



# 鲲鹏HPC应用调优实践



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# 1 旗舰店环境使用说明

## 1.1 旗舰店登陆指导



鲲鹏创新中心旗舰店HPC集群用户使用

参考：5.1 章节

### 5.1 VPN 登录

步骤1 下载VPN Client

<https://www.leagsoft.com/doc/article/103107.html>

| WINDOWS  |   |
|--|---|
| 软件版本信息   | V10781.2.555.0330   |
| 软件包相关说明  | 版本：正式版<br>MD5：8C0B99546276807934B82FA12FE0BE9A<br>更新时间：2022-03-31<br>系统平台：Win7/Win8.1/Win10兼容软件，X86架构 |
| 软件版本更新说明                                       | 2022-03-31正式发布V10781.2.555.0330   |
| <a href="#">点击软件包下载</a> <a href="#">点击文档下载</a> |   |

#### 说明

如客户端非Windows，可选择对应系统的版本进行下载安装

## 1.2 使用分配的 VPN 账号登陆 VPN

请使用各自VPN账号进行登录。



HPC\_fae\_vpn.xlsx



123.60.114.62.ini

### 1.3 连接 VPN 后，使用统一服务器账号密码登陆测试服务器

服务器登陆节点地址：175.200.19.12 账号：weibohong 密码：Openlab@123

在当前目录新建个人用户目录进行考试。如：/workspace/home/nws/weibohong/wbc

### 1.4 考试内容安装包路径

/workspace/home/nws/weibohong/opt-case

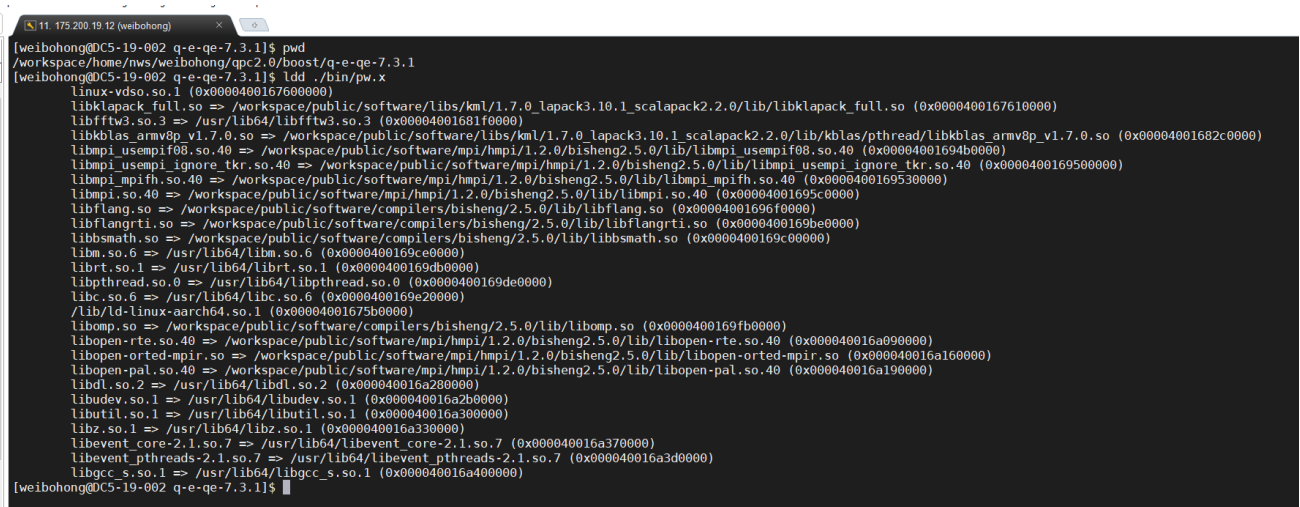
## 2 鲲鹏 HPC 应用 QE 调优

迁移指导：[https://www.hikunpeng.com/document/detail/zh/kunpenghpcs/prtg\\_osc/kunpengquantumesspresso\\_02\\_0001.html](https://www.hikunpeng.com/document/detail/zh/kunpenghpcs/prtg_osc/kunpengquantumesspresso_02_0001.html)

