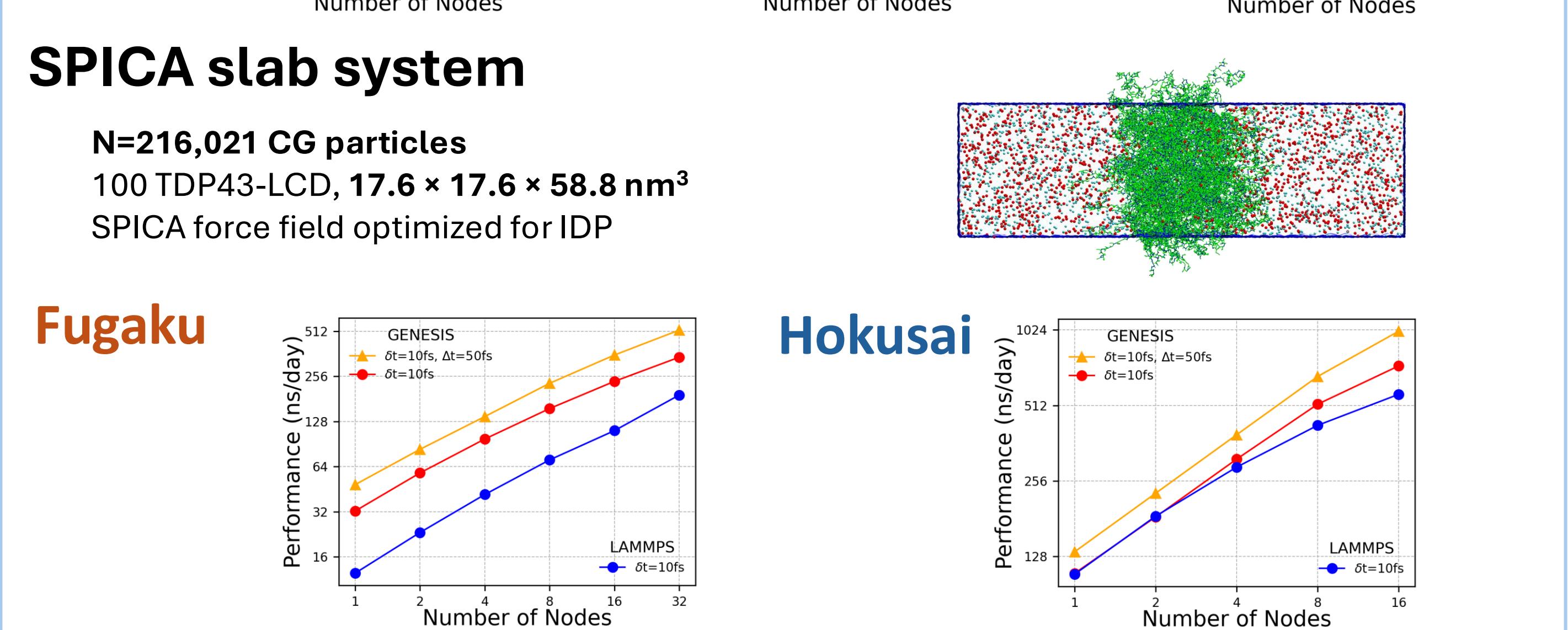
