

# 从头开始用 VASP 做结构优化

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登入 **Linux**

编辑文件

**VASP** 输入文件解读

执行 **VASP** 计算

解读结构优化过程

## 登入 Linux

# 计算机通信协议

- ▶ 安全 Shell 协议 (SSH)
- ▶ 远程桌面类型 (VNC, RDP)
- ▶ 文件传输协议 (FTP)

# 基于 SSH 协议的 SSH 客户端

## 基本需求

1. 通过命令行的方式操作远端的电脑 (投任务, 编辑文本, 编译程序, ...)
2. 上传下载文件
3. 支持 Linux 上的窗口化的程序 (比如 `xmgrace`)

# 微软 Windows 下的 SSH 客户端

## 1. 自带的 ssh 客户端工具

优点: Windows10 原生程序, 不需要第三方的程序

缺点: 文件互传不便, 默认不支持 Linux 上窗口化程序

## 2. 第三方 ssh 客户端, 例如MobaXterm

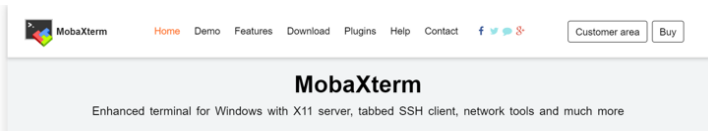


Figure 1: MobaXterm

优点: 免费软件, 拖拽式文件上传下载, 支持 X Windows 窗口软件

缺点: 并不是总能跟上 Windows 的更新频率

# 自带 SSH 客户端 I

← 设置

## 管理可选功能

可选功能

[查看可选功能历史记录](#)



添加功能



Internet Explorer 11

1.74 MB



Microsoft 快速助手

1.52 MB



OpenSSH 客户端

5.70 MB



Windows Media Player

61.1 MB



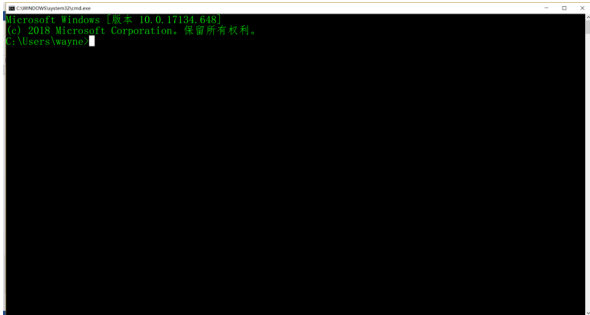
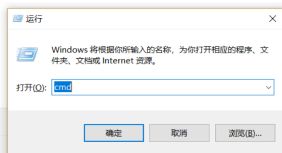
XPS Viewer

16.1 MB

Figure 2: 安装 SSH 客户端

# 自带 SSH 客户端 II

打开 Windows 的命令提示符窗口: Win+R → cmd



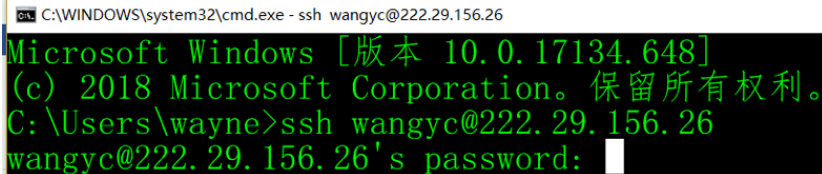


# 自带 SSH 客户端 III

## 1. 输入 ssh 登录的命令

@ 前面是用户名, @ 后面是远端服务器的 IP

## 2. 输入密码



```
C:\WINDOWS\system32\cmd.exe - ssh wangyc@222.29.156.26
Microsoft Windows [版本 10.0.17134.648]
(c) 2018 Microsoft Corporation。保留所有权利。
C:\Users\wayne>ssh wangyc@222.29.156.26
wangyc@222.29.156.26's password: 
```

Figure 3: 登录命令

# 自带 SSH 客户端 IV

登录成功! 可以在命令行下控制远端设备了

wangyc@b214: ~

```
C:\Users\wayne>ssh wangyc@222.29.156.26
```

```
wangyc@222.29.156.26's password:
```

```
Welcome to Ubuntu 18.04.2 LTS (GNU/Linux 4.15.0-47-generic x86_64)
```

```
* Documentation:  https://help.ubuntu.com
* Management:    https://landscape.canonical.com
* Support:        https://ubuntu.com/advantage
```

```
* Ubuntu's Kubernetes 1.14 distributions can bypass Docker and use containerd
  directly, see https://bit.ly/ubuntu-containerd or try it now with
```

```
    snap install microk8s --classic
```

```
* Canonical Livepatch is available for installation.
  - Reduce system reboots and improve kernel security. Activate at:
    https://ubuntu.com/livepatch
```

```
82 packages can be updated.
```

