KNL Performance Comparison: *LAMMPS*

March 2017

1. Compilation, Setup and Input

Compilation

You can obtain a copy of LAMMPS from the official repository:
`git clone http://git.icms.temple.edu/lammps-ro.git lammps`

The modules and library versions used to compile LAMMPS are shown in the table below:

Compiler/Library	ARCHER Xeon	ARCHER KNL
Intel Compiler	Intel/ 15.0.2.164	intel/ 17.0.0.098

and the following user changes to the Makefile scripts were required

ARCHER

```
CC =          CC
OPTFLAGS =    -xHost -O2 -fp-model fast=2 -no-prec-div -qoverride-limits
CCFLAGS =     -g -qopenmp -DLAMMPS_MEMALIGN=64 -qno-offload -fno-alias -
ansi-alias -restrict $(OPTFLAGS)
SHFLAGS =
DEPFLAGS =    -M

LINK =        CC -dynamic
LINKFLAGS =   -O2 -g -qopenmp  $(OPTFLAGS)
LIB =            -ltbbmalloc
SIZE =        size

ARCHIVE =     ar
ARFLAGS =     -rc
SHLIBFLAGS = -shared
```

KNL

```
CC =          CC
OPTFLAGS =       -xMIC-AVX512 -O2 -fp-model fast=2 -no-prec-div -qoverride-
limits
CCFLAGS =     -O2 -qopenmp -DLAMMPS_MEMALIGN=64 -qno-offload \
                  -fno-alias -ansi-alias -restrict

SHFLAGS =
DEPFLAGS =    -M

LINK =        CC
LINKFLAGS =   -O2 -g -qopenmp
LIB =
SIZE =        size

ARCHIVE =     ar
ARFLAGS =     -rc
SHLIBFLAGS = -shared
SHLIBFLAGS = -shared
```

Once the previous changes have been completed, we can procced to configure LAMMPS:

```
make package-status
#Add the new makefile to the list
make makelist
#Add modules to the install list
make yes-asphere yes-body yes-class2 yes-colloid yes-compress yes-
coreshell yes-dipole yes-fld yes-granular yes-mc yes-misc yes-
mpiio yes-opt yes-peri yes-qeq yes-replica yes-rigid yes-shock yes-
snap yes-srd yes-xtc yes-kspace yes-manybody yes-misc yes-molecule

make yes-user-omp yes-user-intel
```

and finally build it with

```
make knl
```

Setup

ARCHER KNL nodes in “quad_100” mode were used in all cases.

Input

We have used the Intel input data provided in the LAMMPS USER-INTEL package (located at src/USER-INTEL/TEST) with 512000 atoms and 7900 timsteps:

- Lennard-Jones potential benchmarks (in.intel.lj) using "-v m 0.1" at run time and "atom_modify sort 100 2.8" was added to the input script.
- Stillinger-Weber potential (in.intel.sw) run using "-v m 0.1". For KNL, "atom_modify sort 100 4.77" was added to the input script.
- Tersoff potential (in.intel.tersoff) was run using "-v m 0.2". For KNL, "atom_modify sort 100 4.2" was added to the input script.

2. Performance Data

Figure 1 represents the best performance obtained of the Lennard-Jones potential benchmark for each user package on an ARCHER –Xeon and –KNL node. This means that each bar of Figure 1 may have a different combination of MPI processes, OpenMP threads (T) and hyperthreads (HT).

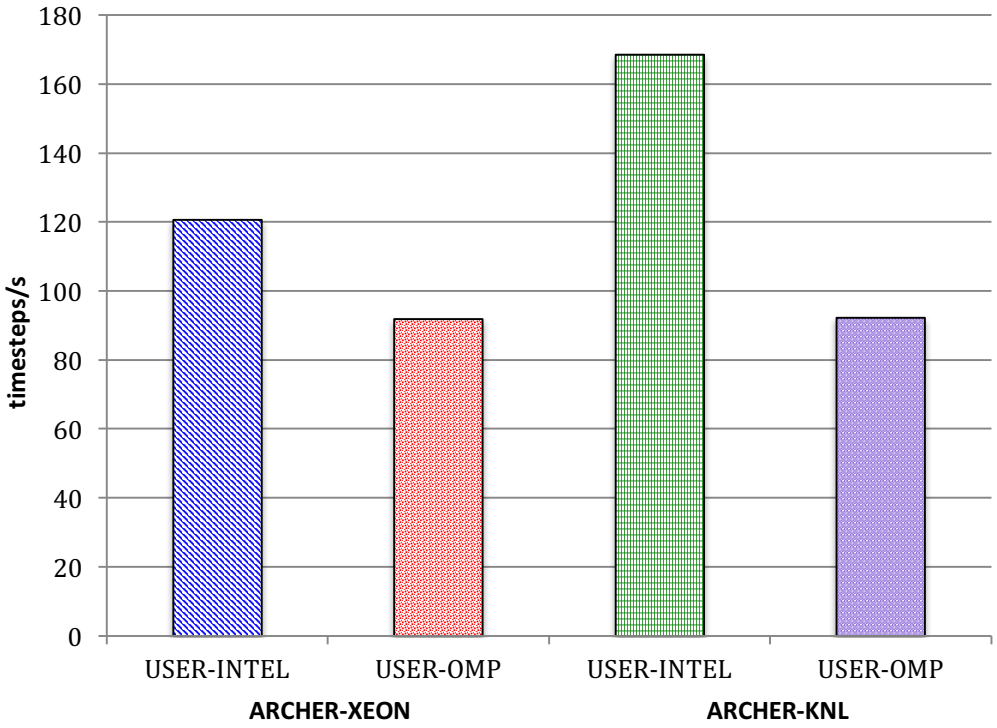

Figure 1 -Performance for the Lennard-Jones potential benchmarks run on a single ARCHER Xeon and KNL node.

The legend of this graph is as follow:

ARCHER-Xeon

- **USER-INTEL**: 48 MPI processes, 1 OpenMP thread and 2 hyperthread.
- **USER-OMP**: 48 MPI processes, 1 OpenMP thread and 2 hyperthread.

ARCHER-KNL

- **USER-INTEL**: 128 MPI processes, 1 OpenMP thread and 2 hyperthreads.
- **USER-OMP**: 64 MPI processes, 4 OpenMP thread and 4 hyperthreads.

Similarly, Figure 2 shows only the best performance for the Stillinger-Weber potential benchmark on a single ARCHER –Xeon and –KNL node.

