Parallel Barnes-Hut N-body Toy Galaxy Simulation for Outreach

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Introduction

Motivation:

- Simulations enhance understanding of galaxy evolution and interactions.
- Current methods require extensive resources, limiting accessibility.
- Need for efficient simulations on resource-constrained systems.

Objective:

- Develop a Barnes-Hut N-body simulation for WeeArchie (a Raspberry Pi cluster).
- Use hybrid MPI + OpenMP for better efficiency and memory use.
- Make simulations accessible for education and outreach.

Context

N-body Method:

- Simulates dynamics of physical systems using discrete particles.
- Widely applied in astrophysics to model star clusters, galaxies, etc.

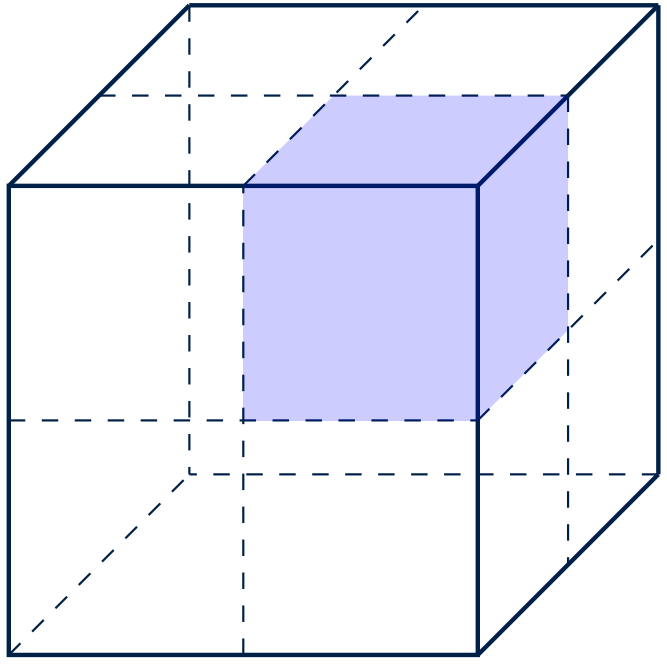
Barnes-Hut (BH) Algorithm:

- Approximates distant particle groups as single entities.
- Reduces complexity from $O(n^2)$ to $O(n \log n)$ using hierarchical tree structure.
- Enhanced through parallelization for better performance.

BH Algorithm (cont.)

Tree Construction (3D Space):

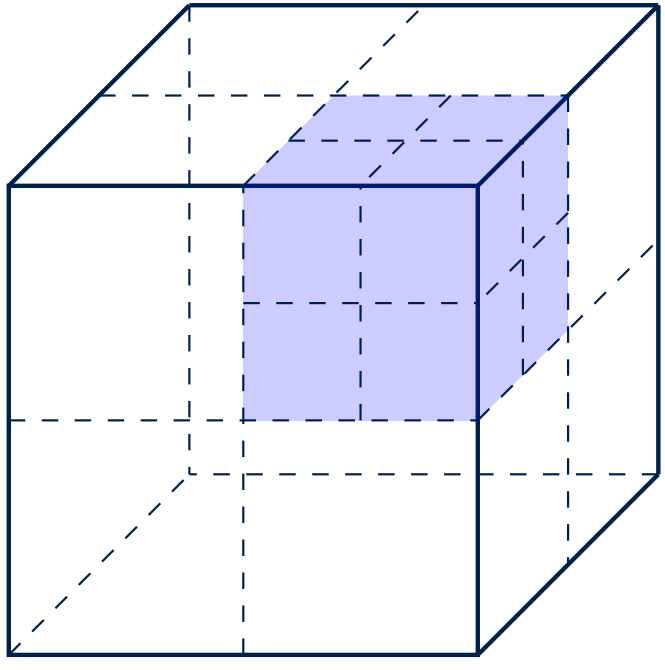
- Space is recursively divided into 8 sub-spaces.
- Each region is represented as a node in an octree.



BH Algorithm (cont.)

Octree Construction (3D Space):