### 2.1 QE 应用全栈编译完成

基于毕昇2.5+hmpi1.2.0+KML 1.7.0完成QE 7.3.1版本的编译

ldd qe/bin/pw.x



```
[weibohong@DC5-19-002 q-e-qe-7.3.1] pwd
/workspace/home/nws/weibohong/qpc2.0/boost/q-e-qe-7.3.1
[weibohong@DC5-19-002 q-e-qe-7.3.1] ldd ./bin/pw.x
linux-vdso.so.1 (0x0000400167600000)
libklapack_full.so => /workspace/public/software/libs/kml/1.7.0/lapack3.10.1_scalapack2.2.0/lib/libklapack_full.so (0x0000400167610000)
libfftw3.so.3 => /usr/lib64/libfftw3.so.3 (0x00004001681f0000)
libblas_armv8p_v1.7.0.so => /workspace/public/software/libs/kml/1.7.0/lapack3.10.1_scalapack2.2.0/lib/blas/pthread/libblas_armv8p_v1.7.0.so (0x00004001682c0000)
libmpi_usempif08.so.40 => /workspace/public/software/mpi/hmpi/1.2.0/bisheng2.5.0/lib/libmpi_usempif08.so.40 (0x00004001694b0000)
libmpi_ignore_tkr.so.40 => /workspace/public/software/mpi/hmpi/1.2.0/bisheng2.5.0/lib/libmpi_ignore_tkr.so.40 (0x00004001695f0000)
libmpi_mpih.so.40 => /workspace/public/software/mpi/hmpi/1.2.0/bisheng2.5.0/lib/libmpi_mpih.so.40 (0x0000400169530000)
libmpi.so.40 => /workspace/public/software/mpi/hmpi/1.2.0/bisheng2.5.0/lib/libmpi.so.40 (0x00004001695c0000)
libflang.so => /workspace/public/software/compilers/bisheng/2.5.0/lib/libflang.so (0x00004001696f0000)
libflangrti.so => /workspace/public/software/compilers/bisheng/2.5.0/lib/libflangrti.so (0x0000400169be0000)
libbmath.so => /workspace/public/software/compilers/bisheng/2.5.0/lib/libbmath.so (0x0000400169ce0000)
libm.so.6 => /usr/lib64/libm.so.6 (0x0000400169ce0000)
librt.so.1 => /usr/lib64/librt.so.1 (0x0000400169db0000)
libpthread.so.0 => /usr/lib64/libpthread.so.0 (0x0000400169de0000)
libc.so.6 => /usr/lib64/libc.so.6 (0x0000400169e20000)
/lib/ld-linux-aarch64.so.1 (0x00004001675b0000)
libomp.so => /workspace/public/software/compilers/bisheng/2.5.0/lib/libomp.so (0x0000400169fb0000)
libopen-rte.so.40 => /workspace/public/software/mpi/hmpi/1.2.0/bisheng2.5.0/lib/libopen-rte.so.40 (0x000040016a090000)
libopen-orted-mpir.so => /workspace/public/software/mpi/hmpi/1.2.0/bisheng2.5.0/lib/libopen-orted-mpir.so (0x000040016a160000)
libopen-pal.so.40 => /workspace/public/software/mpi/hmpi/1.2.0/bisheng2.5.0/lib/libopen-pal.so.40 (0x000040016a190000)
libdl.so.2 => /usr/lib64/libdl.so.2 (0x000040016a280000)
libudev.so.1 => /usr/lib64/libudev.so.1 (0x000040016a2b0000)
libutil.so.1 => /usr/lib64/libutil.so.1 (0x000040016a300000)
libz.so.1 => /usr/lib64/libz.so.1 (0x000040016a330000)
libevent_core-2.1.so.7 => /usr/lib64/libevent_core-2.1.so.7 (0x000040016a370000)
libevent_pthreads-2.1.so.7 => /usr/lib64/libevent_pthreads-2.1.so.7 (0x000040016a3d0000)
libgcc_s.so.1 => /usr/lib64/libgcc_s.so.1 (0x000040016a400000)
[weibohong@DC5-19-002 q-e-qe-7.3.1] █
```



