Angara-based hybrid supercomputer for efficient acceleration of computational materials science studies

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In this paper, we describe the supercomputer Desmos consisting of 32 hybrid nodes connected by a low-latency high-bandwidth torus interconnect. This supercomputer is aimed at classical molecular dynamics calculations and is able to speed-up efficiently electronic structure calculations as well. In this report, we present scalability benchmarks for a representative set of models in LAMMPS, GROMACS, VASP and CP2K. We compare the benchmark results with other HPC systems. This supercomputer is based on the Angara interconnect developed by JSC NICEVT that supports 3D and 4D torus topologies. The observed parallel scaling of the benchmarks on the supercomputer Desmos illustrates the capability of the Angara interconnect to speedup efficiently MPI-based applications on MPP systems.