

Materials Studio 软件使用规定

超算中心为了规范集群中 Materials Studio 软件的使用，现作出如下规定：

1. 集群上安装的 Materials Studio 软件版本为 6.0，包含 CASTEP 和 DMol3 两个模块。
2. 为方便集群账户的管理和使用，从即日起限制利用 Gateway 进行 MS 作业提交，改为利用作业调度系统进行 MS 作业的提交及运算状态查看，具体方法见附件。
3. 若对于软件使用有任何问题，请电话咨询 0631-5688813 程雨芊，杨浩志；或加入群 143029839 进行交流。

利用作业调度系统进行 MS 作业提交——以 CASTEP 为例

方法一

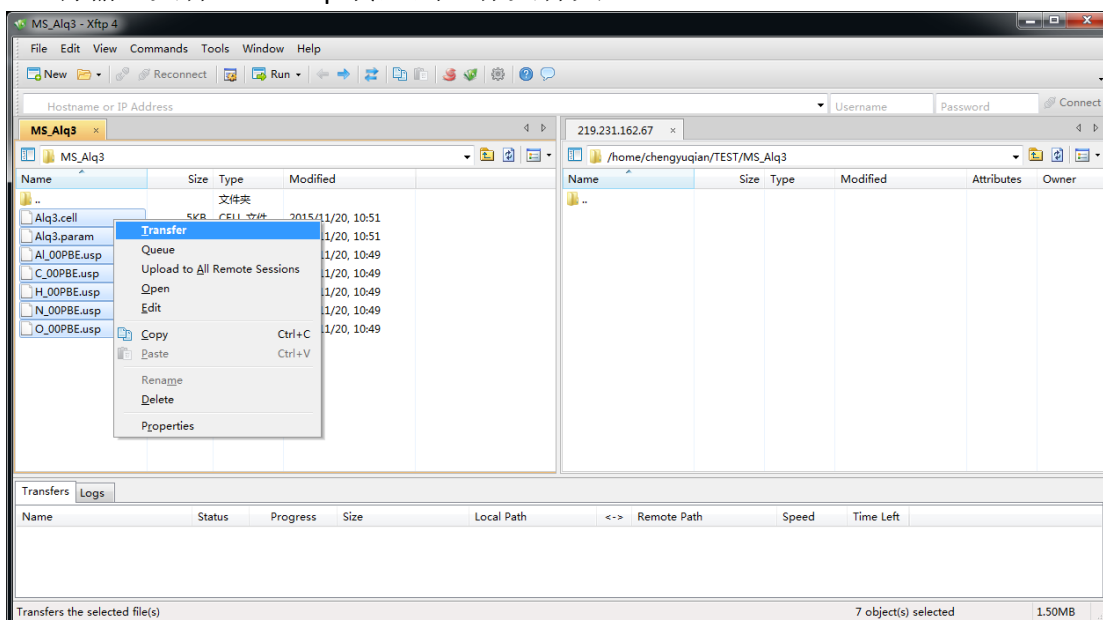
1. 打开 Xshell 软件，利用个人账户登陆集群节点 ln01:219.231.162.66。

```
Type 'help' to learn how to use Xshell prompt.
Xshell:\>

Connecting to 219.231.162.67:22...
Connection established.
Escape character is '^@]'.

Last login: Sat Nov 21 08:09:38 2015 from 219.231.162.52
[chengyuqian@mu01 ~]$
```

2. 将输入文件通过 Xftp 传入到工作文件夹。



```
[chengyuqian@mu01 MS_Alq3]$ ll
total 4
-rw-rw-r-- 1 chengyuqian chengyuqian 353002 Nov 21 10:03 Al_00PBE.usp
-rw-rw-r-- 1 chengyuqian chengyuqian 4805 Nov 21 10:03 Alq3.cell
-rw-rw-r-- 1 chengyuqian chengyuqian 1022 Nov 21 10:03 Alq3.param
-rw-rw-r-- 1 chengyuqian chengyuqian 336106 Nov 21 10:03 C_00PBE.usp
-rw-rw-r-- 1 chengyuqian chengyuqian 164133 Nov 21 10:03 H_00PBE.usp
-rw-rw-r-- 1 chengyuqian chengyuqian 371434 Nov 21 10:03 N_00PBE.usp
-rw-rw-r-- 1 chengyuqian chengyuqian 343270 Nov 21 10:03 O_00PBE.usp
[chengyuqian@mu01 MS_Alq3]$
```

