

WE HAVE RUN THE FOLLOWING COMMAND TO RUN AMBER12 SIMULATON USING pmemd.cuda.MPI FOR TWO NVIDIA K20M GPU. BUT WE GETTING FOLLOWING ERROR (NO2)

```
#export AMBERHOME=/opt/testamber/amber12/;$AMBERHOME  
#export DO_PARALLEL="mpirun -np 20"
```

```
#mpirun -np 20 /opt/testamber/amber12/bin/pmemd.cuda.MPI -O -i density-eqm.in -o density-eqm.out  
-p peptide-wat.prmtop -c heat-final-300K-0t.rst -r density-eqm.rst -x density-eqm.mdcrd
```

NO 2: ERROR

Currently only GPU SM Revisions 1.3 and 2.X are supported.  
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```
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```

- = BAD TERMINATION OF ONE OF YOUR APPLICATION PROCESSES
- = PID 1088 RUNNING AT localhost.localdomain
- = EXIT CODE: 255
- = CLEANING UP REMAINING PROCESSES
- = YOU CAN IGNORE THE BELOW CLEANUP MESSAGES

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#### Nvidia GPU K20m CARD DETAILS

Detected 2 CUDA Capable device(s)

Device 0: "Tesla K20m"

CUDA Driver Version / Runtime Version      6.0 / 6.0  
CUDA Capability Major/Minor version number:  3.5  
Total amount of global memory:              4800 MBytes (5032706048 bytes)  
(13) Multiprocessors, (192) CUDA Cores/MP:  2496 CUDA Cores  
GPU Clock rate:                              706 MHz (0.71 GHz)  
Memory Clock rate:                            2600 Mhz

Device 1: "Tesla K20m"

CUDA Driver Version / Runtime Version      6.0 / 6.0  
CUDA Capability Major/Minor version number:  3.5  
Total amount of global memory:              4800 MBytes (5032706048 bytes)  
(13) Multiprocessors, (192) CUDA Cores/MP:  2496 CUDA Cores  
GPU Clock rate:                              706 MHz (0.71 GHz)

deviceQuery, CUDA Driver = CUDART, CUDA Driver Version = 6.0, CUDA Runtime Version = 6.0,  
NumDevs = 2, Device0 = Tesla K20m, Device1 = Tesla K20m  
Result = PASS