

安装记录

vasp.6.4.1+vtstcode6.4安装

基本运行环境

- module load gcc/14.1.0
- module load mpi/2021.12
- module load mkl/2024.1
- module load compiler/2024.1.0

1.vtstcode6.4文件配置

解压两个软件的安装包，将vtstcode所有文件拷贝至vasp的src下，并修改以下文件：

修改src目录下main.F文件

①第一处修改

%将最后一行修改

```
CALL CHAIN_FORCE(T_INFO%NIONS,DYN%POSITION,TOTEN,TIFOR, &  
    LATT_CUR%A,LATT_CUR%B,IO%IU6)
```

%修改后

```
CALL CHAIN_FORCE(T_INFO%NIONS,DYN%POSITION,TOTEN,TIFOR, &  
    TSIF,LATT_CUR%A,LATT_CUR%B,IO%IU6)
```

②第二处修改

%修改前

```
IF (LCHAIN) CALL chain_init( T_INFO, IO)
```

%修改后

```
CALL chain_init( T_INFO, IO)
```

修改src目录下.objects文件，在chain.o前添加内容：

```
bfgs.o dynmat.o instanton.o lbfgs.o sd.o cg.o dimer.o bbm.o \  
fire.o lanczos.o neb.o qm.o \  
pyamff_fortran/*.o ml_pyamff.o \  
opt.o
```

```
bfgs.o dynmat.o instanton.o lbfgs.o sd.o cg.o dimer.o bbm.o \  
fire.o lanczos.o neb.o qm.o \  
pyamff_fortran/*.o ml_pyamff.o \  
opt.o \  
chain.o \  
_
```

修改src同级目录下的makefile文件

```
LIB= lib parser pyamff_fortran
```

2.vasp文件配置

修改vasp目录下makefile.include文件中的内容：

```
FC          = mpiifx
FCL         = mpiifx
```

```
CC_LIB      = icx
```

```
CXX_PARS 0 = icpx
```

注意，下图中的MKLROOT，INCS中的mpi路径，填写根据环境准备module load后的实际路径。

```
FCL      += -qmk=sequential -xCORE-avx2
MKLROOT  ?=/gpfs/opt/intel/oneapi/mkl/latest
LLIBS    += -L$(MKLROOT)/lib/intel64 -lmkl_scalapack_lp64 -lmkl_blacs_intelmpi_lp64
INCS     -= I$(MKLROOT)/include/fftw -I/gpfs/opt/intel/oneapi/mpi/2021.12/include
```

3.vasp安装及环境变量配置

在vasp目录下使用make all命令，并在~/.bashrc 将新生成可执行的vasp文件添加到环境变量中。

```
%路径根据实际情况调整
export PATH=$PATH:/opt/vasp_and_tools/vasp/6.4.1/bin
```

4.运行测试

准备好输入文件，测试vasp_std命令。

```
LDA part: xc-table for Pade appr. of Perdew
POSCAR found type information on POSCAR LiFeSiO
POSCAR found : 4 types and 32 ions
```

```
W  W  AA  RRRRR  N  N  II  N  N  GGGG  !!!
W  W  A  A  R  R  NN  N  II  NN  N  G  G  !!!
W  W  A  A  R  R  NN  N  II  NN  N  G  G  !!!
W WW W AAAAAA RRRRR  N  N  N  II  N  NN  G  GGG  !
WW WW A  A  R  R  N  NN  II  N  NN  G  G
W  W  A  A  R  R  N  N  II  N  N  GGGG  !!!
```

```
The requested file could not be found or opened for reading
k-point information. Automatic k-point generation is used as a
fallback, which may lead to unwanted results.
```

```
POSCAR, INCAR and KPOINTS ok, starting setup
```

```
FFT: planning ... GRIDC
```

```
FFT: planning ... GRID_SOFT
```

```
FFT: planning ... GRID
```

```
WAVECAR not read
```

```
entering main loop
```

	N	E	dE	d eps	ncg	rms	rms(c)
DAV:	1	0.163622707046E+04	0.16362E+04	-0.65786E+04	3296	0.141E+03	0.952E+01
DAV:	2	-0.910777460859E+02	-0.17273E+04	-0.18798E+04	3925	0.436E+02	0.517E+01

