# 如果手动安装，各种bug，环境问题

Problem setting up the Intel(R) Compiler compilation environment. Requires 'install path' setting gathered from 'g++'

dnf install gcc-c++

mpi run命令找不到

yum install mpich不对

应该是. /opt/intel/oneapi/setvars.sh

source /opt/intel/oneapi/setvars.sh

??

icc：命令未找到

准备文件

vasp.6.3.0.tgz

l\_BaseKit\_p\_2022.1.1.119\_offline.sh

l\_HPCKit\_p\_2022.1.1.97\_offline.sh

# 安装路径

cd /vasplocal/

# 已经下载到本地了，就不用wget了

#wget --no-check-certificate <https://registrationcenter-download.intel.com/akdlm/irc_nas/18445/l_BaseKit_p_2022.1.1.119_offline.sh>

sh ./l\_BaseKit\_p\_2022.1.1.119\_offline.sh -a -s --eula accept --components intel.oneapi.lin.mkl.devel

#wget --no-check-certificate <https://registrationcenter-download.intel.com/akdlm/irc_nas/18438/l_HPCKit_p_2022.1.1.97_offline.sh>

sh ./l\_HPCKit\_p\_2022.1.1.97\_offline.sh -a -s --eula accept --components intel.oneapi.lin.mpi.devel:intel.oneapi.lin.ifort-compiler:intel.oneapi.lin.dpcpp-cpp-compiler-pro

. /opt/intel/oneapi/setvars.sh

(**该命令之后，就出现了icc**)

cd /opt/intel/oneapi/mkl/latest/interfaces/fftw3xf/ && make libintel64

~~(icc找不到,把makefile里的某个icc 改成gcc就好了)~~

# 正式安装vasp：

cd /vasplocal/

tar -zxf vasp.6.3.0.tgz

cd /vasplocal/vasp.6.3.0/

cp arch/makefile.include.intel makefile.include

sed -i 's/\/path\/to\/your\/mkl\/installation//' makefile.include

. /opt/intel/oneapi/setvars.sh（一个初始化脚本，一定要输入，不然vasp-std找不到/vasp\_std: error while loading shared libraries: libmkl\_intel\_lp64.so.2: cannot open shared object file: No such file or directory）

make

RUN rm -rf /var/lib/apt/lists/\* && cp /vasp.6.3.0/bin/\* /bin/ && rm -rf l\_\* vasp\*

ENV LD\_LIBRARY\_PATH='/opt/intel/oneapi/mpi/2021.5.0//libfabric/lib:/opt/intel/oneapi/mpi/2021.5.0//lib/release:/opt/intel/oneapi/mpi/2021.5.0//lib:/opt/intel/oneapi/mkl/2022.0.1/lib/intel64' \

FI\_PROVIDER\_PATH='/opt/intel/oneapi/mpi/2021.5.0//libfabric/lib/prov:/usr/lib64/libfabric' \

CPATH='/opt/intel/oneapi/mpi/2021.5.0//include:/opt/intel/oneapi/mkl/2022.0.1/include' \

PATH='/opt/intel/oneapi/mpi/2021.5.0//libfabric/bin:/opt/intel/oneapi/mpi/2021.5.0//bin:/opt/intel/oneapi/mkl/2022.0.1/bin/intel64:/usr/local/sbin:/usr/local/bin:/usr/sbin:/usr/bin:/sbin:/bin:'

# slurm提交任务脚本

#!/bin/bash

#SBATCH --job-name=sl\_vasp#作业名任取

#SBATCH --partition=debug#提交到哪个分区

#SBATCH --nodes=1 #节点数

#SBATCH --ntasks=40 #总核数

#SBATCH --ntasks-per-node=40#每节点核数

#SBATCH --output=%j.out

#SBATCH --error=%j.err

#正式计算，其会读取当前文件夹内的4输入文件

mpirun -n $SLURM\_NTASKS vasp\_std

#mpirun -np $SLURM\_NPROCS vasp\_std

# VMware虚拟机CentOS8新系统，安装vasp的history

[root@vasp630 bin]# history

CentOS8initial.sh

1 mkdir vasplocal

3 cp l\_\* vasplocal/

4 cp vasp.6.3.0.tgz vasplocal/

5 cd vasplocal/

7 sh ./l\_BaseKit\_p\_2022.1.1.119\_offline.sh -a -s --eula accept --components intel.oneapi.lin.mkl.devel

8 sh ./l\_HPCKit\_p\_2022.1.1.97\_offline.sh -a -s --eula accept --components intel.oneapi.lin.mpi.devel:intel.oneapi.lin.ifort-compiler:intel.oneapi.lin.dpcpp-cpp-compiler-pro

10 . /opt/intel/oneapi/setvars.sh

11 cd /opt/intel/oneapi/mkl/latest/interfaces/fftw3xf/ && make libintel64

28 cd /vasplocal/

30 tar -zxf vasp.6.3.0.tgz

32 cd vasp.6.3.0/

~~33 cd /opt/intel/oneapi/mkl/latest/interfaces/fftw3xf/ && make libintel64~~

34 cd /vasplocal/vasp.6.3.0/

36 cp arch/makefile.include.intel makefile.include

37 vi makefile.include#将MKLROOT ？=，其余未动

38 . /opt/intel/oneapi/setvars.sh

39 make#发现缺少g++

42 dnf install gcc-c++

43 cd /

45 cd /opt/intel/oneapi/mkl/latest/interfaces/fftw3xf/ && make libintel64

47 reboot

48 cd /opt/intel/oneapi/mkl/latest/interfaces/fftw3xf/ && make libintel64

53 cd /vasplocal/

55 cd vasp.6.3.0/

57 make

58 . /opt/intel/oneapi/setvars.sh

59 cd /opt/intel/oneapi/mkl/latest/interfaces/fftw3xf/ && make libintel64

60 cd /vasplocal/

62 cd vasp.6.3.0/

64 . /opt/intel/oneapi/setvars.sh && make

65 make

67 cd bin

69 vasp\_std

70 ./vasp\_std

72 history