EuroHPC User Days
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Scaling and performance aspects of the P3M method on multiple GPUs

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HPC Architecture Landscape

- Multiple CPU Architectures
- Multiple GPU vendors
- Multiple programming models

alpaka RAJA CUDA OpenMP HIP SYCL kokkos OpenACC pSTL OpenCL



Source: EuroHPC JU

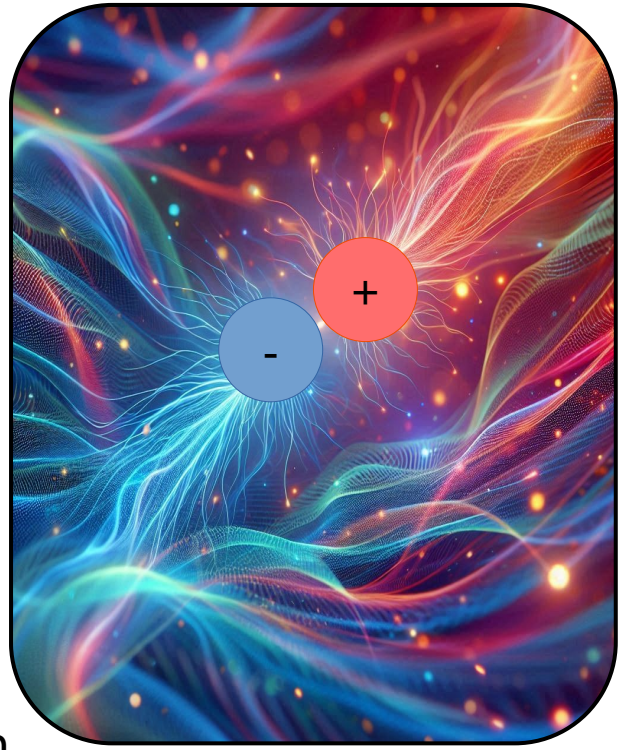
Electrostatics

- Molecular Dynamics and Soft Matter
- Long range interactions
- Periodic Boundary Conditions

$$E = \frac{1}{2} \sum_{i,j=1}^{N} {\sum_{\boldsymbol{n} \in Z}}' \frac{q_i q_j}{\left| \boldsymbol{r}_{ij} + n L \right|}$$

$\tilde{\rho}\left(\vec{\boldsymbol{k}}\right)$ Ewald Summation

$\rho_M\left(\boldsymbol{r}_p\right)$ Particle-Particle Particle-Mesh



Why does it matter for scaling?

