物质学院集群及常用软件介绍

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Outline

- vasp编译及使用

Flow chart of compiling

load environment vars

prepare makefile

make

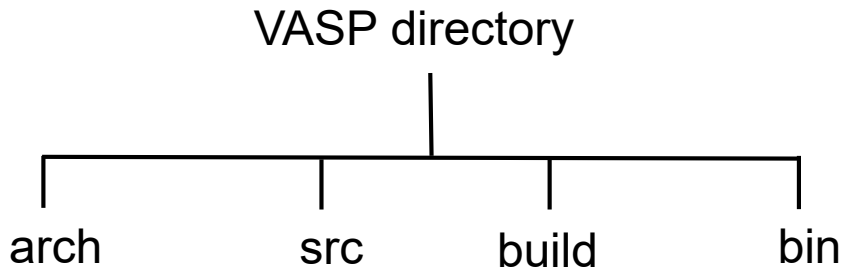
```
module load compiler/intel/composer_xe_2015.2.164
module load mpi/intelmpi/5.0.2.044
echo  $MKLROOT
echo  $I_MPI_ROOT
```

copy makefile from template

```
make / make xxx
```

See **README** file for the detail of the make options

File structure of VASP



Directory name	Containing
arch	Templates of makefile.include
src	source files
build	copy of src and compiled files for different version
bin	executable file

Compiling VASP.5.4.4

Steps:

- 加载环境变量

```
module load compiler/intel/composer_xe_2015.2.164
module load mpi/intelmpi/5.0.2.044
module load compiler/cuda/6/9.0    # 目前110节点为centos6系统
```

Note: 这里默认登录节点为10.15.22.110，若登录节点为10.15.22.190，需注意部分环境变量的变化

- 复制makefile.include文件模板

```
cp arch/makefile.include.linux_intel    makefile.include
```

- 编辑makefile.include (gpu)

```
vi makefile.include
```

修改:1) CUDA_ROOT = /public/software/compiler/cuda/6/cuda-9.0 (版本与前面module加载保持一致)
2) 在GENCODE_ARCH行添加: -gencode=arch=compute_70,code=\“sm_70,compute_70\“ (此参数对应V100 GPU卡，其他型号需查看对应计算能力)。目前vasp的GPU加速建议使用6以上的版本。

- 编译

```
make
```

Compiling VASP.5.4.4

Options	comment
make	vasp_std, vasp_gam, and vasp_ncl
make std	vasp_std
make gam	vasp_gam
make ncl	vasp_ncl
make all	vasp_std, vasp_gam, vasp_ncl, vasp_gpu, vasp_gpu_ncl
make gpu	vasp_gpu
make gpu_ncl	vasp_gpu_ncl

Compiling VASP.5.4.4

Compile with shell script (cpu version):

1. Put the file vasp.5.4.4.tar.gz and patch.5.4.4.16052018.gz in the same directory;
2. Run the following shell script.

```
#!/bin/bash
tar -zxvf vasp.5.4.4.tar.gz
cd ./vasp.5.4.4
cp arch/makefile.include.linux_intel ./makefile.include
module load compiler/intel/composer_xe_2015.2.164
module load mpi/intelmpi/5.0.2.044
nohup make std>make.log 2>&1 &
```

Example - Fcc Si band

https://www.vasp.at/wiki/index.php/Fcc_Si_bandstructure

SCF

INCAR

```
System = fcc Si
ICHARG=2
ENCUT  =    240
ISMEAR = 0
SIGMA = 0.1
EDIFF = 1e-6

LWAVE =.T.
LCHARG =.T.
```

POSCAR

```
fcc Si:
 3.9
 0.5 0.5 0.0
 0.0 0.5 0.5
 0.5 0.0 0.5
 Si
  1
cartesian
0 0 0
```

KPOINTS

```
K-POINTS
0
Gamma
15  15  15
0.0  0.0  0.0
```

POTCAR is provided by VASP

Example - Fcc Si band

https://www.vasp.at/wiki/index.php/Fcc_Si_bandstructure

Band structure

```
System = fcc Si
ICHARG=11
ENCUT  =    240
ISMEAR = 0
SIGMA = 0.1
EDIFF = 1e-6
LORBIT=11

LWAVE= F
LCHARG = F
```

INCAR

```
fcc Si:
 3.9
 0.5 0.5 0.0
 0.0 0.5 0.5
 0.5 0.0 0.5
 Si
  1
cartesian
0 0 0
```

POSCAR

```
K-Path Generated by VASPKIT.
  20
Line-Mode
Reciprocal
  0.50000  0.50000  0.50000    L
  0.00000  0.00000  0.00000    GAMMA

  0.00000  0.00000  0.00000    GAMMA
  0.00000  0.50000  0.50000    X

  0.00000  0.50000  0.50000    X
  0.25000  0.62500  0.62500    U

  0.37500  0.7500   0.37500    K
  0.00000  0.00000  0.00000    GAMMA
```

KPOINTS

The command description can be found in vasp wiki:
https://www.vasp.at/wiki/index.php/The_VASP_Manual

Example - Fcc Si band

- Input files of VASP
  - INCAR
  - POSCAR
  - POTCAR
  - KPOINTS

PBS script (sub.pbs)