5.添加module并测试

在安装目录下添加modulefile文件内容见下：

```
proc ModulesHelp { } {
    puts stderr "Using moudle load to load this module."
}
module-whatis "vasp 6.4.1, compiled with Intel® oneAPI Compiler 2024, Intel MKL 2019 (for
lapack scalapack fftw ...)"

conflict vasp

module load gcc/14.1.0 mpi/2021.12 mkl/2024.1

#setenv MKL_THREADING_LAYER INTEL
setenv OMP_NUM_THREADS 1
setenv OMP_PLACES cores
setenv OMP_PROC_BIND close
setenv OMP_STACKSIZE 10GB

prepend-path PATH /opt/vasp_and_tools/vasp-6.4.1_vtstcode.6.4/vasp6.4.1/bin
```

module purge后对新添加的模块进行测试：

```
(base) lijinyou22@hanhai22-01:/opt/vasp_and_tools/vasp-6.4.1_vtstcode.6.4/vasp6.4.1/testCase$ vasp_std
vasp_std: error while loading shared libraries: libmkl_intel_lp64.so.2: cannot open shared object file: No such file or directory
(base) lijinyou22@hanhai22-01:/opt/vasp_and_tools/vasp-6.4.1_vtstcode.6.4/vasp6.4.1/testCase$ module load /opt/vasp_and_tools/vasp/6.4.1/intel_mpi
Loading /opt/vasp_and_tools/vasp/6.4.1/intel_mpi
Loading requirement: gcc/14.1.0 mpi/2021.12 tbb/latest compiler-rt/latest mkl/2024.1
(base) lijinyou22@hanhai22-01:/opt/vasp_and_tools/vasp-6.4.1_vtstcode.6.4/vasp6.4.1/testCase$ vasp_std
running 1 mpi-ranks, on 1 nodes
distrk: each k-point on 1 cores, 1 groups
distr: one band on 1 cores, 1 groups
vasp.6.4.1 05Apr23 (build Mar 08 2025 12:24:21) complex

POSCAR found type information on POSCAR LiFeSiO
POSCAR found : 4 types and 32 ions
scaLAPACK will be used

-----
      W  W  AA  RRRRR  N  N  II  N  N  GGGG  !!!
      W  W  A  A  R  R  NN  N  II  NN  N  G  G  !!!
      W  W  A  A  R  R  N  N  N  II  N  N  N  G  !!!
      W  WW  W  AAAAAA  RRRRR  N  N  N  II  N  N  N  G  GGG  !
      WW  WW  A  A  R  R  N  NN  II  N  NN  G  G  G
      W  W  A  A  R  R  N  N  II  N  N  GGGG  !!!

The value NCORE = 8 specified in the INCAR file was overwritten,
because it was not compatible with the 1 processes available:
NCORE = 1
was used instead, please check that this makes sense for your
machine.
-----
```

vaspkit 1.4.1安装

配置要求见下：Python 3.5 or higher

- Numpy 1.15.4 or higher
- Scipy 1.1.0 or higher
- matplotlib 3.0.1 or higher

1.安装conda环境

```
module load anaconda/3/24.06
```

2.换conda镜像源

利用conda config --add channels的命令添加新源和删除默认default源不奏效。以下是通过修改.condarc的方法进行换源。

```
conda config --show-sources
```

```
(base) lijinyou22@hanhai22-01:/opt/vasp_and_tools$ conda config --show-source  
==> /home/wszhanggroup/lijinyou22/.condarc <==
```

