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| #!/bin/bash#SBATCH --tasks-**per-node=16** --mem 100Gsource /usr/modules/init/bashmodule load openmpi/2.1.6mpirun **-n 8** lmp < input.txt | Total # of neighbors = 137107294Ave neighs/atom = 708.14Neighbor list builds = 528Dangerous builds = 515Total wall time: **6:17:11** |
| #!/bin/bash#SBATCH --tasks-**per-node=16** --mem 100Gsource /usr/modules/init/bashmodule load openmpi/2.1.6mpirun **-n 10** lmp < input.txt | Total # of neighbors = 137107294Ave neighs/atom = 708.14Neighbor list builds = 528Dangerous builds = 515Total wall time: **6:15:31** |
| #!/bin/bash#SBATCH --tasks-**per-node=16** --mem 100Gsource /usr/modules/init/bashmodule load openmpi/2.1.6mpirun **-n 12** lmp < input.txt | Total # of neighbors = 137107294Ave neighs/atom = 708.14Neighbor list builds = 528Dangerous builds = 515Total wall time**: 6:15:21** |
| #!/bin/bash#SBATCH --tasks-**per-node=16** --mem 100Gsource /usr/modules/init/bashmodule load openmpi/2.1.6mpirun **-n 16** lmp < input.txt | Total # of neighbors = 137107294Ave neighs/atom = 708.14Neighbor list builds = 528Dangerous builds = 515Total wall time: **6:15:23** |
| #!/bin/bash#SBATCH --tasks-**per-node=16** --mem 100Gsource /usr/modules/init/bashmodule load openmpi/2.1.6mpirun **-n 2** lmp < input.txt | Total # of neighbors = 137107294Ave neighs/atom = 708.14Neighbor list builds = 528Dangerous builds = 515Total wall time**: 6:12:59** |
| #!/bin/bash#SBATCH --tasks-**per-node=16** --mem 100Gsource /usr/modules/init/bashmodule load openmpi/2.1.6mpirun **-n 4** lmp < input.txt | Total # of neighbors = 137107294Ave neighs/atom = 708.14Neighbor list builds = 528Dangerous builds = 515Total wall time: **6:17:35** |