Amber18 benchmark on ASPIRE1

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Case:

1. **Explicit Solvent (PME)**
   - DHFR NVE HMR 4fs (23,558 atoms)
   - DHFR NPT HMR 4fs (23,558 atoms)
   - DHFR NVE 2fs (23,558 atoms)
   - DHFR NPT 2fs (23,558 atoms)
   - FactorIX NVE 2fs (90,906 atoms)
   - FactorIX NPT 2fs (90,906 atoms)
   - Cellulose NVE 2fs (408,609 atoms)
   - Cellulose NPT 2fs (408,609 atoms)
   - STMV NPT HMR 4fs (1,067,095 atoms)
2. **Implicit Solvent (GB)**
   - TRPCage 2fs (304 atoms)
   - Myoglobin (2,492 atoms)
   - Nucleosome (25,095 atoms)

Source: http://ambermd.org/Amber18_Benchmark_Suite_RCW.tar.bz2

DGX-1 (8 GPUs)
Software stack: CentOS7, GNU 4.8.5, OpenMPI 1.10.7, CUDA 9.0, Singularity 2.6.0, Amber18 (update.9), AmberTools18 (update.11)

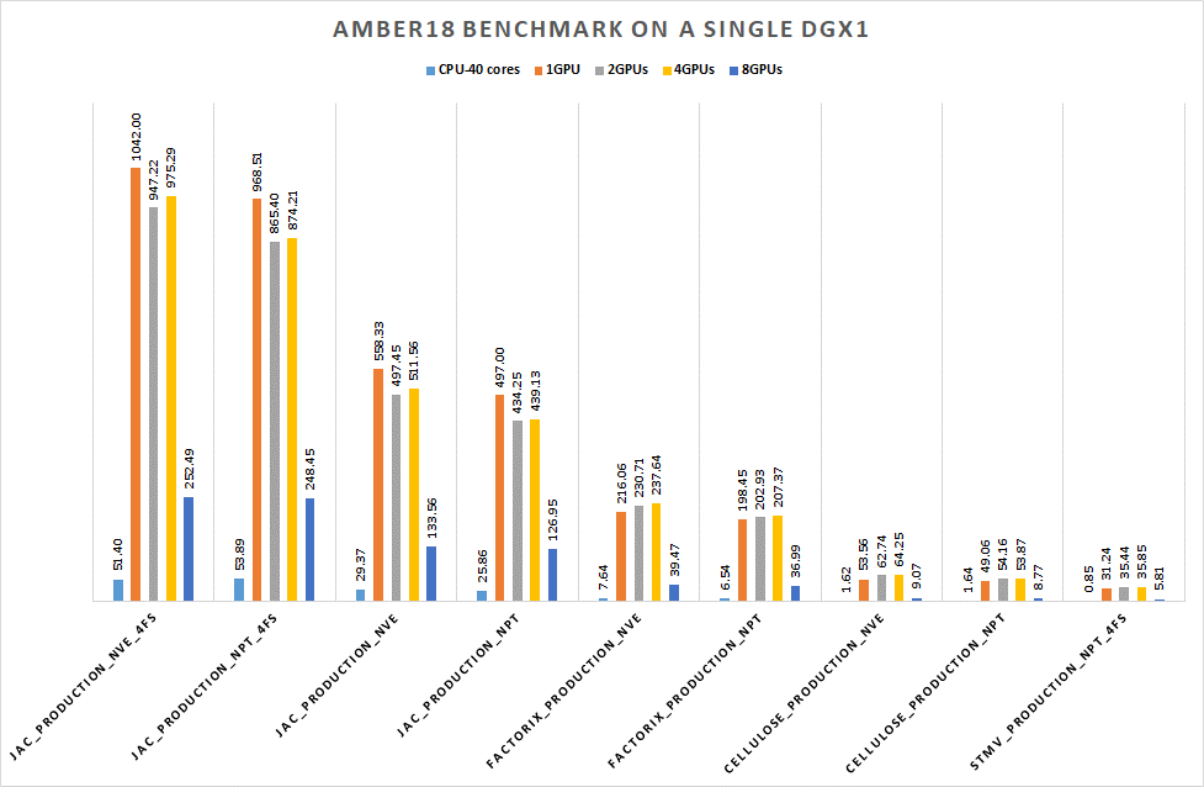
Amber18 binaries: pmemd.MPI (CPU), pmemd.cuda (SPFP, single GPU), pmemd.cuda.MPI (SPFP, multi-GPUs)

Results:

