NAMD

NAMD 2.12 (2016-12-22)

- /fs00/software/namd/2.12

例: 输入文件为当前目录下的 in.conf, 申请 48个核提交到 e5v3ib队列

```
#BSUB -n 48
#BSUB -q e5v3ib

input=in.conf
#bindir=/fs00/software/namd/2.12/verbs/
bindir=/fs00/software/namd/2.12/ibverbs/

nodefile=nodelist
echo "group main" > $nodefile
for i in `echo $LSB_HOSTS`
do
echo "host $i" >> $nodefile
done

${bindir}charmrun ++remote-shell ssh ++nodelist $nodefile +p$LSB_DJOB_NUMPROC ${bindir}namd2
$input
```

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