PERFORMANCE-PORTABLE ELECTROSTATICS FOR EXASCALE ATOMISTIC SIMULATIONS

SIMULATION AND DATA LABORATORY COMPLEX PARTICLE SYSTEMS

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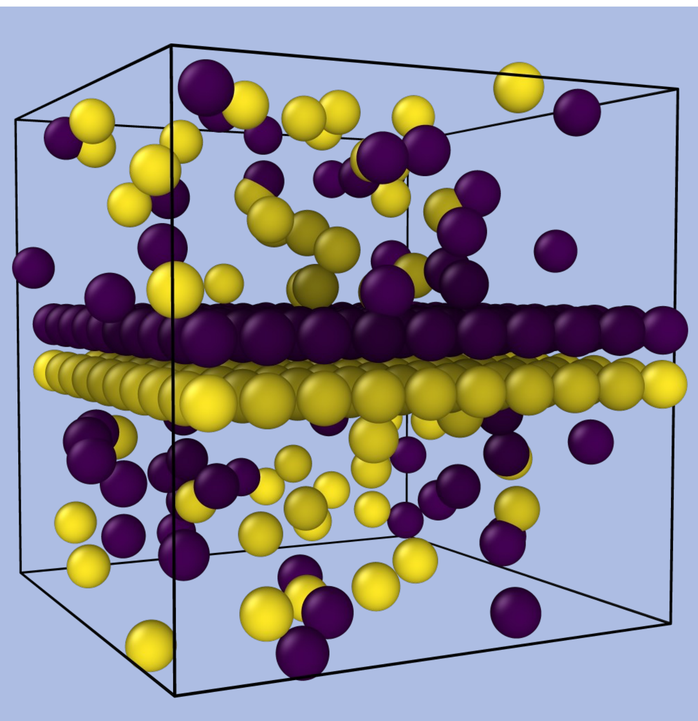


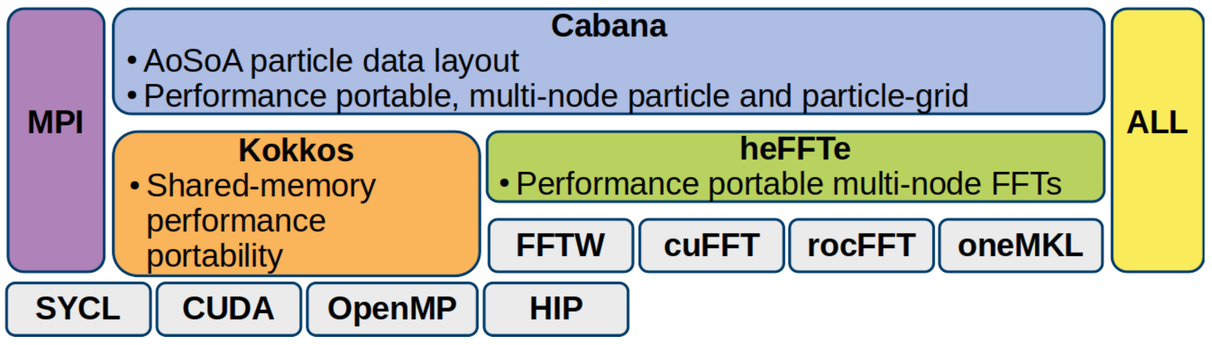
Visualization of the Cloud Wall system (300 charges)[1].

Long-range interactions remains a central challenge in molecular dynamics, soft-matter physics and materials science, especially in Exascale architectures with complex memory hierarchies and heterogeneous computing resources.

We present an Exascale-ready library that provides performance-portable implementations of the Particle–Particle Particle–Mesh (P3M) method and the Ewald summation method. These are designed to operate efficiently across diverse hardware platforms.

- Single, performance portable implementation for long-range electrostatics
- Modular design and ecosystem integration
- Short-range and long-range electrostatic calculations to be separated into distinct computational partitions

Dependecies and backends

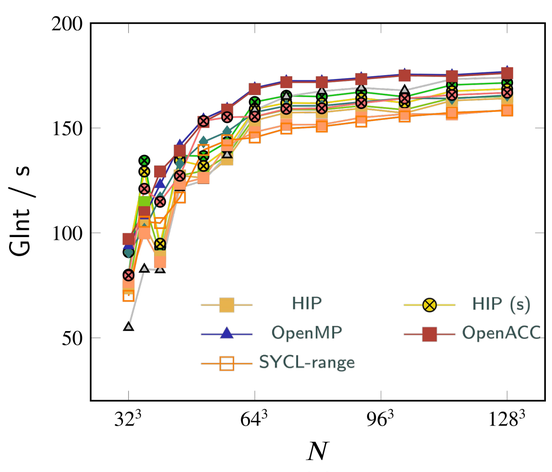


Long-Range Interactions

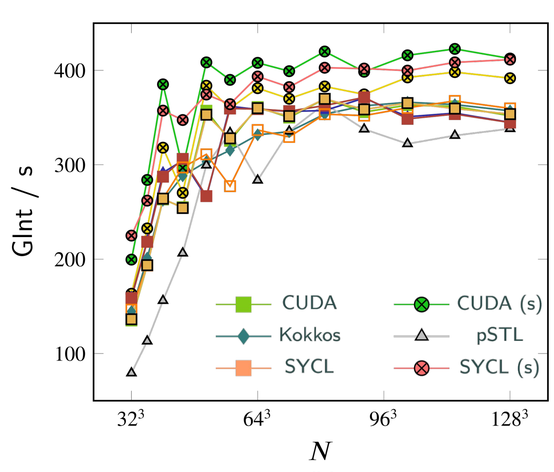
- Scalable Fast Coulomb Solvers (ScaFaCos)[2]
- Optimized particle-mesh transfer
- Electrostatics (Ewald Sum and Particle-Mesh algorithms)
- Sub-communicators for short- and long-range partitions
- Capable of tuning real and reciprocal-space in heterogeneous architectures[3]