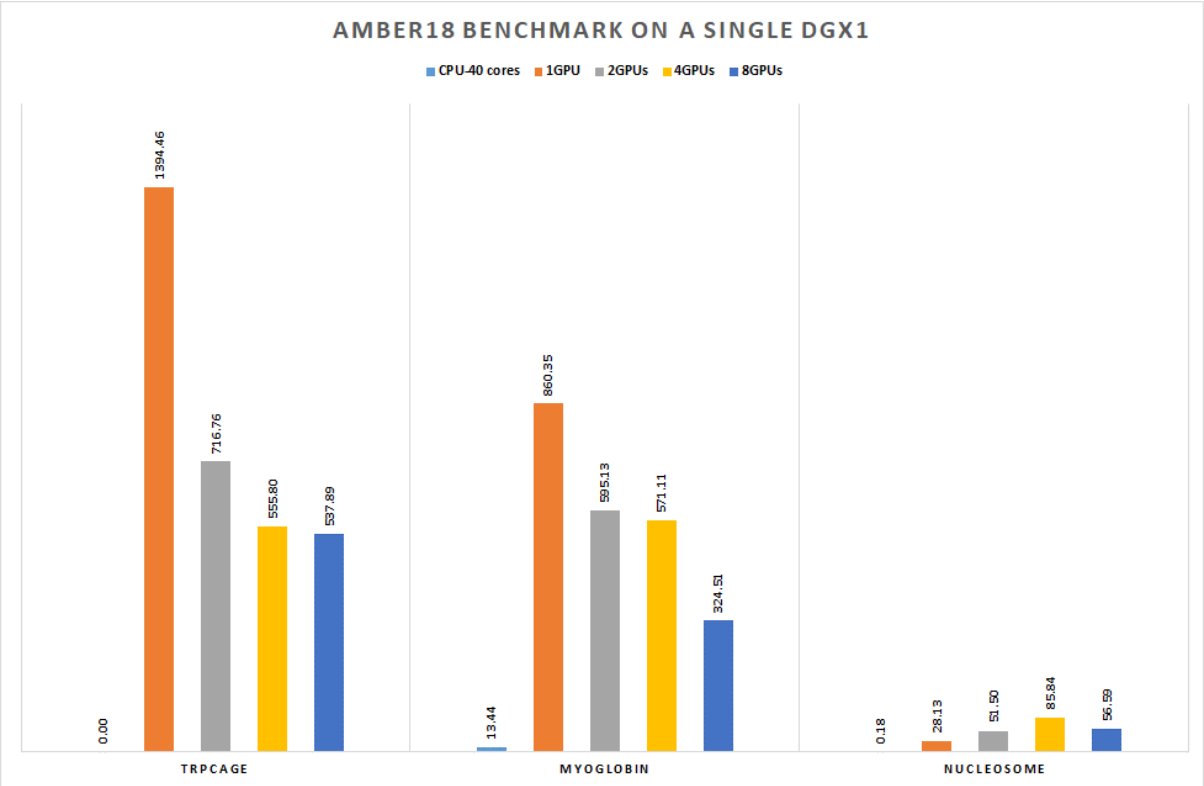
Solvent	Case	Performance of the average timings for all steps (ns/day)				
		40-core CPU	1-GPU	2-GPU	4-GPU	8-GPU
PME	JAC_production_NVE_4fs	51.40	1042.00	947.22	975.29	252.49
PME	JAC_production_NPT_4fs	53.89	968.51	865.40	874.21	248.45
PME	JAC_production_NVE	29.37	558.33	497.45	511.56	133.56
PME	JAC_production_NPT	25.86	497.00	434.25	439.13	126.95
PME	FactorIX_production_NVE	7.64	216.06	230.71	237.64	39.47
PME	FactorIX_production_NPT	6.54	198.45	202.93	207.37	36.99
PME	Cellulose_production_NVE	1.62	53.56	62.74	64.25	9.07
PME	Cellulose_production_NPT	1.64	49.06	54.16	53.87	8.77
PME	STMV_production_NPT_4fs	0.85	31.24	35.44	35.85	5.81
GB	TRPCage	N.A.*	1394.46	716.76	555.80	537.89
GB	myoglobin	13.44	860.35	595.13	571.11	324.51
GB	nucleosome	0.18	28.13	51.50	85.84	56.59

* ERROR: Must have 10x more atoms than processors.

PME solvent



GB solvent



Reference scripts:

1. Settings in the benchmark script

```
[jamesche@nscc02 Amber18_Benchmark_Suite]$ head run_bench_CPU+GPU.sh
#!/bin/bash

#------ SET FOR YOUR SYSTEM -------
#
GPU_COUNT=8
CPU_COUNT=40
#Should we run large STMV 1 million atom + test?
RUN_LARGE_BENCH=true
#
#-----------------------------------
```

2. Job script for PBS queuing ststem

```
[jamesche@nscc02 Amber18_Benchmark_Suite]$ cat pbs-gpu.sh
#!/bin/bash
#PBS -N amber-bm
#PBS -q dgx
#PBS -l select=1:ncpus=40:mpiprocs=40:ompthreads=2:ngpus=8
#PBS -l walltime=24:00:00
#PBS -P Personal
#PBS -j oe
cd $PBS_O_WORKDIR

echo '====================================================='
echo Working directory is $PBS_O_WORKDIR
echo "Starting on `hostname` at `date`"


ulimit -a ## check the limit of kernel parameters
export SINGULARITYENV_LD_LIBRARY_PATH=/home/users/astar/scei/jamesche/mylib/openmpi-1.10.7-cuda9-gnu4/:$SING
ULARITYENV_LD_LIBRARY_PATH
export SINGULARITYENV_AMBERHOME=/usr/local/src/amber18
export SINGULARITYENV_OMP_NUM_THREADS=2

/opt/singularity/bin/singularity exec --nv /home/users/astar/scei/jamesche/dl-image/amber18-gnu-openmpi1-cud
a9-centos7-gpu.simg /home/projects/41000001/jamesche/amber18-gpu4/Amber18_Benchmark_Suite/run_bench_CPU+GPU.
sh

echo "Job Ended at `date`"
echo '====================================================='
```

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