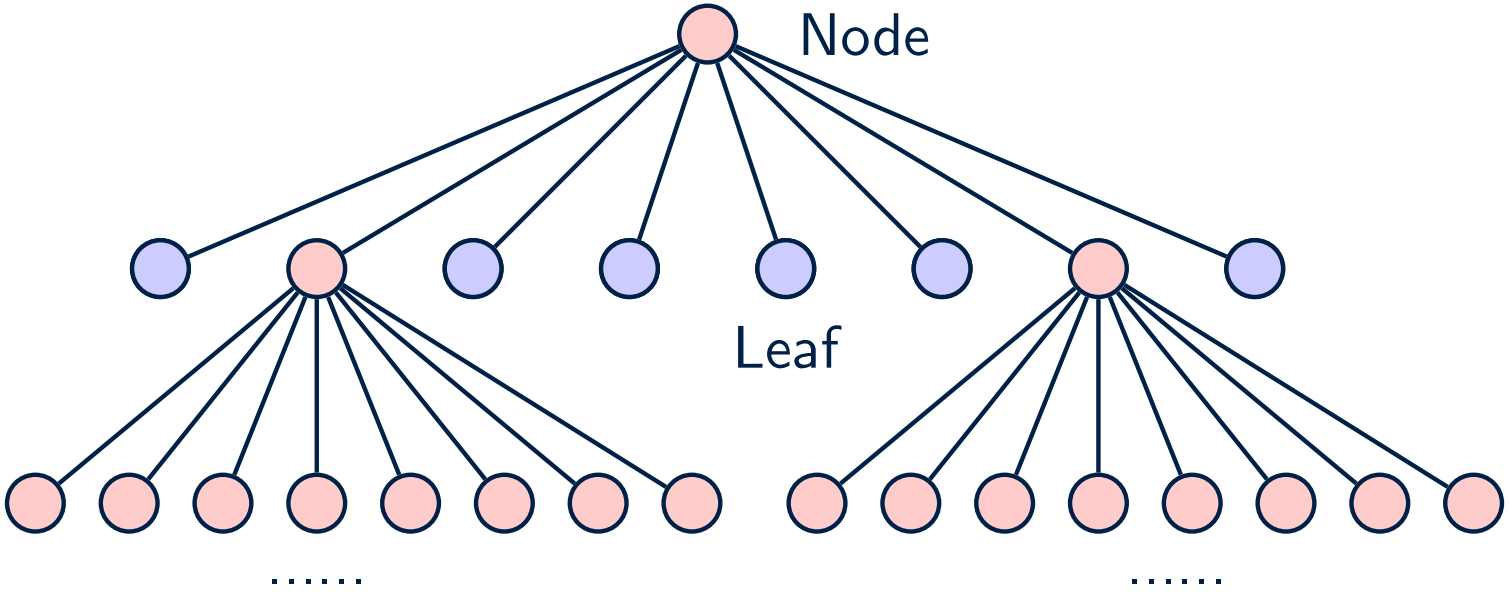
- Space is recursively divided into 8 sub-spaces.
- Each region is represented as a node in an octree.
- Each region with more than 1 particle can be continuous divided into 8 parts.



BH Algorithm (cont.)

Tree Construction (Octree):

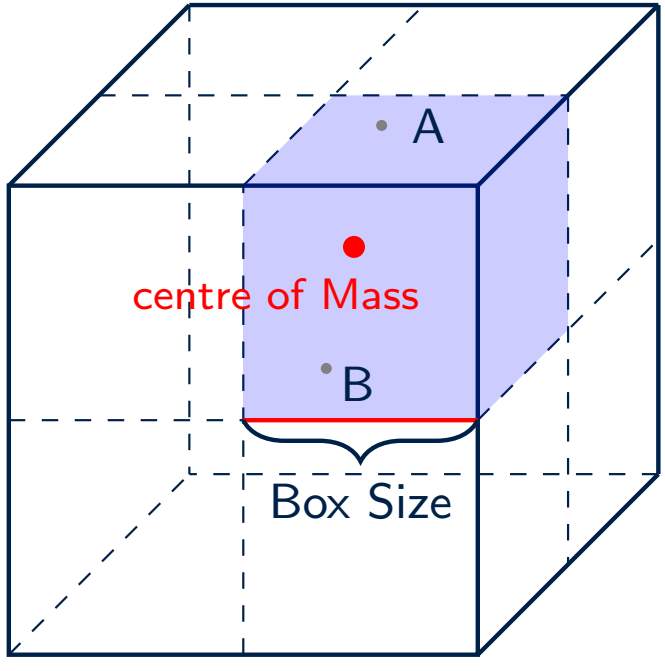
- Nodes containing a single particle are leaves
- Nodes with multiple particles are further subdivided.



BH Algorithm (cont.)

Force Calculation:

- For each octree node, the node is simplified to a single mass at its center of mass if the box size to distance ratio is less than a predefined threshold `THETA`.
- Otherwise, the algorithm recursively evaluates child nodes for detailed force calculations.



Galaxy Simulation - Initialization

- **Supermassive Black Hole (SMBH)**: Central massive object around which the galaxy is modeled.
- **Disk-like Galaxy**: Modeled as a circular approximation for ease of simulation.
- **Initial Velocity**: Each particle is given an initial velocity to simulate circular orbits around the SMBH.

