UNIVERSITÀ
DEGLI STUDI
DI PADOVA

N-Body Simulation: Design, Optimizations and Benchmarking

M. Sc. Physics of Data, University of Padova

Alessio

July 23, 2025

Outline

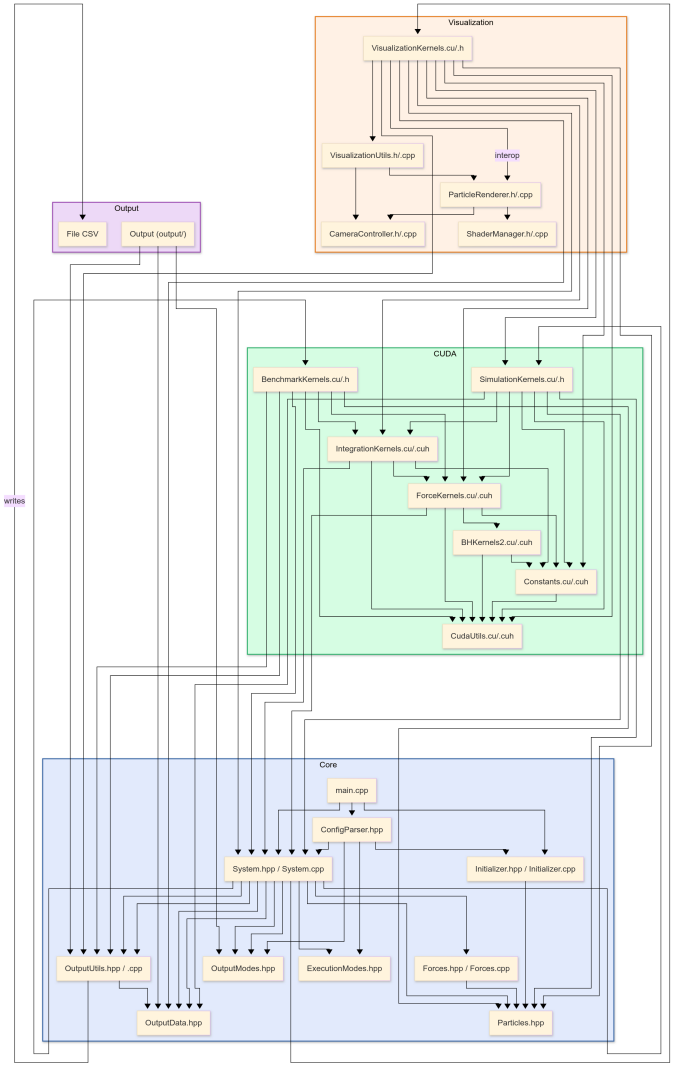
Introduction and Motivation

- Started as a simple single-file C++ code for Voyager II trajectory
- Evolved into a modular, configurable N-body simulator
- Main goals:
  - Flexible and extensible framework
  - Fair CPU vs GPU performance comparison
  - Advanced optimizations and interactive visualization

Project Evolution

- Initial single-file C++ implementation
- Output separation and modularization
- Integration of OpenMP, CUDA, (AVX2)
- Refactoring, CMake build system, JSON configuration
- Interactive visualization with OpenGL