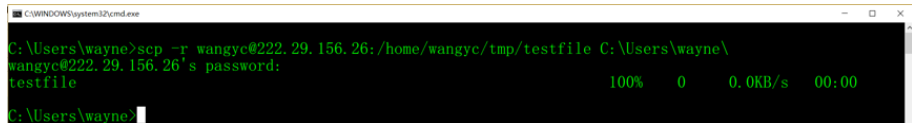
```
0 updates are security updates.
```

```
Last login: Mon Apr  8 18:50:38 2019 from 222.29.156.16
```

```
wangyc@b214: ~$
```

# 自带 SSH 客户端 V

传输文件: 使用 `scp` 命令



```
C:\WINDOWS\system32\cmd.exe
C:\Users\wayne>scp -r wangyc@222.29.156.26:/home/wangyc/tmp/testfile C:\Users\wayne\
wangyc@222.29.156.26's password:
testfile
100% 0 0.0KB/s 00:00
C:\Users\wayne>
```

含义:

将用户 wangyc 在

222.29.156.26 机器上的 `/home/wangyc/tmp/testfile` 文件

拷贝到 `C:\Users\wayne\` 目录下

# 自带 SSH 客户端 VI

免密码登录: 使用 `ssh-keygen` 命令

一路回车下去, 创建公钥和私钥

在远端服务器上已进行相同的操作, 产生 `~/.ssh/` 目录

```
C:\WINDOWS\system32\cmd.exe

C:\Users\wayne>ssh-keygen
Generating public/private rsa key pair.
Enter file in which to save the key (C:\Users\wayne\.ssh\id_rsa):
Enter passphrase (empty for no passphrase):
Enter same passphrase again:
Your identification has been saved in C:\Users\wayne\.ssh\id_rsa.
Your public key has been saved in C:\Users\wayne\.ssh\id_rsa.pub.
The key fingerprint is:
SHA256:REcZFsio/HUj4fjMLm6qC9I7jpuApUR45o4X9MPFMHM wayne@my-laptop
The key's randomart image is:
+---[RSA 2048]-----+
|
| o+oE..
| . . oB =
| oo+ o * .
| o* + * +
| . = 0 o S
| o* o =
| B + .
| ++. + .
| B=*o.
+---[SHA256]-----+

C:\Users\wayne>
```

# 自带 SSH 客户端 VII

将 .ssh 目录下的 id\_rsa.pub 上传到远端服务器

C:\WINDOWS\system32\cmd.exe

```
C:\Users\wayne>cd .ssh/
```

```
C:\Users\wayne\.ssh>dir
```

驱动器 C 中的卷是 OS  
卷的序列号是 826C-9374

C:\Users\wayne\.ssh 的目录

```
2019/04/08  19:28    <DIR>          .
2019/04/08  19:28    <DIR>          ..
2019/04/08  19:23             1,679 id_rsa
2019/04/08  19:23             398 id_rsa.pub
2018/12/21  19:27             2,121 known_hosts
                3 个文件             4,198 字节
                2 个目录    6,832,545,792 可用字节
```

```
C:\Users\wayne\.ssh>scp id_rsa.pub wangyc@222.29.156.26:~/
```