进入第一行显示路径，写入全新的./condarc镜像源：

```
channels:  
- http://mirrors.tuna.tsinghua.edu.cn/anaconda/pkgs/free/  
- http://mirrors.tuna.tsinghua.edu.cn/anaconda/cloud/conda-forge/  
- http://mirrors.tuna.tsinghua.edu.cn/anaconda/cloud/msys2/  
show_channel_urls: true  
default_channels:  
- http://mirrors.tuna.tsinghua.edu.cn/anaconda/pkgs/main  
- http://mirrors.tuna.tsinghua.edu.cn/anaconda/pkgs/free  
- http://mirrors.tuna.tsinghua.edu.cn/anaconda/pkgs/r  
- http://mirrors.tuna.tsinghua.edu.cn/anaconda/pkgs/pro  
- http://mirrors.tuna.tsinghua.edu.cn/anaconda/pkgs/msys2  
custom_channels:  
conda-forge: http://mirrors.tuna.tsinghua.edu.cn/anaconda/cloud  
msys2: http://mirrors.tuna.tsinghua.edu.cn/anaconda/cloud  
bioconda: http://mirrors.tuna.tsinghua.edu.cn/anaconda/cloud  
menpo: http://mirrors.tuna.tsinghua.edu.cn/anaconda/cloud  
pytorch: http://mirrors.tuna.tsinghua.edu.cn/anaconda/cloud  
simpleitk: http://mirrors.tuna.tsinghua.edu.cn/anaconda/cloud  
ssl_verify: false
```

3.指定目录下创建conda环境

```
conda create -p /opt/vasp_and_tools/.conda/vaspkitEnv python=3.10
```

可能出现的问题：第一次在该目录下建立虚拟环境时，conda env list得到的环境未命名。

```
lijinyou22@hanhai22-01:/opt/vasp_and_tools/.conda$ conda env list  
# conda environments:  
#  
base /opt/anaconda3/2024.06-1  
/opt/vasp_and_tools/.conda/vaspkitEnv
```

通过复制该环境得到命名新环境：

```
conda create -n vaspkit --clone /opt/vasp_and_tools/.conda/vaspkitEnv
```

```
(/opt/vasp_and_tools/.conda/vaspkitEnv) lijinyou22@hanhai22-01:/opt$ conda env list
# conda environments:
#
base                                /opt/anaconda3/2024.06-1
* vaspkit                          /opt/vasp_and_tools/.conda/vaspkitEnv
vaspkit                            /opt/vasp_and_tools/.conda/vaspkitEnv/vaspkit
```

4.激活并进入环境

```
conda activate vaspkit
```

利用pip安装所需其他工具：

```
pip install -i https://pypi.tuna.tsinghua.edu.cn/simple spicy
pip install -i https://pypi.tuna.tsinghua.edu.cn/simple numpy
pip install -i https://pypi.tuna.tsinghua.edu.cn/simple matplotlib
```

5.vaspkit安装

安装包解压后按要求复制文件并修改

```
cp -f how_to_set_environment_variable ~/.vaspkit//
```

后者路径固定，由官方安装脚本决定

```
# All environment variables are case sensitive.
VASP5                                = .TRUE.                                # .TRUE. or .FALSE.; Set .FALSE. if you are using vasp.4.x
LDA_PATH                            = ~/POTCAR/LDA                        # Path of LDA potential
PBE_PATH                            = ~/POTCAR/PBE                        # Path of PBE potential
GGA_PATH                            = ~/POTCAR/GGA                        # Path of PW91 potential
VASPKIT_UTILITIES_PATH              = ~/vaspkit/utilities                # Path of VASPKIT
PYTHON_BIN                          = /opt/anaconda3/2024.06-1/bin/python  # Python executable program with its installation path.
```

在解压缩包的安装目录下运行vaspkit，成功界面如下：

```
(base) lijinyou22@hanhai22-01:/opt/vasp_and_tools$ vaspkit
```

```

      /\//\
      /  \
    (| (o)(o) |)
o-----.000o--( )--o000.-----o
|          VASPKIT Standard Edition 1.4.1 (26 Apr. 2023)          |
|          Core Developer: Vei WANG (wangvei@icloud.com)          |
|          Main Contributors: Gang TANG, Nan XU & Jin-Cheng LIU    |
|          Online Tutorials Available on Website: https://vaspkit.com |
o-----.000o-----o
      (  )    0ooo.
      \ (    (  )
      \_)    ) /
      (_/

Hey, you must know what you are doing.
Otherwise you might get wrong results.

===== Structural Utilities =====
1) VASP Input-Files Generator      2) Mechanical Properties
3) K-Path for Band-Structure      4) Structure Editor
5) Catalysis-ElectroChem Kit      6) Symmetry Analysis
7) Materials Databases            8) Advanced Structure Models
===== Electronic Utilities =====
11) Density-of-States             21) Band-Structure
23) 3D Band-Structure             25) Hybrid-DFT Band-Structure
26) Fermi-Surface                 28) Band-Structure Unfolding
31) Charge-Density Analysis       42) Potential Analysis
51) Wave-Function Analysis        62) Magnetic Properties
65) Spin-Texture                  68) Transport Properties
===== Misc Utilities =====
71) Optical Properties            72) Molecular-Dynamics Kit
74) User Interface               78) VASP2other Interface
91) Semiconductor Kit            92) 2D-Material Kit
0) Quit
----->>
```