$O\left(N^2\right)$

- Direct Summation

$O\left(N^{3/2}\right)$

- Ewald Summation

$O\left(N \log N\right)$

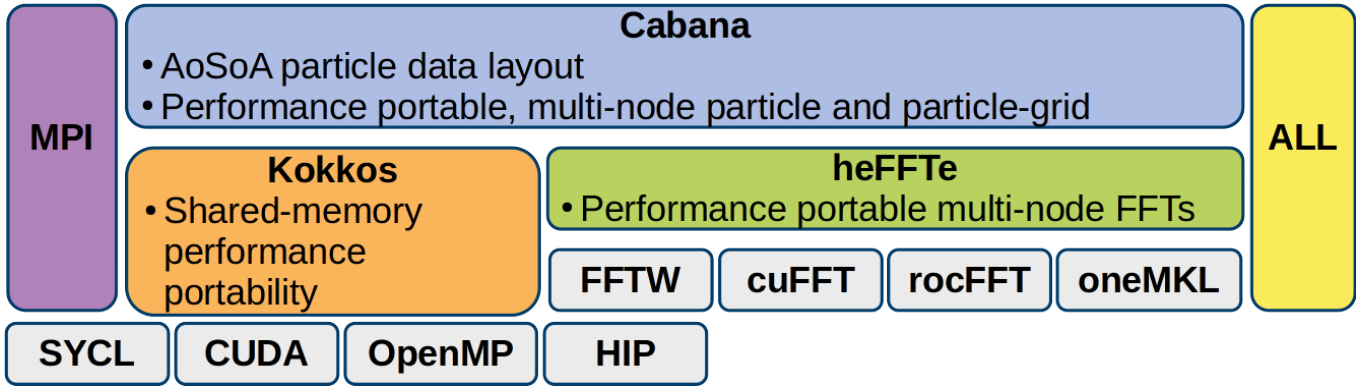
- Mesh based
- P3M
- PME
- SPME

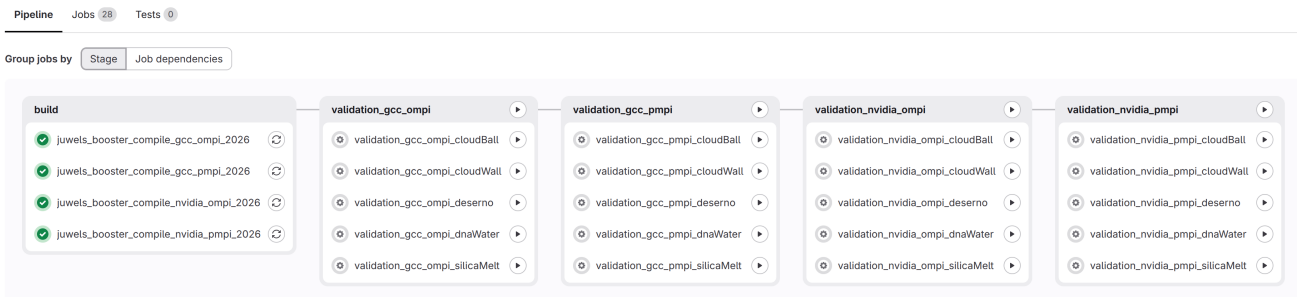
- Fast Fourier Transforms

$$\boldsymbol{E}\left(\boldsymbol{r}_p\right) = \overleftarrow{FFT}\left[-ik \cdot \overrightarrow{FFT}\left[\rho_M\right] \cdot \hat{G}_{opt}\right]\left(\boldsymbol{r}_p\right)$$

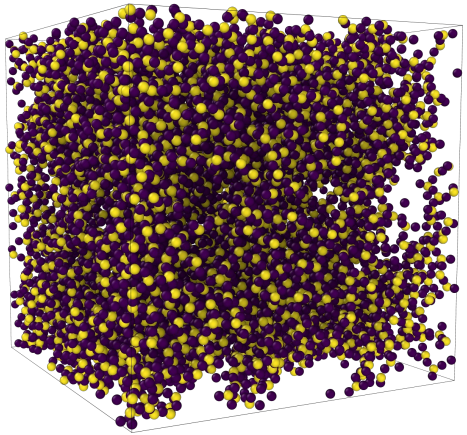
GROMACS ; AMBER ; LAMMPS

Dependencies and CI CD

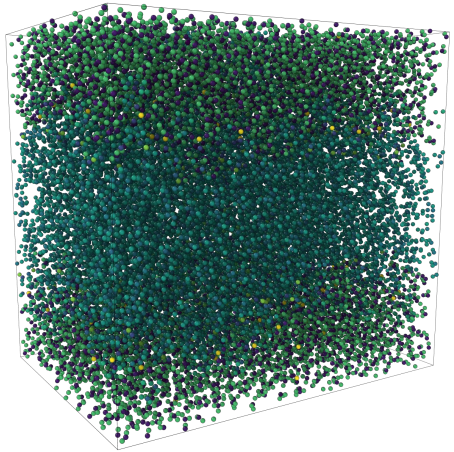




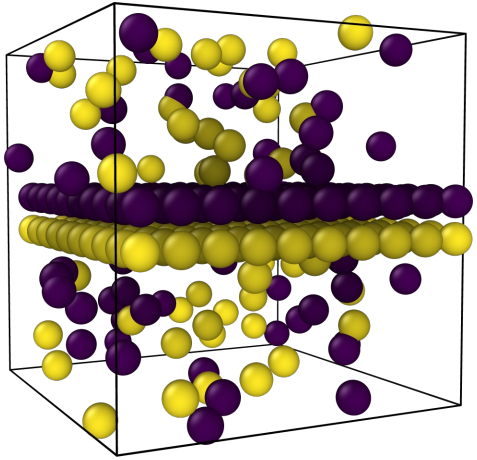
Validation Systems



Silica Melt (12960 particles)



Rhodopsin(32000 particles)



Cloud Wall (300 particles)

Setup

- EuroHPC JU Developer access
- Software stack
  - GCC 13.2.0
  - CUDA 12.8
  - Kokkos 4.7.2
  - Cabana 0.8.0
  - heFFTe 2.4.1 (cuFFT backend)
- –02 optimization
- Host parallelization: OpenMP
- Device execution: CUDA