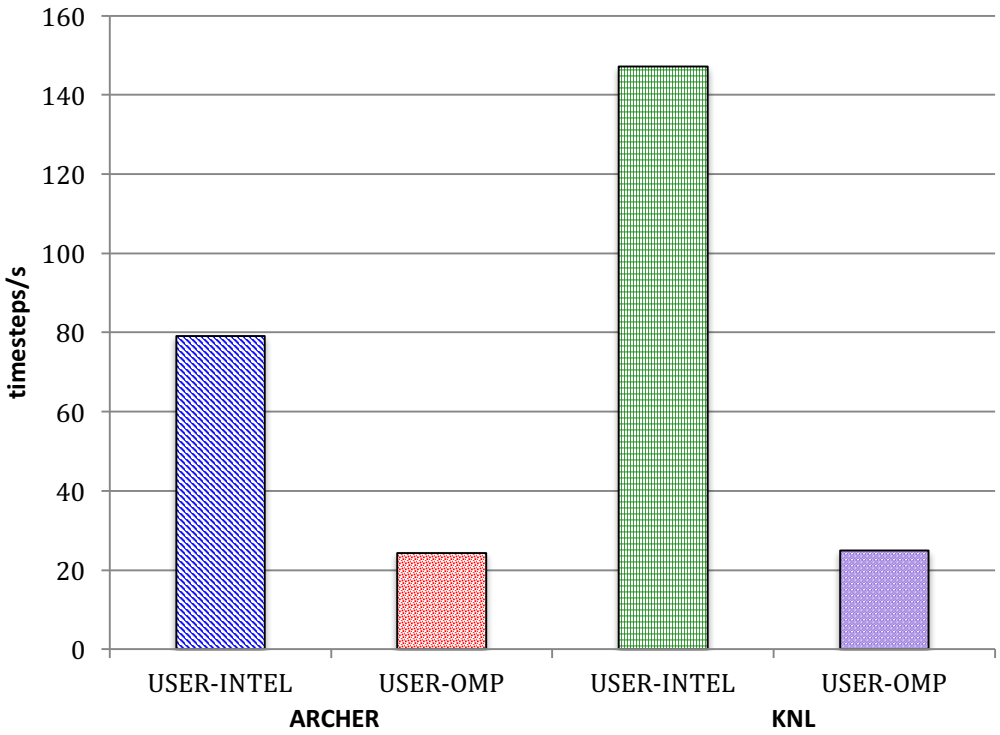

Figure 2 - Performance for the Stillinger- Weber potential benchmark run on a single ARCHER -Xeon and -KNL node.

The legend of Figure 2:

ARCHER-Xeon

- **USER-INTEL**: 48 MPI processes, 1 OpenMP thread and 2 hyperthread.
- **USER-OMP**: 48 MPI processes, 1 OpenMP thread and 2 hyperthread.

ARCHER-KNL

- **USER-INTEL**: 64 MPI processes, 4 OpenMP thread and 4 hyperthreads.
- **USER-OMP**: 64 MPI processes, 4 OpenMP thread and 4 hyperthreads

Finally, Figure 3 shows the best performance for the Tersoff potential.
The legend of this graph is as follow:

ARCHER-Xeon

- **USER-INTEL**: 48 MPI processes, 1 OpenMP thread and 2 hyperthread.
- **USER-OMP**: 48 MPI processes, 1 OpenMP thread and 2 hyperthread.

ARCHER-KNL

- **USER-INTEL**: 64 MPI processes, 4 OpenMP thread and 4 hyperthreads.
- **USER-OMP**: 64 MPI processes, 4 OpenMP thread and 4 hyperthreads

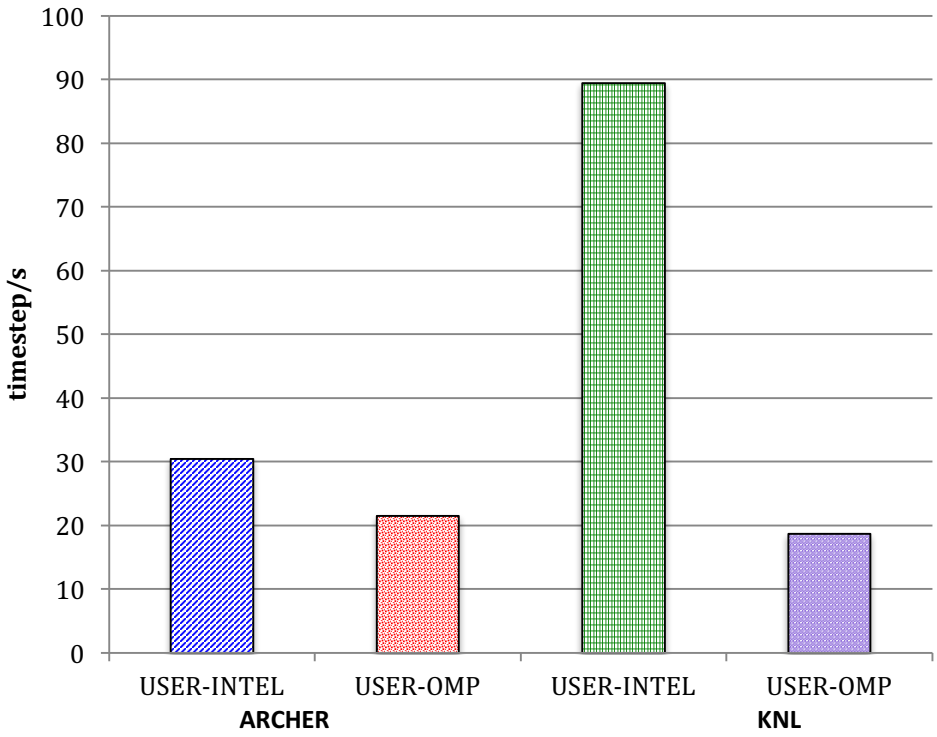

Figure 3 - Performance for the Tersoff potential benchmark run on a single ARCHER -Xeon and -KNL node.

We have also run the benchmarks on a multi-node mode for both USER-INTEL and USER-OMP packages. The performance figures of the Lennard-Jones benchmark with USER-OMP are shown in Figure 4.