3. 建立脚本文件（详见附录）。

```
#!/bin/bash
task -N MS_Alq3
task -i nodes=ippamd
task -q cu
project_name=Alq3
source /opt/intel/mpi/5.0.3.044/intel64/bin/mpivars.sh
cd $PBS_O_WORKDIR
NP=$(cat $PBS_NODEFILE) | wc -l
/home/mai/accelrys/materialstudio6.0/bin/mpiexec -f mpd.hosts -machinefile $PBS_NODEFILE --np $NP --env ACCELRY_LICENSE_PACK_DIR /home/mai/accelrys/licensepack --env MSI_LICENSE_FILE /home/mai/accelrys/licensepack/licenses --env LD_LIBRARY_PATH /home/mai/accelrys/materialstudio6.0/lib:/home/mai/accelrys/materialstudio6.0/lib/64:/home/mai/accelrys/licensepack/linux/lib:/home/mai/accelrys/materialstudio6.0/lib/64:/x86_64-linux-thread-multi/CORE:/home/mai/accelrys/materialstudio6.0/lib:/home/mai/accelrys/materialstudio6.0/lib/64:/x86_64-linux-thread-multi/CORE:/home/mai/accelrys/materialstudio6.0/bin/./lib/ --env ACCELRY_LICENSE_USER_NAME root --env PATH /home/mai/accelrys/materialstudio6.0/bin:/home/mai/accelrys/licensepack/linux/bin:/home/mai/accelrys/materialstudio6.0/bin:/opt/tscs/share/bin:/opt/tscs/share/sbin:/opt/tscs/share/jdk1.8.0_10/bin:/opt/tscs/share/jdk1.8.0_10/jre/bin:/usr/lib64/qt.5.9/bin:/usr/kerberos/sbin:/usr/kerberos/bin:/usr/local/sbin:/usr/local/bin:/bin:/usr/sbin:/usr/bin:/opt/ibutils/bin:/root/bin:/home/mai/accelrys/materialstudio6.0/bin --env I_MPI_ROOT /home/mai/accelrys/materialstudio6.0/bin --env FUPNTENDIAN big --env OMP_NUM_THREADS 1 --env TMPDIR /tmp --env PSPOT_DIR /home/mai/accelrys/materialstudio6.0/share/Resources/Quantum/Castep/Potentials /home/mai/accelrys/materialstudio6.0/bin/castep.exe $project_name
exit 0
```

```
[chengyuqian@mu01 MS_Alq3]$ ll
total 1560
-rw-rw-r-- 1 chengyuqian chengyuqian 353002 Nov 21 10:03 Al_00PBE.usp
-rw-rw-r-- 1 chengyuqian chengyuqian 4805 Nov 21 10:03 Alq3.cell
-rw-rw-r-- 1 chengyuqian chengyuqian 1022 Nov 21 10:03 Alq3.param
-rw-rw-r-- 1 chengyuqian chengyuqian 336106 Nov 21 10:03 C_00PBE.usp
-rw-rw-r-- 1 chengyuqian chengyuqian 164133 Nov 21 10:03 H_00PBE.usp
-rw-rw-r-- 1 chengyuqian chengyuqian 635 Nov 21 10:09 MS_Alq3.sh
-rw-rw-r-- 1 chengyuqian chengyuqian 371434 Nov 21 10:03 N_00PBE.usp
-rw-rw-r-- 1 chengyuqian chengyuqian 343270 Nov 21 10:03 O_00PBE.usp
[chengyuqian@mu01 MS_Alq3]$
```

4. 提交脚本文件，生成作业号。

```
[chengyuqian@mu01 MS_Alq3]$ qsub MS_Alq3.sh
4714.mu01
[chengyuqian@mu01 MS_Alq3]$
```