## 2.2 QE 应用全栈使能运行

截图QE成功运行：（注意，登陆节点禁止mpirun运行作业，请通过run.sh调度脚本提交dsub -s run.sh）

```
11. 175.200.19.12 (weibohong) x
hartree contribution = 863.15689177 Ry
xc contribution = -819.46734564 Ry
ewald contribution = -4328.08423805 Ry

convergence has been achieved in 15 iterations

Writing all to output data dir /tmp/pwscf.save/ :
XML data file, charge density, pseudopotentials, collected wavefunctions

init_run : 0.70s CPU 0.77s WALL ( 1 calls)
electrons : 59.75s CPU 60.83s WALL ( 1 calls)

Called by init_run:
wfcinit : 0.38s CPU 0.39s WALL ( 1 calls)
potinit : 0.01s CPU 0.02s WALL ( 1 calls)
hinit0 : 0.06s CPU 0.10s WALL ( 1 calls)

Called by electrons:
c_bands : 56.88s CPU 57.78s WALL ( 15 calls)
sum_band : 1.93s CPU 1.97s WALL ( 15 calls)
v_of_rho : 0.09s CPU 0.09s WALL ( 16 calls)
newd : 0.73s CPU 0.81s WALL ( 16 calls)
mix_rho : 0.08s CPU 0.09s WALL ( 15 calls)

Called by c_bands:
init_us_2 : 0.05s CPU 0.05s WALL ( 31 calls)
regterg : 56.75s CPU 57.62s WALL ( 15 calls)

Called by *egterg:
rdiagh : 47.75s CPU 48.19s WALL ( 156 calls)
h_psi : 5.40s CPU 5.69s WALL ( 157 calls)
s_psi : 0.90s CPU 0.92s WALL ( 157 calls)
g_psi : 0.02s CPU 0.02s WALL ( 141 calls)

Called by h_psi:
h_psi:calbec : 1.37s CPU 1.45s WALL ( 157 calls)
vloc_psi : 3.00s CPU 3.17s WALL ( 157 calls)
vloc_psi:tg : 0.01s CPU 0.01s WALL ( 157 calls)
add_vuspsi : 1.01s CPU 1.05s WALL ( 157 calls)

General routines
calbec : 1.84s CPU 1.92s WALL ( 172 calls)
fft : 0.23s CPU 0.26s WALL ( 93 calls)
ffts : 0.02s CPU 0.03s WALL ( 31 calls)
fftw : 3.37s CPU 3.55s WALL ( 18149 calls)
interpolate : 0.05s CPU 0.05s WALL ( 16 calls)

Parallel routines
fft_scatt_xy : 0.14s CPU 0.14s WALL ( 18273 calls)
fft_scatt_yz : 2.21s CPU 2.38s WALL ( 18273 calls)
fft_scatt_tg : 0.03s CPU 0.03s WALL ( 18149 calls)

PWSCF : 1m 1.74s CPU 1m 3.53s WALL

This run was terminated on: 15: 7:15 30May2024

-----
JOB DONE.
-----
```

优化点1: 使用 毕昇2.5+hmpi1.2.0+KML 1.7.0 三件套

```
module purge
```

```
module load compilers/bisheng/2.5.0/bisheng2.5.0 mpi/hmpi/1.2.0/bisheng2.5.0
```

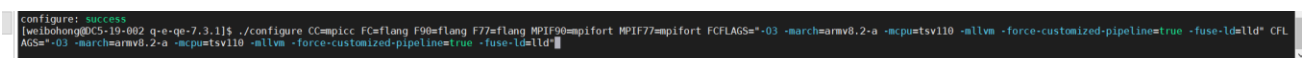
```
libs/kml/1.7.0/kml_1.7.0_lapack3.10.1_scalapack2.2.0_bisheng2.4.0
```