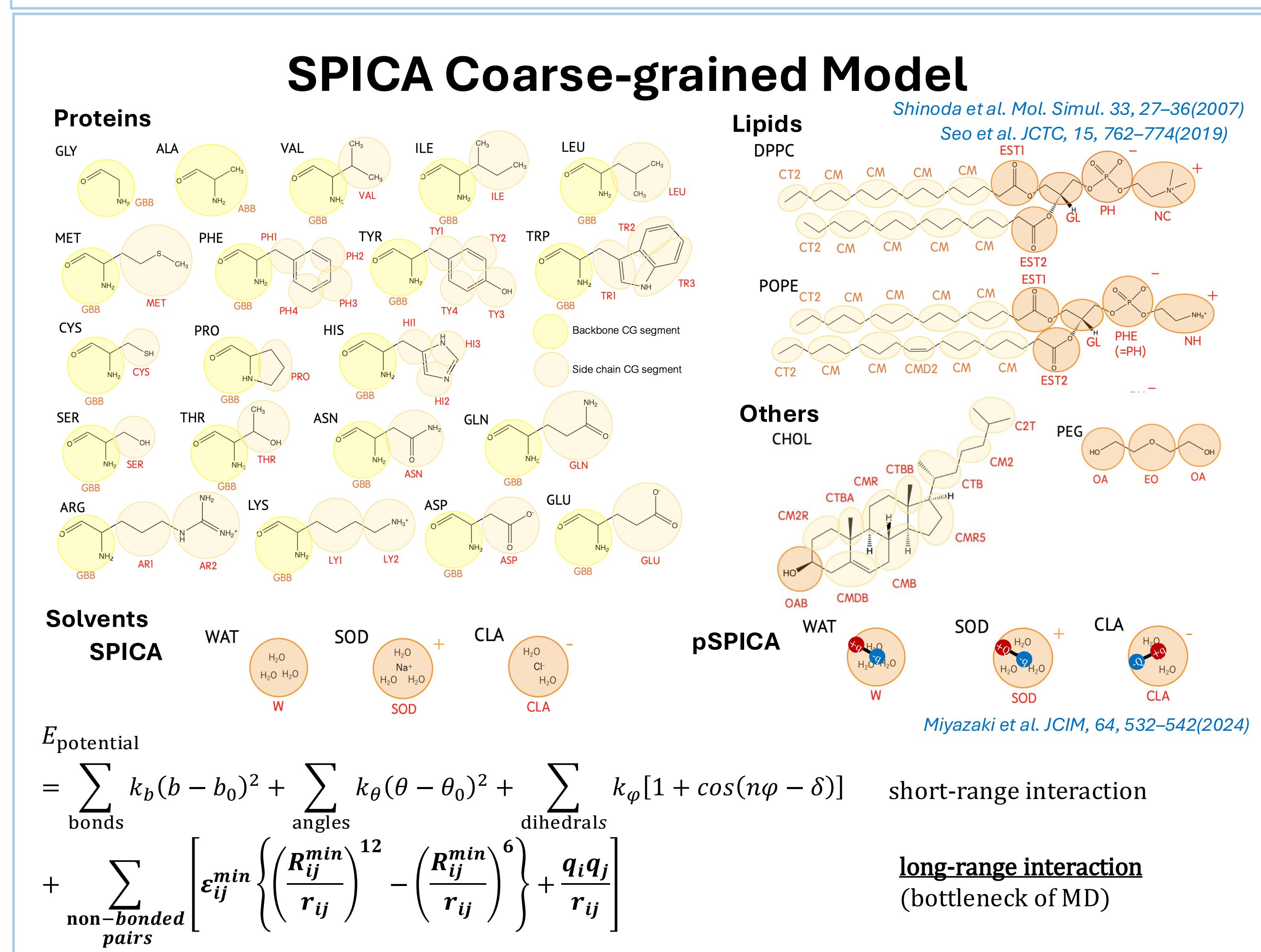