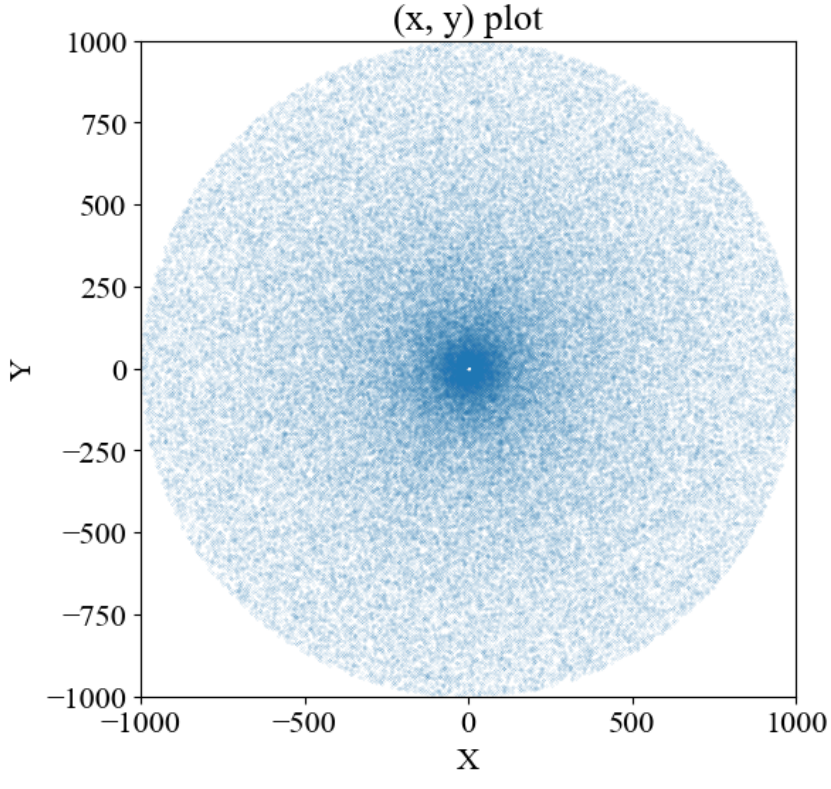


Figure: Initialization of the galaxy.

Hybrid MPI + OpenMP Parallelization

Data Decomposition: Particles are statically assigned to processes based on their index, promoting an even distribution of work across processes.

MPI Communication:

- **Broadcast**: Initial particle states are shared using `MPI_Bcast`.
- **Updates**: Updates are gathered with `MPI_Gather` and redistributed via `MPI_Bcast` to minimize data exchanges.
- **Synchronization**: `MPI_Barrier` ensures all processes are synchronized after updates.

Hybrid MPI + OpenMP Parallelization (cont.)

OpenMP Implementation

- **Octree Insertion**:
  - `pragma omp parallel for` parallelizes particle insertion into the octree.
  - `pragma omp critical` prevents data races during octree updates.
- **Force Calculation and Particle Update**:
  - `pragma omp parallel for` parallelizes force calculations and updates, with threads handling separate subsets of particles.

Test Hardware Changed

Original Plan:

- Develop and test the galaxy simulation on WeeArchie.

Challenges:

- WeeArchie was temporarily unavailable.
- Replicating WeeArchie on an EIDF VM was complex and time-consuming.

Solution - Cirrus Supercomputer:

- Switched to Cirrus for its high-performance computing.
- Cirrus' powerful CPUs were ideal for intensive simulations.
- Ensured timely development and testing.

Performance Results

Testing Framework:

- Simulated 10^5 particles over 50 iterations.
- Each test was repeated three times to get average runtime.

Optimal Configuration:

- Used 2 MPI processes with 18 threads each, spread over 8 nodes.
- Achieved a runtime of 31 seconds for 50 iterations.
- This parallel setup is 15 times faster than the baseline.

Performance Result - Scaling

Strong Scaling:

- Conducted with optimal configuration across varying numbers of nodes.