5. 利用 qstat 命令查看作业状态。

```
[chengyuqian@mu01 MS_Alq3]$ qstat -an 4714
mu01:
Job ID          Username      Queue        Jobname      SessID NDS      Req'd  Req'd   Elap
-----
4714.mu01      chengyuqian  cu          MS_Alq3      --      2         40    --    --  R  --
cu17/19+cu17/18+cu17/17+cu17/16+cu17/15+cu17/14+cu17/13+cu17/12+cu17/11
+cu17/10+cu17/9+cu17/8+cu17/7+cu17/6+cu17/5+cu17/4+cu17/3+cu17/2+cu17/1
+cu17/0+cu16/19+cu16/18+cu16/17+cu16/16+cu16/15+cu16/14+cu16/13+cu16/12
+cu16/11+cu16/10+cu16/9+cu16/8+cu16/7+cu16/6+cu16/5+cu16/4+cu16/3+cu16/2
+cu16/1+cu16/0
[chengyuqian@mu01 MS_Alq3]$
```

```
[chengyuqian@mu01 MS_Alq3]$ qstat -a 4714
mu01:
Job ID          Username      Queue        Jobname      SessID NDS      Req'd  Req'd   Elap
-----
4714.mu01      chengyuqian  cu          MS_Alq3      29913  2         40    --    --  R  00:00
[chengyuqian@mu01 MS_Alq3]$
```

```
[chengyuqian@mu01 MS_Alq3]$ qstat -a 4714
mu01:
Job ID          Username      Queue        Jobname      SessID NDS      Req'd  Req'd   Elap
-----
4714.mu01      chengyuqian  cu          MS_Alq3      29913  2         40    --    --  C  01:44
```

6. 作业完成后，请通过 Xftp 将结果下载到个人计算机。

```
[chengyuqian@mu01 MS_Alq3]$ ll
total 173320
-rw-rw-r-- 1 chengyuqian chengyuqian          7 Nov 21 10:01 030317.pid
-rw-rw-r-- 1 chengyuqian chengyuqian    353002 Nov 21 10:03 Al_00PBE.usp
-rw-rw-r-- 1 chengyuqian chengyuqian     1580 Nov 21 11:45 Alq3.bands
-rw-rw-r-- 1 chengyuqian chengyuqian     1706 Nov 21 11:45 Alq3.bib
-rw-rw-r-- 1 chengyuqian chengyuqian    221295 Nov 21 11:45 Alq3.castep
-rw-rw-r-- 1 chengyuqian chengyuqian  20816283 Nov 21 11:45 Alq3.castep_bin
-rw-rw-r-- 1 chengyuqian chengyuqian     4704 Nov 21 10:01 Alq3.cell
-rw-rw-r-- 1 chengyuqian chengyuqian  134313497 Nov 21 11:45 Alq3.check
-rw-rw-r-- 1 chengyuqian chengyuqian  20342048 Nov 21 11:45 Alq3.cst_esp
-rw-rw-r-- 1 chengyuqian chengyuqian    127703 Nov 21 11:45 Alq3.geom
-rw-rw-r-- 1 chengyuqian chengyuqian     989 Nov 21 10:01 Alq3.param
-rw-rw-r-- 1 chengyuqian chengyuqian     917 Nov 21 11:45 Alq3.status.dat
-rw-rw-r-- 1 chengyuqian chengyuqian   336106 Nov 21 10:03 C_00PBE.usp
-rw-rw-r-- 1 chengyuqian chengyuqian     206 Nov 21 11:45 Castepexe.log
-rw-rw-r-- 1 chengyuqian chengyuqian  164133 Nov 21 10:03 H_00PBE.usp
-rw----- 1 chengyuqian chengyuqian      99 Nov 21 11:54 MS_Alq3.e4714
-rw----- 1 chengyuqian chengyuqian      0 Nov 21 10:10 MS_Alq3.o4714
-rw-rw-r-- 1 chengyuqian chengyuqian     650 Nov 21 11:09 MS_Alq3.sh
-rw-rw-r-- 1 chengyuqian chengyuqian  371434 Nov 21 10:03 N_00PBE.usp
-rw-rw-r-- 1 chengyuqian chengyuqian  343270 Nov 21 10:03 O_00PBE.usp
-rw-rw-r-- 1 chengyuqian chengyuqian      0 Nov 21 10:01 std.err
-rw-rw-r-- 1 chengyuqian chengyuqian      0 Nov 21 10:01 std_err.txt
-rw-rw-r-- 1 chengyuqian chengyuqian     77 Nov 21 11:45 std_out.txt
[chengyuqian@mu01 MS_Alq3]$
```

