

Gromacs 2018 benchmark on ASPIRE1

James Jen-Chang CHEN

james@nscg.sg

Case: lignocellulose

Source: http://www.prace-ri.eu/UEABS/GROMACS/1.2/GROMACS_TestCaseB.tar.gz

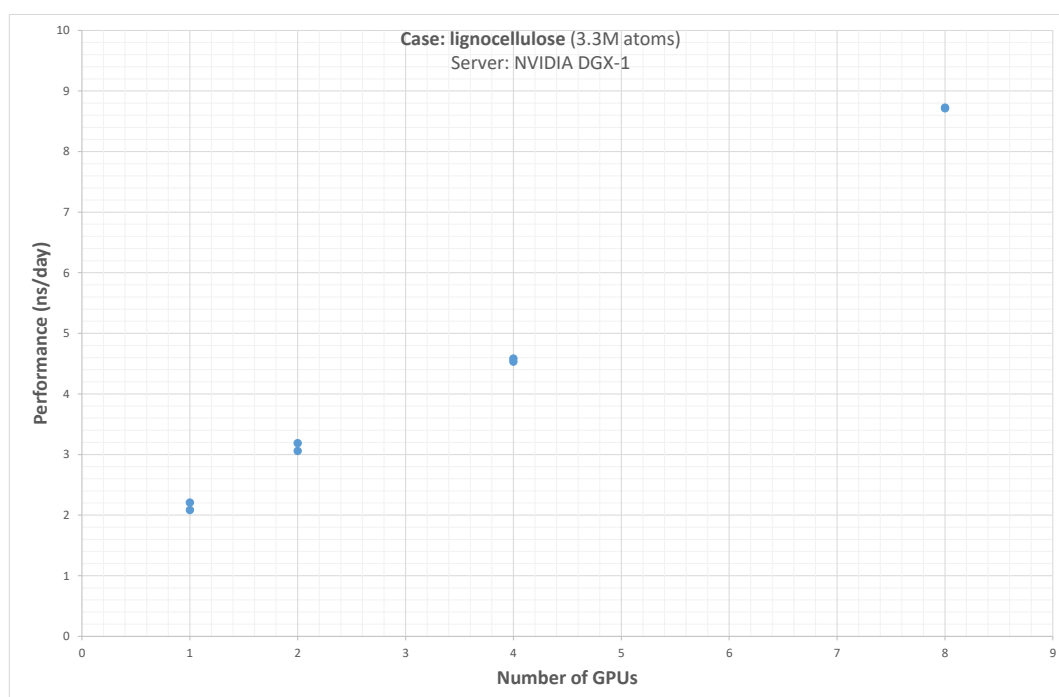
3.3M atoms, PRACE Unified European Applications Benchmark Suite (UEABS).

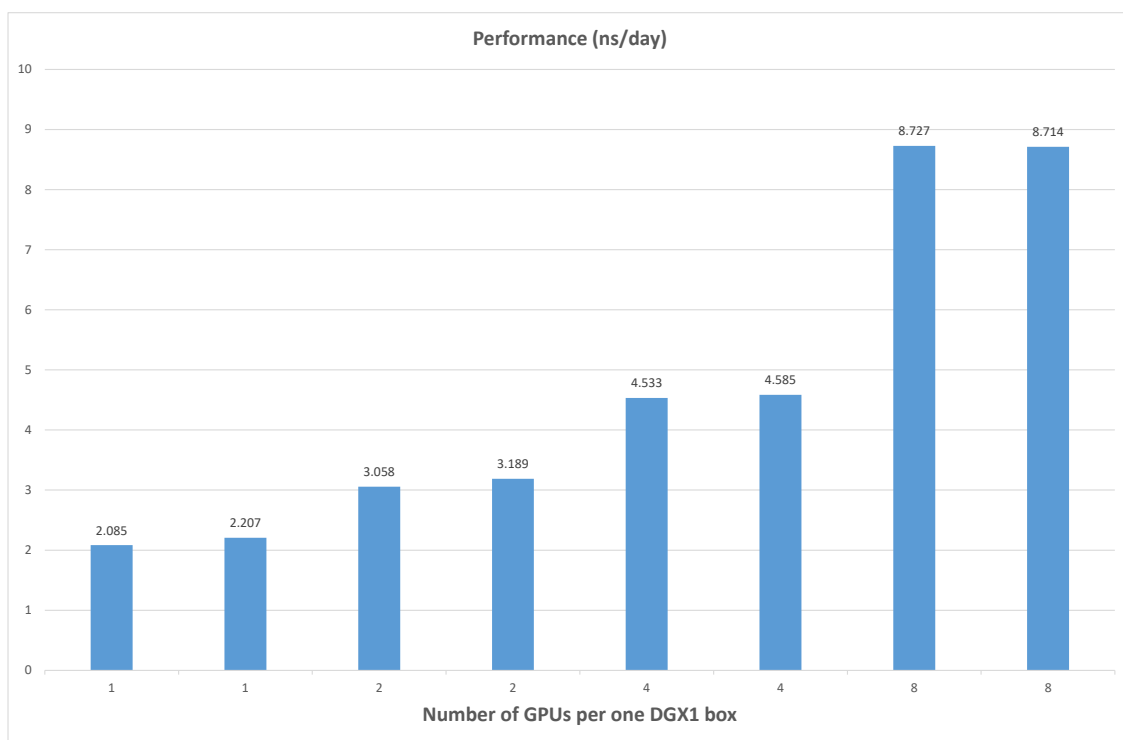
DGX-1 (8 GPUs)

Software stack: CentOS7, GNU 4.8.5, OpenMPI 1.10.7, CUDA 9.0, Singularity 2.6.0, Gromacs 2018.4

