

Different versions on the same machine:

lammps@12.1.0

lammps@12.1.0+cuda

lammps@12.1.0+mpi

lammps@12.1.0+cuda+mpi

lammps@12.2.1

lammps@12.2.1+cuda

lammps@12.2.1+mpi

lammps@12.2.1+cuda+mpi

lammps@12.1.0%gcc (loaded)

lammps@12.1.0%gcc@8.3.0

lammps@12.1.0%intel (loaded)

lammps@12.1.0%intel@2023.0.0

@ = version name

% = compiler

+ = dependencies

~ = remove default dependencies

lammps@12.1.0%gcc@8.3.0~mpi

spack installation steps:

git clone <https://github.com/spack/spack.git>

cd spack

source /home/cdacapps01/himanshu/spack/share/spack/setup-env.sh

spack --version

spack list

spack list | grep hpctoolkit

spack find (get list of installed packages using spack)

spack info hpctoolkit (get info about specific package in spack)

spack spec -l hpctoolkit

spack install -v -j40 hpctoolkit

spack install -v -j40 hpctoolkit+cuda

spack load hpctoolkit

spack install -v -j40 gcc@8.3.0

On shavak: to load already installed spack and applications from root account  
source /home/apps/spack/share/spack/setup-env.sh  
spack find hpctoolkit  
spack load hpctoolkit@2021.10.15