方法二

1. 打开超算中心网站首页，利用个人账户登陆 ClusterEngine HPC 云服务平台。

山东大学 (威海) 超级计算中心

服务科学计算 促进人才培养

学校首页 网站首页 通知公告 规章制度 资料手册 用户申请

通知公告

- 高性能计算高级培训 第一期 2015-06-02
- 超级计算中心用户培训内容及时间安排 2015-04-28
- 超算中心HPC集群简介 2015-04-28

规章制度

- Materials Studio软件使用说明 2015-11-23
- 山东大学 (威海) 超级计算中心超算用户申请... 2015-07-30
- 作业排队申请表 (校内用户) 2015-05-21
- 山东大学 (威海) 超级计算中心服务管理办法... 2015-04-28
- 管理员操作流程 2015-04-28
- 用户递交流程 2015-04-28

资料手册

- 高性能集群已安装计算软件清单 2015-05-26
- 集群作业调度软件使用培训 2015-11-06
- linux基本命令操作 2015-05-26
- 高性能集群系统基础 2015-05-26
- 高性能集群搭建使用运维 2015-05-26
- 密度泛函理论与从头计算分子动力学 2015-05-21

用户登录

ClusterEngine HPC云服务平台

相关链接

- 中国科学院超级计算环境
- 中国科学院超级计算中心
- 超级计算创新联盟
- 国家超级计算济南中心
- 中国科学院计算技术研究所

联系方式

办公电话: 0631-568(0311)

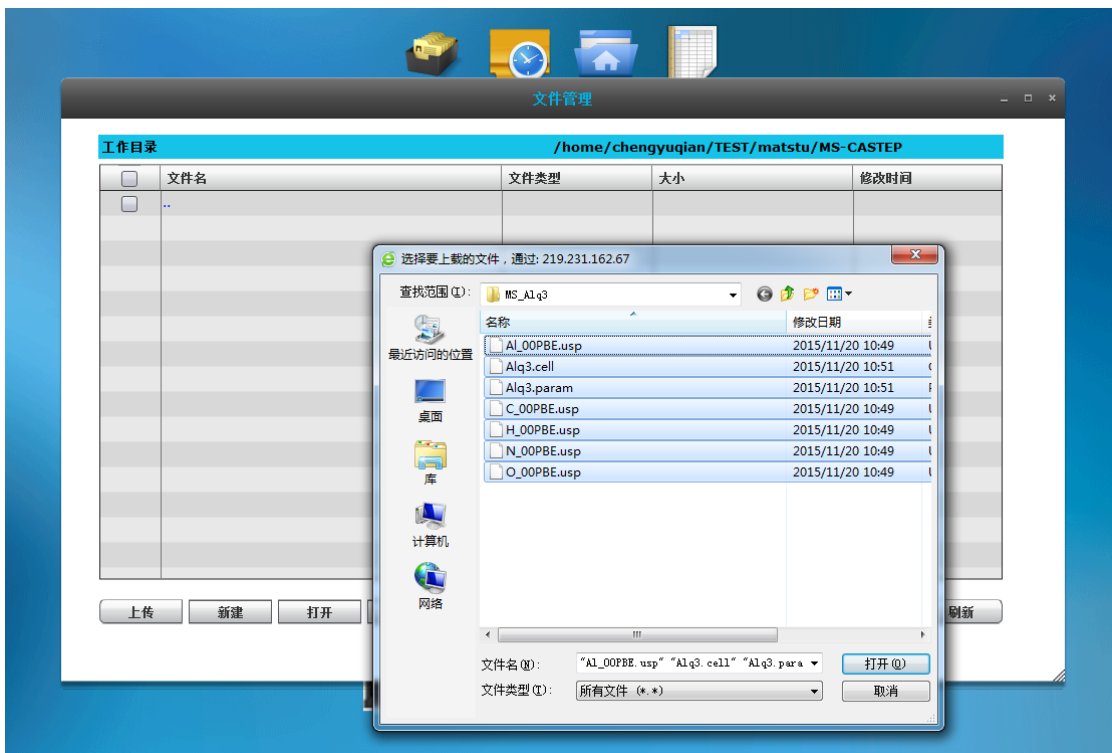
机房电话: 0631-568(6907)