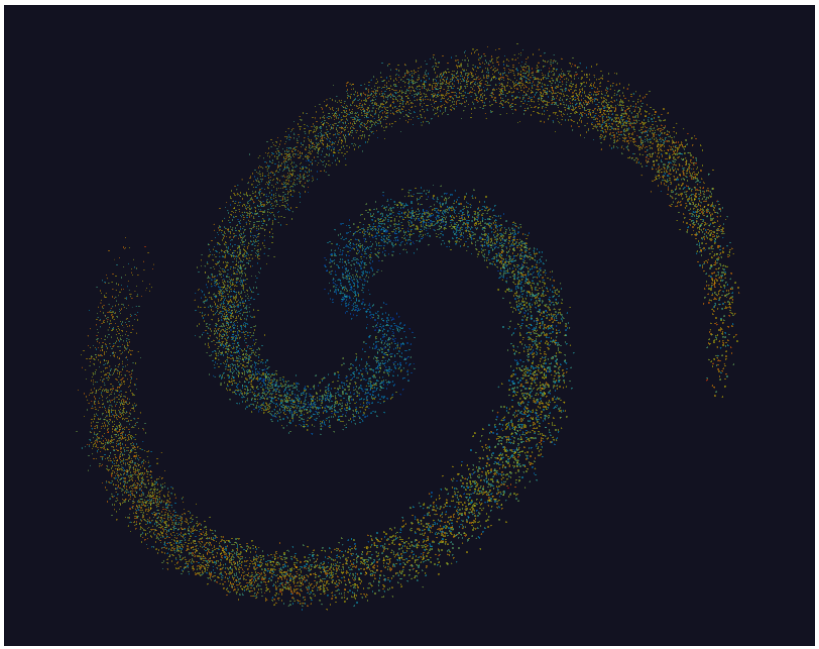
General Architecture



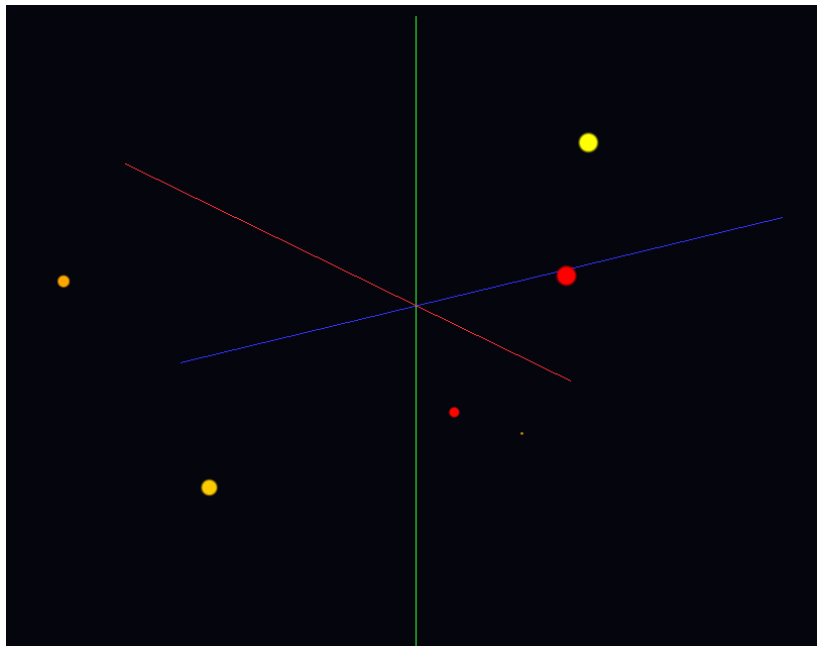
- **Core**: simulation logic, data structures, and CPU part
- **CUDA**: GPU kernels, utilities and host functions
- **Visualization**: OpenGL and OpenGL/CUDA interop
- **Output**: CSV output, dynamical buffer to use for other integrations
- **Configuration**: single JSON file

Configuration and Initialization

- Single JSON configuration file
- Flexible initialization: random, file-based, or custom implementations (galaxy, stellar systems, etc.)



Example of a galaxy configuration



Example of random initialization

Memory Management and Optimizations

- Structure of Arrays (SoA) for efficient access and fully coalesced memory with double4
- Pinned memory and CUDA streams
- AVX2 vectorization and OpenMP threading
- Low-ish memory footprint: 1.1 GiB for 1B particles
- In CSV output mode, System is copied only at the start $\rightarrow$ multiple cuda streams for memory and compute management.
- In visualization mode, System is copied every frame to a dynamic buffer, which is then used for rendering $\rightarrow$ worst case scenario $\Rightarrow$ OpenGL-cuda interop and separate rendering stream $\rightarrow$ less bottleneck.

Force and Integration Methods

- Pairwise, Adaptive Mutual Softening, Barnes-Hut (no GPU implementation)
- Configurable physical constants and softening
- Multiple integration schemes: Euler (not symplectic), Velocity Verlet (symplectic)

Pairwise Newtonian:

$$\vec{a}_i = G \sum_{j \neq i} m_j \frac{\vec{r}_j - \vec{r}_i}{|\vec{r}_j - \vec{r}_i|^3}$$

Adaptive Mutual Softening:

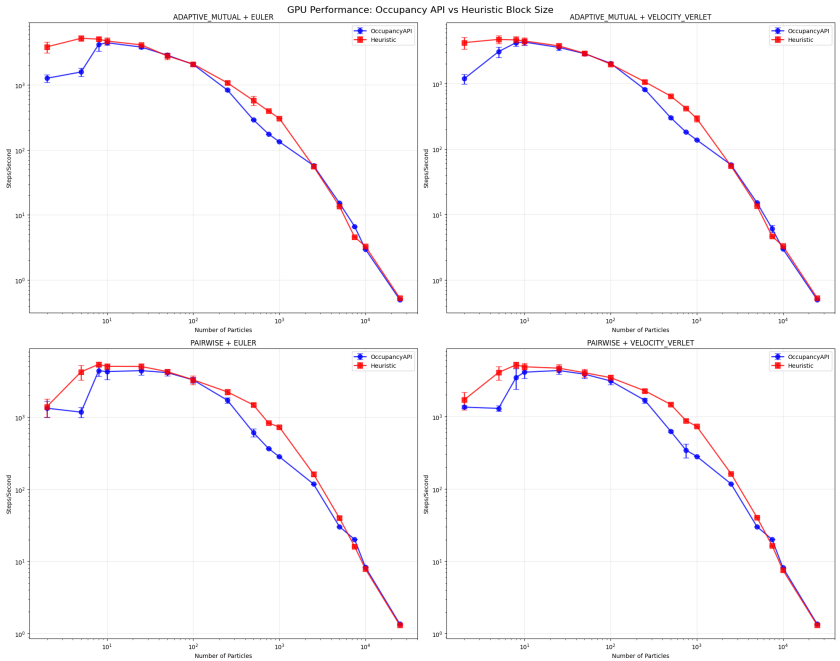
$$\vec{a}_i = G \sum_{j \neq i} m_j \frac{\vec{r}_j - \vec{r}_i}{\left(|\vec{r}_j - \vec{r}_i|^2 + \epsilon_{ij}^2\right)^{3/2}}$$