优化点2: 编译参数调优

```
./configure CC=mpicc FC=flang F90=flang F77=flang MPIF90=mpifort MPIF77=mpifort FCFLAGS="-
```

```
O3 -march=armv8.2-a -mcpu=tsv110 -mllvm -force-customized-pipeline=true -fuse-ld=lld"
```

```
CFLAGS="-O3 -march=armv8.2-a -mcpu=tsv110 -mllvm -force-customized-pipeline=true -fuse-ld=lld"
```



```
configure: success  
[weiboheng@DC5-19-892 q-e-qe-7.3.ll]$ ./configure CC=mpicc FC=flang F90=flang F77=flang MPIF90=mpifort MPIF77=mpifort FCFLAGS="-O3 -march=armv8.2-a -mcpu=tsv110 -mllvm -force-customized-pipeline=true -fuse-ld=lld" CFL
```

ipplit MultiExec Tunneling Packages Settings Help

11. 175.200.19.12 (weibohong)

```
hartree contribution = 863.15689177 Ry
xc contribution      = -819.46734564 Ry
ewald contribution   = -4328.08423805 Ry
```

convergence has been achieved in 15 iterations

Writing all to output data dir /tmp/pwscf.save/ :  
XML data file, charge density, pseudopotentials, collected wavefunctions

```
init_run   : 0.75s CPU 0.77s WALL ( 1 calls)
electrons  : 59.94s CPU 61.35s WALL ( 1 calls)
```

Called by init\_run:

```
wfcinit   : 0.39s CPU 0.40s WALL ( 1 calls)
potinit   : 0.02s CPU 0.02s WALL ( 1 calls)
hinit0    : 0.08s CPU 0.09s WALL ( 1 calls)
```

Called by electrons:

```
c_bands   : 56.96s CPU 58.21s WALL ( 15 calls)
sum_band  : 1.93s CPU 2.00s WALL ( 15 calls)
v_of_rho  : 0.11s CPU 0.11s WALL ( 16 calls)
newd      : 0.80s CPU 0.81s WALL ( 16 calls)
mix_rho   : 0.09s CPU 0.10s WALL ( 15 calls)
```

Called by c\_bands:

```
init_us_2 : 0.05s CPU 0.05s WALL ( 31 calls)
regterg   : 56.83s CPU 58.01s WALL ( 15 calls)
```

Called by \*egterg:

```
rdiaghg   : 47.47s CPU 48.19s WALL ( 156 calls)
h_psi     : 5.65s CPU 5.90s WALL ( 157 calls)
s_psi     : 0.89s CPU 0.96s WALL ( 157 calls)
g_psi     : 0.02s CPU 0.02s WALL ( 141 calls)
```

Called by h\_psi:

```
h_psi:calbec : 1.43s CPU 1.49s WALL ( 157 calls)
vloc_psi     : 3.20s CPU 3.34s WALL ( 157 calls)
vloc_psi:tg_ : 0.01s CPU 0.01s WALL ( 157 calls)
add_vuspsi   : 1.02s CPU 1.06s WALL ( 157 calls)
```

General routines

```
calbec   : 1.90s CPU 1.98s WALL ( 172 calls)
fft       : 0.28s CPU 0.30s WALL ( 93 calls)
ffts      : 0.02s CPU 0.02s WALL ( 31 calls)
fftw      : 3.56s CPU 3.72s WALL ( 18149 calls)
interpolate : 0.05s CPU 0.05s WALL ( 16 calls)
```

Parallel routines

```
fft_scatt_xy : 0.14s CPU 0.15s WALL ( 18273 calls)
fft_scatt_yz : 2.41s CPU 2.53s WALL ( 18273 calls)
fft_scatt_tg : 0.03s CPU 0.03s WALL ( 18149 calls)
```

```
PWSCF      : 1m 2.06s CPU 1m 4.46s WALL
```

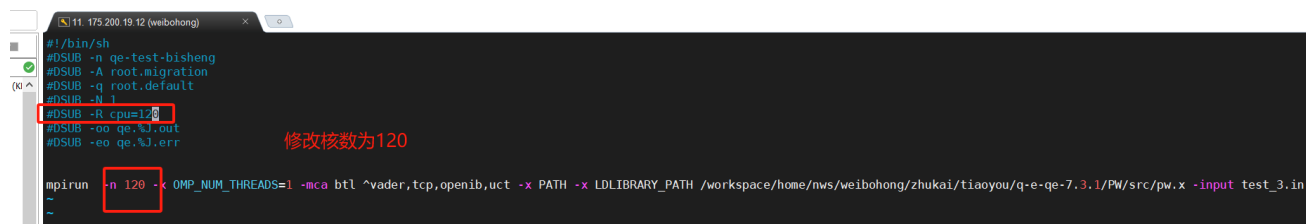
This run was terminated on: 16:10:16 30May2024

```
=====  
JOB DONE.  
=====
```

