

Breakout session: Acceleration packages

Stan Moore
Sandia National Laboratories

5th LAMMPS Workshop and Symposium
August 2017 - Albuquerque, NM

LAMMPS resources for performance acceleration

- **Hardware support**
 - CPU including OpenMP
 - GPU via Cuda
 - KNL via OpenMP
- **Website:** Benchmarking page (discussed in this session)
 - input files, Makefiles, run commands, log files, plots & tables
- **Distro**
 - bench directory
- **Manual**
 - Section 5 = Accelerating LAMMPS performance
 - Section 5.3.1 = GPU package
 - Section 5.3.2 = USER-INTEL package
 - Section 5.3.3 = KOKKOS package
 - Section 5.3.4 = USER-OMP package
 - Section 5.3.5 = OPT package
 - Section 8 = Performance and Scalability

LAMMPS resources (continued)

- **Packages**
 - GPU, KOKKOS, OPT, USER-INTEL, USER-OMP
- **Makefiles** in src/MAKE/OPTIONS dir
 - Makefile.kokkos, several variants: Cuda, KNL, OpenMP
 - Makefile.intel, several variants: CPU and KNL
 - Makefile.omp
- **Commands**
 - balance, fix balance, processors, run_style verlet/split
- **Example** dirs
 - balance