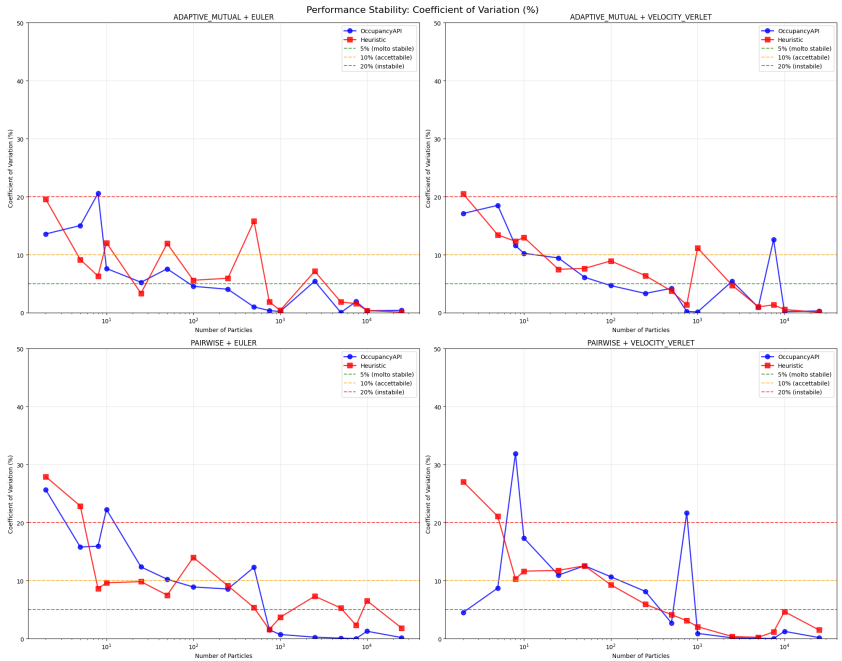
$$\epsilon_{ij} = \max\left(\eta \, |\vec{r}_j - \vec{r}_i| \left(\frac{m_i + m_j}{3\langle m \rangle}\right)^{1/3}, \epsilon_{\min}\right)$$

where G is the gravitational constant, ϵ_{ij} is the adaptive softening, η and $\epsilon_{\min}$ are tunable parameters, and $\langle m \rangle$ is the average mass.

Block Size Auto-Tuning

- **block size selection** is crucial for GPU efficiency in these problems.
- Two strategies compared:
  - Occupancy API (NVIDIA)
  - Heuristic (custom, optimized for this workload)



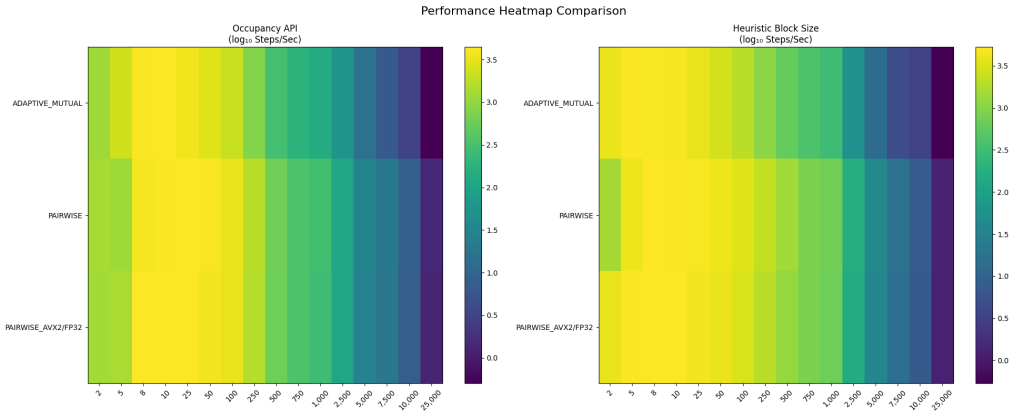


Block Size Auto-Tuning

Grid size:

