

1. 上传安装文件并解压

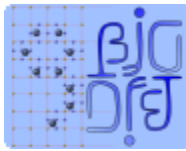
```
[caoao@c01n01 ~]$ mkdir /gpfsHOME/home/student/caoao/BigDFT
[caoao@c01n01 ~]$ cd /gpfsHOME/home/student/caoao/BigDFT/
[caoao@c01n01 BigDFT]$ ls
bigdft-1.7-dev.28.tar.bz2
[caoao@c01n01 BigDFT]$ tar jxf bigdft-1.7-dev.28.tar.bz2
[caoao@c01n01 BigDFT]$ ls
bigdft-1.7-dev.28  bigdft-1.7-dev.28.tar.bz2
[caoao@c01n01 BigDFT]$ cd bigdft-1.7-dev.28
[caoao@c01n01 bigdft-1.7-dev.28]$ pwd
/gpfsHOME/home/student/caoao/BigDFT/bigdft-1.7-dev.28
```

2. 安装节点环境变量设置（此处以 c01n01 节点为例，用户为 caoao）

```
[caoao@c01n01 bigdft-1.7-dev.28]$ vi ~/.bashrc    //在文件尾部添加以下语句
source /opt/intel2012/impi/4.0.3.008/bin/mpivars.sh intel64
source /opt/intel2012/composer_xe_2011_sp1.6.233/bin/iccvars.sh intel64
source /opt/intel2012/composer_xe_2011_sp1.6.233/mkl/bin/mklvars.sh intel64
source /opt/intel2012/composer_xe_2011_sp1.6.233/bin/ifortvars.sh intel64
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/usr/local/cuda-5.5/lib64
[caoao@c01n01 ~]$ source ~/.bashrc
```

3. 测试安装环境是否完整

```
[caoao@c01n01 ~]$ which icc
/opt/intel2012/composer_xe_2011_sp1.6.233/bin/intel64/icc
[caoao@c01n01 ~]$ which mpicc
/opt/intel2012/impi/4.0.3.008/intel64/bin/mpicc
[caoao@c01n01 ~]$ which ifort
/opt/intel2012/composer_xe_2011_sp1.6.233/bin/intel64/ifort
[caoao@c01n01 ~]$ which mpiifort
/opt/intel2012/impi/4.0.3.008/intel64/bin/mpiifort
[caoao@c01n01 ~]$ which mpirun
/opt/intel2012/impi/4.0.3.008/intel64/bin/mpirun
```



4. CPU 上编译 BigDFT

- 切换至 BigDFT 软件解压后的目录

```
[caoao@c01n01 ~]$ cd BigDFT/bigdft-1.7-dev.28
```

- 新建 build 目录用于存放在 CPU 上编译产生的文件

```
[caoao@c01n01 bigdft-1.7-dev.28]$ mkdir build
```

- 切换至 build 目录进行指定参数的 configure 环境编译

```
[caoao@c01n01 bulid]$ ../configure
```

```
--prefix=/gpfsHOME/home/student/caoao/bigdft_1 CC=mpiicc CXX=mpiicpc
```

```
F77=mpiifort FC=mpiifort FCFLAGS="-O2 -xsse4.2" FFLAGS=-O2 CFLAGS=-O2
```

```
CXXFLAGS=-O2
```

```
--with-ext-linalg="/opt/intel2012/composer_xe_2011_sp1.6.233/mkl/lib/intel64/libmkl_
solver_lp64_sequential.a -Wl,--start-group
```

```
/opt/intel2012/composer_xe_2011_sp1.6.233/mkl/lib/intel64/libmkl_intel_lp64.a
```

```
/opt/intel2012/composer_xe_2011_sp1.6.233/mkl/lib/intel64/libmkl_scalapack_lp64.a
```

```
/opt/intel2012/composer_xe_2011_sp1.6.233/mkl/lib/intel64/libmkl_blacs_lp64.a
```

```
/opt/intel2012/composer_xe_2011_sp1.6.233/mkl/lib/intel64/libmkl_intel_thread.a
```

```
/opt/intel2012/composer_xe_2011_sp1.6.233/mkl/lib/intel64/libmkl_lapack95_lp64.a
```

```
/opt/intel2012/composer_xe_2011_sp1.6.233/mkl/lib/intel64/libmkl_core.a
```

```
-Wl,--end-group -liomp5 -lpthread -limf -lm"
```

```
--with-ext-linalg-path=-L/opt/intel2012/composer_xe_2011_sp1.6.233/mkl/lib/intel64/
```

- 切换至 S_GPU 目录，执行以下操作（官方建议）

```
[caoao@c01n01 S_GPU]$ cd S_GPU/
```

```
[caoao@c01n01 S_GPU]$ make clean
```

```
[caoao@c01n01 S_GPU]$ make LDFLAGS=""
```

```
[caoao@c01n01 S_GPU]$ cd -
```

- 编译并安装 BigDFT

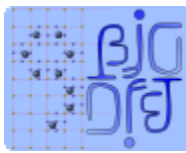
```
[caoao@c01n01 bulid]$ make
```

```
[caoao@c01n01 build]$ make install
```