# 自带 SSH 客户端 VIII

```
wangyc@b214: ~/.ssh$ cat ~/.ssh/id_rsa.pub >> authorized_keys
```

即可无密码访问远端服务器

# MobaXterm I

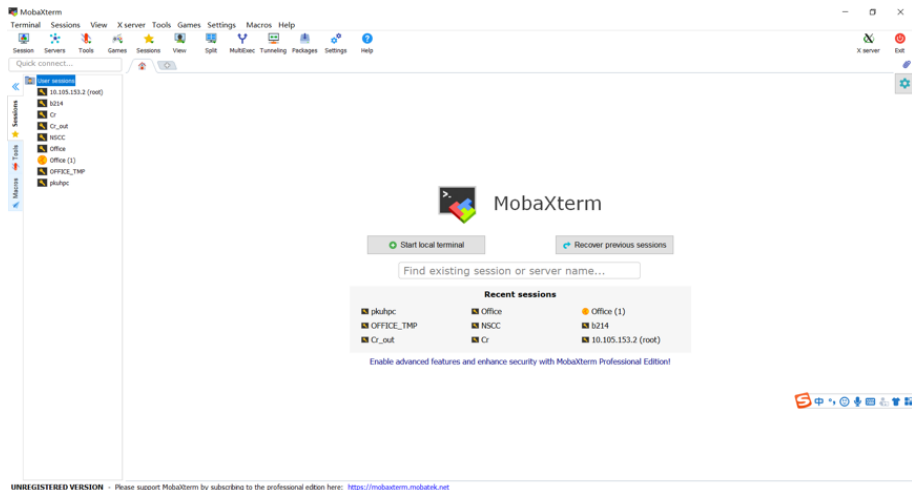


Figure 4: MobaXterm 界面

# MobaXterm II

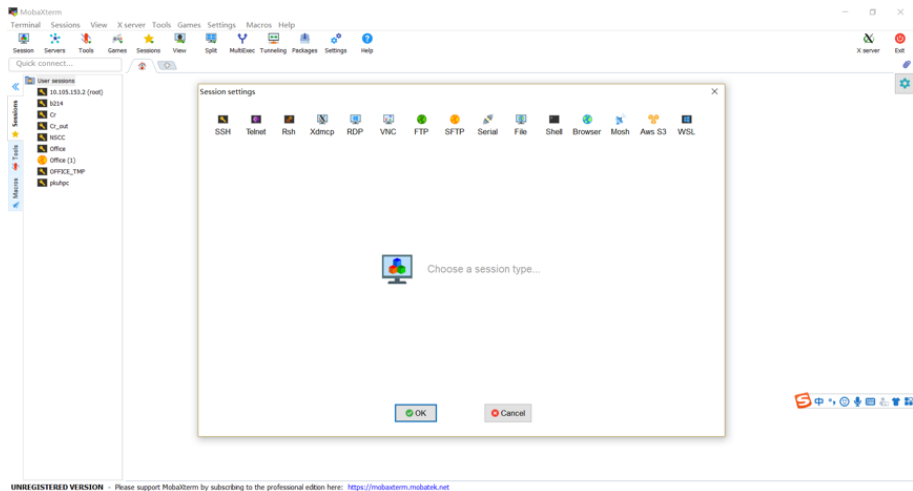
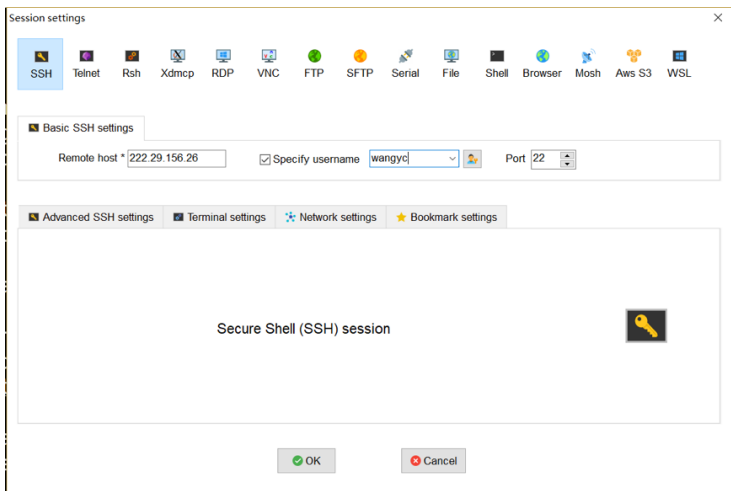


Figure 5: sessions → new session 对话框

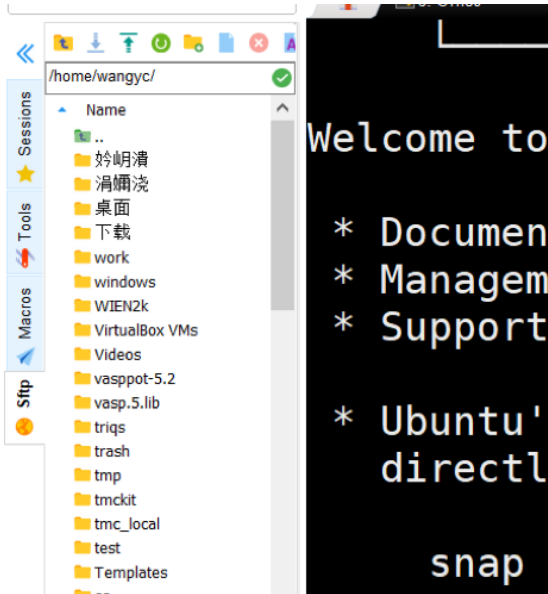


# MobaXterm III

选择中间对话框左上角的 SSH 标签, 填好远端的 IP 和用户名, 点击 OK, 第一次登陆会询问是否记住密码, 选择记住之后登陆就不用输入密码了



# MobaXterm IV



登陆之后左侧出现文件列表  
可以通过拖拽的方式进行文  
件的上传和下载

# 常用计算平台

平台	IP	备注
未名一号	162.105.133.134	用户名与密码为一卡通
教学一号	162.105.133.209	用户名与密码为一卡通 自助开通
天津中心	192.168.2.101	需 VPN
组内服务器	TBA	小型工作站