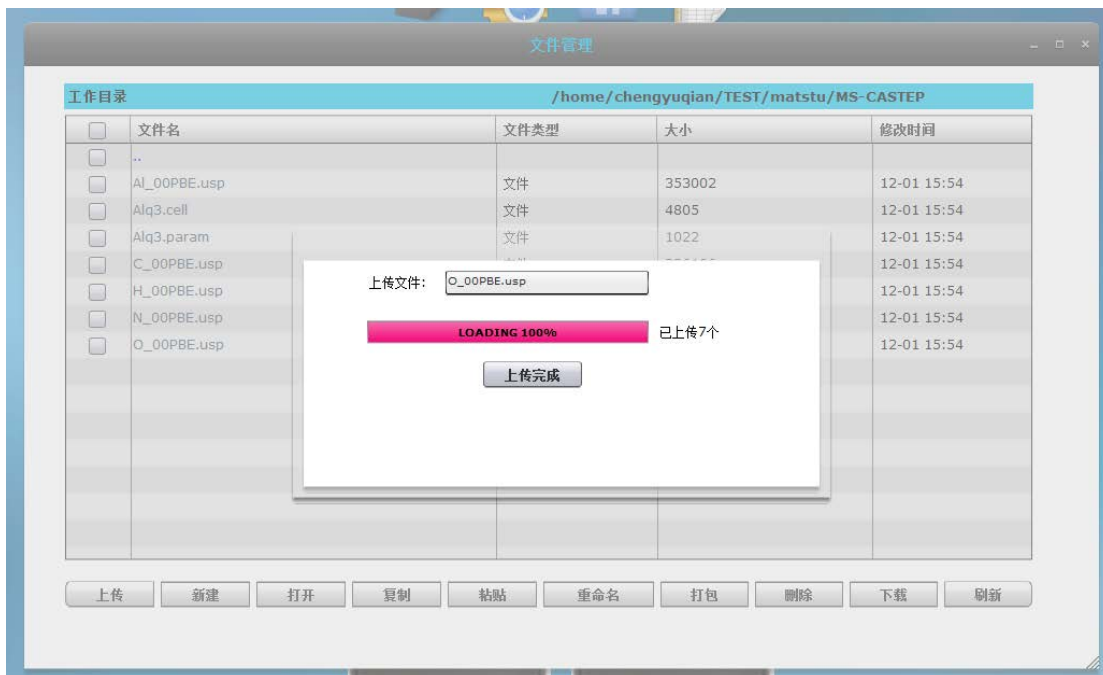
Email: hpc@wh.sdu.edu.cn

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2.在文件管理中，上传 CASTEP 计算相关的文件。





3.选择作业提交中的 MS_CASTEP (MS_DMol3) 应用类型，修改作业名称、队列、工作目录、使用节点数和项目名称。**注：工作目录为参数文件所在的目录，项目名称必须与相应的参数文件名相同。**