编译参数调优



优化点3: 设置为120个核



```
#! /bin/sh
#DSUB -n qe-test-bisheng
#DSUB -A root:migration
#DSUB -q root.default
#DSUB -N 1
#DSUB -R cpu=120
#DSUB -oo qe.%j.out
#DSUB -eo qe.%j.err

mpirun -n 120 -x OMP_NUM_THREADS=1 -mca btl ^vader,tcp,openib,uct -x PATH -x LD_LIBRARY_PATH /workspace/home/nws/weibohong/zhukai/tiaoyou/q-e-qe-7.3.1/PW/src/pw.x -input test_3.in
```

修改核数为 120

```
mpirun -n 120 -x OMP_NUM_THREADS=1 -mca btl ^vader,tcp,openib,uct -x PATH -x
```

```
LD_LIBRARY_PATH /workspace/home/nws/weibohong/zhukai/tiaoyou/q-e-qe-7.3.1/PW/src/pw.x -input
```

```
test_3.in
```



Split MultiExec Tunneling Packages Settings Help

11. 175.200.19.12 (weibohong)

```
xc contribution      = -819.46738598 Ry
ewald contribution   = -4328.08423805 Ry
```

convergence has been achieved in 16 iterations

Writing all to output data dir /tmp/pwscf.save/ :  
XML data file, charge density, pseudopotentials, collected wavefunctions

```
init_run      :      0.77s CPU      0.79s WALL (      1 calls)
electrons     :     53.02s CPU     53.53s WALL (      1 calls)
```

Called by init\_run:

```
wfcinit      :      0.41s CPU      0.41s WALL (      1 calls)
potinit      :      0.02s CPU      0.03s WALL (      1 calls)
hinit0       :      0.06s CPU      0.08s WALL (      1 calls)
```

Called by electrons:

```
c_bands      :     49.79s CPU     50.27s WALL (     16 calls)
sum_band     :      2.12s CPU      2.13s WALL (     16 calls)
v_of_rho     :      0.14s CPU      0.14s WALL (     17 calls)
newd         :      0.79s CPU      0.81s WALL (     17 calls)
mix_rho      :      0.12s CPU      0.12s WALL (     16 calls)
```

Called by c\_bands:

```
init_us_2    :      0.06s CPU      0.06s WALL (     33 calls)
regterg      :     49.65s CPU     50.11s WALL (     16 calls)
```

Called by \*egterg:

```
rdiaghg     :     40.00s CPU     40.25s WALL (    135 calls)
h_psi       :      5.90s CPU      6.02s WALL (    136 calls)
s_psi       :      1.03s CPU      1.03s WALL (    136 calls)
g_psi       :      0.02s CPU      0.02s WALL (    119 calls)
```

Called by h\_psi:

```
h_psi:calbec :      1.46s CPU      1.47s WALL (    136 calls)
vloc_psi     :      3.26s CPU      3.36s WALL (    136 calls)
vloc_psi:tg_ :      0.01s CPU      0.01s WALL (    136 calls)
add_vuspsi   :      1.15s CPU      1.17s WALL (    136 calls)
```

General routines

```
calbec      :      1.98s CPU      1.99s WALL (    152 calls)
fft         :      0.28s CPU      0.31s WALL (     99 calls)
ffts        :      0.03s CPU      0.03s WALL (     33 calls)
fftw        :      3.65s CPU      3.75s WALL (  19500 calls)
interpolate :      0.07s CPU      0.08s WALL (     17 calls)
```

Parallel routines

```
fft_scatt_xy :      0.16s CPU      0.16s WALL (  19632 calls)
fft_scatt_yz :      2.36s CPU      2.45s WALL (  19632 calls)
fft_scatt_tg :      0.03s CPU      0.04s WALL (  19500 calls)
```

```
PWSCF       :     55.14s CPU     56.11s WALL
```

This run was terminated on: 16: 3:11 30May2024

```
-----
JOB DONE.
-----
```

^C

```
[weibohong@DC5-19-002 test-case]$
```



### 3 附录：修订记录

| 版本   | 发布日期      | 修订记录 |
|------|-----------|------|
| V1.0 | 2024-5-20 | init |
|      |           |      |