临时平台: dft003@222.29.156.125

## 编辑文件

# Linux 下常用文本编辑器: Vim

- ▶ 语法高亮
- ▶ 简单的自动补全
- ▶ 列编辑和多文件编辑
- ▶ 通过键盘输入命令实现, 同时支持鼠标操作

# 学习 Vim

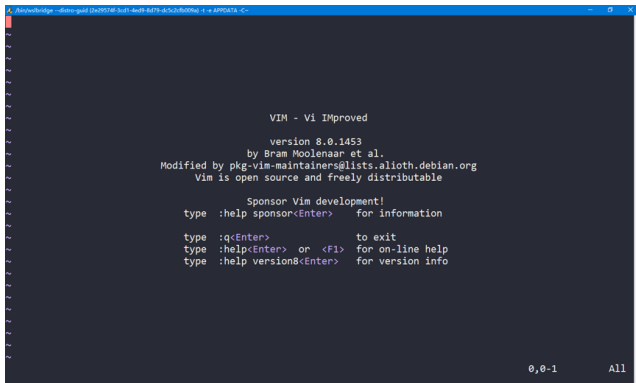
- ▶ 善用搜索引擎 (百度, Google, ...)

想知道 vim 如何查找替换  $\Rightarrow$  搜 “vim 查找替换”

- ▶ Linux 下各种命令与程序的用法: CSDN 博客, 脚本之家

## 启动,保存与退出 I

命令行输入 `vim`, 回车, 会出现 `vim` 的一个界面

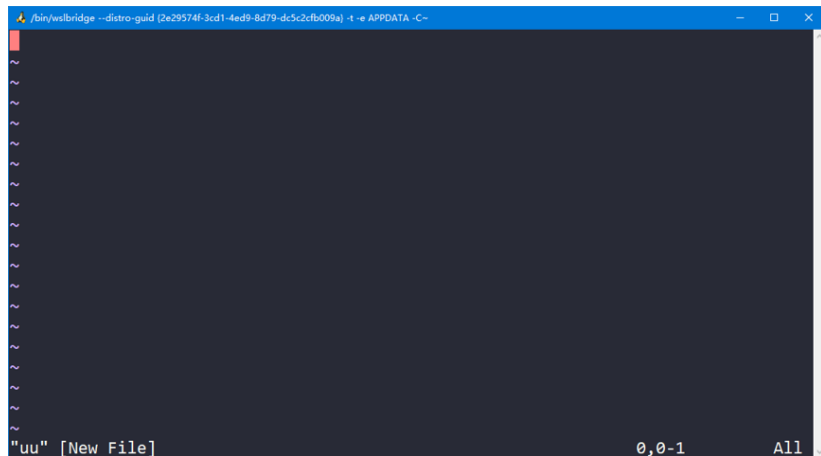


### Figure 6: Vim 界面

如果后面加上文件名就会打开相应的文件,若该文件不存在则创建一个新文件

# 启动, 保存与退出 II

此时你在键盘上的任何输入一般都是无效的

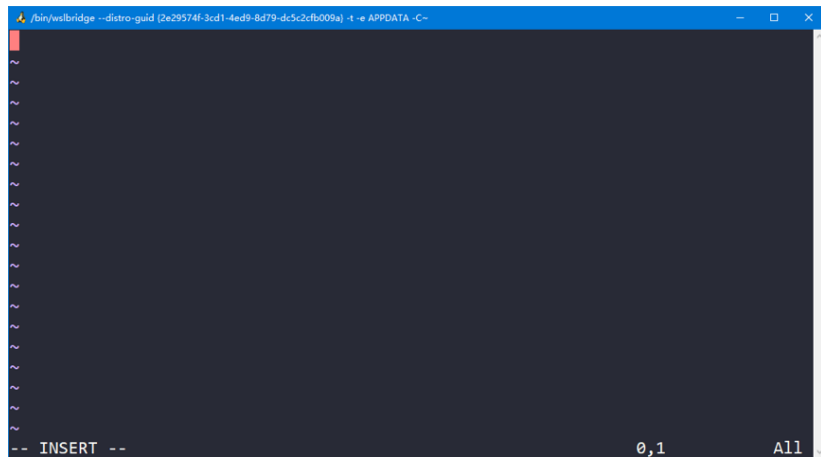


The screenshot shows a terminal window with a blue title bar. The title bar text is `/bin/wslbridge --distro-guid [2e29574f-3cd1-4ed9-8d79-dc5c2cfb009a] -t -e APPDATA -C-`. The terminal content shows a Vim editor interface. On the left side, there is a vertical column of tilde characters (~). At the bottom left, the text `"uu" [New File]` is visible. At the bottom right, the text `0,0-1` and `All` are visible. The terminal background is dark blue, and the text is light blue.