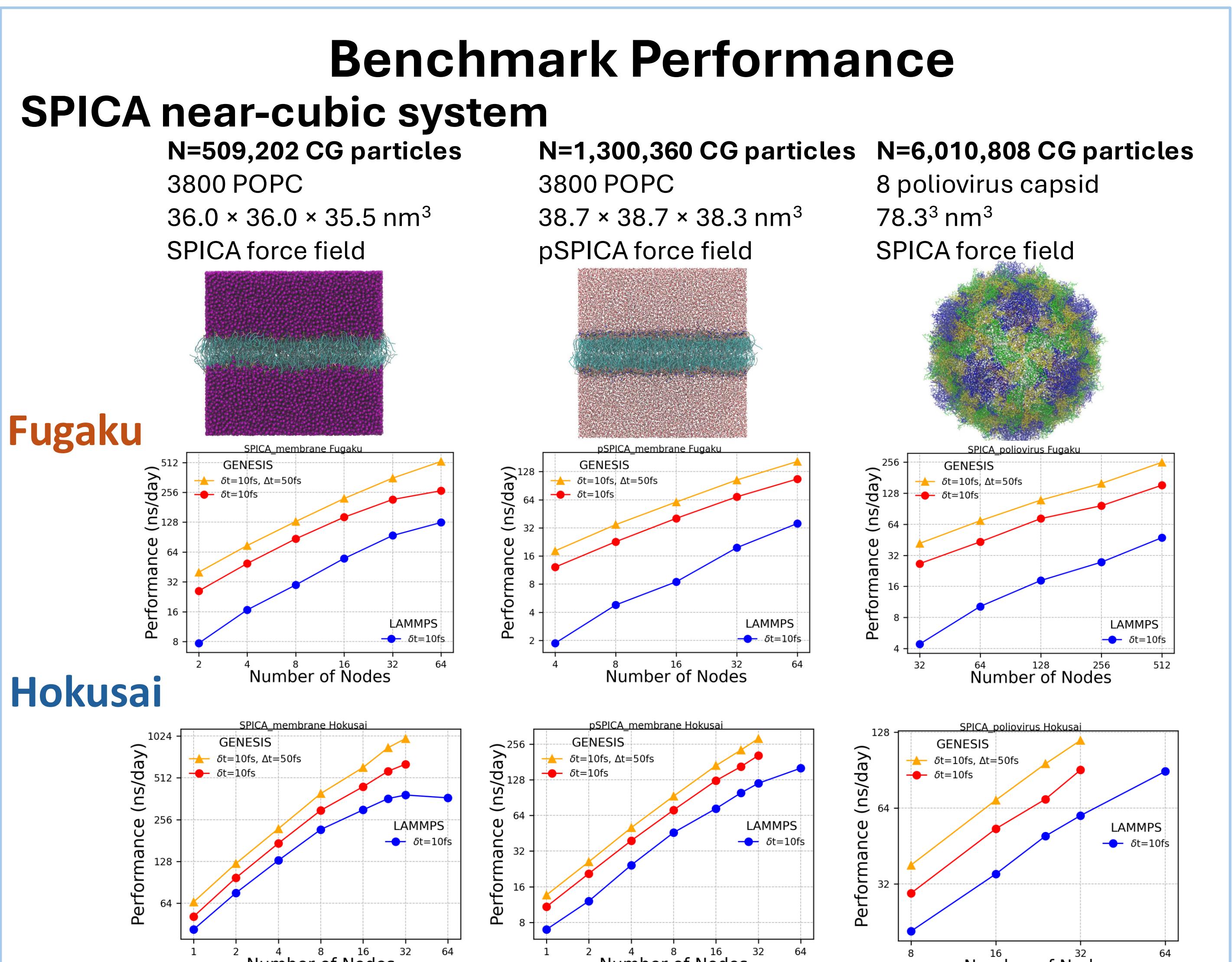
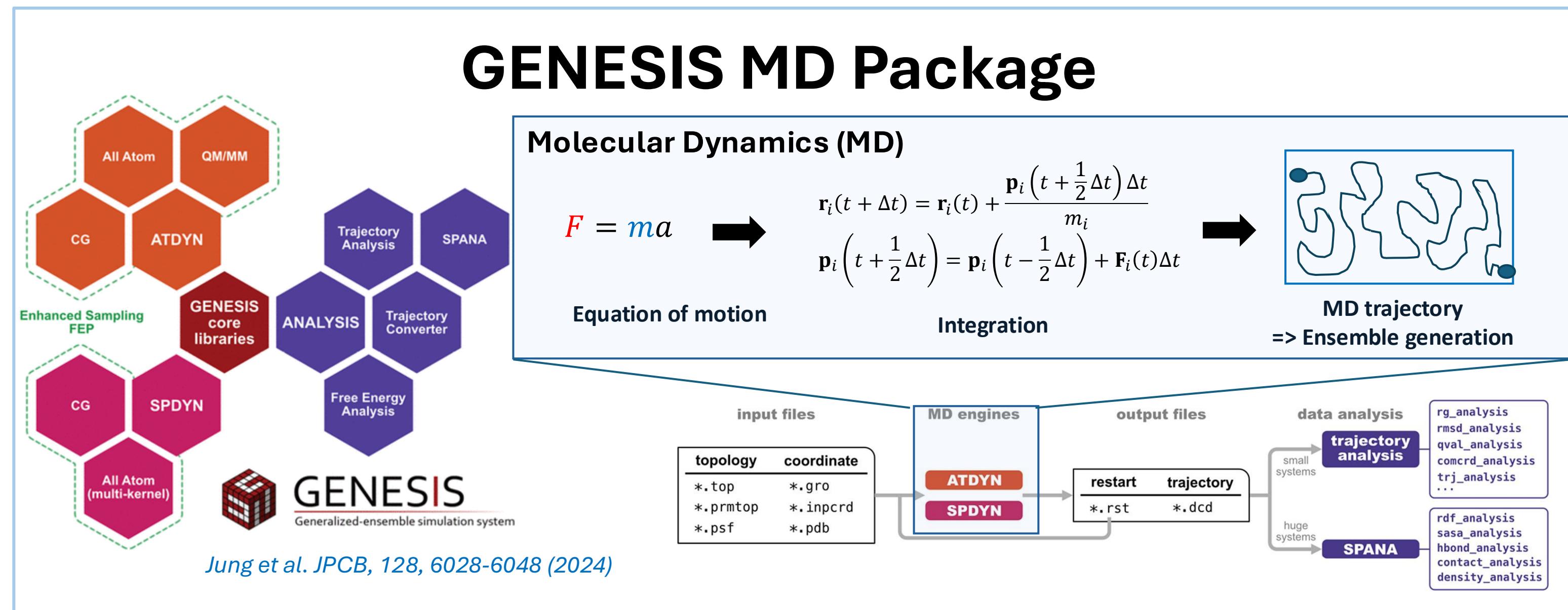