6.添加module并测试

在安装目录下添加modulefile文件内容见下：

```
##Module1.0

proc ModulesHelp {} {
  puts stderr "Using moudle load to load this module. Before running vaspkit, please run
  setup.sh to setup your environment."
}

module-whatis "VASPKIT v1.4.1"

prepend-path PATH /opt/vasp_and_tools/vaspkit-1.4.1/bin
```

module purge后对新添加的模块进行测试：

```
(base) lijinyou22@hanhai22-01:~$ vaspkit
vaspkit: command not found
(base) lijinyou22@hanhai22-01:~$ module load /opt/vasp_and_tools/vaspkit/1.4.1
(base) lijinyou22@hanhai22-01:~$ vaspkit
```

```

      /\//
     /  \
    (| (o)(o) |)      Hey, you must know what you are doing.
                        Otherwise you might get wrong results.
o-----.000o--()--o000.-----o
|          VASPKIT Standard Edition 1.4.1 (26 Apr. 2023)          |
|          Core Developer: Vei WANG (wangvei@icloud.com)         |
|          Main Contributors: Gang TANG, Nan XU & Jin-Cheng LIU   |
|          Online Tutorials Available on Website: https://vaspkit.com |
o-----.0000-----o
|          ( )      0ooo.          VASPKIT Made Simple          |
|          \ (      ( )          |
|          \_)      ) /          |
|          (_/      (_/          |
===== Structural Utilities =====
1) VASP Input-Files Generator      2) Mechanical Properties
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51) Wave-Function Analysis        62) Magnetic Properties
65) Spin-Texture                  68) Transport Properties
===== Misc Utilities =====
71) Optical Properties            72) Molecular-Dynamics Kit
74) User Interface               78) VASP2other Interface
91) Semiconductor Kit            92) 2D-Material Kit
0) Quit
----->>
```

vtstscripts安装

1.赋予可执行权限：

解压文件包，赋执行权限 `chmod +x vtstscripts-1033`

```
(base) lijinyou22@hanhai22-01:/opt/vasp_and_tools/vtstscripts$ ls -l
total 8
drwxr-xr-x 4 lijinyou22 wszhanggroup 8192  3月  5 15:05 vtstscripts-1033
```

2.添加环境变量~/.bashrc：

```
export PATH=$PATH:/opt/vasp_and_tools/vtstscripts/vtstscripts-1033
```

3.添加至module

在安装目录下添加modulefile文件内容见下：

```
#%Module1.0

proc ModulesHelp { } {
    puts stderr "Using moudle load to load this module. Before running vtstscripts-1033, please run setup.sh to
    setup your environment."
}

module-whatis "VTSTSCRIPTS 1033"

prepend-path PATH /opt/vasp_and_tools/vtstscripts-1033/vtstscripts-1033
```

lobster.5.1.0安装

1.赋予执行权限

解压安装包后内容如下：

```
(base) lijinyou22@hanhai22-01:/opt/vasp_and_tools/lobster-5.1.0$ ls -l
total 14788
drwxr-xr-x 8 lijinyou22 wszhanggroup      4096  6月 11  2024 ABINIT
-rw-r--r-- 1 lijinyou22 wszhanggroup    133317  6月 11  2024 CHANGELOG.pdf
drwxr-xr-x 3 lijinyou22 wszhanggroup      4096  6月 11  2024 Custom_Basis
drwxr-xr-x 3 lijinyou22 wszhanggroup      4096  6月 11  2024 Generic
-rw-r--r-- 1 lijinyou22 wszhanggroup  12590064  6月 11  2024 lobster-5.1.0
-rw-r--r-- 1 lijinyou22 wszhanggroup    361460  6月 12  2024 Lobster_FAQ_5.1.0.pdf
-rw-r--r-- 1 lijinyou22 wszhanggroup   1849288  6月 12  2024 Lobster_Users_Guide_5.1.0.pdf
drwxr-xr-x 2 lijinyou22 wszhanggroup      4096  6月 11  2024 OSX
drwxr-xr-x 8 lijinyou22 wszhanggroup      4096  6月 11  2024 QE
drwxr-xr-x 8 lijinyou22 wszhanggroup      4096  6月 11  2024 VASP
drwxr-xr-x 2 lijinyou22 wszhanggroup      4096  6月 11  2024 win64
```