$$\text{gridSize} = \left\lceil \frac{n}{\text{blockSize}} \right\rceil$$

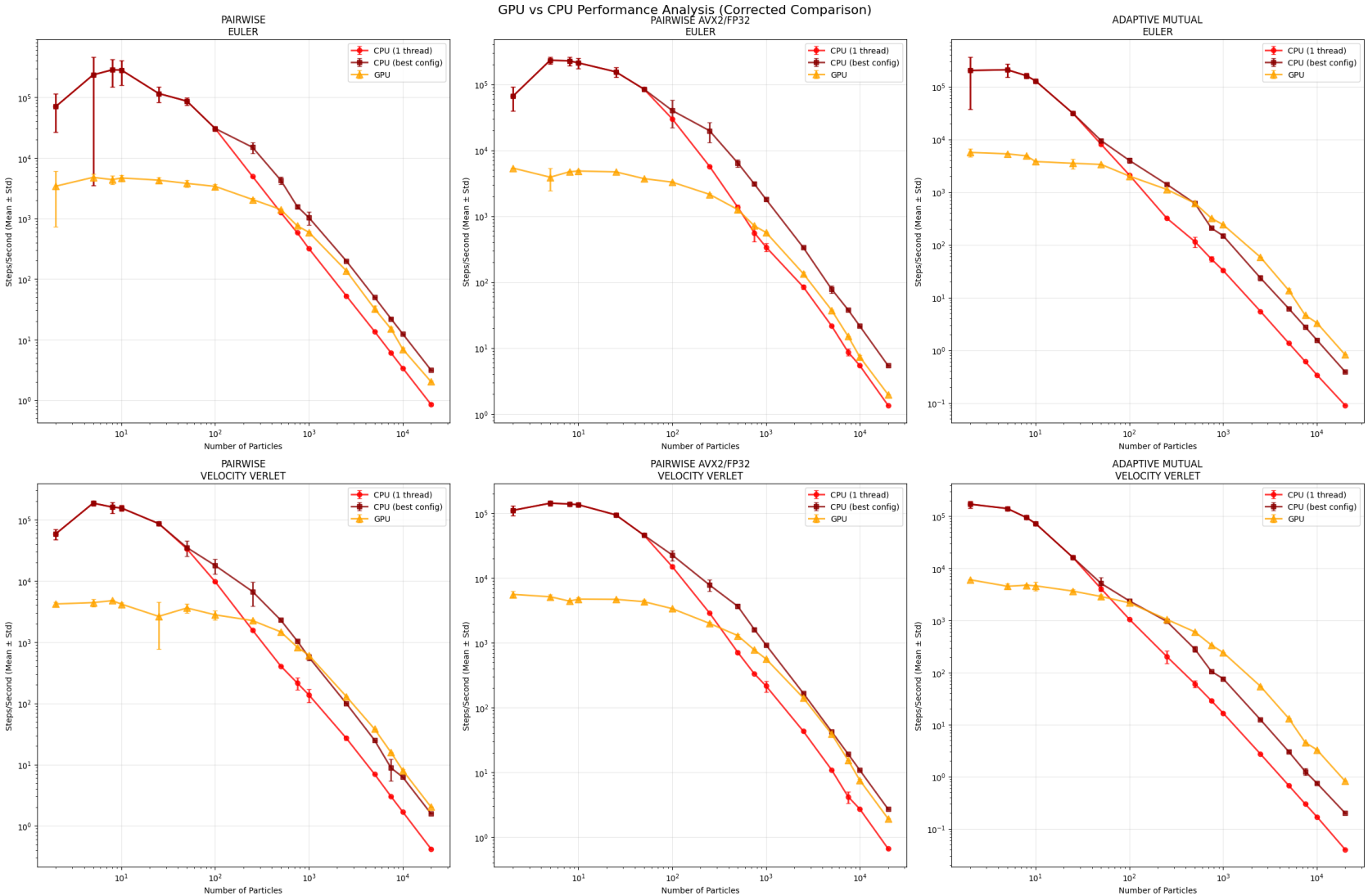
The heuristic is robust, saturates SMs, and respects shared memory limits. The grid size formula is exact for 1D N-body kernels.