# 启动, 保存与退出 III

需要按一下 `i` 键变成可输入状态, 然后向里面输入内容



The screenshot shows a terminal window with a blue title bar. The terminal content is a dark gray area representing a Vim editor. On the left side, there is a vertical column of tilde (~) characters. At the bottom left, the text "-- INSERT --" indicates the current mode. At the bottom right, the text "0,1" and "All" are visible, likely representing line numbers or a range. The terminal window has standard window controls (minimize, maximize, close) in the top right corner.

# 启动, 保存与退出 IV

- ▶ vim 的很多操作是通过“命令”进行的
- ▶ 在--INSERT--状态下, 任何键盘输入都成为了输入的内容



# 启动, 保存与退出 VI

输入命令

- ▶ :wq(write and quit), 回车  $\Rightarrow$  保存并退出
- ▶ :q!, 回车  $\Rightarrow$  直接退出, 不保存

注意: 两个命令都以一个冒号开头

# 复制, 粘贴和删除文本

**Table 2:** Vim 常用命令

命令	作用
yy	复制当前一整行的内容
p	把复制的内容粘贴到光标所在行的下一行
dd	删除光标所在的一整行内
u	撤销上次输入
.	恢复上次输入

- ▶ Vim 不支持鼠标光标选中后 Delete
- ▶ 注意上面这些都是按了 Esc 之后执行, 不需要加冒号, 在--INSERT--状态无法执行

# 文本定位, 查找和替换 I

## 跳转

- ▶ `Shift + G` 跳转到文件末尾
- ▶ 按两次 `[` 可以跳转到文件开头
- ▶ `:n` 跳转到某一行使用命令, `n` 是一个行号
- ▶ 使用命令 `:set nu` 显示行号

# 文本定位, 查找和替换 II

## 查找文本

- ▶ 以 FORCE 为例, 在非插入状态下输入/FORCE, 光标即可跳转到 FORCE 所在的位置
- ▶ 按一下 n 键 (next) 跳转到下一个 FORCE 文本所在的位置
- ▶ 要想从文件末尾查找, 则先按下 Shift + G 跳转到文件末尾, 然后按 Shift + N, 即可跳转到从末尾数的第一个 FORCE 所在位置

# 文本定位, 查找和替换 III

替换: 与 sed 命令类似

- ▶ 在非插入状态下输入命令:`%s/FORCE/force/g`, 把所有 FORCE 替换成 force
- ▶ 如果没有前面的百分号, 则每次只替换一个

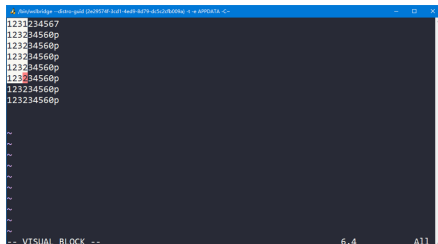


# 列编辑 I

非插入状态下按下 `Ctrl + V` 即进入列选择状态

按住方向键上下左右即可按列选择文本

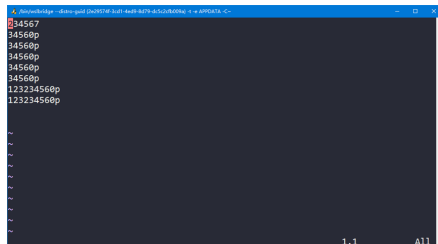
按一下 `d` 键则删除按列选中的文本



A terminal window titled `bincodebridge --data-god [0x017f-buff-4e09-8c5c0b609e, 1 + APPDATA, C-]`. The text content is as follows:

```
1231234567
123204560p
123204560p
123204560p
123204560p
123204560p
123204560p
123234560p
123234560p
123234560p
```

The first column of the first line is selected, indicated by a red vertical bar. The status bar at the bottom shows `-- VISUAL BLOCK --`, `6,4`, and `All`.