4.点击提交作业，返回相应的作业号。

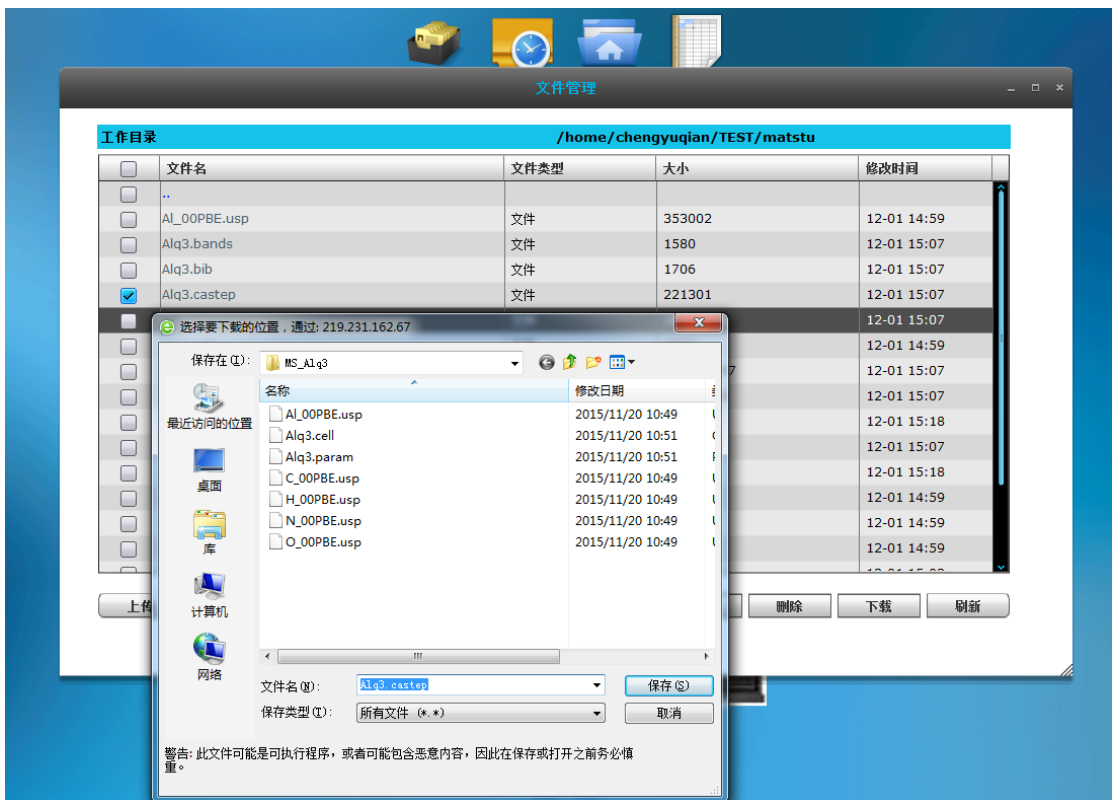


5.在作业管理中查看作业的详细信息、作业输出等状态。





6. 计算完成后，在文件管理中可以下载相应文件。



附录一：MS 软件脚本 CASTEP 示例——只需修改红色斜体部分的内容

```
#!/bin/bash
#PBS -N filename
#PBS -l nodes=1:ppn=5
#PBS -q cu
#PBS -V

project_name=Alq3

source /opt/intel/impi/5.0.2.044/intel64/bin/mpivars.sh

cd $PBS_O_WORKDIR
NP=`cat ${PBS_NODEFILE} | wc -l`

/home/msi/Accelrys/MaterialsStudio6.0/bin/mpirun -f mpd.hosts -machinefile $PBS_NODEFILE -
np $NP -env ACCELRY_S_LIC_PACK_DIR /home/msi/Accelrys/LicensePack -env MSI_LICENSE_FILE
/home/msi/Accelrys/LicensePack/Licenses -env LD_LIBRARY_PATH
/home/msi/Accelrys/MaterialsStudio6.0/lib:/home/msi/Accelrys/MaterialsStudio6.0/lib/32:/hom
e/msi/Accelrys/LicensePack/linux/lib:/home/msi/Accelrys/MaterialsStudio6.0/lib/5.8.9/x86_64-
linux-thread-
multi/CORE:/home/msi/Accelrys/MaterialsStudio6.0/lib:/home/msi/Accelrys/MaterialsStudio6.0
/lib/32:/home/msi/Accelrys/MaterialsStudio6.0/lib/5.8.9/x86_64-linux-thread-
multi/CORE:/home/msi/Accelrys/MaterialsStudio6.0/bin/./lib/ -env
ACCELRY_S_LICENSE_USERNAME $USER -env PATH
/home/msi/Accelrys/MaterialsStudio6.0/bin:/home/msi/Accelrys/LicensePack/linux/bin:/home/
msi/Accelrys/MaterialsStudio6.0/bin:/opt/tsce/share/bin:/opt/tsce/share/sbin:/opt/tsce/share/j
dk1.6.0_10/bin:/opt/tsce/share/jdk1.6.0_10/jre/bin:/usr/lib64/qt-
3.3/bin:/usr/kerberos/sbin:/usr/kerberos/bin:/usr/local/sbin:/usr/local/bin:/sbin:/bin:/usr/sbin:/
usr/bin:/opt/ibutils/bin:./home/msi/Accelrys/MaterialsStudio6.0/bin -env I_MPI_ROOT
/home/msi/Accelrys/MaterialsStudio6.0/bin -env F_UFMTENDIAN big -env OMP_NUM_THREADS
1 -env TMPDIR /tmp -env PSPOT_DIR
/home/msi/Accelrys/MaterialsStudio6.0/share/Resources/Quantum/Castep/Potentials
/home/msi/Accelrys/MaterialsStudio6.0/bin/castepexe.exe $project_name

rm -f *.pid
```