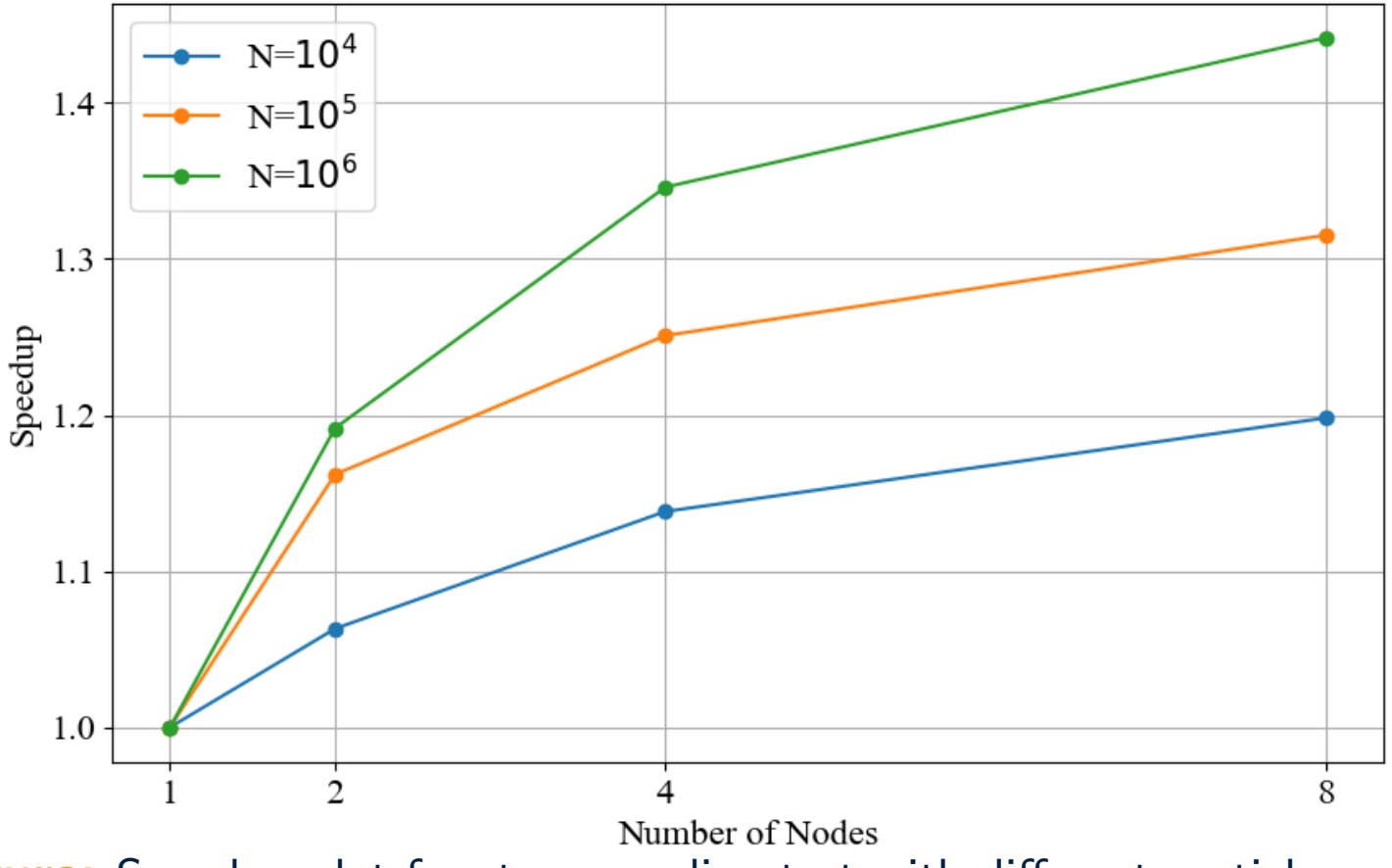


Figure: Speedup plot for strong scaling test with different particle counts.

Conclusion

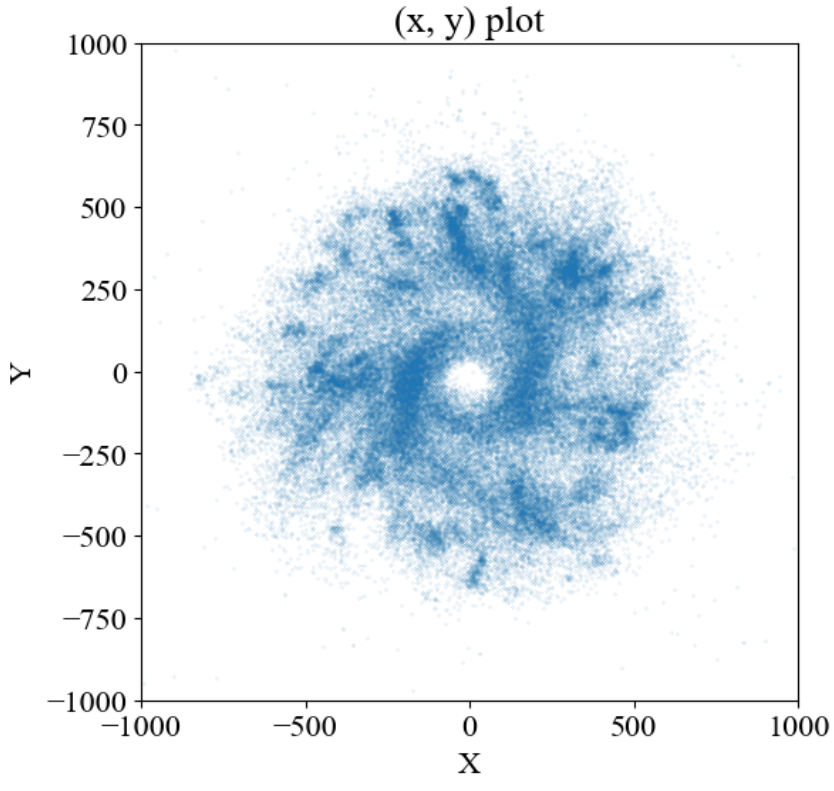
- Successfully developed a hybrid parallelized galaxy simulation model.
- Tested on Cirrus due to WeeArchie's unavailability, demonstrating scalability and performance improvements.
- Laid groundwork for using low-cost hardware for complex simulations.
- Future adaptations needed for WeeArchie's limited resources to fully meet project objectives.