The same terminal window after deleting the selected column. The text content is now:

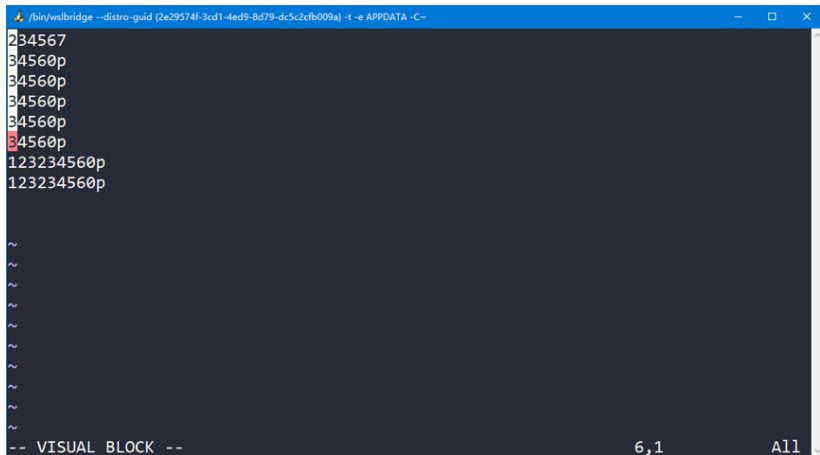
```
234567
34560p
34560p
34560p
34560p
34560p
34560p
123234560p
123234560p
```

The first column has been removed. The status bar at the bottom shows `1,1` and `All`.

## 列编辑 II

另一个常用的操作是给很多行加注释

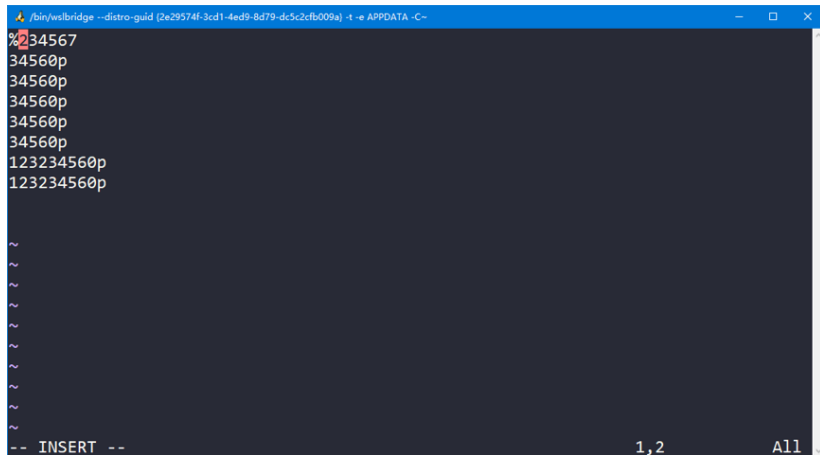
按 `Esc` 键进入非插入状态, 按 `Ctrl + V` 进入列选择状态, 然后选择要插入的列范围



```
/bin/wslbridge --distro-guid [2e29574f-3cd1-4ed9-8d79-dc5c2cfb009a] -t -e APPDATA -C~
234567
34560p
34560p
34560p
34560p
34560p
34560p
123234560p
123234560p
~
~
~
~
~
~
~
~
~
~
-- VISUAL BLOCK --                               6,1                               All
```

# 列编辑 III

按下 Shift + i 键, 输入文本



```
/bin/wslbridge --distro-guid [2e29574f-3cd1-4ed9-8d79-dc5c2cfb009a] -t -e APPDATA -C-  
%234567  
34560p  
34560p  
34560p  
34560p  
34560p  
123234560p  
123234560p  
~  
~  
~  
~  
~  
~  
~  
~  
~  
~  
-- INSERT -- 1,2 All
```

再连按两次 Esc, 前面选择过的行前都出现了相同的内容

# VASP 输入文件解读

# 输入文件

文件名	用途
POSCAR	结构文件
POTCAR	原子势
INCAR	计算参数控制
KPOINTS	倒空间中的 k 点取样网格

# POSCAR: 晶体结构文件

```
1 system Si # a comment line, usually the name of the system
2 1.000000 # a universe scaling factor
3 2.71500000 2.71500000 0.00000000 # the 1st lattice vector
4 0.00000000 2.71500000 2.71500000 # the 2nd lattice vector
5 2.71500000 0.00000000 2.71500000 # the 3rd lattice vector
6 Si # atomic species
7 2 # the number of atoms per atomic species
8 Direct # Fractional coordinates or cartesian coordinates
9 0.000000000 0.000000000 0.000000000 # three coordinates for the 1st Si atom
10 0.250000000 0.250000000 0.250000000 # three coordinates for the 2nd Si atom
```