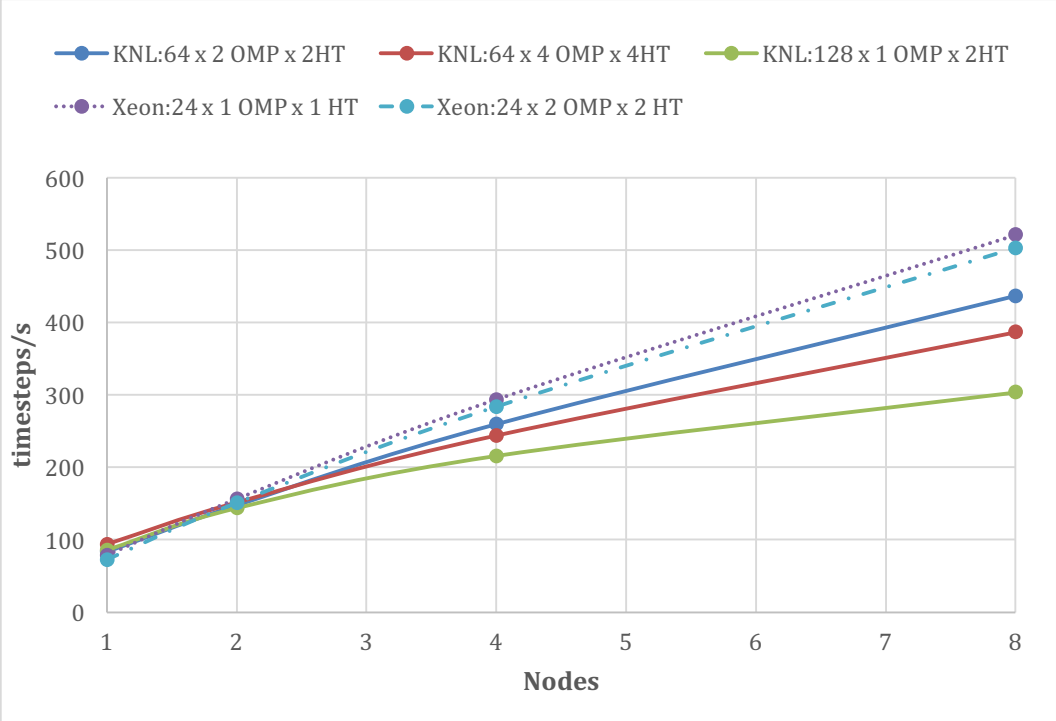

Figure 4 - Performance for the Lennard-Jones potential benchmark run on 8 nodes with the USER-OMP package. Dashed lines correspond to the Xeon performance whereas the solid lines represent the KNL performance

Similarly, Figure 5 shows the performance results of the Lennard-Jones benchmark run with the USER-INTEL package.

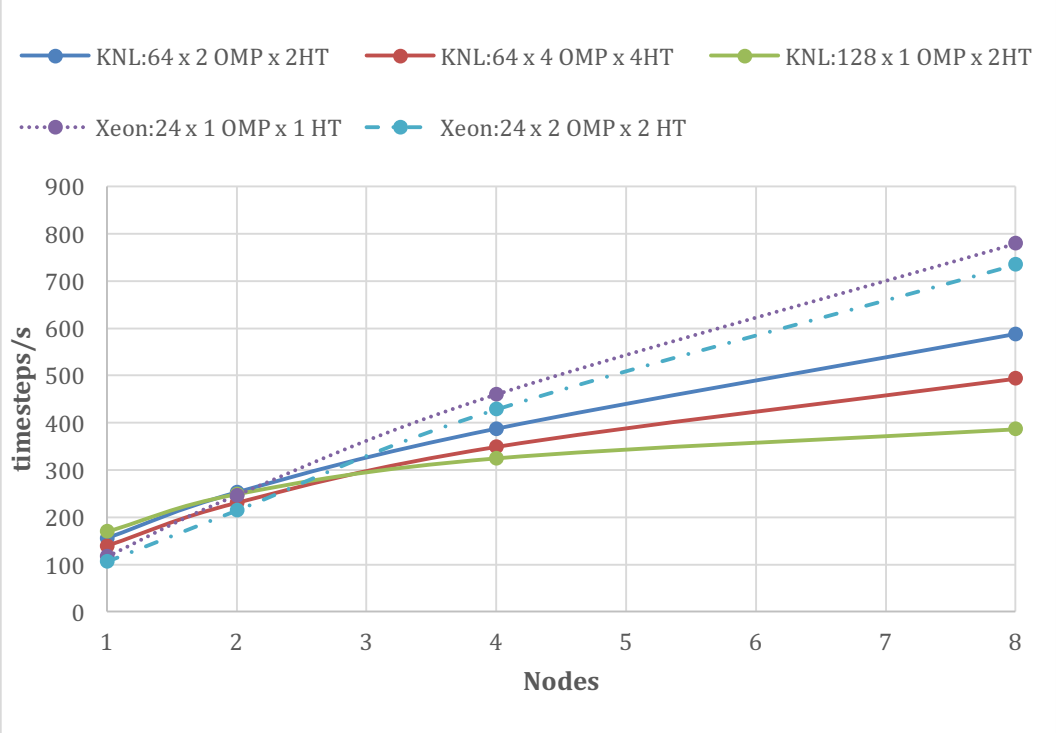

Figure 5 - Performance for the Lennard-Jones potential benchmark run on ARCHER -Xeon and -KNL in multi-node mode with the USER-INTEL package. Dashed lines correspond to the Xeon performance whereas the solid lines represent the KNL performance.

Figure 6 - Performance for the Stillinger-Weber potential benchmark run on ARCHER -Xeon and -KNL in multi-node mode with the USER-OMP package. Dashed lines correspond to the Xeon performance whereas the solid lines represent the KNL performance.Figure 6 and Figure 7 show the performance ofr the Stillinger-Weber potential benchmark.