添加lobster-5.1.0的权限

```
chmod +x lobster-5.1.0
```

```
(base) lijinyou22@hanhai22-01:/opt/vasp_and_tools/lobster-5.1.0$ ls -l
total 14788
drwxr-xr-x 8 lijinyou22 wszhanggroup      4096  6月 11  2024 ABINIT
-rw-r--r-- 1 lijinyou22 wszhanggroup    133317  6月 11  2024 CHANGELOG.pdf
drwxr-xr-x 3 lijinyou22 wszhanggroup      4096  6月 11  2024 Custom_Basis
drwxr-xr-x 3 lijinyou22 wszhanggroup      4096  6月 11  2024 Generic
-rwxr-xr-x 1 lijinyou22 wszhanggroup  12590064  6月 11  2024 lobster-5.1.0
-rw-r--r-- 1 lijinyou22 wszhanggroup    361460  6月 12  2024 Lobster_FAQ_5.1.0.pdf
-rw-r--r-- 1 lijinyou22 wszhanggroup   1849288  6月 12  2024 Lobster_Users_Guide_5.1.0.pdf
drwxr-xr-x 2 lijinyou22 wszhanggroup      4096  6月 11  2024 OSX
drwxr-xr-x 8 lijinyou22 wszhanggroup      4096  6月 11  2024 QE
drwxr-xr-x 8 lijinyou22 wszhanggroup      4096  6月 11  2024 VASP
drwxr-xr-x 2 lijinyou22 wszhanggroup      4096  6月 11  2024 win64
```

2.添加环境变量~/.bashrc

```
export PATH=$PATH:/opt/vasp_and_tools/lobster-5.1.0
```

可在输入目录下运行 ./lobster-5.1.0

3.直接运行可执行文件

/opt/vasp_and_tools/lobster/5.1.0

qvasp安装

1.启动安装脚本：

解压软件包，启动安装脚本报错：

```
sh install.sh
```

```
(base) lijinyou22@hanhai22-01:/opt/vasp_and_tools/qvasp-v2.24/qvasp-v2.24$ ls
documents Examples exefile fix-program.sh install.sh qvasp README source-code todoto uninstall.sh update.log
(base) lijinyou22@hanhai22-01:/opt/vasp_and_tools/qvasp-v2.24/qvasp-v2.24$ sh install.sh
```

```
(base) lijinyou22@hanhai22-01:/opt/vasp_and_tools/qvasp-v2.24/qvasp-v2.24$ sh install.sh
do you wish the installer to prepend the qvasp location to PATH in /home/wszhanggroup/lijinyou22/.bashrc ? (yes or no):yes
install.sh: 17: [: yesx: unexpected operator
install.sh: 25: [: yesx: unexpected operator
install.sh: 34: [: yesx: unexpected operator
```

选择直接修改环境变量的方式：

```
export qvasppath=/opt/vasp_and_tools/qvasp-v2.24/qvasp-v2.24
export PATH=$qvasppath:$PATH
export PATH=$qvasppath/exefile/Tools/USERTools/vtstscripts:$PATH
```

3.添加至module

在安装目录下添加modulefile文件内容见下：

```
#%Module1.0
```

```
proc ModulesHelp { }
```

```
puts stderr "Using moudle load to load this module. Before running qvasp-v2.24, please run setup.sh to
setup your environment."
```

```
}
```

```
module-whatis "QVASP-V2.24"
```

```
prepend-path PATH /opt/vasp_and_tools/qvasp-v2.24/qvasp-v2.24
```

```
prepend-path PATH /opt/vasp_and_tools/qvasp-v2.24/qvasp-v2.24/exefile/Tools/USERTools/vtstscripts
```