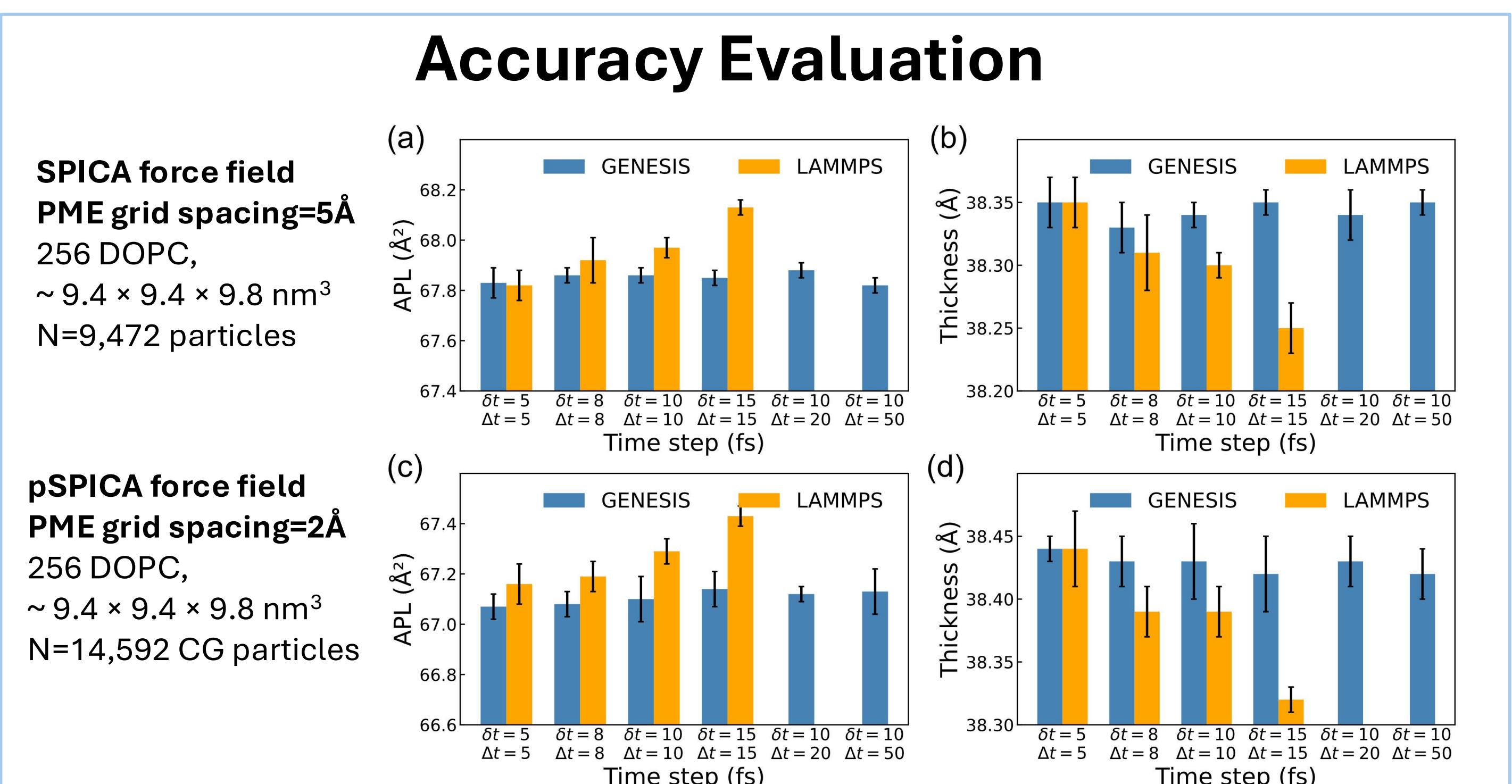