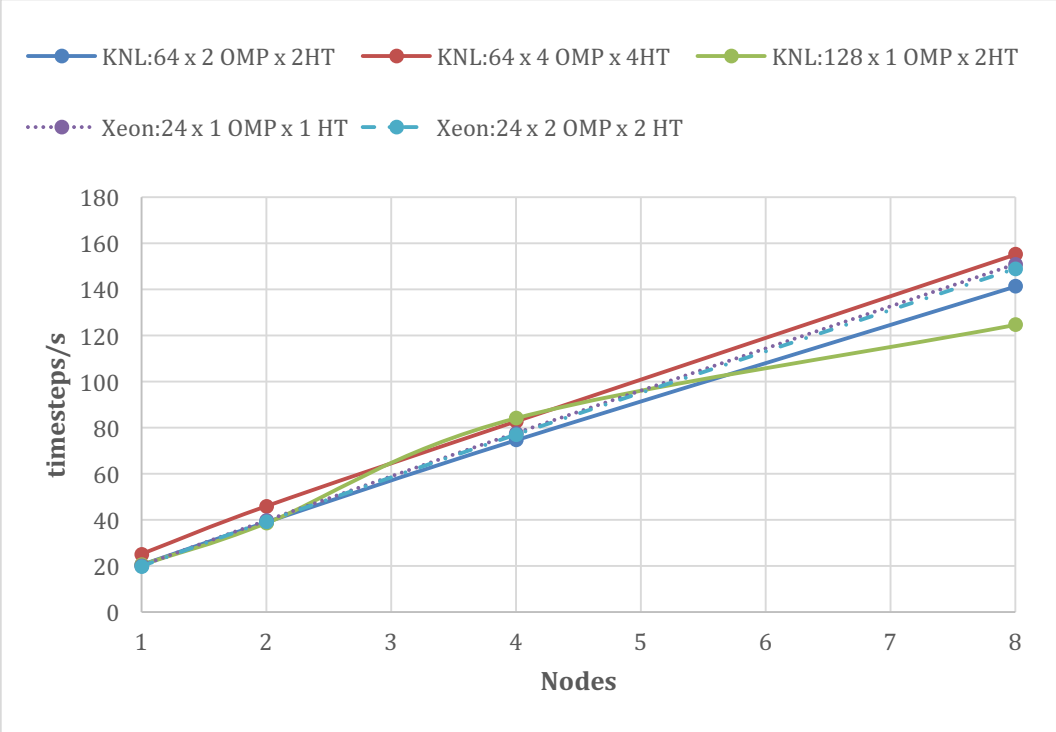

Figure 6 - Performance for the Stillinger-Weber potential benchmark run on ARCHER -Xeon and -KNL in multi-node mode with the USER-OMP package. Dashed lines correspond to the Xeon performance whereas the solid lines represent the KNL performance.

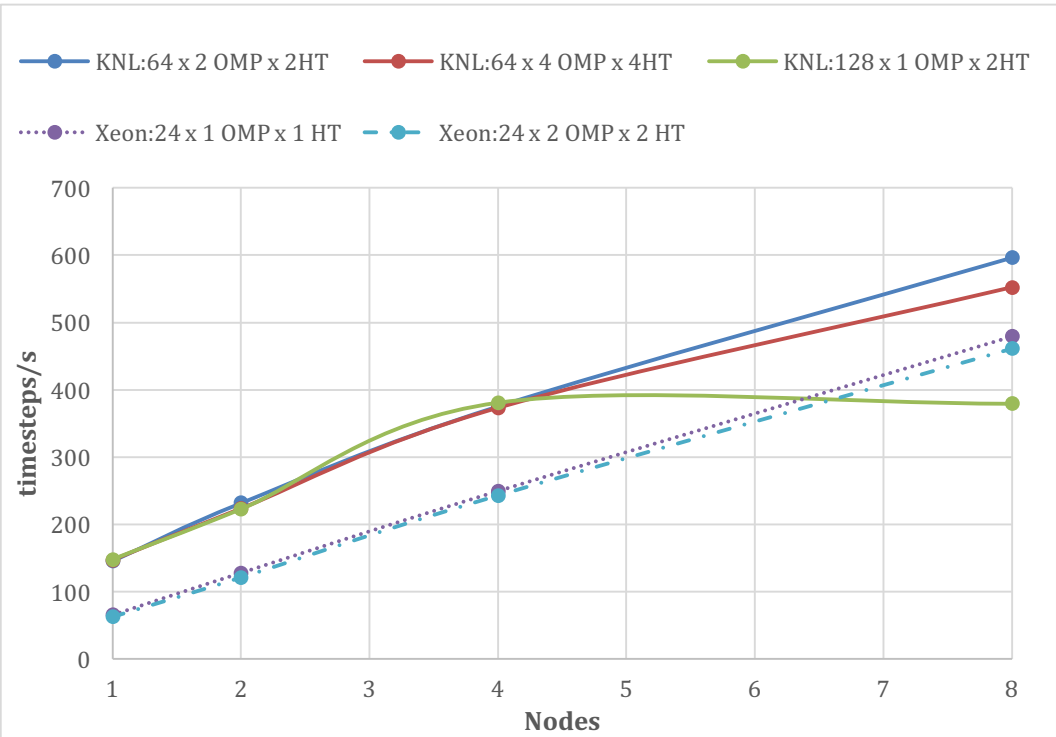

Figure 7 - Performance for the Stillinger-Weber potential benchmark run on ARCHER -Xeon and -KNL in multi-node mode with the USER-INTEL package. Dashed lines correspond to the Xeon performance whereas the solid lines represent the KNL performance.

Finally, Figure 8 and Figure 9 represent the performance figures for the Tersoff potential benchmarks.