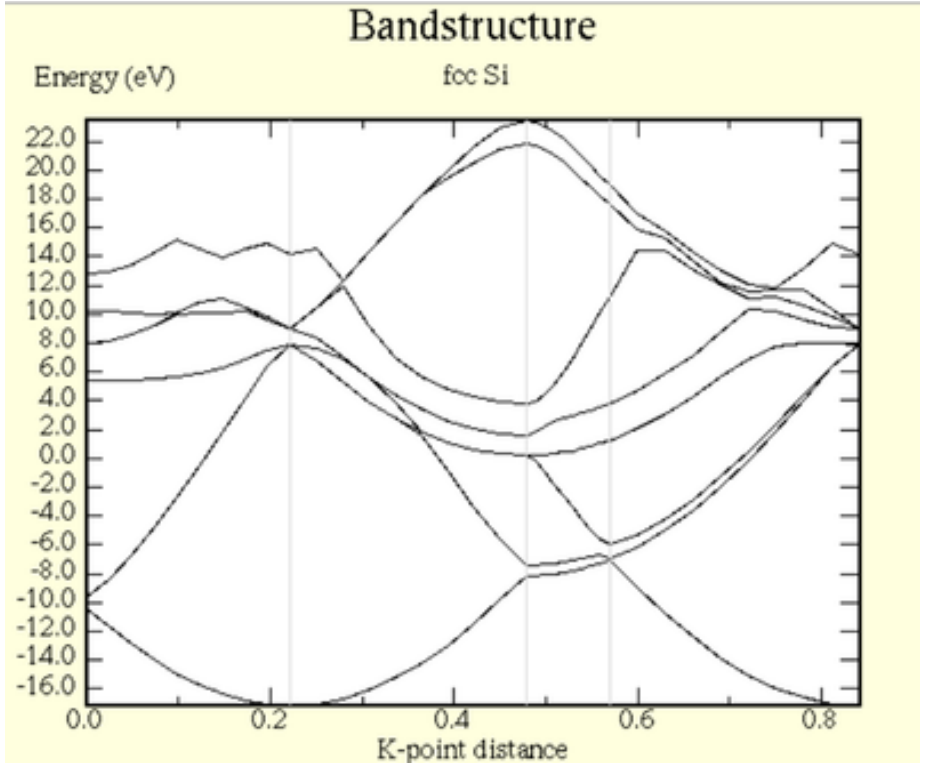
```
#PBS -N vasp
#PBS -l nodes=1:ppn=28
#PBS -S /bin/bash
#PBS -j oe
#PBS -q queue_name

cd $PBS_O_WORKDIR
NPROCS=`wc -l < $PBS_NODEFILE`

module load mpi/intelmpi/2017.4.239
module load compiler/intel/intel-compiler-2017.5.239

export vasp=/public/home/yourname/vasp/bin/vasp_std
mpirun -np $NPROCS  $vasp >output
```

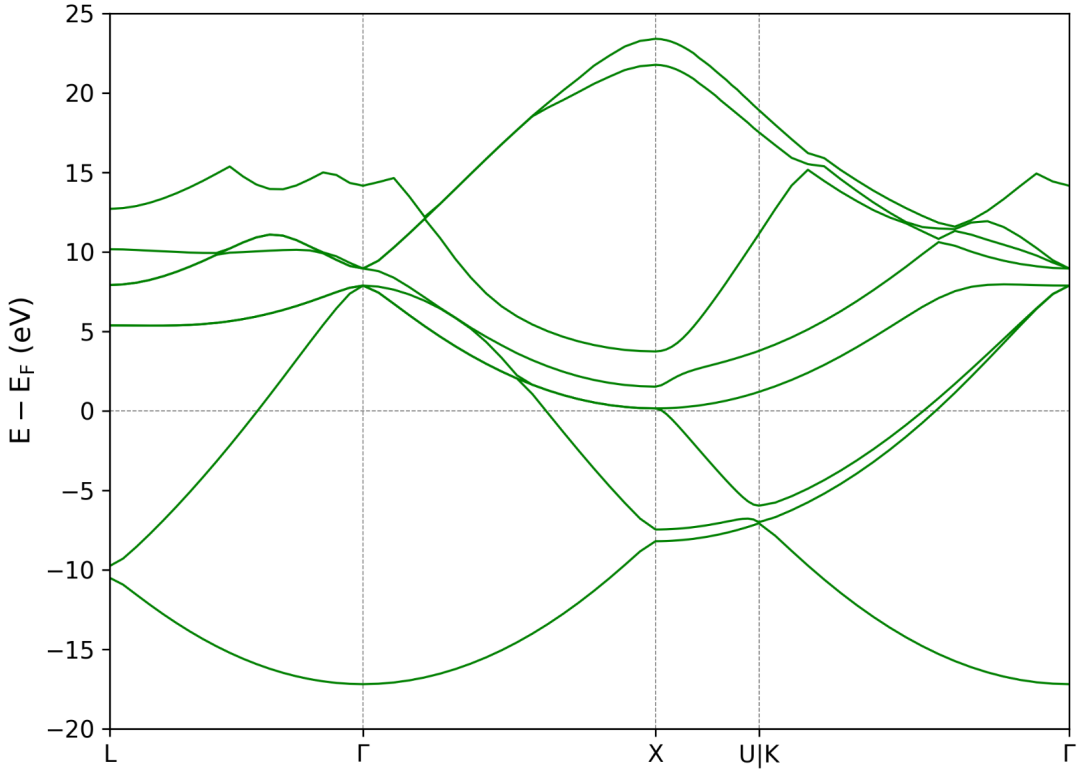
submit job:

```
qsub sub.pbs
```

Example - Fcc Si band

Plot the band structure





Example - Fcc Si band

Some useful tools and websites for VASP

https://www.vasp.at/wiki/index.php/The_VASP_Manual (VASP Manual)

https://www.bigbrosci.com/

https://vaspkit.com/