

从头开始用 VASP 做结构优化

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解读结构优化过程

登入 Linux

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

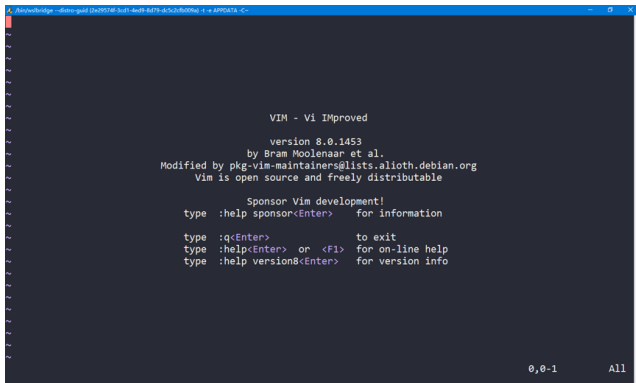
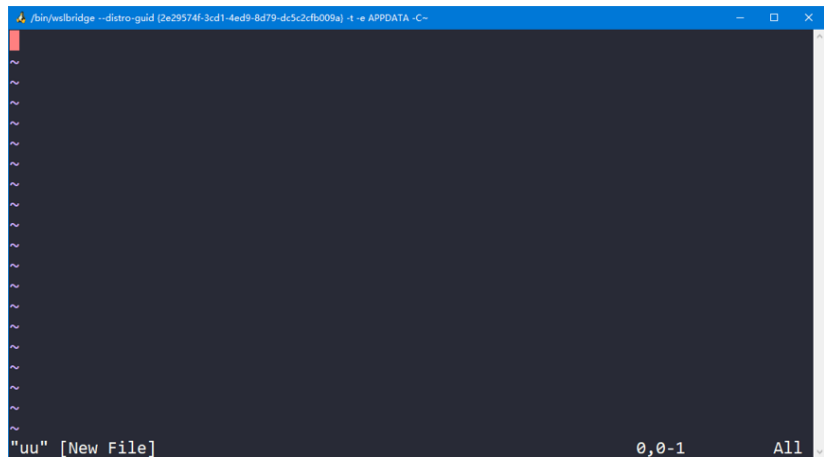


Figure 1: vim 界面

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

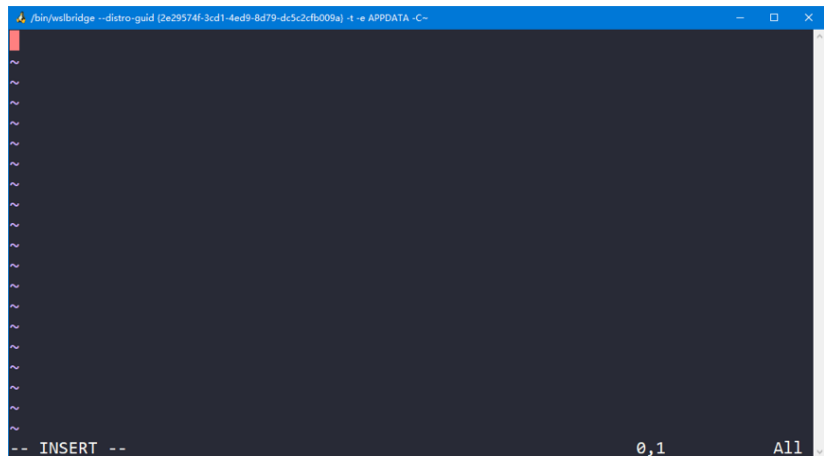
此时你在键盘上的任何输入一般都是无效的



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 area has a dark background. On the left side, there is a vertical column of approximately 15 tilde (~) characters, indicating a busy prompt. 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 window has standard minimize, maximize, and close buttons in the top right corner.

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



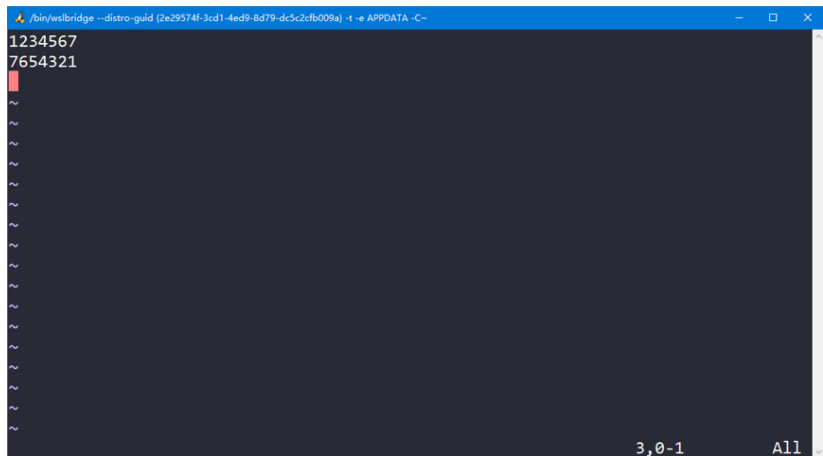
The screenshot shows a terminal window with a blue title bar. The title bar text is `/bin/wslbridge --distro-guid [2e29574f-3cd1-4ed9-8d79-dc5c2cfb009a] -t -e APPDATA -C-`. The terminal content is a dark blue background with a red cursor at the top left. The left margin has a vertical line of tilde characters (~). The bottom status bar shows `-- INSERT --` on the left, `0,1` in the center, and `All` on the right.