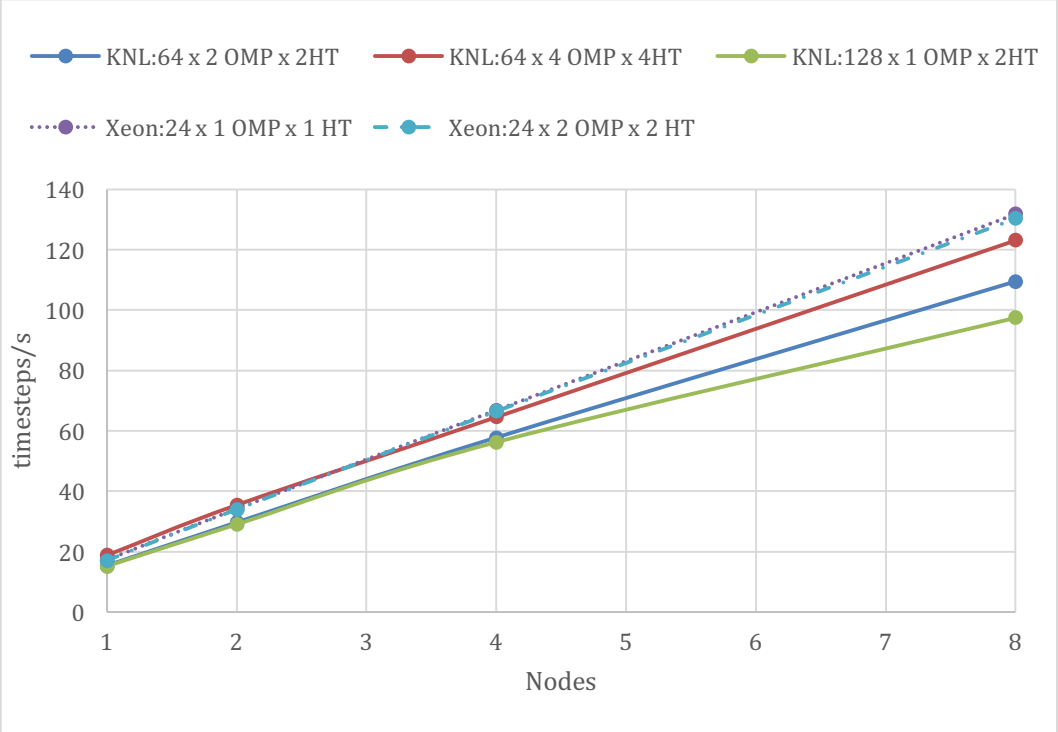

Figure 8 - Performance for the Tersoff potential benchmark run on ARCHER -Xeon and -KNL in multi-node mode with the USER-OMP package. Dashed lines correspond to the Xeon performance whereas the solid lines represent the KNL performance.

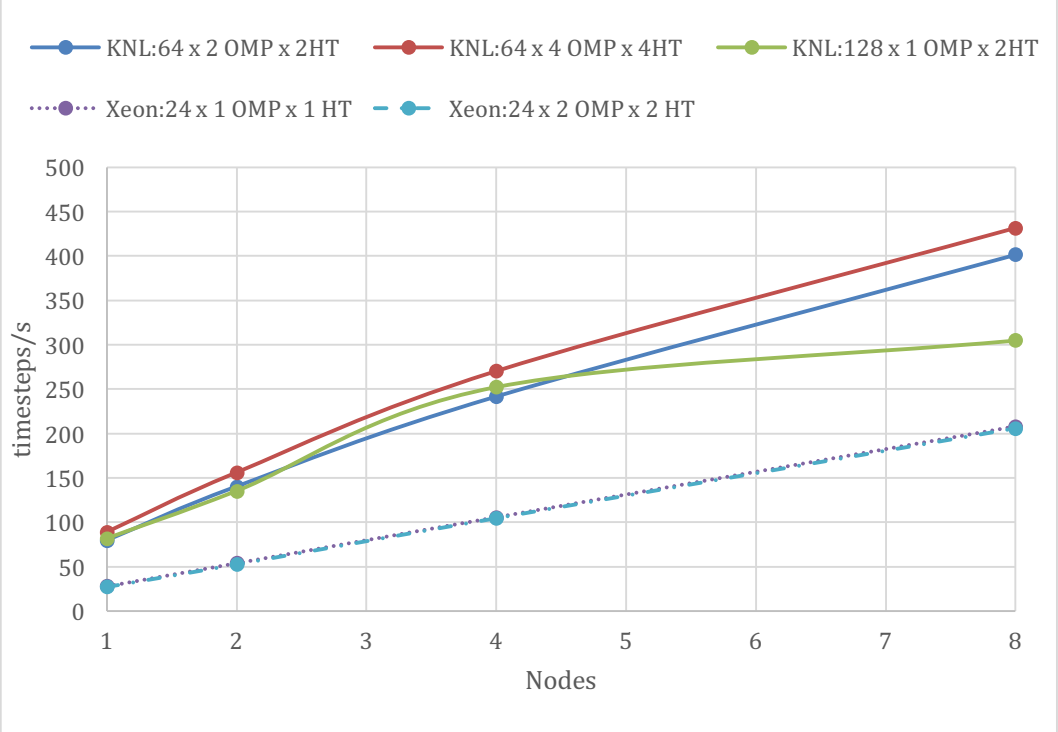

Figure 9 - Performance for the Tersoff potential benchmark run on ARCHER -Xeon and -KNL in multi-node mode with the USER-INTEL package. Dashed lines correspond to the Xeon performance whereas the solid lines represent the KNL performance.

3. Summary and Conclusions

- Results are strongly dependent on the benchmark case.
- KNL performs better than Xeon on all single node cases.
- The USER-INTEL package gives the best performance in all cases.
- The 64 MPI processes x 4 HT x 4 T and the 64 MPI processes x 2 HT x 2 T combinations seem to provide the best performance in all KNL benchmarks.
- KNL shows better performance than Xeon for the Stillinger-Weber and Tersoff benchmarks (USER-INTEL), but it is not the case for the Lennard-Jones benchmarks where Xeon's performance seems to overcome KNL's performance.

4. Full Performance Results

KNL

Lennar-Jones (USER-INTEL)

nodes	Processes	PPN	HT	T	timesteps/s
1	1	1	1	64	18.891
1	1	1	2	128	13.9487
1	1	1	4	256	9.023
1	2	2	1	32	31.6553
1	2	2	2	64	24.231
1	2	2	4	128	17.6887
1	4	4	1	16	49.564
1	4	4	2	32	42.0983
1	4	4	4	64	29.6713
1	8	8	1	8	74.6463
1	8	8	2	16	67.1357
1	8	8	4	32	49.067
1	16	16	1	4	102.499
1	16	16	2	8	101.016
1	16	16	4	16	75.475
1	32	32	1	2	126.291
1	32	32	2	4	135.099
1	32	32	4	8	107.913
1	64	64	1	1	143.503
1	64	64	2	2	155.196
1	64	64	4	4	139.368
1	128	128	2	1	169.354
1	128	128	4	2	151.535
1	256	256	4	1	129.78
2	2	1	1	64	34.5993
2	2	1	2	128	28.6343
2	2	1	4	256	19.1707
2	4	2	1	32	55.1237
2	4	2	2	64	47.471
2	4	2	4	128	34.3133
2	8	4	1	16	86.2117
2	8	4	2	32	77.0177
2	8	4	4	64	56.46
2	16	8	1	8	129.59
2	16	8	2	16	119.879
2	16	8	4	32	91.194