- 检查安装情况(安装目录下需要有四个文件夹，分别为 bin/ include/ lib/ share/)

```
[caoao@c01n01 build]$ cd /gpfsHOME/home/student/caoao/bigdft_1/
```

```
[caoao@c01n01 bigdft_1]$ ls
```



bin include lib share

- 将 BigDFT 软件的环境变量添加到用户 (caoao) 环境中

```
[caoao@c01n01 bin]$ echo "export PATH=$PATH:/gpfsHOME/home/student
/caoao/bigdft_1/bin">> ~/.bashrc
[caoao@c01n01 bin]$ source ~/.bashrc
[caoao@c01n01 bin]$ which bigdft
~/bigdft_1/bin/bigdft
```

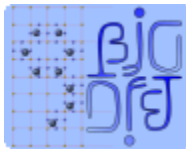
- 在家目录下新建 BigDFT-test/cpu 文档(通过 SFTP 上传测试所需文件至此目录), 并在此目录下编写测试脚本 run_cpu.sh 和节点文件 hostfile

```
[caoao@c01n01 ~]$ mkdir -p $HOME/BigDFT-test/cpu
[caoao@c01n01 ~]$ cd BigDFT-test/cpu
[caoao@c01n01 cpu]$ ls
posinp.ascii      input.dft  malloc.prc      time.yaml
[caoao@c01n01 cpu]$ vi run_cpu.sh
#!/bin/bash
mpdboot -f hostfile -n 6
nohup mpirun -genv I_MPI_DEVICE rdma --hostfile hostfile -ppn 8 -np 48 bigdft >
cpulog 2>&1 &
[caoao@c01n01 cpu]$ chmod +x run_cpu.sh
[caoao@c01n01 cpu]$ vi hostfile
c06n01
c06n02
c06n03
c06n04
c06n05
c06n06
c06n07
c06n08
```

测试所用节点为 6 号刀箱的 6 个刀片节点 (c06n01-c06n06 每个节点用 8 个核)

结果输出文件为 cpu_log

- 开始进行测试



```
[caoao@c01n01 cpu]$ ./run_cpu.sh &
```

```
[1] 2284
```

- 登录任意一个测试节点（此处为 c6n01）(top 命令)是否有相应进程产生

```
top - 16:53:57 up 14 days, 36 min, 1 user, load average: 7.29, 3.08, 1.16
Tasks: 444 total, 9 running, 435 sleeping, 0 stopped, 0 zombie
Cpu(s): 50.0%us, 0.0%sy, 0.0%ni, 49.9%id, 0.0%wa, 0.0%hi, 0.0%si, 0.0%st
Mem: 132129388k total, 28601440k used, 103527948k free, 172260k buffers
Swap: 33816560k total, 0k used, 33816560k free, 263816k cached
```

| PID | USER | PR | NI | VIRT | RES | SHR | S | %CPU | %MEM | TIME+ | COMMAND |
|------|-------|----|----|-------|------|-----|---|-------|------|---------|---------|
| 6547 | caoao | 20 | 0 | 3337m | 3.1g | 14m | R | 100.0 | 2.4 | 2:24.90 | bigdft |
| 6542 | caoao | 20 | 0 | 3335m | 3.1g | 13m | R | 99.6 | 2.4 | 2:23.81 | bigdft |
| 6543 | caoao | 20 | 0 | 3335m | 3.1g | 13m | R | 99.6 | 2.4 | 2:24.87 | bigdft |
| 6544 | caoao | 20 | 0 | 3336m | 3.1g | 14m | R | 99.6 | 2.4 | 2:24.85 | bigdft |
| 6545 | caoao | 20 | 0 | 3336m | 3.1g | 14m | R | 99.6 | 2.4 | 2:24.01 | bigdft |
| 6546 | caoao | 20 | 0 | 3337m | 3.1g | 14m | R | 99.6 | 2.4 | 2:24.79 | bigdft |
| 6548 | caoao | 20 | 0 | 3338m | 3.1g | 15m | R | 99.6 | 2.4 | 2:24.92 | bigdft |
| 6549 | caoao | 20 | 0 | 3338m | 3.1g | 15m | R | 99.6 | 2.4 | 2:24.84 | bigdft |