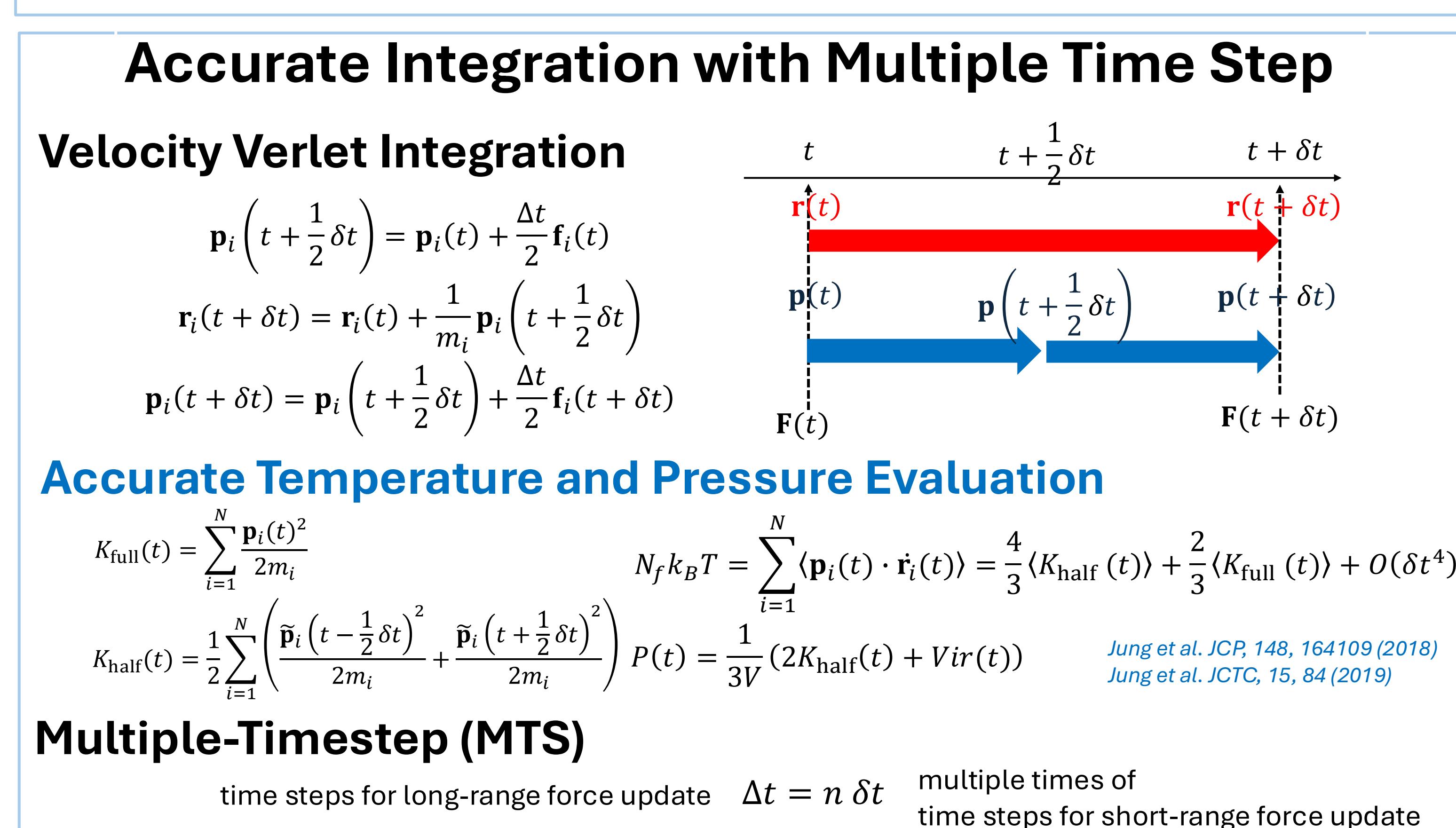


