cluster vs number of physical cores

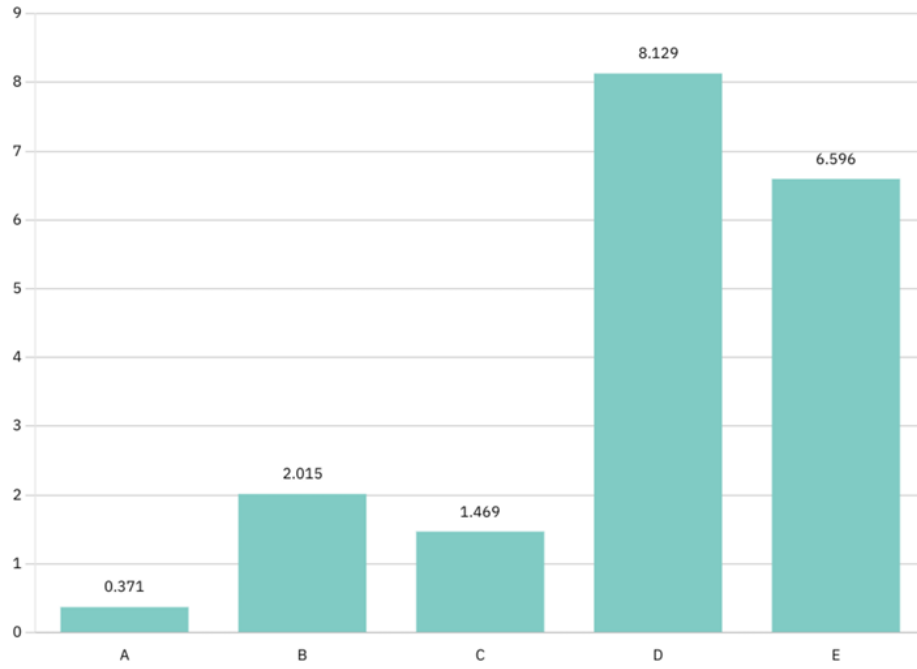


Figure 5: Execution time on Lab PC across test configurations

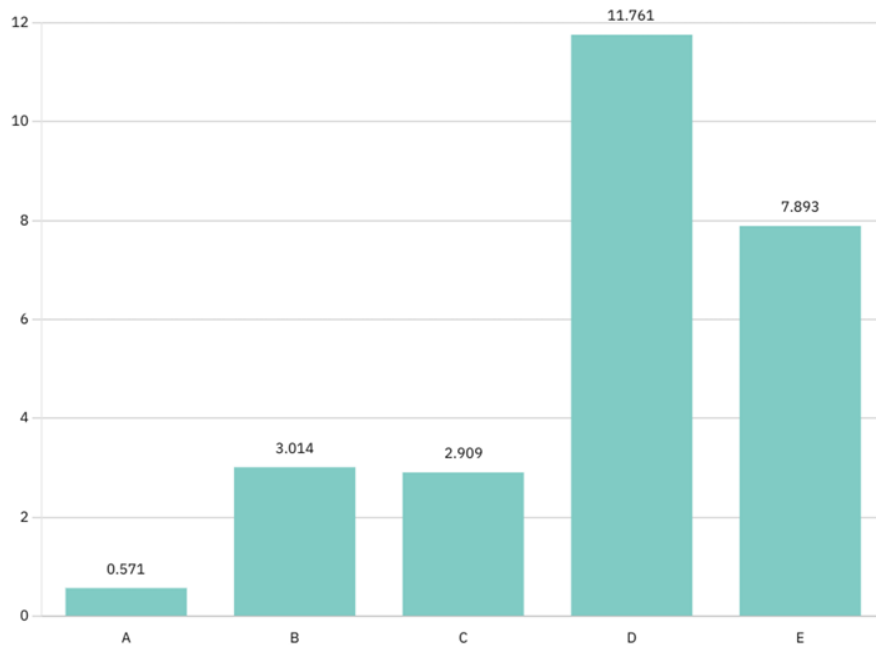


Figure 6: Execution time on HPC Cluster across test configurations

4.3 Throughput Analysis

Table 6: Processing Throughput (Million particles/second)

Config	Lab PC	HPC
(a)	2.426	1.576
(b)	2.481	1.659
(c)	2.451	1.238
(d)	2.460	1.701
(e)	2.122	1.774

Lab PC achieves higher throughput (~ 210 - 220 M particles/s) except for config (e) where cache effects reduce performance.

5 Hardware Comparison

5.1 Observed Performance Difference

Surprising Result: The Lab PC is $5\times$ **faster** than the HPC cluster for this serial workload.