附录二：MS 软件脚本 DMol3 示例——只需修改红色斜体部分的内容

```
#!/bin/bash
#PBS -N filename
#PBS -l nodes=1:ppn=20
#PBS -q cu
#PBS -V

project_name=ee-a2

source /opt/intel/impi/5.0.2.044/intel64/bin/mpivars.sh

cd $PBS_O_WORKDIR
NP=`cat ${PBS_NODEFILE} | wc -l`

/home/msi/Accelrys/MaterialsStudio6.0/bin/mpirun -f mpd.hosts -machinefile $PBS_NODEFILE -
np $NP -env ACCELRY_S_LIC_PACK_DIR /home/msi/Accelrys/LicensePack -env MSI_LICENSE_FILE
/home/msi/Accelrys/LicensePack/Licenses -env LD_LIBRARY_PATH
/home/msi/Accelrys/MaterialsStudio6.0/lib:/home/msi/Accelrys/MaterialsStudio6.0/lib/32:/hom
e/msi/Accelrys/LicensePack/linux/lib:/home/msi/Accelrys/MaterialsStudio6.0/lib/5.8.9/x86_64-
linux-thread-
multi/CORE:/home/msi/Accelrys/MaterialsStudio6.0/lib:/home/msi/Accelrys/MaterialsStudio6.0
/lib/32:/opt/intel//impi/5.0.2.044/intel64/lib:/opt/intel/composer_xe_2015.1.133/compiler/lib/i
ntel64:/opt/intel/mic/coi/host-linux-
release/lib:/opt/intel/mic/myo/lib:/opt/intel/composer_xe_2015.1.133/mpirt/lib/intel64:/opt/in
tel/composer_xe_2015.1.133/ipp/./compiler/lib/intel64:/opt/intel/composer_xe_2015.1.133/ip
p/lib/intel64:/opt/intel/mic/coi/host-linux-
release/lib:/opt/intel/mic/myo/lib:/opt/intel/composer_xe_2015.1.133/compiler/lib/intel64:/opt
/intel/composer_xe_2015.1.133/mkl/lib/intel64:/opt/intel/composer_xe_2015.1.133/tbb/lib/int
el64/gcc4.4:/opt/intel/composer_xe_2015.1.133/compiler/lib:/home/msi/Accelrys/MaterialsStu
dio6.0/lib/5.8.9/x86_64-linux-thread-
multi/CORE:/home/msi/Accelrys/MaterialsStudio6.0/bin/./lib/ -env
ACCELRY_S_LICENSE_USERNAME $USER -env PATH
/home/msi/Accelrys/MaterialsStudio6.0/bin:/home/msi/Accelrys/LicensePack/linux/bin:/home/
msi/Accelrys/MaterialsStudio6.0/bin:/opt/intel//impi/5.0.2.044/intel64/bin:/opt/intel/composer
_xe_2015.1.133/bin/intel64:/opt/intel/composer_xe_2015.1.133/debugger/gdb/intel64_mic/bin
:/usr/local/maui/sbin:/usr/local/maui/bin:/opt/tsce/share/bin:/opt/tsce/share/sbin:/opt/tsce/sh
are/jdk1.6.0_10/bin:/opt/tsce/share/jdk1.6.0_10/jre/bin:/usr/lib64/qt-
3.3/bin:/usr/kerberos/sbin:/usr/kerberos/bin:/usr/local/bin:/bin:/usr/bin:/usr/local/sbin:/usr/sbi
n:/sbin:/opt/ibutils/bin:./home/msi/Accelrys/MaterialsStudio6.0/bin -env I_MPI_ROOT
/home/msi/Accelrys/MaterialsStudio6.0/bin -env F_UFMTENDIAN big -env OMP_NUM_THREADS
1 -env DMOL_TMP /tmp/ -env TMPDIR /tmp/ -env DMOL_BIN
/home/msi/Accelrys/MaterialsStudio6.0/bin/dmol3.exe -env DMOL3_DATA
/home/msi/Accelrys/MaterialsStudio6.0/share/Resources/Quantum/DMol3
/home/msi/Accelrys/MaterialsStudio6.0/bin/dmol3.exe $project_name
```