Results:

# of GPUs	Performance (ns/day)	Remarks
1	2.085	GPU ID:0
1	2.207	GPU ID:7
2	3.058	GPU ID:0,1
2	3.189	GPU ID:0,4
4	4.533	GPU ID:0,1,4,5
4	4.585	GPU ID:0,1,2,3
8	8.727	ALL GPUs
8	8.714	ALL GPUs





Reference scripts:

1-GPU case

```
/opt/singularity/bin/singularity exec --nv /home/users/astar/scei/jamesche/dl-
image/gromacs2018-gnu-openmpi1-cuda9-centos7-gpu.simg mpirun -np 1 -bind-to none -
map-by slot /usr/local/gromacs/bin/gmx_mpi mdrun -ntomp 4 -pin on -gpu_id 0 -s
lignocellulose-rf.tpr -nsteps 10000 -g logfile
```

2-GPU case

```
/opt/singularity/bin/singularity exec --nv /home/users/astar/scei/jamesche/dl-
image/gromacs2018-gnu-openmpi1-cuda9-centos7-gpu.simg mpirun -np 2 -bind-to none -
map-by slot /usr/local/gromacs/bin/gmx_mpi mdrun -ntomp 4 -pin on -gpu_id 01 -s
lignocellulose-rf.tpr -nsteps 10000 -g logfile
```

4-GPU case

```
/opt/singularity/bin/singularity exec --nv /home/users/astar/scei/jamesche/dl-
image/gromacs2018-gnu-openmpi1-cuda9-centos7-gpu.simg mpirun -np 4 -bind-to none -
map-by slot /usr/local/gromacs/bin/gmx_mpi mdrun -ntomp 4 -pin on -gpu_id 0145 -s
lignocellulose-rf.tpr -nsteps 10000 -g logfile
```

8-GPU case

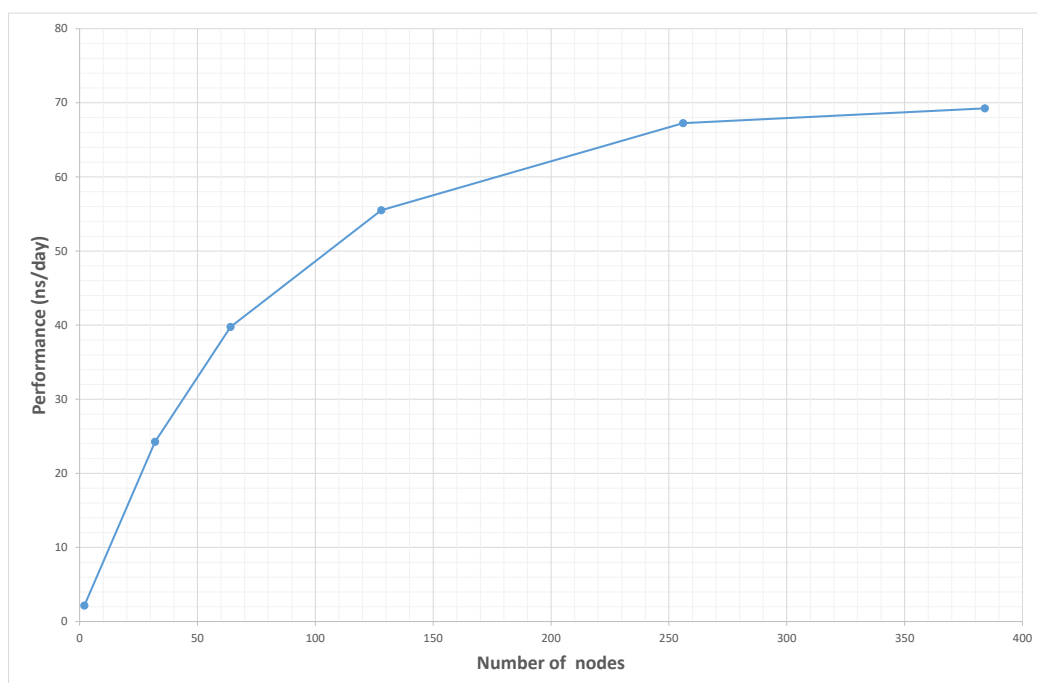
```
/opt/singularity/bin/singularity exec --nv /home/users/astar/scei/jamesche/dl-
image/gromacs2018-gnu-openmpi1-cuda9-centos7-gpu.simg mpirun -np 8 -bind-to none -
map-by slot /usr/local/gromacs/bin/gmx_mpi mdrun -ntomp 4 -pin on -s lignocellulose-rf.tpr
-nsteps 10000 -g logfile
```

PURE CPU node (Intel Xeon E5-2690v3 cluster)

Software stack: CentOS6, Intel compiler suite 2017, Intel MPI, Gromacs 2018.1

Results:

Platform/Compiler	Performance (ns/day)	Remarks
ASPIRE1/Intel 2017	2.161	2 nodes
ASPIRE1/Intel 2017	24.272	32 nodes
ASPIRE1/Intel 2017	39.758	64 nodes
ASPIRE1/Intel 2017	55.496	128 nodes
ASPIRE1/Intel 2017	67.248	256 nodes
ASPIRE1/Intel 2017	69.260	384 nodes



Machine description

Platform	Hardware
DGX1	Single Node only CPU: Dual Intel Xeon E5-2698V4 GPU: 8 NVIDIA V100-SXM2 (16GB) RAM: 512GB DDR4 Filesystem: GPFS via NFS NIC: Mellanox IB EDR x 4
Intel Xeon E5-2690v3 cluster	Cluster CPU: Dual Intel Xeon E5-2690V3 RAM: 128GB DDR4 Filesystem: Lustre NIC: Mellanox IB EDR