GENESIS (GENeralized Ensemble SImulation System) is a high-performance molecular dynamics (MD) software featuring efficient CPU parallelization and a validated multiple-timestep (MTS) integrator. We recently extended GENESIS to support the SPICA coarse-grained (CG) model, originally developed in LAMMPS MD software package. SPICA explicitly include solvent beads and treats electrostatic interactions by decomposing real- and reciprocal-space ones, limiting the performance with large number of processes. We implemented SPICA model in GENESIS with three-dimensional decomposition of fast Fourier transform (FFT).

Benchmarks on Fugaku and Hokusai BigWaterfall 2 were performed for lipid membranes, a viral capsid, and a protein condensate slab system. With single timestep integrator, GENESIS showed good CPU parallelization scaling and about twice better performance than LAMMPS for most systems. MTS further improves performance without compromising accuracy, highlighting GENESIS as a scalable platform for large-scale MD simulation of CG models and future GPU acceleration.



1. With a single-timestep (ST) integrator, GENESIS shows good CPU scaling and achieves about twice higher performance than LAMMPS for most systems. For the slab systems, GENESIS and LAMMPS exhibit comparable performance up to 1 to 2 nodes, after which GENESIS achieves higher parallel efficiency.
2. The multiple-timestep (MTS) integrator provides an additional acceleration while maintaining stable and accurate dynamics.



Under otherwise identical conditions, **as the timestep is increased**:
GENESIS preserves APL and membrane thickness within statistical uncertainty, including with MTS

Including with MTS. **LAMMPS**, by contrast, shows **monotonic, timestep-dependent** deviations, characterized by increasing APL and decreasing membrane thickness.

Conclusions

We implemented the SPICA coarse-grained force field in GENESIS and benchmarked its performance and accuracy against LAMMPS

performance and accuracy against LAMMPS. For SPICA systems, GENESIS achieves higher performance at the same timestep. Moreover, GENESIS supports larger timesteps, including MTS, without compromising accuracy.

accuracy. Overall, GENESIS provides a scalable and numerically stable MD framework for SPICA coarse-grained simulations, combining high performance with robust accuracy.

Acknowledgement

Project Information