Performance Portability study

- Benchmark suite for Performance Portable Frameworks
- Evaluation of architecture independent programming models (smooth transition between CPU / GPU)[4]

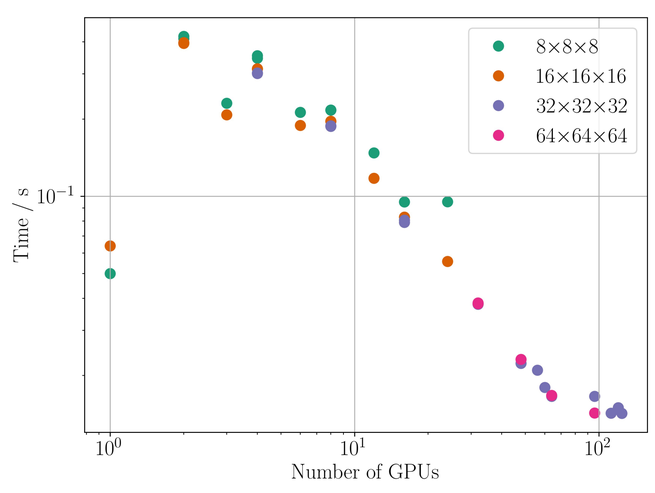


(a) A100



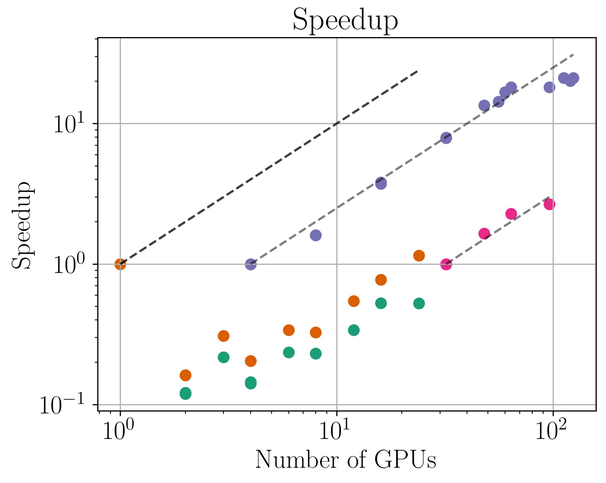
(b) GH200

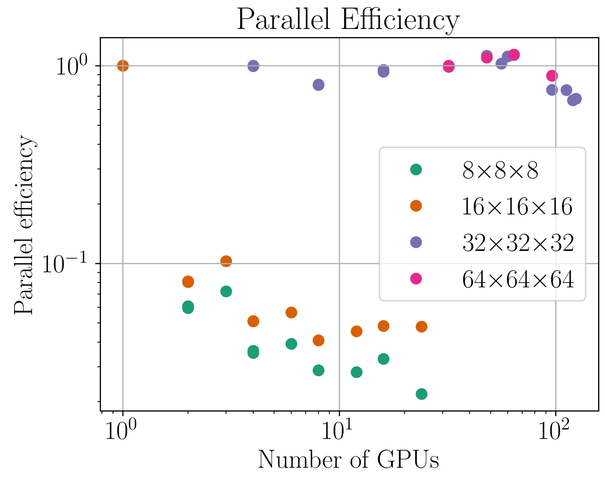
Benchmarks



- MareNostrum 5 Accelerated partition
- Node configuration
  2 x Intel Xeon Platinum 8460Y CPUs
  4 x NVIDIA H100 64GB GPUs

No. of Charges	Grid size	No. of Nodes
153600	256	1;2;4;8
1228800	512	1;2;4;8
9830400	1024	16;32
78643200	2048	16;32





Speedup (left) and Parallel efficiency (right) of strong-scaling benchmark results for different system replication numbers (8 to 64) on 1 to 128 GPUs (1 to 32 nodes).

- Optimal scalability for large systems
- Multi-GPU parallel overhead cannot be compensated for small configurations

[1] A. Arnold e*t al.* Comparison of scalable fast methods for long-range interactions, Phys. Rev. E 88 (2013).

[2] G. Sutmann, P. Gibbon, and T. Lippert (eds.): Fast Methods for Long Range Interactions in Complex Systems, Jülich, (2009).

[3] R. A. C. Bartolomeu and G. Sutmann, Technical report on performance-portable electrostatics. Zenodo, (2025).

[4] R. A. C. Bartolomeu, R. Halver, J. H. Meinke and G. Sutmann. Effect of implementations of the n-body problem on the performance and portability across gpu vendors, Future Gener. Comput. Syst. 169 (2025)

[5] R. A. C. Bartolomeu, R. Halver and G. Sutmann. Scaling and performance aspects of the P3M method on multiple GPUs. EuroHPC User Days 2026 (Submitted).*

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