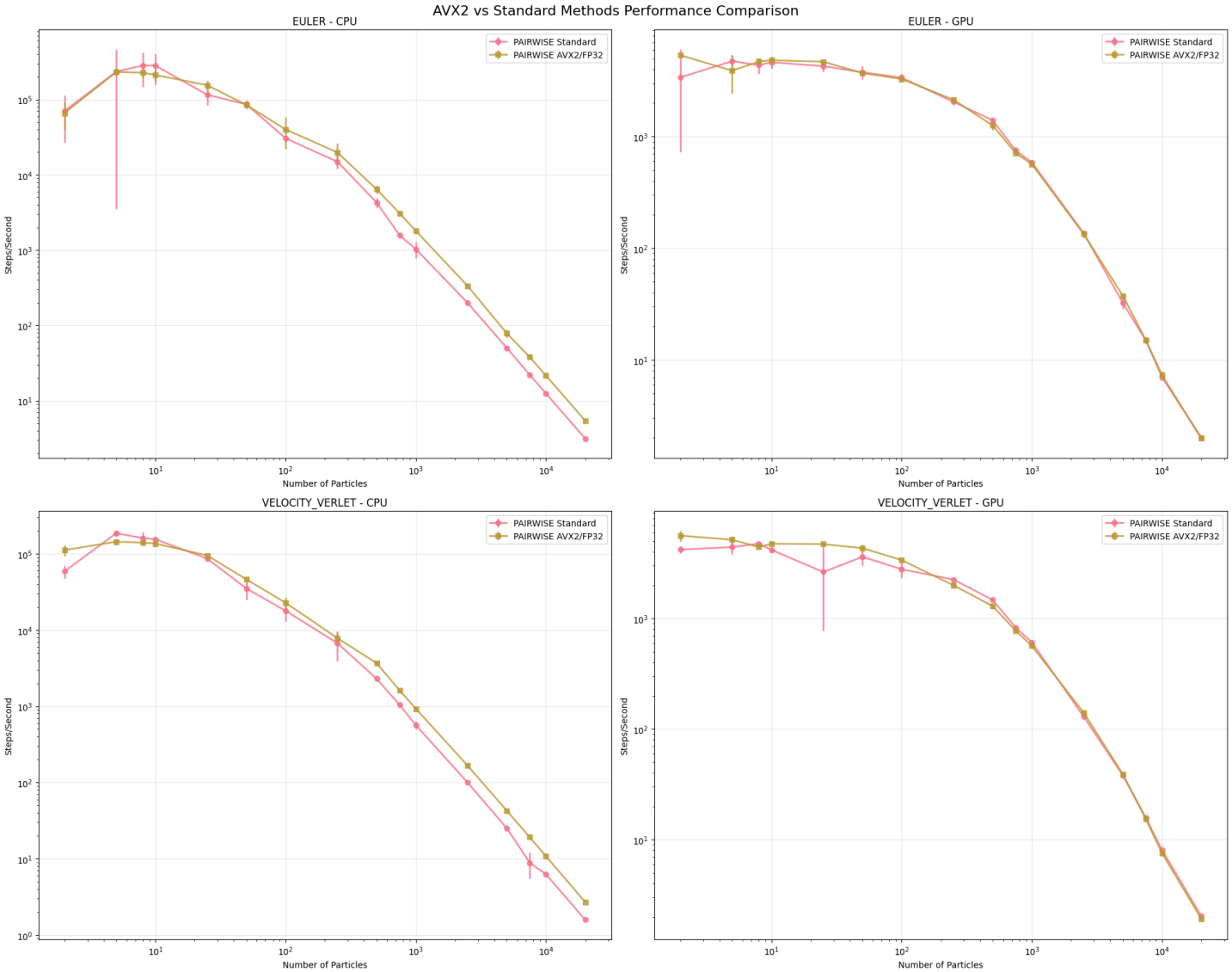
Heuristic Block Size Selection (pseudocode)

```
blockSize = 1024
if n ≤ 32:  return 32
while sharedMem(blockSize)
> maxShared && blockSize
> warp:
    blockSize //= 2
blockSize = min(blockSize,
maxThreads)
while numBlocks(blockSize)
< 2*numSMs && blockSize
> warp:
    blockSize //= 2
blockSize = max(blockSize,
warp)
return blockSize
```