2	32	16	1	4	169.294
2	32	16	2	8	165.533
2	32	16	4	16	125.719
2	64	32	1	2	209.936
2	64	32	2	4	217.027
2	64	32	4	8	173.403
2	128	64	1	1	247.659
2	128	64	2	2	252.141
2	128	64	4	4	230.403
2	256	128	2	1	248.847
2	256	128	4	2	208.006
2	512	256	4	1	150.226
4	4	1	1	64	57.2893
4	4	1	2	128	48.063
4	4	1	4	256	33.8697
4	8	2	1	32	90.9337
4	8	2	2	64	80.0057
4	8	2	4	128	56.241
4	16	4	1	16	143.292
4	16	4	2	32	128.522
4	16	4	4	64	96.3427
4	32	8	1	8	208.229
4	32	8	2	16	190.499
4	32	8	4	32	141.369
4	64	16	1	4	276.528
4	64	16	2	8	271.582
4	64	16	4	16	212.854
4	128	32	1	2	343.187
4	128	32	2	4	347.674
4	128	32	4	8	290.41
4	256	64	1	1	403.187
4	256	64	2	2	386.945
4	256	64	4	4	348.999
4	512	128	2	1	324.995
4	512	128	4	2	265.604
4	1024	256	4	1	200.737
6	6	1	1	64	77.9587
6	6	1	2	128	66.188
6	6	1	4	256	46.4043
6	12	2	1	32	122.102
6	12	2	2	64	107.753
6	12	2	4	128	77.96

6	24	4	1	16	180.685
6	24	4	2	32	164.867
6	24	4	4	64	122.955
6	48	8	1	8	256.746
6	48	8	2	16	234.654
6	48	8	4	32	174.683
6	96	16	1	4	363.547
6	96	16	2	8	341.319
6	96	16	4	16	273.914
6	192	32	1	2	415.34
6	192	32	2	4	415.105
6	192	32	4	8	342.007
6	384	64	1	1	521.965
6	384	64	2	2	500.611
6	384	64	4	4	451.472
6	768	128	2	1	337.691
6	768	128	4	2	269.357
6	1536	256	4	1	99.4053
8	8	1	1	64	93.5603
8	8	1	2	128	79.1157
8	8	1	4	256	55.395
8	16	2	1	32	146.193
8	16	2	2	64	130.011
8	16	2	4	128	92.3347
8	32	4	1	16	213.356
8	32	4	2	32	194.129
8	32	4	4	64	144.471
8	64	8	1	8	304.208
8	64	8	2	16	277.942
8	64	8	4	32	205.267
8	128	16	1	4	428.949
8	128	16	2	8	398.894
8	128	16	4	16	313.381
8	256	32	1	2	518.552
8	256	32	2	4	514.395
8	256	32	4	8	432.606
8	512	64	1	1	622.003
8	512	64	2	2	587.466
8	512	64	4	4	493.462
8	1024	128	2	1	386.55
8	1024	128	4	2	323.159
8	2048	256	4	1	84.8763

Lennard-Jones (USER-OMP)

nodes	Processes	PPN	HT	T	timesteps/s
1	1	1	1	64	20.249
1	1	1	2	128	13.619
1	1	1	4	256	7.55133
1	2	2	1	32	32.322
1	2	2	2	64	23.7353
1	2	2	4	128	14.5137
1	4	4	1	16	40.5493
1	4	4	2	32	35.324
1	4	4	4	64	25.497
1	8	8	1	8	49.0017
1	8	8	2	16	54.5657
1	8	8	4	32	40.5163
1	16	16	1	4	56.2377
1	16	16	2	8	68.608
1	16	16	4	16	59.1793
1	32	32	1	2	60.393
1	32	32	2	4	78.625
1	32	32	4	8	82.5787
1	64	64	1	1	62.196
1	64	64	2	2	83.224
1	64	64	4	4	93.325
1	128	128	2	1	85.728
1	128	128	4	2	99.3573
1	256	256	4	1	85.6467
2	2	1	1	64	35.2687
2	2	1	2	128	23.8253
2	2	1	4	256	13.5113
2	4	2	1	32	55.415
2	4	2	2	64	40.451
2	4	2	4	128	25.4697
2	8	4	1	16	72.8593
2	8	4	2	32	59.7277
2	8	4	4	64	43.954
2	16	8	1	8	91.0687
2	16	8	2	16	99.23
2	16	8	4	32	72.8053
2	32	16	1	4	103.703
2	32	16	2	8	120.515
2	32	16	4	16	100.374

2	64	32	1	2	112.167
2	64	32	2	4	127.312
2	64	32	4	8	136.601
2	128	64	1	1	116.052
2	128	64	2	2	147.407
2	128	64	4	4	151.066
2	256	128	2	1	143.507
2	256	128	4	2	151.262
2	512	256	4	1	114.031
4	4	1	1	64	58.7367
4	4	1	2	128	40.887
4	4	1	4	256	22.8897
4	8	2	1	32	92.203
4	8	2	2	64	67.8257
4	8	2	4	128	44.016
4	16	4	1	16	130.15
4	16	4	2	32	107.093
4	16	4	4	64	77.3737
4	32	8	1	8	162.908
4	32	8	2	16	171.628
4	32	8	4	32	119.996
4	64	16	1	4	187.469
4	64	16	2	8	209.791
4	64	16	4	16	168.997
4	128	32	1	2	204.908
4	128	32	2	4	217.306
4	128	32	4	8	231.132
4	256	64	1	1	214.832
4	256	64	2	2	259.478
4	256	64	4	4	243.703
4	512	128	2	1	215.676
4	512	128	4	2	217.6
4	1024	256	4	1	163.839
6	6	1	1	64	78.4717
6	6	1	2	128	56.748
6	6	1	4	256	33.968
6	12	2	1	32	125.157
6	12	2	2	64	93.5937
6	12	2	4	128	61.624
6	24	4	1	16	172.356
6	24	4	2	32	142.806
6	24	4	4	64	106.044

6	48	8	1	8	216.752
6	48	8	2	16	219.379
6	48	8	4	32	159.67
6	96	16	1	4	258.684
6	96	16	2	8	281.521
6	96	16	4	16	221.168
6	192	32	1	2	268.186
6	192	32	2	4	275.315
6	192	32	4	8	283.858
6	384	64	1	1	302.145
6	384	64	2	2	350.383
6	384	64	4	4	329.767
6	768	128	2	1	245.729
6	768	128	4	2	258.75
6	1536	256	4	1	92.0093
8	8	1	1	64	92.9847
8	8	1	2	128	69.573
8	8	1	4	256	42.4197
8	16	2	1	32	154.774
8	16	2	2	64	116.951
8	16	2	4	128	75.1287
8	32	4	1	16	204.092
8	32	4	2	32	175.253
8	32	4	4	64	129.191
8	64	8	1	8	260.692
8	64	8	2	16	266.229
8	64	8	4	32	188.787
8	128	16	1	4	317.06
8	128	16	2	8	333.854
8	128	16	4	16	260.679
8	256	32	1	2	347.782
8	256	32	2	4	348.326
8	256	32	4	8	355.979
8	512	64	1	1	382.595
8	512	64	2	2	436.648
8	512	64	4	4	386.524
8	1024	128	2	1	303.315
8	1024	128	4	2	267.58
8	2048	256	4	1	79.637

