Examining performance portability with Kokkos for an Ewald Sum Coulomb Solver

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We have implemented the computation of Coulomb interactions in particle systems using the performance portable C++ framework Kokkos. Coulomb interactions are evaluated with an Ewald-sum-based solver, where the interactions are split into long- and short-range contributions. The short-range contributions are calculated using pair-wise contributions of particles while long-range interactions are calculated using Fourier sums. We evaluate the performance portability of the implementation on Intel CPUs, including Intel Xeon Phi, and Nvidia GPUs.

Keywords: performance portability, Kokkos, GPU, KNL, particle simulation.