- 查看运行结果文件 cpulog 是否正确

```
[caoao@c01n01 cpu]$ cat cpulog
```

```
Reference Paper : The Journal of Chemical Physics 129, 014109 (2008)
Version Number : 1.7-dev.28
Timestamp of this run : 2014-02-21 17:00:12.731
Root process Hostname : c06n01
Number of MPI tasks : 48
OpenMP parallelization : No
MPI tasks of root process node : 8
#----- Code compiling options
Compilation options:
Configure arguments:
" '--prefix=/gpfsHOME/home/student/caoao/bigdft_1' 'CC=mpicc' 'CXX=mpicpc'
'F77=mpiifort' 'FC=mpiifort' 'FCFLAGS=-O2 -xsse4.2' 'FFLAGS=-O2' 'CFLAGS=-O2'
'CXXFLAGS=-O2'
Compilers (CC, FC, CXX) : [ mpicc, mpiifort, mpicpc ]
Compiler flags:
CFLAGS : -O2
FCFLAGS : -O2 -xsse4.2
CXXFLAGS : -O2
CPPFLAGS :
#----- Timing for root process
Timings for root process:
CPU time (s) : 2363.15
Elapsed time (s) : 2377.70
Memory Consumption Report:
Tot. No. of Allocations : 257086
Tot. No. of Deallocations : 257086
Remaining Memory (B) : 0
Memory occupation:
Peak Value (MB) : 4507
for the array : psiw
in the routine : LDiagHam
```

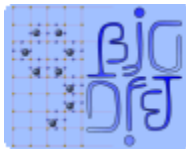
5. GPU 上编译 BigDFT

- 切换至 BigDFT 软件解压后的目录

```
[caoao@gpu02 ~]$ cd BigDFT/bigdft-1.7-dev.28
```

- 新建 build 目录用于存放在 CPU 上编译产生的文件

```
[caoao@gpu02 bigdft-1.7-dev.28]$ mkdir build
```



- 切换至 build 目录进行指定参数的 configure 环境编译

```
[caoao@gpu02 bigdft-1.7-dev.28]$ cd build/
[caoao@gpu02 build]$ ../configure
--prefix=/gpfsHOME/home/student/caoao/bigdft_2 CC=mpiicc CXX=mpiicpc
F77=mpiifort FC=mpiifort FCFLAGS="-O2 -openmp -g -traceback -xsse4.2"
FFLAGS=-O2 CFLAGS=-O2 CXXFLAGS=-O2
--with-ext-linalg="/opt/intel2012/composer_xe_2011_sp1.6.233/mkl/lib/intel64/libmkl_
solver_lp64_sequential.a -Wl,--start-group
/opt/intel2012/composer_xe_2011_sp1.6.233/mkl/lib/intel64/libmkl_intel_lp64.a
/opt/intel2012/composer_xe_2011_sp1.6.233/mkl/lib/intel64/libmkl_scalapack_lp64.a
/opt/intel2012/composer_xe_2011_sp1.6.233/mkl/lib/intel64/libmkl_blacs_lp64.a
/opt/intel2012/composer_xe_2011_sp1.6.233/mkl/lib/intel64/libmkl_intel_thread.a
/opt/intel2012/composer_xe_2011_sp1.6.233/mkl/lib/intel64/libmkl_lapack95_lp64.a
/opt/intel2012/composer_xe_2011_sp1.6.233/mkl/lib/intel64/libmkl_core.a
-Wl,--end-group -liomp5 -lpthread -limf -lm" --enable-cuda-gpu
--with-cuda-path=/usr/local/cuda-5.5 --enable-opencl
--with-ocl-path=/usr/local/cuda-5.5
```

- 切换至 S_GPU 目录，执行以下操作（官方建议）

```
[caoao@gpu02 build]$ cd S_GPU/
[caoao@gpu02 S_GPU]$ make clean
[caoao@gpu02 S_GPU]$ make LDFLAGS=""
[caoao@gpu02 S_GPU]$ cd -
/gpfsHOME/home/student/caoao/BigDFT/bigdft-1.7-dev.28/build
```

- 编译并安装 BigDFT

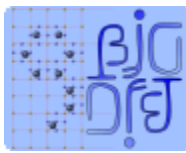
```
[caoao@gpu02 build]$ make
[caoao@gpu02 build]$ make install
```

- 检查安装情况(安装目录下需要有四个文件夹，分别为 bin/ include/ lib/ share/)

```
[caoao@gpu02 ~]$ cd $HOME/bigdft_2
[caoao@gpu02 bigdft_2]$ ls
```

bin examples include lib share

- 将 BigDFT 软件的环境变量添加到用户（caoao）环境中(需注释掉 cpu 的，或者不添加，直



[caoao@gpu02 gpu]\$ top

```
top - 22:04:16 up 14 days, 5:48, 1 user, load average: 9.15, 7.52, 4.15
Tasks: 439 total, 5 running, 433 sleeping, 0 stopped, 1 zombie
Cpu(s): 0.0%us, 0.0%sy, 0.0%ni, 99.9%id, 0.0%wa, 0.0%hi, 0.0%si, 0.0%st
Mem: 132131812k total, 3774476k used, 128357336k free, 11788k buffers
Swap: 33816560k total, 30956k used, 33785604k free, 118404k cached

  PID USER      PR  NI  VIRT  RES  SHR S %CPU  %MEM    TIME+  COMMAND
  6077 caoao      20   0   297g 617m  78m R 789.4   0.5   35:44.30 bigdft
  6078 caoao      20   0   297g 604m  78m R 785.5   0.5   36:01.02 bigdft
```

➤ 查看运行结果文件 gpulog 是否正确

[caoao@gpu02 gpu]\$ cat gpulog

还在运行中...