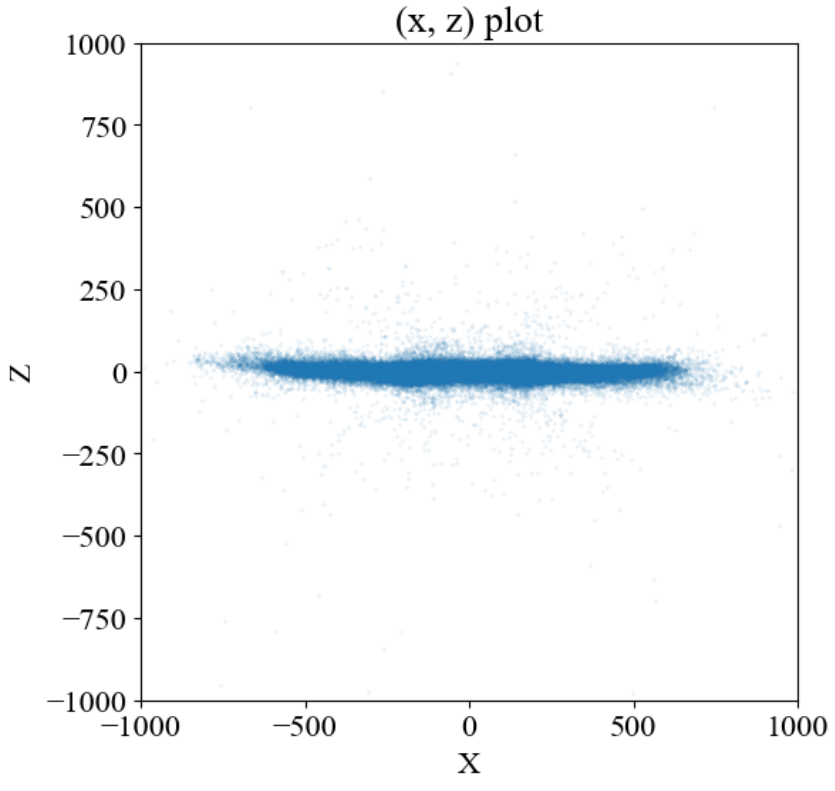
Future Work

- Adapt the simulation model for efficient execution on WeeArchie.
- Optimize MPI communication, exploring non-blocking methods and efficient data aggregation.
- Develop a user-friendly interface to enhance accessibility for educators and researchers.

Thank you!

Q&A





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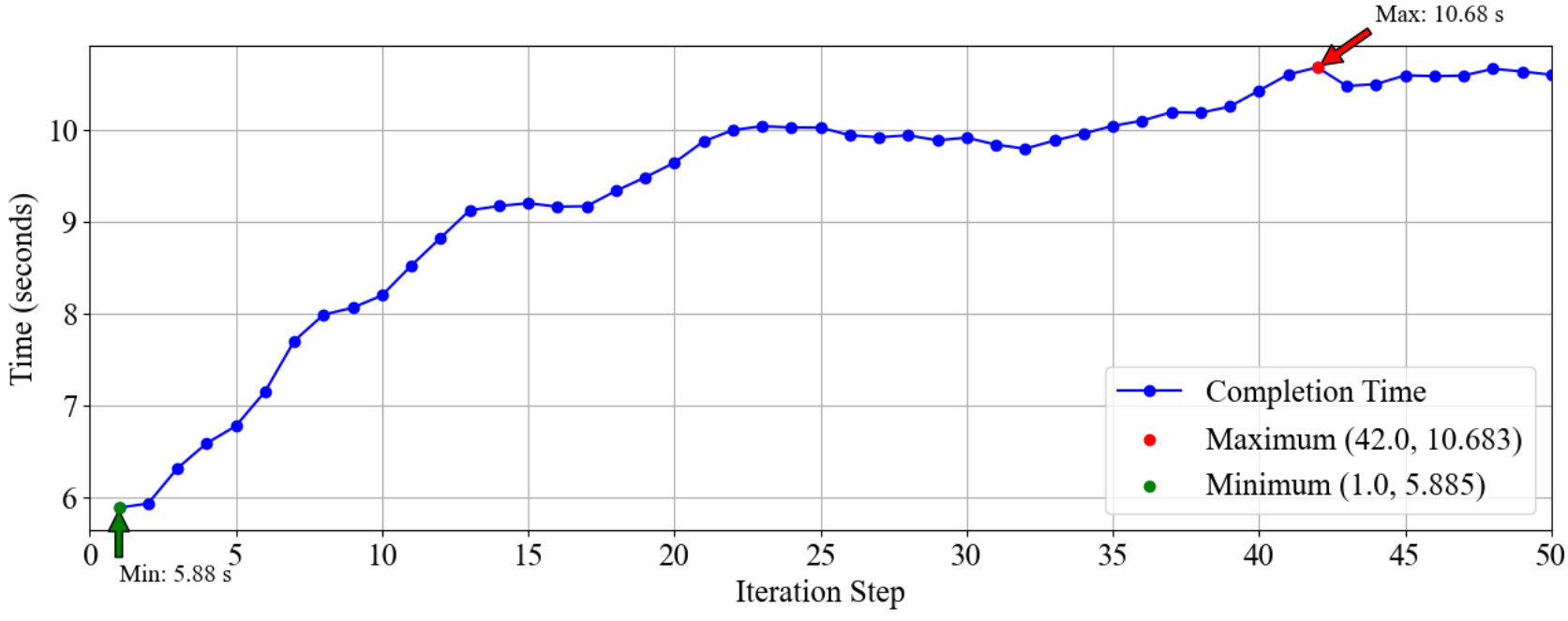
[1] Alternative access to video: Galaxy Simulation Video