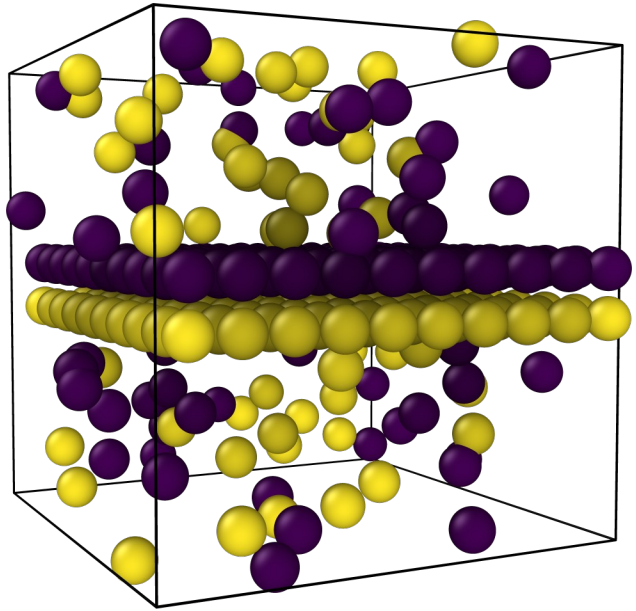
- Node configuration
- 2 Xeon Platinum 8460Y CPUs
- 4 H100 64GB HBM2 GPUs
- 512 GB of 4800MHz DDR5



Source: EuroHPC JU

System and parameters

- Creates an artificial dipole
- High long-range contribution



Base system: Cloud Wall (300 particles)

Reciprocal space parameters of the P3M solver:

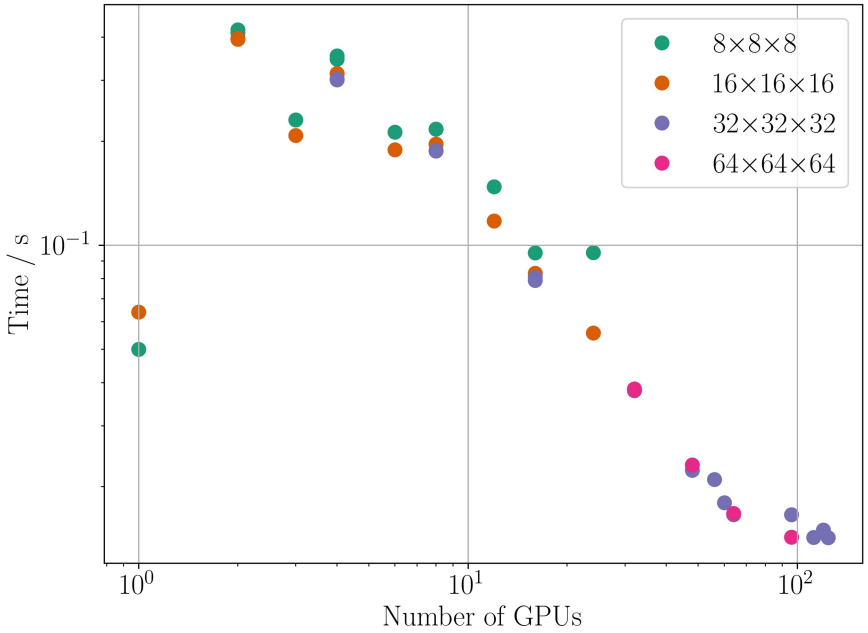
Charge assignment order = 7, $\alpha = 0.846208$, and $r_{cut} = 4.6172$

Replication	No. of charges	Grid size	No. of nodes	No. of GPUs for k-space
8 × 8 × 8	153600	256	1, 2, 4 and 8	1;2;3;4;6;8;12;16;24
16 × 16 × 16	1228800	512	1, 2, 4 and 8	1;2;3;4;6;8;12;16;24
32 × 32 × 32	9830400	1024	16 and 32	4;8;16;32;48;64;80;96;112;120;124
64 × 64 × 64	78643200	2048	16 and 32	32;48;64;96

Validation at large scale

```
tuned Ewald values:
        r_max:  6.30579
        k_max (1D / 3D):        240 / 240 240 240
        alpha:  0.871125
        estimated RMS error in forces: 4.84886e-14
tuned P3M values:
        r_max:  4.6172
        FFT grid size (3D):     512 512 512
        charge assignment order:        7
        alpha:  0.846208
        h * alpha:      0.26444
        estimated RMS error in forces: 3.15284e-07
RMS potential :  4.02801676349598e-07
RMS fields:  7.64805475718963e-08 8.4353410644898e-08 3.97391771302327e-07
Time spent in run [Ewald] (avg, min, max): 2086.3770867 s  2085.901671 s 2086.535621 s
Time spent in run [P3M]   (avg, min, max):    0.5853885 s     0.585388 s    0.585389 s
```