10,84

All

# 获取晶体结构 I

## Inorganic Crystal Structure Database: 实验结构

**ICSD** Welcome to ICSD Web. IP authenticated (222.29.116.46). Peking Univ. FZ Karlsruhe | Contact  
Close session

**Login**

Logint:

Password:

☐ Lost password? ☐ Personalize account

**Content Selection**

☒ Experimental Structures only  
☐ Theoretical Structures only  
☐ All Structures

**Navigation**

Q Basic search & retrieve

**Advanced search & retrieve**

Q Bibliography

Q Cell

Q Chemistry

Q Symmetry

Q Crystal Chemistry

Q Structure Type

Q Experimental Information

Q DB Info

**Query Management**

☐ Manage Queries

☐ List Combined Queries

☐ Create Combined Query

**Basic Search & Retrieve**

**Bibliography**

Authors  Year of Publication

Title of Journal

Title of Article

**Chemistry**

Composition   Number of Elements

**Cell**

Cell Parameters

Cell Volume  Tolerance +/-  %

**Symmetry**

Space Group Symbol  Space Group Number

Crystal System  Centering

**Exp. Info. & Ref. Data**

New Data Only ☐

PDF Number  Temperature  K

ICSD Collection Code  Pressure  MPa

**Search Action**

**Search Summary**

Basic Search: -

**Query History**

Number of queries: 0

Figure 7: ICSD 搜索页面

# 获取晶体结构 II

**AFLOW**: Duke 材料基因组学数据库

The image shows the AFLOW search interface. The header includes the AFLOW logo and navigation links: HOME, CONSORTIUM, PUBLICATIONS, FORUM, SRC, and SEARCH. Below the header is a search bar with the text "Search Aflow" and a "Search" button. The main content area displays a periodic table of elements, with a search filter set to "icad". The periodic table includes element symbols, atomic numbers, and names. A search results summary shows "80375 Compounds". At the bottom, there are filters for "Results Per Page" (40), "Total # of Results" (1000), and "# of Species".

Figure 8: AFLOW 搜索页面



# 获取晶体结构 III

Materials Project: 基于 pymatgen 的材料基因组学数据库

The screenshot displays the Materials Project search page. At the top, there is a navigation bar with links for Home, About, Apps, Documentation, API, Tutorials, and Dashboard. Below this is a search bar with the text "Search for materials information by chemistry, composition, or property". The main content area is titled "Explore Materials" and features a periodic table of elements. The search bar is set to "by Elements" and contains the text "Na-O". To the right of the periodic table, there are several filters: "# of elements" (with a dropdown menu showing "e.g., 4 or >2 & <8"), "excluded elements" (with a dropdown menu showing "C, Br"), "Material Tags" (with a dropdown menu showing "e.g., Inorganic"), "Band Gap (eV)" (with a range from 0 to 10), "Energy Above Hull" (with a range from 0 to 8), and "Formation Energy" (with a range from -4 to 4). The periodic table itself is color-coded by groups, with elements like H, He, Li, Be, Na, Mg, K, Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Ga, Ge, As, Se, Br, Kr, Rb, Sr, Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Cd, In, Sn, Sb, Te, I, Xe, Cs, Ba, La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Fr, Ra, Ac, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, and Lr.

Figure 9: MaterialsProject 搜索页面

# POTCAR: 原子势 I

- ▶ ENMAX, ENMIN: 平面波基组的截断能
- ▶ LEXCH: 产生赝势所使用的泛函
- ▶ ZVAL: 价电子数目

# POTCAR: 原子势 II

## 推荐赝势

### Recommended PAW potentials for DFT calculations using vasp.5.2

The following table reports in bold face the recommended potentials for calculations using vasp.5.2. This list of potentials is fully compatible with the MedeA user interface distributed by Materials Design (<http://www.materialsdesign.com/>) facilitating a simple migration between the standard VASP version and the Materials Design MedeA user interface.

More details on the potentials are reported in the follow up sections. All distributed potentials have been tested using standard DFT-"benchmark" runs (see the `data_base` file in the released tar files). In most cases, the potentials are literally identical to the previous releases, but all potentials have been recalculated using a new version of the PAW generation code to include additional information allowing for calculations using meta-GGA functionals. The present potentials can be used in VASP.4.6, but we strongly recommend to use them only in VASP.5.X, since some compatibility issues might emerge (specifically LDA+U results might differ substantially between vasp.5.2 and vasp.4.6 using these new potentials, since a different PAW sphere radius is used by both version for these new potentials).

The reported default cutoffs (in eV) are for the PBE potentials, and might differ slightly for LDA potentials. The corresponding distribution directory of the potential is created by adding underscores between the elemental name and the extensions "\_", e.g Li sv becomes `Li_sv`.