Stillinger- Weber (USER-INTEL)

nodes	Processes	PPN	HT	T	timesteps/s
1	16	16	1	4	91.984
1	32	32	1	2	111.879
1	32	32	2	4	128.566
1	64	64	1	1	123.306
1	64	64	2	2	145.901
1	64	64	4	4	147.208
1	128	128	2	1	148.079
1	128	128	4	2	148.288
1	256	256	4	1	128.02
2	32	16	1	4	157.074
2	64	32	1	2	186.589
2	64	32	2	4	211.761
2	128	64	1	1	209.495
2	128	64	2	2	232.026
2	128	64	4	4	223.668
2	256	128	2	1	222.706
2	256	128	4	2	197.047
2	512	256	4	1	211.564
4	64	16	1	4	261.159
4	128	32	1	2	301.125
4	128	32	2	4	323.425
4	256	64	1	1	361.489
4	256	64	2	2	375.638
4	256	64	4	4	373.166
4	512	128	2	1	380.871
4	512	128	4	2	362.321
4	1024	256	4	1	84.9583
6	96	16	1	4	325.876
6	192	32	1	2	397.289
6	192	32	2	4	418.289
6	384	64	1	1	471.117
6	384	64	2	2	475.556
6	384	64	4	4	459.005
6	768	128	2	1	309.056
6	768	128	4	2	275.836
6	1536	256	4	1	70.8533
8	128	16	1	4	381.025
8	256	32	1	2	471.155
8	256	32	2	4	497.012
8	512	64	1	1	600.178

8	512	64	2	2	596.486
8	512	64	4	4	552.221
8	1024	128	2	1	379.335
8	1024	128	4	2	309.856
8	2048	256	4	1	67.2017

Stillinger-Weber (USER-OMP)

nodes	Processes	PPN	HT	T	timesteps/s
1	16	16	1	4	12.6607
1	32	32	1	2	12.865
1	32	32	2	4	20.044
1	64	64	1	1	12.9327
1	64	64	2	2	20.503
1	64	64	4	4	25.066
1	128	128	2	1	20.4987
1	128	128	4	2	25.0327
1	256	256	4	1	23.094
2	32	16	1	4	24.5907
2	64	32	1	2	25.0103
2	64	32	2	4	35.4753
2	128	64	1	1	25.1397
2	128	64	2	2	39.0193
2	128	64	4	4	45.864
2	256	128	2	1	38.6327
2	256	128	4	2	45.5663
2	512	256	4	1	45.4727
4	64	16	1	4	47.2753
4	128	32	1	2	47.8377
4	128	32	2	4	68.3067
4	256	64	1	1	48.7327
4	256	64	2	2	74.6163
4	256	64	4	4	82.73
4	512	128	2	1	74.4233
4	512	128	4	2	84.188
4	1024	256	4	1	49.262
6	96	16	1	4	68.443
6	192	32	1	2	70.3827
6	192	32	2	4	94.5133
6	384	64	1	1	70.9083
6	384	64	2	2	107.173
6	384	64	4	4	114.463
6	768	128	2	1	95.8217

6	768	128	4	2	103.961
6	1536	256	4	1	49.856
8	128	16	1	4	89.5603
8	256	32	1	2	92.2593
8	256	32	2	4	121.547
8	512	64	1	1	93.9573
8	512	64	2	2	141.335
8	512	64	4	4	155.279
8	1024	128	2	1	124.714
8	1024	128	4	2	133.385
8	2048	256	4	1	49.2703

Tersoff (USER-INTEL)

nodes	Processes	PPN	HT	T	timesteps/s
1	16	16	1	4	50.5527
1	32	32	1	2	55.8857
1	32	32	2	4	74.4163
1	64	64	1	1	58.0737
1	64	64	2	2	79.4283
1	64	64	4	4	88.9327
1	128	128	2	1	81.6897
1	128	128	4	2	90.9323
1	256	256	4	1	83.3387
2	32	16	1	4	92.1537
2	64	32	1	2	101.748
2	64	32	2	4	132.154
2	128	64	1	1	108.785
2	128	64	2	2	140.192
2	128	64	4	4	155.995
2	256	128	2	1	135.209
2	256	128	4	2	139.189
2	512	256	4	1	151.251
4	64	16	1	4	164.701
4	128	32	1	2	183.016
4	128	32	2	4	225.83
4	256	64	1	1	199.598
4	256	64	2	2	241.551
4	256	64	4	4	270.088
4	512	128	2	1	252.23
4	512	128	4	2	271.626
4	1024	256	4	1	79.4453
6	96	16	1	4	217.426

6	192	32	1	2	248.782
6	192	32	2	4	290.953
6	384	64	1	1	277.623
6	384	64	2	2	312.596
6	384	64	4	4	341.442
6	768	128	2	1	265.757
6	768	128	4	2	256.642
6	1536	256	4	1	63.647
8	128	16	1	4	266.931
8	256	32	1	2	302.287
8	256	32	2	4	357.015
8	512	64	1	1	362.021
8	512	64	2	2	401.355
8	512	64	4	4	431.28
8	1024	128	2	1	304.682
8	1024	128	4	2	277.554
8	2048	256	4	1	50.6127

Tersoff (USER-OMP)

nodes	Processes	PPN	HT	T	timesteps/s
1	16	16	1	4	9.84867
1	32	32	1	2	9.97933
1	32	32	2	4	14.775
1	64	64	1	1	10.0353
1	64	64	2	2	15.265
1	64	64	4	4	18.8247
1	128	128	2	1	15.1437
1	128	128	4	2	18.8767
1	256	256	4	1	18.0263
2	32	16	1	4	19.31
2	64	32	1	2	19.629
2	64	32	2	4	26.7383
2	128	64	1	1	19.863
2	128	64	2	2	29.5737
2	128	64	4	4	35.4823
2	256	128	2	1	29.0307
2	256	128	4	2	34.4523
2	512	256	4	1	34.6127
4	64	16	1	4	37.7153
4	128	32	1	2	38.6843
4	128	32	2	4	52.3617
4	256	64	1	1	39.0163