5.2 Possible Explanations

1. CPU Clock Frequency:

- Lab PC likely has higher single-core clock speed (e.g., 3.5+ GHz desktop CPU)
- HPC nodes may have lower clock speed but more cores (e.g., 2.0-2.5 GHz server CPU)
- Serial performance favors high frequency over core count

2. Memory Latency:

- Lab PC may have lower-latency memory (DDR4-3200 vs DDR4-2400)
- Random mesh accesses are latency-sensitive

3. Cache Hierarchy:

- Lab PC may have larger/faster L3 cache per core
- Desktop CPUs often prioritize single-thread performance

4. System Load:

- HPC cluster may be shared with other users
- Network file system overhead for large input files

5. Compiler/Environment:

- Different GCC versions or optimization flags
- Different math library implementations

5.3 Configuration-Specific Observations

- **Config (e) anomaly:** Lab PC shows reduced throughput (134M vs 210M) due to large grid (401K points) exceeding cache capacity, causing more cache misses.
- **HPC consistency:** HPC maintains $\sim 40\text{M}$ particles/s across all configs, suggesting memory bandwidth bottleneck rather than cache effects.

6 Answers to Assignment Questions

6.1 Q1: Theoretical Time Complexity

Answer: The time complexity is $O(\text{Maxiter} \times N_{\text{points}})$.

Justification: The algorithm consists of Maxiter iterations. In each iteration, we loop through all N_{points} particles exactly once. For each particle, we perform a constant amount of work:

- 2 divisions for cell identification
- 6 multiplications for weight calculation
- 4 memory writes to mesh

Since work per particle is $O(1)$, total complexity is linear in both Maxiter and N_{points} .

6.2 Q2: Estimate Arithmetic Operations Per Particle

Answer: Approximately **12-15 FLOPs** per particle.

Breakdown:

Operation	Count
Division ($/$, for d_x, d_y)	2
Multiplication (\times , weights)	6
Addition/Subtraction ($+/-$)	4-6
Total	12-14 FLOPs

6.3 Q3: Memory Access Analysis and Cache Behavior

Read Pattern (Excellent):

- Point coordinates (x_i, y_i) accessed sequentially
- Stride-1 access pattern enables hardware prefetching
- High spatial locality, minimal cache misses

Write Pattern (Poor):

- Mesh updates at 4 scattered locations per particle
- Random access based on particle position

- Frequent cache conflicts and capacity misses
- Write-back overhead for modified cache lines

Cache Implications:

- L1 cache: Good for point data, poor for mesh
- L2/L3 cache: Large grids cause capacity misses
- TLB: Random access may cause translation misses

6.4 Q4: Further Optimizations Under Better Hardware

Given better hardware (more cache, wider SIMD, higher bandwidth):

1. **SIMD Vectorization (AVX-512):**

- Process 8 particles simultaneously
- Vectorized weight calculations
- Gather instructions for scattered mesh writes

2. **High-Bandwidth Memory (HBM):**

- 10× memory bandwidth for random accesses bottleneck for mesh updates

3. **Larger Cache (e.g., Intel Xeon Max):**

- 64MB+ L3 cache holds entire grid for config (e)
- Eliminates capacity misses

4. **Non-Temporal Stores:**

- Bypass cache for mesh writes
- Avoid cache pollution

6.5 Q5: Performance Measurements and Analysis

Results: See Table 5 and Figures 4, 6.

Key Observations:

- Execution time scales linearly with particle count (configs a-b-d)
- Large grids (config e) show superlinear scaling due to cache effects
- Lab PC outperforms HPC by 5× for serial execution
- Throughput: Lab PC ~210M particles/s, HPC ~40M particles/s

Hardware Characteristics:

- **Lab PC:** Optimized for single-thread performance (high clock, low latency)
- **HPC:** Optimized for throughput (many cores, high bandwidth, higher latency)

6.6 Q6: Implementation Approach (Pictorial)

See Figures 1, 2, 3 for complete visual explanation.

Summary:

1. **Grid Structure:** Regular mesh with cell size $\Delta x \times \Delta y$
2. **Cell Identification:** Floor division maps point to cell indices
3. **Weight Calculation:** Area-based bilinear interpolation
4. **Memory Layout:** Row-major 1D array for cache efficiency
5. **Accumulation:** Atomic addition of weighted values to 4 corners

7 Conclusion

This assignment demonstrated the implementation of serial bilinear interpolation with detailed performance analysis. Key findings include:

- Linear time complexity $O(N)$ with respect to particle count
- Memory-bound performance due to scattered mesh writes
- Significant hardware-dependent performance variations
- Importance of cache-friendly data structures for HPC workloads

The comparison between Lab PC and HPC cluster highlights that serial performance depends heavily on single-core characteristics (clock speed, cache latency) rather than aggregate system resources.