Performance and Scaling

Classical/empirical potential MD simulations scale much better than their electronic structure counterparts due the parallel strategy being simpler and more straightforward. Thus, the larger jobs using the most amount of nodes in this project are the MD calculations. We focus below on the scaling and performance of the silica simulations using LAMMPS on Comet (CPU only simulations).

In Figures 3 and 4, we show the benchmark calculations on Comet for both bulk quartz simulations and two-temperature cascade simulations, respectively. In these figures, we show the strong scaling (speedup and parallel efficiency for a fixed problem size), performance (MD steps per second) and weak scaling (fixed number of atoms per node) for each system. For the simulation setup, the system size consists of 648k atoms (Strong scaling: problem size, Weak scaling: atoms / node), we used a Tersoff empirical potential[45,46], and the simulations were for 100 MD steps with a 1 femtosecond timestep.

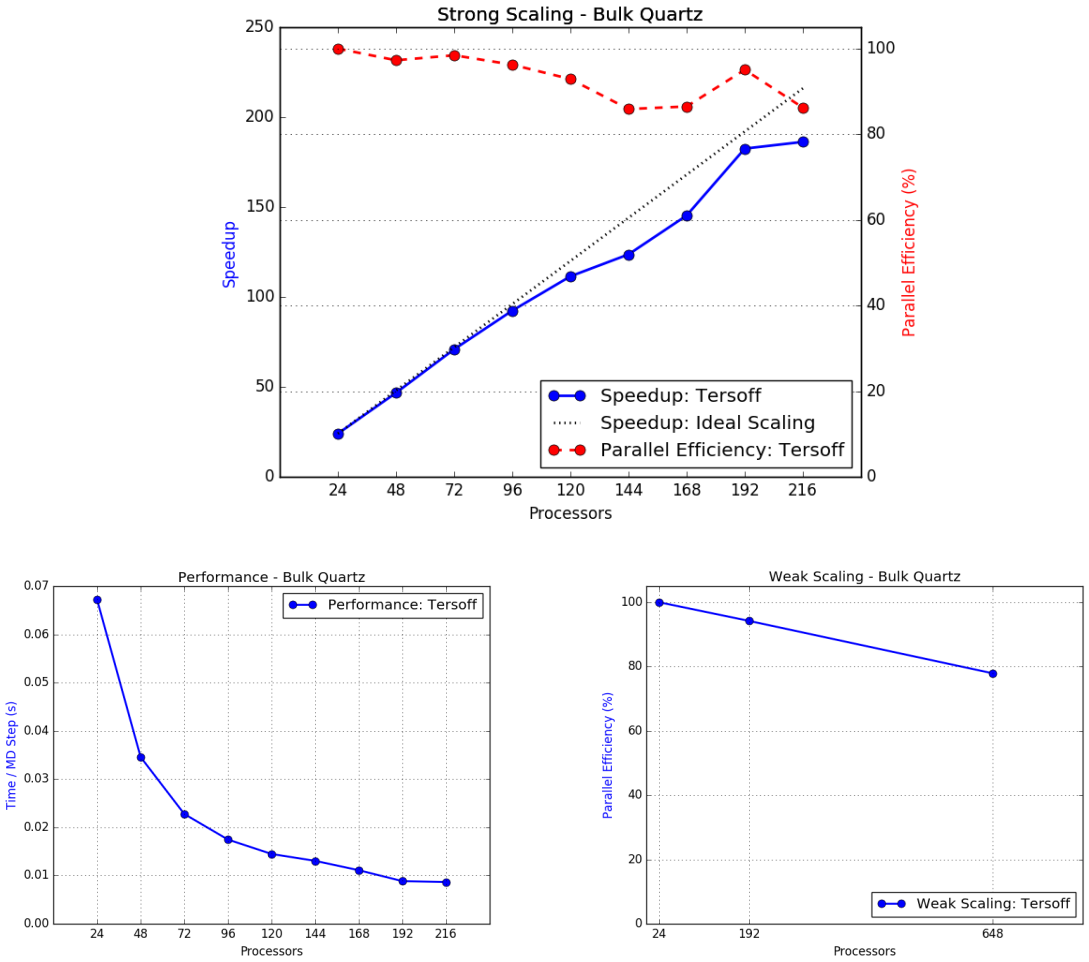

Figure 3: **Performance and Scaling of LAMMPS for Quartz Simulations.** Simulation consists of 640k atoms, Tersoff Potential, Δt = 1 fs, for 100 MD timesteps.