Scaling Runtime

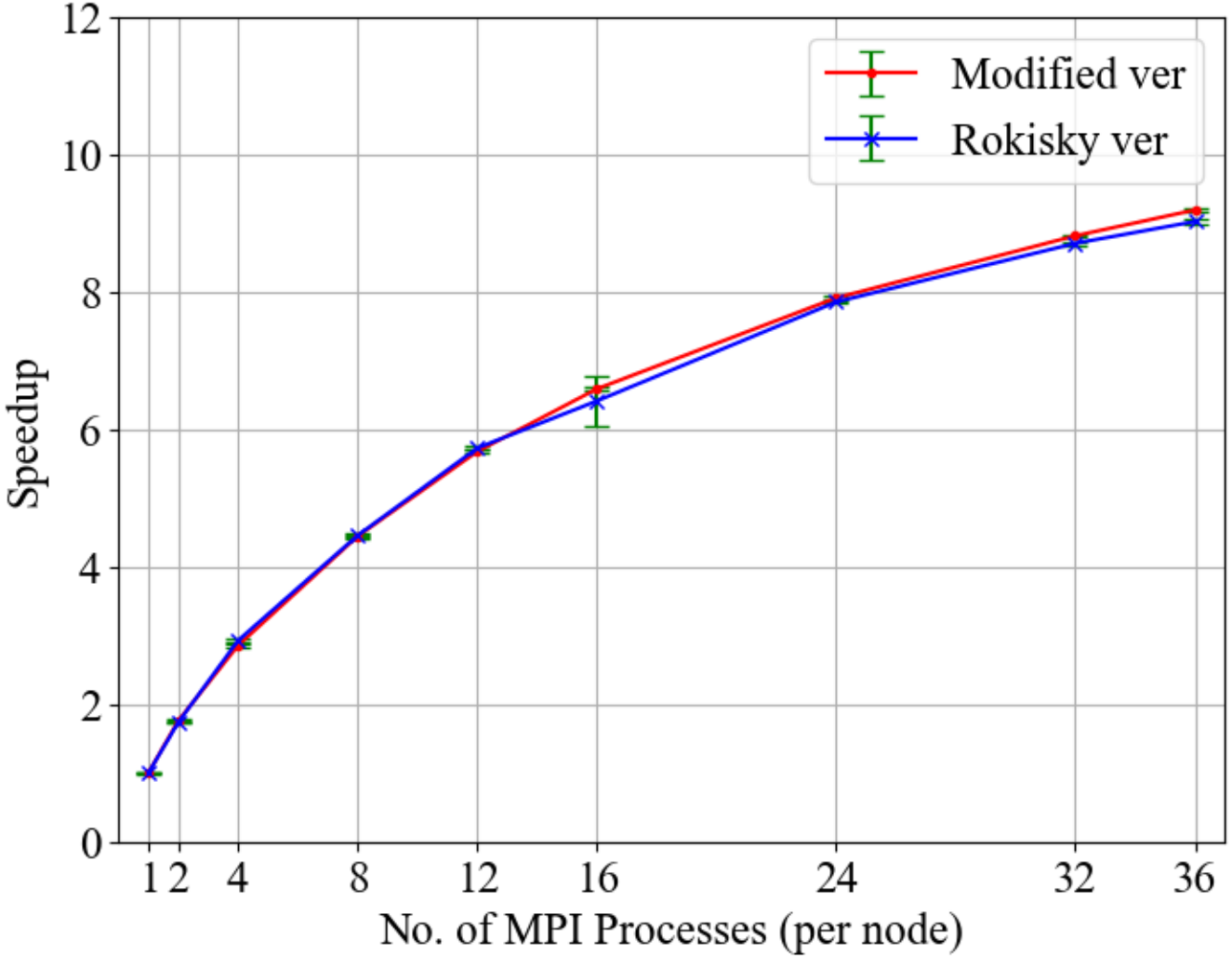
Number of Particles	Nodes = 1 (Avg. Time)	Nodes = 8 (Avg. Time)
10^4	3.87 s	3.23 s
10^5	42.18 s	32.07 s
10^6	517.29 s	358.81 s

Table: Comparison of average runtime for different particle sizes on 1 node and 8 nodes.