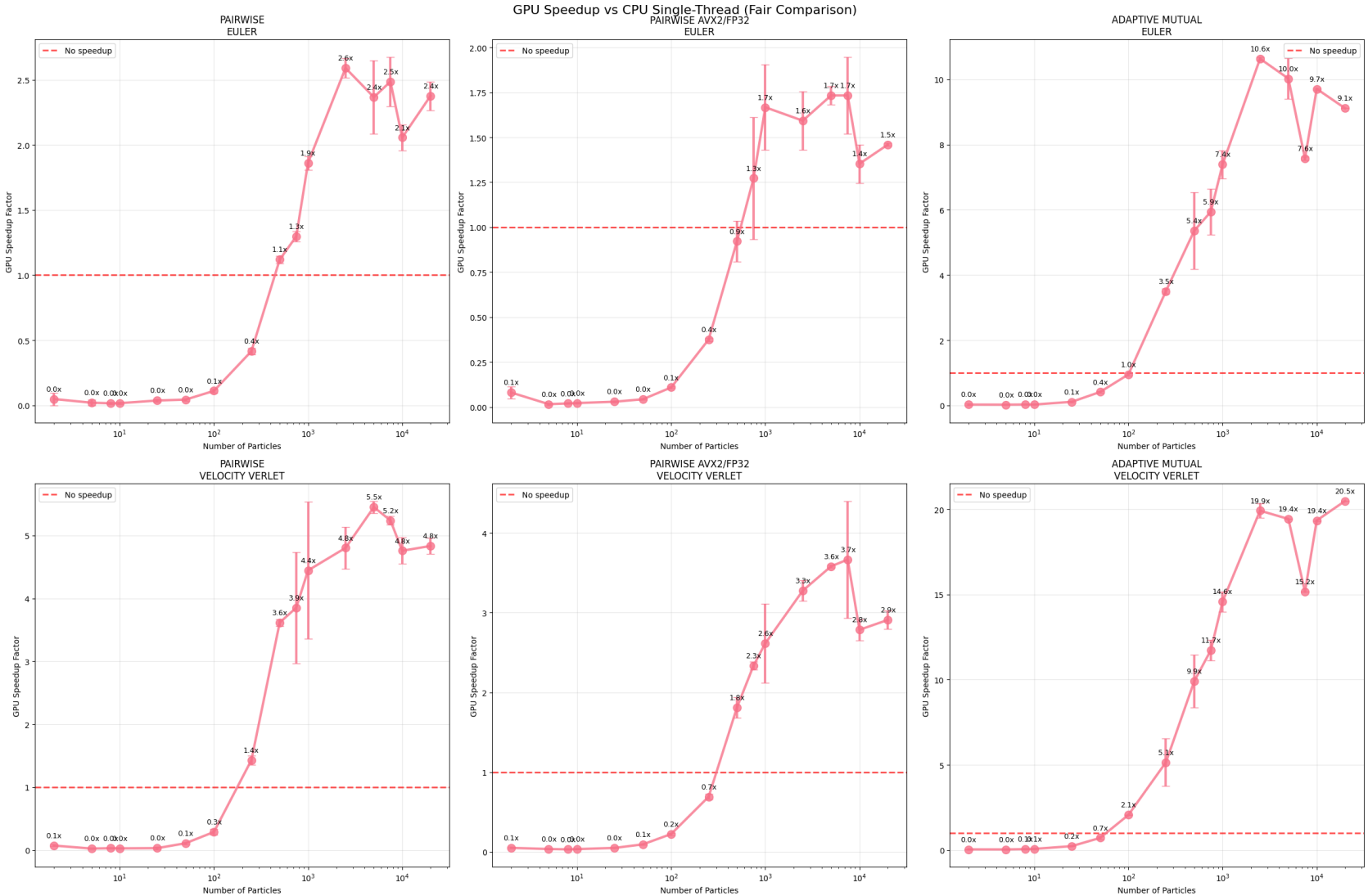
Basic CPU-GPU Comparison Benchmark



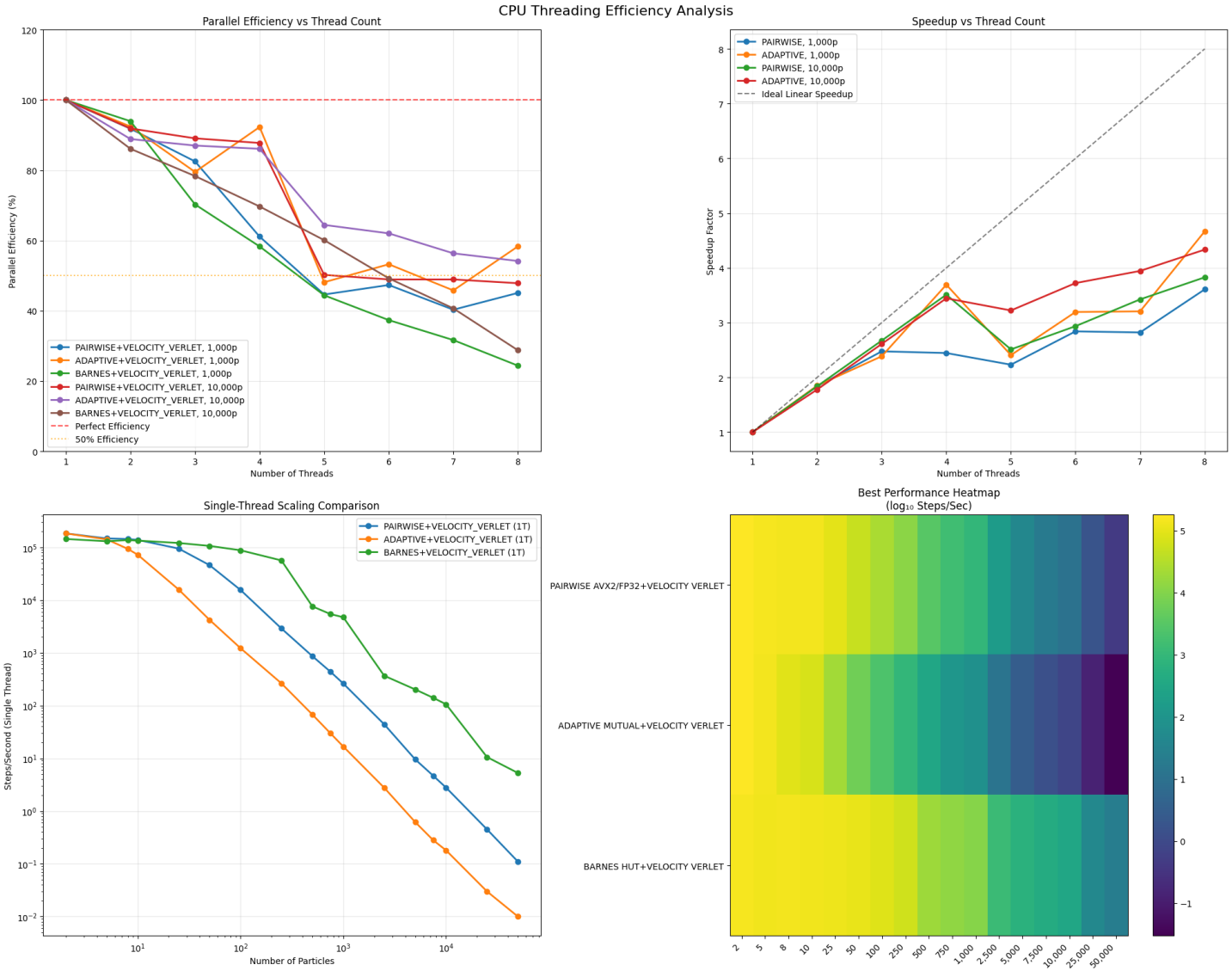
Basic CPU-GPU Comparison Benchmark



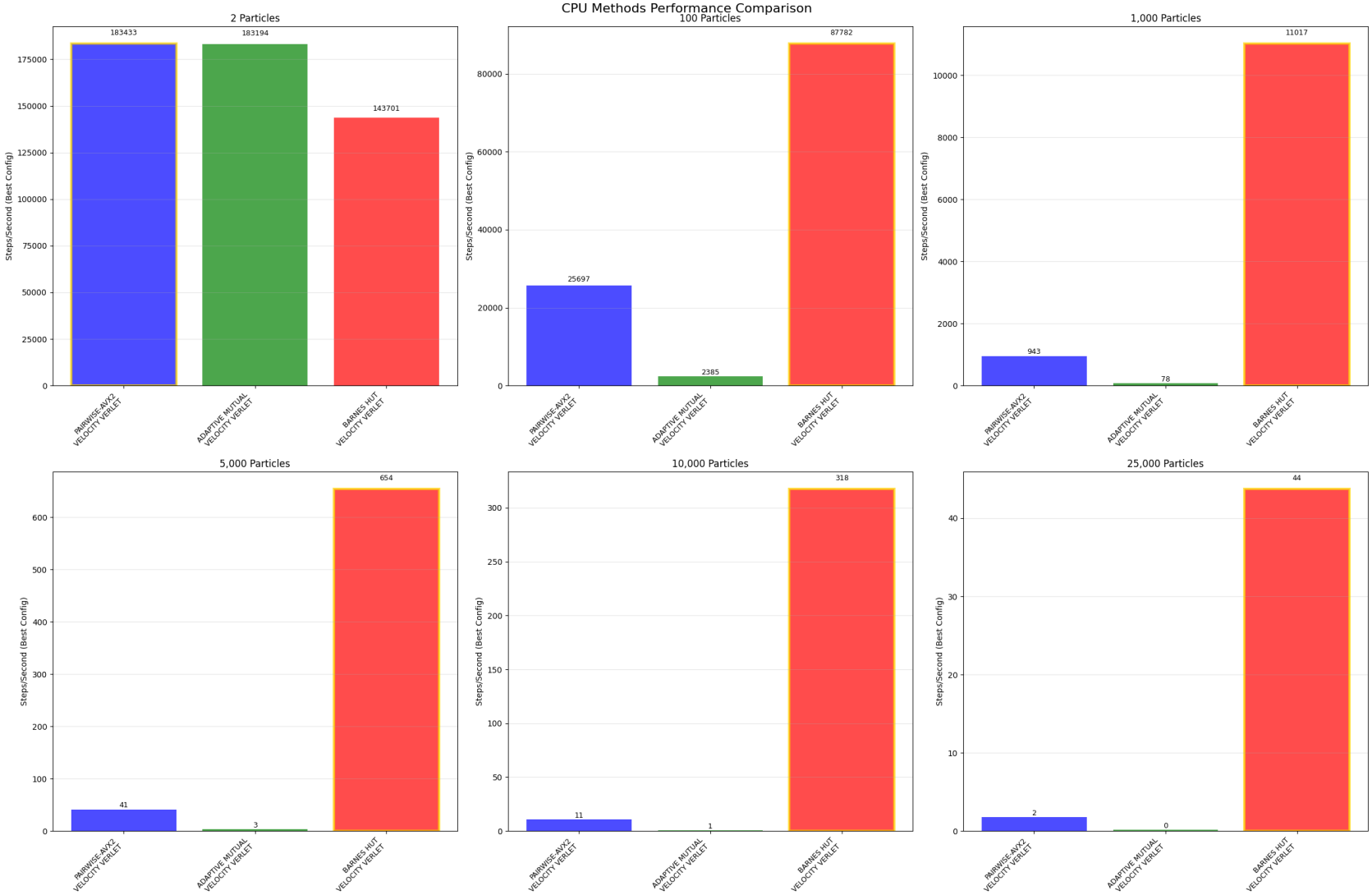
Basic CPU-GPU Comparison Benchmark



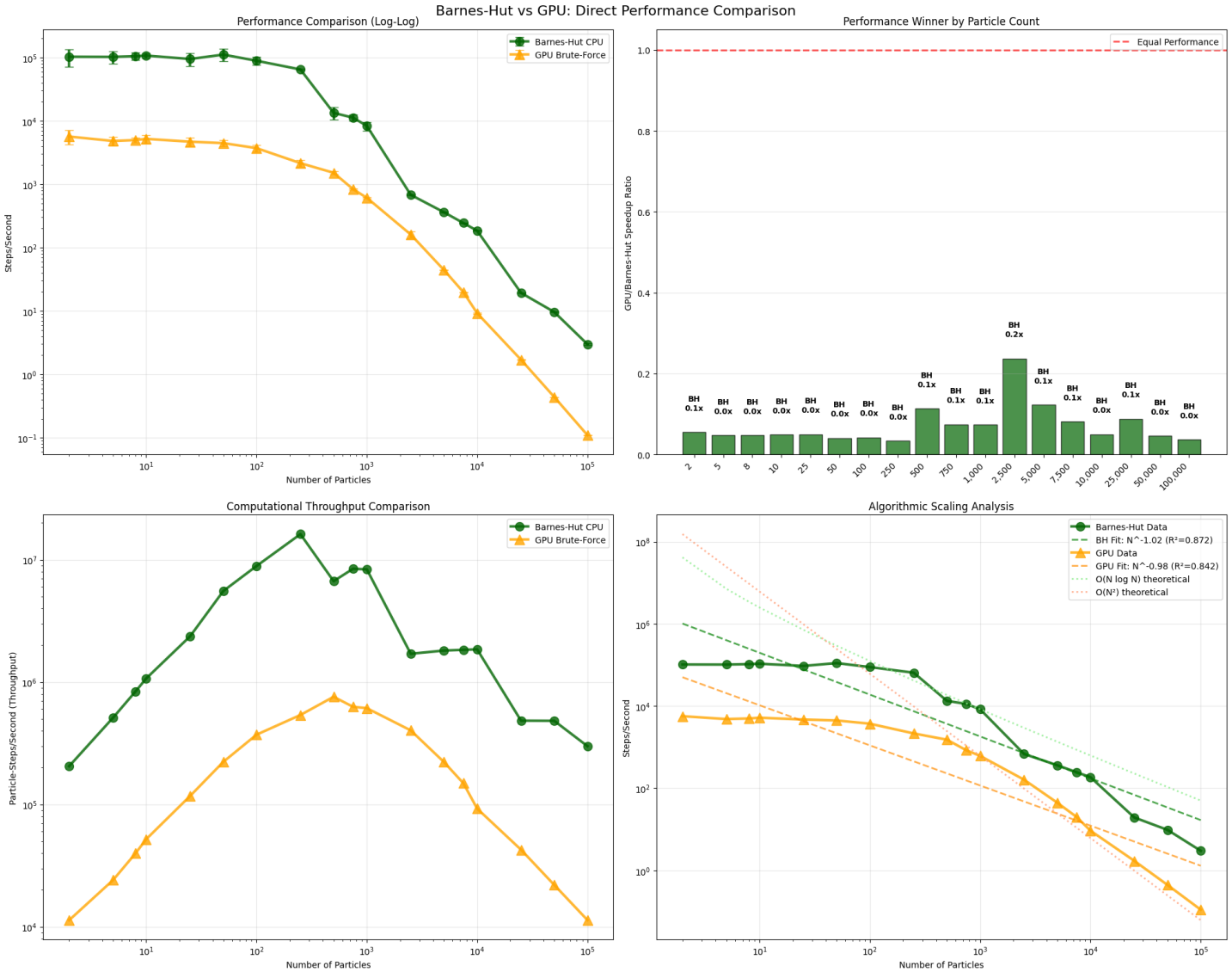
CPU-Methods Comparison Benchmark



CPU-Methods Comparison Benchmark



BH vs GPU Comparison Benchmark



Limitations and Lessons Learned

- Bottlenecks in compute for very large N
- Tradeoffs between accuracy and speed (double in GPU, same memory pattern in CPU).
- Importance of a clear vision at the start of the project
- Need for a robust testing framework
- Make only one main entry point per external library (or as few as possible)
- Future improvements: a running program you can compile without looking at any library requirements

Conclusions

- High-performance, modular N-body simulation achieved
- GPU acceleration enables large-scale experiments
- Framework ready for extension and research

Thank you for your attention!

Questions?

Demo?