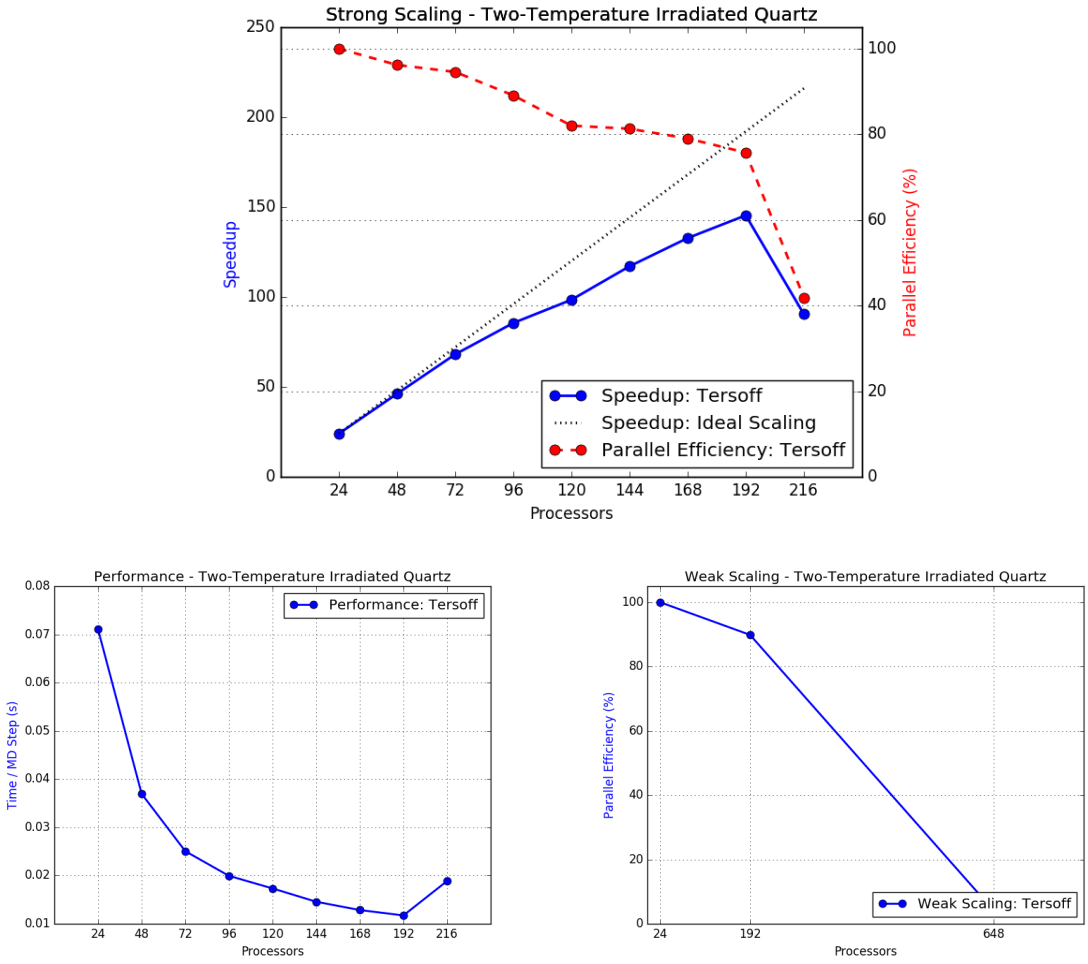

Figure 4: **Performance and Scaling of LAMMPS for Irradiated Quartz via Two-Temperature Modeling Simulations.** Simulation consists of 640k atoms, Tersoff Potential, Δt = 1 fs, for 100 MD timesteps.