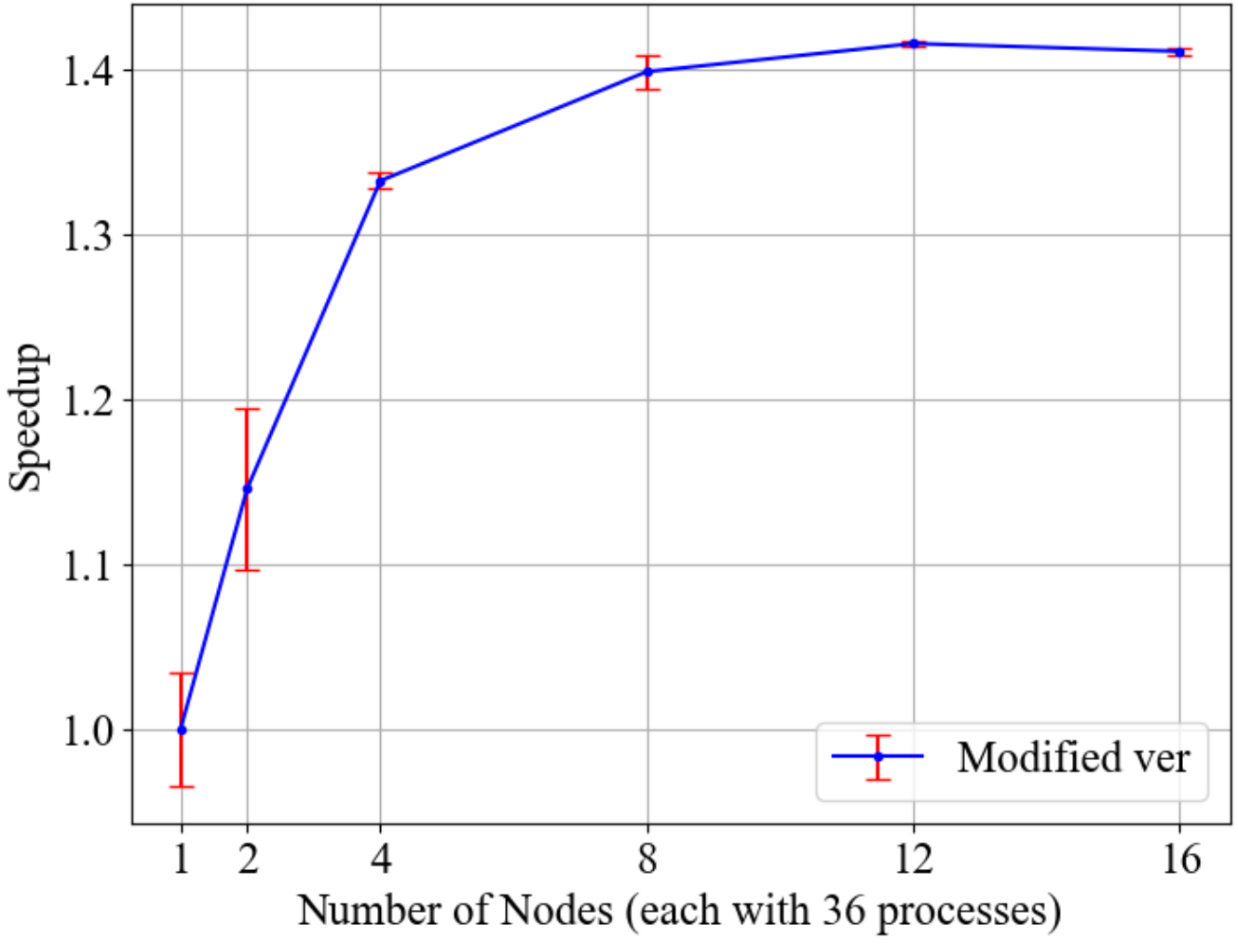
Serial performance at first 50 iterations