Important Note: If dimers with short bonds are present in the compound ( $O_2$ ,  $CO$ ,  $N_2$ ,  $F_2$ ,  $P_2$ ,  $S_2$ ,  $Cl_2$ ), we recommend to use the `_h` potentials. Specifically, `C_h`, `O_h`, `N_h`, `F_h`, `P_h`, `S_h`, `Cl_h`.

Element (and appendix)	default cutoff $E_{MAX}$ (eV)	valency
<b>H</b>	<b>250</b>	<b>1</b>
H AE	1000	1
H h	700	1
H s	200	1
<b>He</b>	<b>479</b>	<b>2</b>

# INCAR: 计算参数控制

```
1 System = Silicon # the title
2 GGA = PE         # the type of generalized-gradient-approximation
3 ENCUT = 184      # the cutoff energy for the planewave basis set in the unit of eV
4 EDIFF = 1e-4     # the break condition for the electronic self-consistent loop
5 ISIF = 3         # which degrees-of-freedom could change in relaxation
6 IBRION = 2       # how the ions are updated and moved
7 NSW = 60        # the maximum number of ionic steps
```

7,54

All

# KPOINTS: 倒空间 K 点取样网格

```
1 Gamma-centered grid    # a comment line
2 0                      # automatic generation mode
3 Gamma                  # generate a \Gamma-centered grid
4 4 4 4                  # k-mesh along three reciprocal lattice vectors
5 0 0 0                  # shift of the mesh
```

5,43

All

## 执行 VASP 计算

# 创建运算目录 I

## ► 教学一号

```
$ ls
sc_run_vasp.sh POSCAR POTCAR INCAR KPOINTS
$ mkdir session-1/
$ cp POSCAR POTCAR INCAR KPOINTS session-1/
$ cp sc_run_vasp.sh session-1/
$ cd session-1/
```

## ► TMC PC

```
$ ls
tests Documents Downloads ...
$ mkdir -p tests/YOUR_NAME
$ cp POSCAR POTCAR INCAR KPOINTS tests/YOUR_NAME
$ cd tests/YOUR_NAME
```

# 创建运算目录 II

命令	用法	作用
ls	ls [.]	显示某路径下文件与文件夹
cd	cd name	进入 name 文件夹
mkdir	mkdir name	新建 name 文件夹
cp	cp file1 file2	复制 file1 为 file2



# 运行 VASP I

与 Windows 桌面不同, 终端下没有程序图标供你双击  
可执行程序的位置

- ▶ 当前路径
- ▶ 环境变量 PATH 中记录的路径

```
$ echo $PATH  
/usr/bin:/bin:...
```

用 which 确认可执行程序位置, 以 ls 为例

```
$ which ls  
/usr/bin/ls
```

# 运行 VASP II

确认可执行程序 vasp\_std 的位置

## ► 教学一号

```
$ which vasp_std  
$ module load vasp/5.4.4-intel18.0  
$ which vasp_std  
/nfs-share/software/vasp/intel18.0/bin/vasp_std
```

## ► TMC PC

```
$ which vasp_std  
/home/dft003/software/vasp.5.4.4/bin/vasp_std
```

# 运行 VASP III

Q: 为什么第一次 `which` 的结果不同?

A: 在教学一号上

```
$ echo $PATH
/nfs-share/software/module/bin:/usr/local/bin:/usr/bin:...
$ module load vasp/5.4.4-intel18.0
$ echo $PATH
/nfs-share/software/vasp/intel18.0/bin:/
/nfs-share/software/module/bin:/usr/local/bin:/usr/bin:
...
```

`module` 来自 [Environment module](#), 一个环境变量管理工具

# 运行 VASP IV

```
$ cat sc_run_vasp.sh
#!/usr/bin/env bash
#SBATCH -A 150xxxxxxx
#SBATCH --nodes=1
#SBATCH -c 2
#SBATCH --partition=compute
#SBATCH -J test
#SBATCH -o stdout

module load intel/2018.0
module load vasp/5.4.4-intel18.0

mpirun -np 2 vasp_std
```

# 解释器  
# 学号  
# 使用一个节点  
# 每个节点使用 2 个核心  
# 指定计算分区  
# 任务名  
  
# 载入 Intel 编译器环境变量  
# 载入 VASP 环境变量 (PATH)  
  
# 运行

# 运行 VASP V

## ► 教学一号

```
$ sbatch sc_run_vasp.sh  
Submitted batch job xxxx  
$ watch -n 1 cat stdout
```

## ► TMC PC

```
$ mpirun -np 2 vasp_std > out &  
$ watch -n 1 cat out
```

## 解读结构优化过程