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 V

按一下 Esc 键, 从--INSERT--状态下退出



The screenshot shows a terminal window with a blue title bar containing the text `/bin/wslbridge --distro-guid {2e29574f-3cd1-4ed9-8d79-dc5c2cfb009a} -t -e APPDATA -C-`. The terminal content shows the first two lines of a file being edited in Vim: `1234567` and `7654321`. A red cursor is positioned at the start of the second line. Below these lines, a series of tilde characters (`~`) are visible, indicating the rest of the file. In the bottom right corner of the terminal, the text `3,0-1` and `All` are displayed, likely representing the current line and column or a search result.

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

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

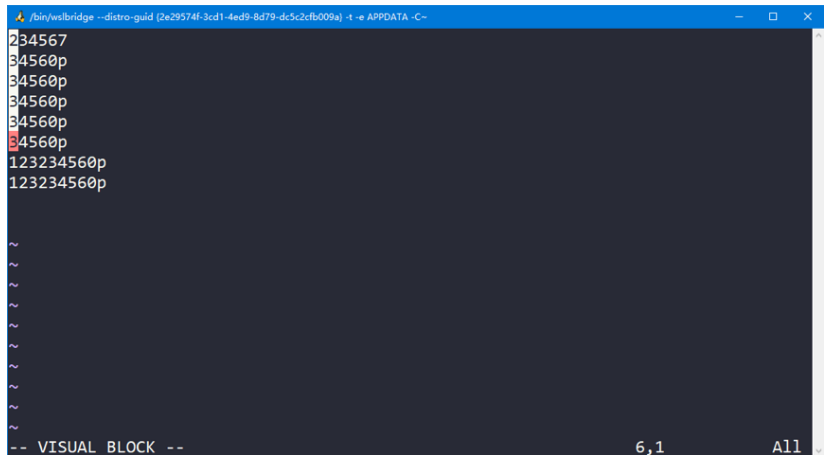
按一下 d 键则删除按列选中的文本

[illegible][illegible]

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

[illegible]

再连接两次 **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

POSCAR: 晶体结构文件

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. FIZ Karlsruhe | Contact Close session

Login

LogInID:

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 2: ICSD 搜索页面

获取晶体结构 II

AFLOW: Duke 材料基因组学数据库

The screenshot shows the AFLOW website's search interface. At the top, the AFLOW logo is displayed with the tagline "Automatic- FLOW for Materials Discovery". Below the logo is a navigation bar with links: HOME | CONSORTIUM | PUBLICATIONS | FORUM | SRC | SEARCH. A search bar is located below the navigation bar, with the text "Search Aflow" and a search button labeled "Search (88375 Compounds)". Below the search bar is a periodic table of elements. The periodic table is color-coded by groups: All Metals (blue), Alkali Metals (orange), Alkaline Earths (yellow), Transition Metals (green), Lanthanides (light blue), Other Metals (light green), Nonmetals (light yellow), Group 3A (light orange), Group 4A (light green), Group 5A (light blue), Chalcogens (pink), and Halogens (red). The periodic table also includes a search bar and a "Search" button. Below the periodic table is a table with columns for "Results Per Page:", "Total # of Results:", and "# of Species:". The table shows "Results Per Page: 40", "Total # of Results: 1000", and "# of Species: 0".

Figure 3: 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 website's search interface. At the top, a navigation bar includes links for Home, About, Apps, Documentation, API, Tutorials, and Dashboard. Below this is a search bar with a magnifying glass icon and a search button. The main content area features a periodic table of elements, with a search bar above it labeled 'Explore Materials' and 'Advanced Search Syntax'. The search bar contains the text 'Na-O' and a search button. To the right of the periodic table, there are several filters and search options: '# of elements' (with a dropdown menu showing 'e.g., 4 or >2 & <5'), 'excluded elements' (with a dropdown menu showing 'e.g., Bi'), 'Material Tags' (with a dropdown menu showing 'e.g., Inorganic'), 'Band Gap (eV)' (with a range slider from 0 to 10), 'Energy Above Hull' (with a range slider from 0 to 5), and 'Formation Energy' (with a range slider 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 4: MaterialsProject 搜索页面

执行 VASP 计算

创建运算目录

► 教学一号

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

► TMC PC

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

运行 VASP I

确认 vasp 可执行程序的位置: which

► 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 II

为什么第一次 `which` 的结果不同?

在教学一号上

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

运行 VASP III

```
$ cat sc_run_vasp.sh
#!/usr/bin/env bash                                # 解释器
#SBATCH -A 150xxxxxxx                               # 学号
#SBATCH --nodes=1                                    # 使用一个节点
#SBATCH -c 2                                          # 每个任务用 2 个核心
#SBATCH --partition=compute                          # 指定计算分区
#SBATCH -J test                                       # 任务名
#SBATCH -o stdout

module load intel/2018.0                            # 载入 Intel 编译器环境变量
module load vasp/5.4.4-intel18.0                    # 载入 VASP 环境变量 (PATH)

mpirun -np 2 vasp_std                                # 运行
```

运行 VASP IV

► 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