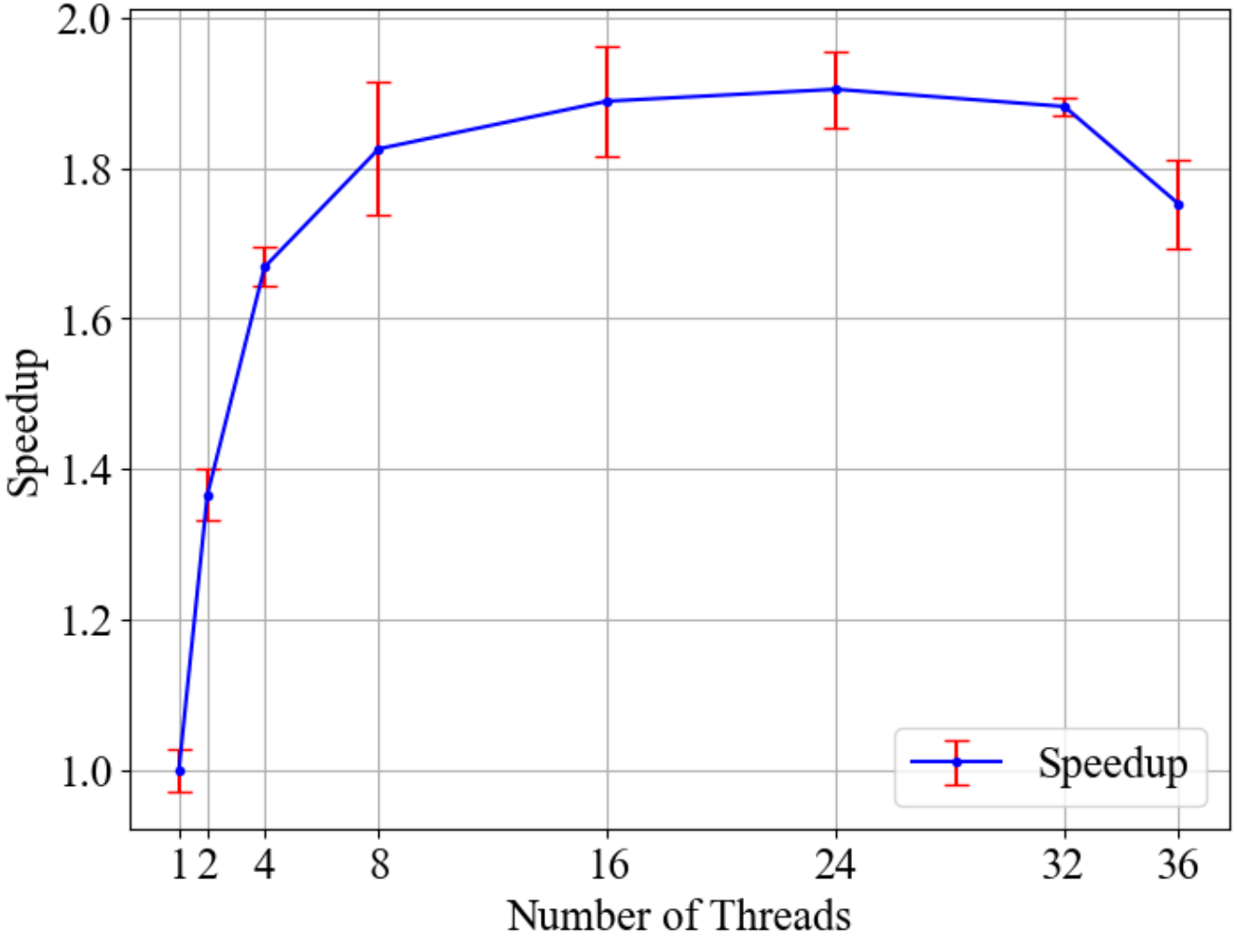
Single Node Performance



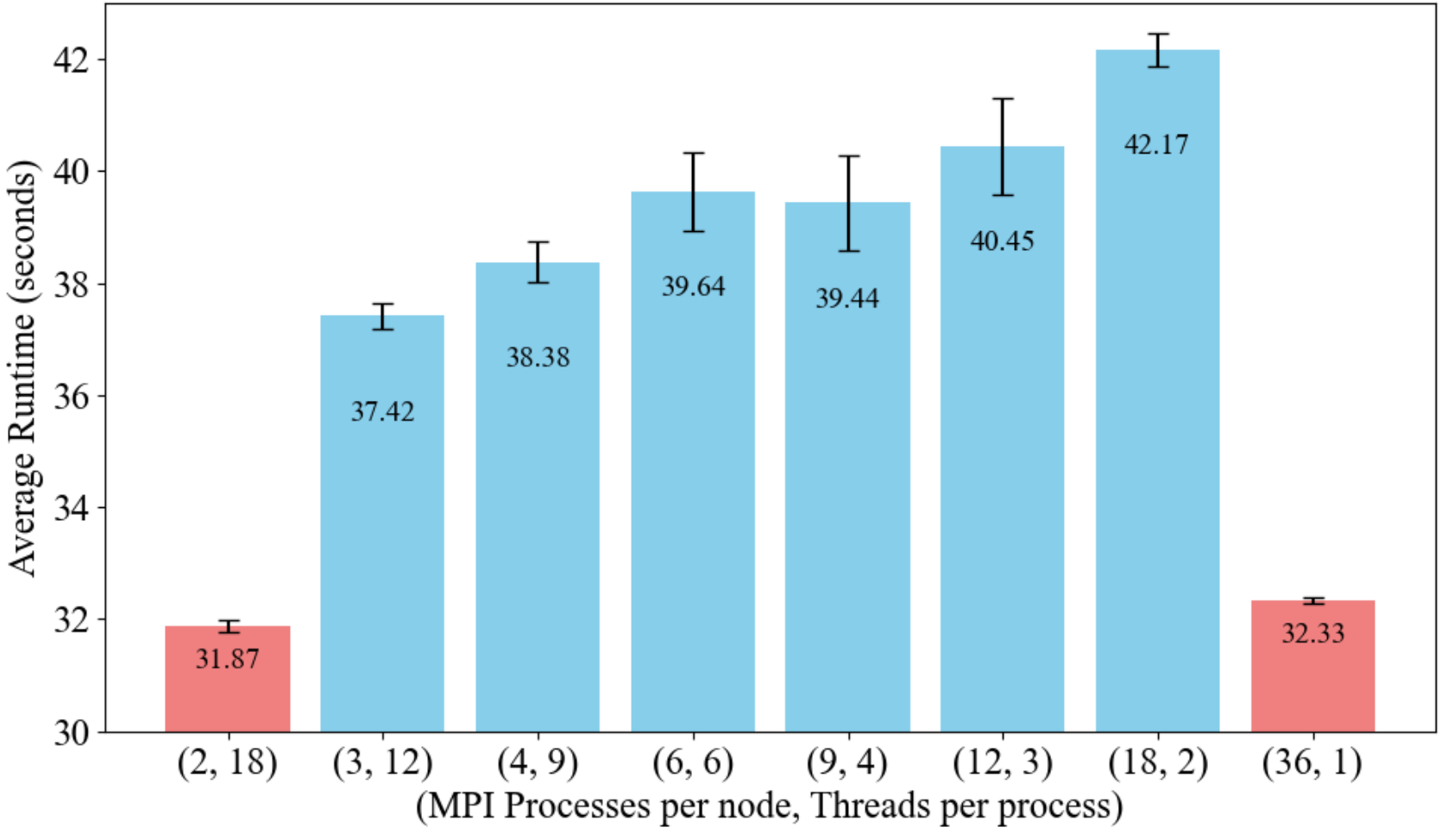
Multiple Nodes Performance



Multiple Threads Performance



8 Nodes with full use of each node



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