The installation of vasp

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The Vienna Ab initio Simulation Package, better known as VASP, is a package for performing ab initio quantum mechanical calculations using either Vanderbilt pseudopotentials, or the projector augmented wave method, and a plane wave basis set. The basic methodology is density functional theory (DFT), but the code also allows use of post-DFT corrections such as hybrid functionals mixing DFT and Hartree-Fock exchange, many-body perturbation theory (the GW method) and dynamical electronic correlations within the random phase approximation.

INTEL COMPILER

First of all, we need to install intel comiler with parallel studio from `https://software.intel.com/zh-cn/parallel-studio-xe`.

```
1 tar -xzvf parallel_studio (Tab)
2 cd parallel_studio (Tab)
3 su root
4 ./install_GUI.sh
```

The destination folder is /opt/intel. The serial number is

$$\text{S4ZD} - \text{XRZCDJ6Z} \tag{1}$$

Then we configurate the environment as root in ∼/.bashrc.

```
1 su root
2 source /opt/intel/parallel_studio (Tab)
  /psxevars.sh
3 source /opt/intel/bin
  /compilervars.sh intel64
4 source /opt/intel/impi/2019 (Tab)
  /intel64/bin/mpivars.sh
5 gedit ~/.bashrc
add at the end
(1) #for mkl mpi
(2) source /opt/intel/parallel_studio (Tab)
  /psxevars.sh
(3) source /opt/intel/bin
  /compilervars.sh intel64
(4) source /opt/intel/impi/2019 (Tab)
  /intel64/bin/mpivars.sh
(5) #end
```

The (Tab) means auto-completion.

FAST FOURIER TRANSFORM ALGORITHM

Before we install vasp, we need to install FFT.

```
1 su root
2 cd /opt/intel
  /compilers_and_libraries_2019 (Tab)
  /linux/mkl/interfaces/fftw3xf
3 make libintel64
```

We suggest that you download fftw from `http://www.fftw.org` at the same time.

```
1 su root
2 tar -xzvf fftw-3.3.8.tar.gz
3 cd ffte-3.3.8
4 ./configure --prefix=/opt/fftw/ CC=icc
  F77=ifort MPICC=mpiicc --enable-mpi
5 make
6 make install
```

VASP INSTALLATION

VASP is business software not open source. We suggest you purchase it through formal channels.

At the beginning, we need to modify the makefile.include. You could use `https://cms.mpi.univie.ac.at/wiki/index.php/Installing_VASP` as a reference.

```
1 su root
2 tar -xzvf vasp.5.4.4.tar.gz
3 cd vasp.5.4.4
4 cp arch/makefile.include.linux.intel
  makefile.include
5 gedit makefile.include
change the content
(14) FC = mpiifort
(15) FCL =mpiifort -mkl
(20) OFLAG = -02 -xhost
(25) BLAS =-L$(MKLPATH) -lmkl_intel_lp64
   -lmkl_sequential -lmkl_core -lpthread
   -lmkl_blacs_intelmpi_lp64
   -lmkl_scalapack_lp64
(30) OBJECTS = fftmpiw.o fftmpi_map.o
   fftw3d.o fft3dlib.o \
(31) /opt/fftw/lib/libfftw3_mpi.a
(32) INCS =-I/opt/fftw/include
```

Then we install the vasp.

```
1 su root
2 make all
3 cd vasp.5.4.4/bin
4 ls
5 gedit ~/.bashrc
add at the end
```

```
#for vasp
export PATH=$PATH:/home/qs/vasp.5.4.4/bin
#end
```

After the installation, there are vasp_gam, vasp_ncl, vasp_std. And you need INCAR, KPOINTS, POSCAR, POTCAR, before run vasp.

```
1 mpirun -np 4 vasp_std
```