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
```

Revision #1
Created 2021-05-11 09:36:42 CST by Yao Ge
Updated 2023-02-08 23:08:01 CST by Yao Ge