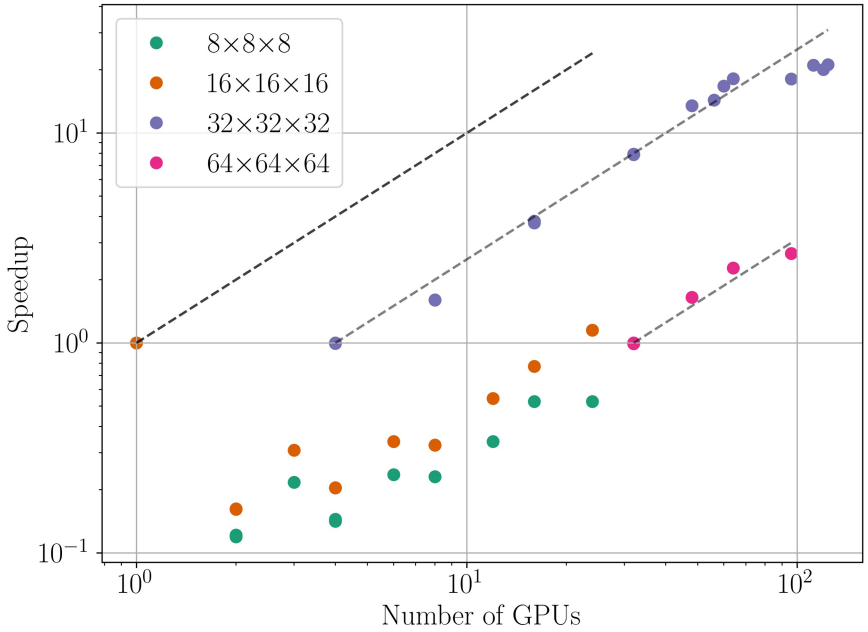
Benchmarks



Strong-scaling benchmark results. Replication numbers (8 to 64) on 1 to 128 GPUs (1 to 32 nodes) on MN5 Acc.

- Normalized to smallest system size
- Parallel overhead
- FFT dominates

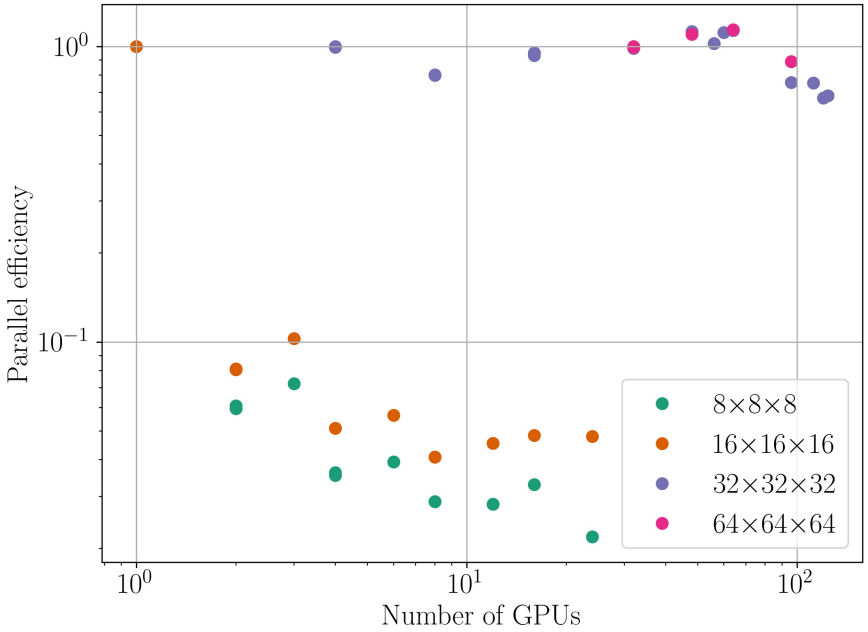
Speedup



Dashed lines represent the ideal speedup taking as reference the smallest amount of resources that could compute the system size.

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

Parallel efficiency



Strong-scaling benchmark results. Replication numbers (8 to 64) on 1 to 128 GPUs (1 to 32 nodes) on MN5 Acc.

- Parallel efficiency remains close to unity for larger systems
- Cache and load-balancing effects
- Computational intensity

  x

  Communication overhead

Conclusions

- P3M solver runs efficiently on MN5
  - Viability on modern GPU-cluster hardware
- FFT grid fits into the memory of a single GPU?
  - single-GPU execution is optimal
  - two or more GPUs adds parallel overhead
- For large grids k-space portion scales
  - adding GPUs can improve performance
- Crossover region is system dependent

Outlook

- Systematic parametric study
  - memory-size vs. parallel-overhead crossover
- Dynamic load-balancing strategies
  - Partition adjustment between real- and k-space
- Real-space splitting parameter
- Coupling the library into ESPResSo
- Comparison with AMD GPUs
  - LUMI Acc access granted (EHPC-DEV-2025D11-078)

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EuroHPC Joint Undertaking

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Multiscale

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