Collaborative Research: Elements: SciMem: Enabling High Performance Multi-Scale Simulation on Big Memory Platforms

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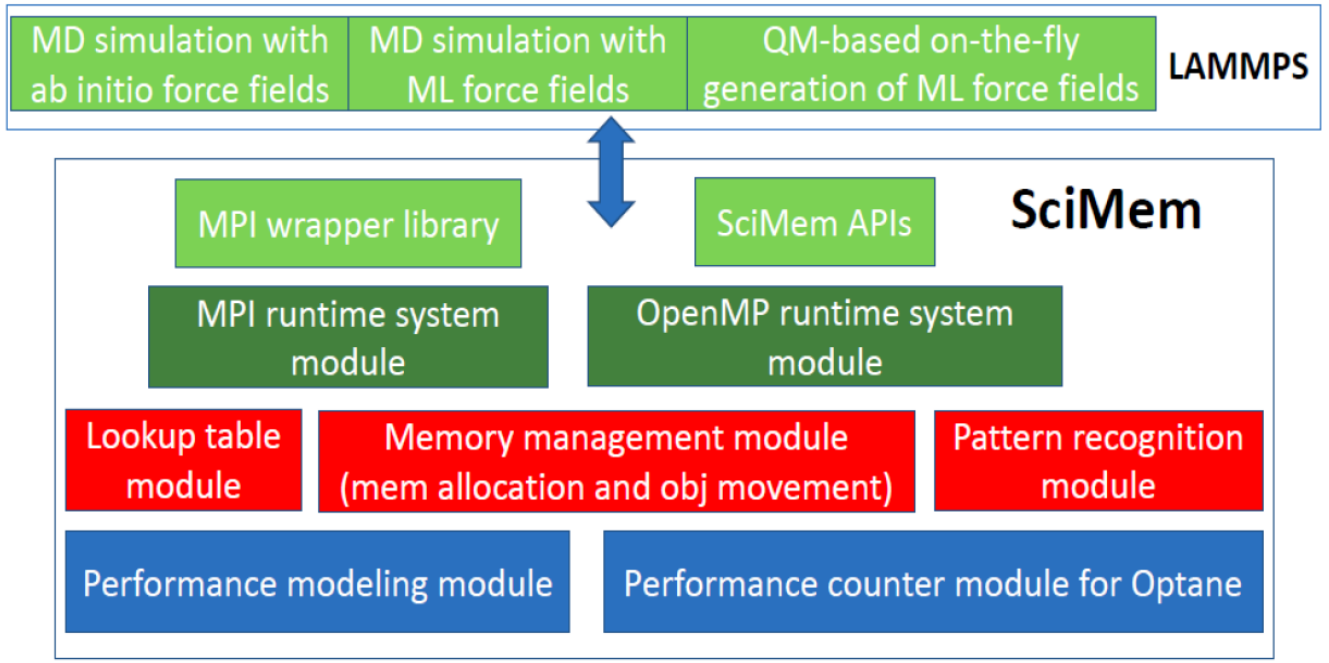
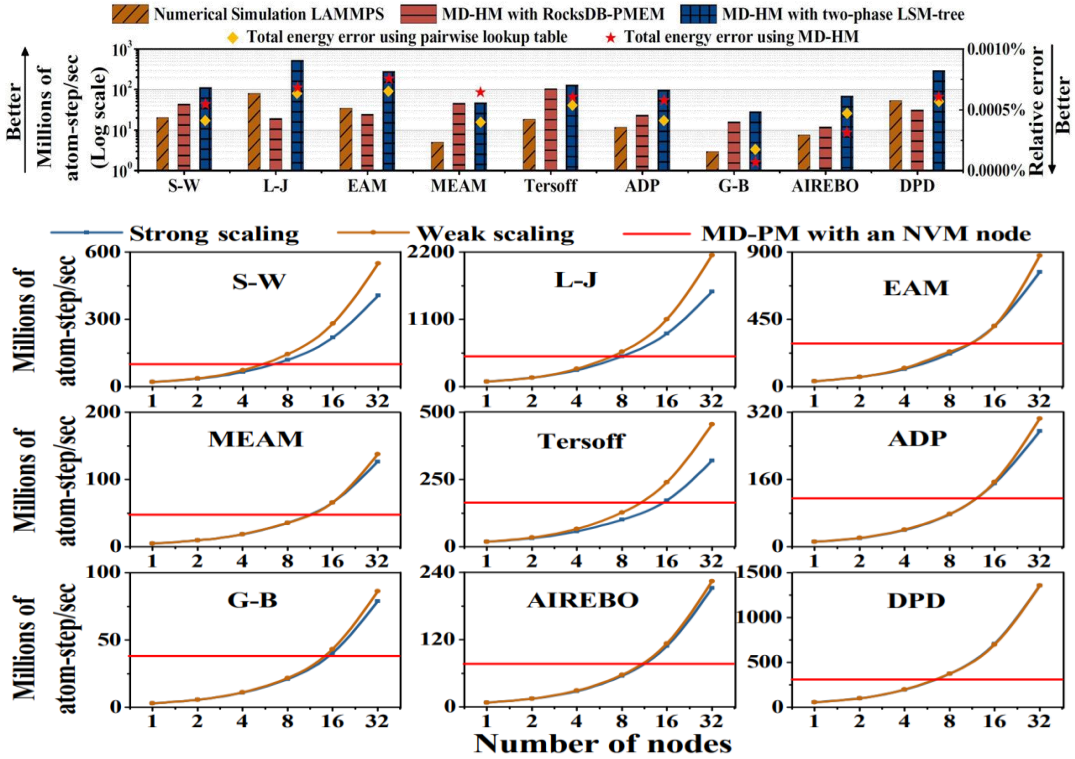
The goal of this project is to create a capability and a software package (named SciMem) that will enable high performance multi-scale simulation on big memory platforms. By designing SciMem as a library, we expect to bring a significant performance improvement for certain larger-scale multi-scale simulations widely applied in the fields of computational chemistry, fluid physics and material science, i.e., quantum mechanical/molecular mechanical-based molecular dynamics (MD) simulations.





References:

1. Xie, Dong, Liu, Peng, Ma and **Dong Li**, *MD-HM: memoization-based molecular dynamics simulations on big memory system,* Proc. Int. Conf. Supercomput., 2021, Pages 215-226.
2. Deng, Tushar, Bravo, Ghoshal, Karniadakis and **Zhen Li**, *Theory and simulation of electrokinetic fluctuations in electrolyte solutions at the mesoscale.* J. Fluid Mech., 2022. 942: A29.