Running Amber GPU jobs

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- Running Amber jobs
To request one GPU card, use SBATCH directives in job script:

```
#SBATCH --gres=gpu:1
#SBATCH --partition=gpu
```

To request a specific card type, use e.g. `--gres=gpu:k80:1` or `--gres=gpu:p1080:1`. As an example, let's submit an Amber job. Amber is a molecular dynamics software package. The recipe is:

```
$ mkdir -p /scratch/$USER/myambertest
$ cd /scratch/$USER/myambertest
$ cp /share/apps/Tutorials/slurm/example/amberGPU/* .
$ sbatch run-amber.s
```

Submitted batch job 14257

From the tutorial example directory we copy over Amber input data files "inpord", "prmtop" and "mdin", and the job script file "run-amber.s". The content of the job script "run-amber.s" is:

```bash
#!/bin/bash
#
#SBATCH --job-name=myAmberJobGPU
#SBATCH --nodes=1
#SBATCH --cpus-per-task=1
#SBATCH --time=00:30:00
#SBATCH --mem=3GB
#SBATCH --gres=gpu:1
#SBATCH --partition=gpu

module purge
module load amber/openmpi/intel/16.06

cd /scratch/$USER/myambertest
pmemd.cuda -O
```

The demo Amber job should take ~2 minutes to finish once it starts running. When the job is done, several output files are generated. Check the one named "mdout", which has a section most relevant here:

```
|--------------------- INFORMATION ----------------------
| GPU (CUDA) Version of PMEMD in use: NVIDIA GPU IN USE. |
|        Version 16.0.0                                    |
|                                                          |
| 02/25/2016                                                |
|                                                          |
|[......]                                                  |

```

```
|------------------- GPU DEVICE INFO -------------------|
| CUDA_VISIBLE_DEVICES: 0 |
| CUDA Capable Devices Detected: 1 |
| CUDA Device ID in use: 0       |
|   CUDA Device Name: Tesla K80   |
| CUDA Device Global Mem Size: 11439 MB |
| CUDA Device Num Multiprocessors: 13 |
|   CUDA Device Core Freq: 0.82 GHz |
```

```