4	256	64	2	2	57.697
4	256	64	4	4	64.602
4	512	128	2	1	56.2607
4	512	128	4	2	64.7477
4	1024	256	4	1	40.0163
6	96	16	1	4	54.3477
6	192	32	1	2	56.3423
6	192	32	2	4	73.1767
6	384	64	1	1	57.06
6	384	64	2	2	83.0393
6	384	64	4	4	91.8603
6	768	128	2	1	77.3543
6	768	128	4	2	88.565
6	1536	256	4	1	43.709
8	128	16	1	4	72.331
8	256	32	1	2	73.752
8	256	32	2	4	94.9073
8	512	64	1	1	76.1527
8	512	64	2	2	109.436
8	512	64	4	4	123.15
8	1024	128	2	1	97.4617
8	1024	128	4	2	108.84
8	2048	256	4	1	39.3653

Xeon

Lennard-Jones (USER-INTEL)

nodes	Processes	PPN	HT	T	timesteps/s
1	6	6	1	4	35.3993
1	12	12	1	2	65.2633
1	12	12	2	4	58.5573
1	24	24	1	1	116.474
1	24	24	2	2	106.088
1	48	48	2	1	128.251
2	12	6	1	4	69.2323
2	24	12	1	2	130.151
2	24	12	2	4	115.389
2	48	24	1	1	246.396
2	48	24	2	2	214.341
2	96	48	2	1	268.153
4	24	6	1	4	139.026
4	48	12	1	2	261.288
4	48	12	2	4	231.252

4	96	24	1	1	459.858
4	96	24	2	2	428.239
4	192	48	2	1	527.699
8	48	6	1	4	265.912
8	96	12	1	2	451.281
8	96	12	2	4	423.331
8	192	24	1	1	779.121
8	192	24	2	2	734.495
8	384	48	2	1	846.531

Lennard-Jones (USER-OMP)

nodes	Processes	PPN	HT	T	timesteps/s
1	6	6	1	4	21.1643
1	12	12	1	2	39.318
1	12	12	2	4	36.4623
1	24	24	1	1	78.481
1	24	24	2	2	72.3877
1	48	48	2	1	92.9933
2	12	6	1	4	42.6343
2	24	12	1	2	79.2043
2	24	12	2	4	75.003
2	48	24	1	1	155.938
2	48	24	2	2	150.714
2	96	48	2	1	185.199
4	24	6	1	4	85.3597
4	48	12	1	2	154.648
4	48	12	2	4	149.722
4	96	24	1	1	293.497
4	96	24	2	2	283.446
4	192	48	2	1	341.125
8	48	6	1	4	161.375
8	96	12	1	2	280.135
8	96	12	2	4	271.54
8	192	24	1	1	520.856
8	192	24	2	2	502.628
8	384	48	2	1	579.728

Stillinger-Weber (USER-INTEL)

nodes	Processes	PPN	HT	T	timesteps/s
1	6	6	1	4	18.9917
1	12	12	1	2	34.6183
1	12	12	2	4	33.1073

1	24	24	1	1	65.7393
1	24	24	2	2	62.937
1	48	48	2	1	81.1807
2	12	6	1	4	37.1723
2	24	12	1	2	68.2453
2	24	12	2	4	64.6273
2	48	24	1	1	128.188
2	48	24	2	2	121.456
2	96	48	2	1	158.202
4	24	6	1	4	74.258
4	48	12	1	2	134.605
4	48	12	2	4	129.237
4	96	24	1	1	249.726
4	96	24	2	2	243.179
4	192	48	2	1	306.951
8	48	6	1	4	142.603
8	96	12	1	2	256.486
8	96	12	2	4	250.843
8	192	24	1	1	479.327
8	192	24	2	2	461.138
8	384	48	2	1	546.597

Stillinger-Weber (USER-OMP)

nodes	Processes	PPN	HT	T	timesteps/s
1	6	6	1	4	5.544
1	12	12	1	2	10.117
1	12	12	2	4	9.93267
1	24	24	1	1	20.0837
1	24	24	2	2	19.7497
1	48	48	2	1	24.802
2	12	6	1	4	11.019
2	24	12	1	2	20.0927
2	24	12	2	4	19.843
2	48	24	1	1	39.613
2	48	24	2	2	39.2133
2	96	48	2	1	49.0167
4	24	6	1	4	21.8183
4	48	12	1	2	39.631
4	48	12	2	4	39.2887
4	96	24	1	1	77.5923
4	96	24	2	2	76.903
4	192	48	2	1	95.184

8	48	6	1	4	43.1563
8	96	12	1	2	77.4037
8	96	12	2	4	76.6723
8	192	24	1	1	150.912
8	192	24	2	2	148.947
8	384	48	2	1	180.252

Tersoff (USER-INTEL)

nodes	Processes	PPN	HT	T	timesteps/s
1	6	6	1	4	7.79267
1	12	12	1	2	14.218
1	12	12	2	4	14.0047
1	24	24	1	1	27.862
1	24	24	2	2	27.4433
1	48	48	2	1	31.644
2	12	6	1	4	15.4307
2	24	12	1	2	28.3037
2	24	12	2	4	27.7317
2	48	24	1	1	53.8843
2	48	24	2	2	52.8353
2	96	48	2	1	60.8467
4	24	6	1	4	30.8563
4	48	12	1	2	56.0103
4	48	12	2	4	55.1203
4	96	24	1	1	105.645
4	96	24	2	2	104.761
4	192	48	2	1	120.291
8	48	6	1	4	60.53
8	96	12	1	2	108.888
8	96	12	2	4	107.526
8	192	24	1	1	207.927
8	192	24	2	2	205.838
8	384	48	2	1	230.501

Tersoff (USER-OMP)

nodes	Processes	PPN	HT	T	timestep/s
1	6	6	1	4	4.63967
1	12	12	1	2	8.64433
1	12	12	2	4	8.34867
1	24	24	1	1	17.218
1	24	24	2	2	17.0257

1	48	48	2	1	21.663
2	12	6	1	4	9.16733
2	24	12	1	2	17.2677
2	24	12	2	4	16.6447
2	48	24	1	1	34.0817
2	48	24	2	2	33.954
2	96	48	2	1	42.735
4	24	6	1	4	18.363
4	48	12	1	2	34.089
4	48	12	2	4	33.1687
4	96	24	1	1	66.809
4	96	24	2	2	66.495
4	192	48	2	1	83.895
8	48	6	1	4	35.966
8	96	12	1	2	66.5653
8	96	12	2	4	64.4057
8	192	24	1	1	131.807
8	192	24	2	2	130.375
8	384	48	2	1	160.9