

VASP Benchmark

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VASP stands for **Vienna Ab-initio Simulation Package** and is a code written in FORTRAN 90 with MPI support that performs **quantum-mechanical molecular dynamics** (MD). This benchmark requires low latency networks to scale (Infiniband over GbE). A free software stack (Open64/MVAPICH2/ACML/ScaLAPACK) performs comparably to the Intel stack.

1 History

Version	Date	Notes
0.1.3	2022-06-14	Shell->bash, changes->history, typos
0.1.2	2020-12-27	Improve link section, line length
0.1.1	2020-05-03	Typos
0.1.0	2016-08-27	Initial release

2 VASP on Bright Cluster Manager

2.1 First Time Preparation

As root

```
cd /root/ckuelker/bm/bin
./speedup
./init-intel-license
./init-intel-compiler

cd /home/hpc/bm-vasp/src/Benchmarks
tar xvzf vasp.tar.gz
mv vasp vasp-007
chown -R hpc:hpc vasp-007
```

2.2 Before Every Run

As user `hpc` :

```
source /cm/shared/apps/intel-ics-2013/bin/compilervars.sh intel64
source /cm/shared/apps/intel-ics-2013/bin/iccvars.sh intel64
source /cm/shared/apps/intel-ics-2013/bin/ifortvars.sh intel64
source
↪ /cm/shared/apps/intel-ics-2013/impi/4.1.0.024/intel64/bin/mpivars.sh
↪ intel64
source /cm/shared/apps/intel-ics-
↪ 2013/composer_xe_2013.1.117/mkl/bin/mklvars.sh
↪ intel64
```

2.3 Build The Benchmark

```
cd /home/hpc/bm-vasp/src/Benchmarks/vasp-007
./build.sh
```

2.4 Run The Benchmark

```
cd /home/hpc/bm-vasp/src/Benchmarks/vasp-007
./run.sh
```

Eventually edit `run.sh` and change core number to be used.

2.5 Optimization

Optimization (changing compiler flags) in the make files:

```
Benchmarks/vasp/src/vasp.5.lib/Makefile
Benchmarks/vasp/src/wannier90-1.2/Makefile
Benchmarks/vasp/src/vasp.5.2.12/makefile
```

3 Example Session Debugging On Intel Cluster

The Intel cluster has 12 core per CPU, Intel(R) Xeon(R) CPU E5645 @ 2.40GHz. Assuming the source is in `~/bm/src/vasp.tar.gz`

```
tar xvzf bm/src/vasp.tar.gz
cd bm/src/vasp-5.2.12
module load intel/cs-xe-2013--binary
module load intelmpi/4.1.1--binary
module load blas/2011--intel--cs-xe-2013--binary
#module load boost/1.53.0--intel--cs-xe-2013--binary
```

One problem is that the Intel wrapper is not made available for VASP. The file `/lib/intel64/libfftw3xf_intel.a` do not exists. Which will be announced like this:

```
1 make: *** No rule to make target `/lib/intel64/libfftw3xf_intel.a', needed
  by
2 `vasp'. Stop.
```

3.1 Solving

```
mkdir -p ~/bm/build/intel/fftw3xf
cd /prod/compilers/intel/cs-xe-2013/binary/composer_xe_2013.1.117/mkl/\
interfaces/fftw3xf
make libem64t compiler=intel install_to=~/bm/build/intel/fftw3xf

echo "export
↳ LD_LIBRARY_PATH=/new/prod/compilers/intel/cs-xe-2013/binary/impi\
/4.1.1.036/lib64/:/new/prod/compilers/intel/cs-xe-
↳ 2013/binary/lib/intel64/:~/\
bm/build/intel/fftw3xf" > env
source env
```

That do not work, try this

```
cp src/vasp.5.2.12/makefile src/vasp.5.2.12/makefile.original
sed -i -e 's%\$(MKL_PATH)/libfftw3xf_intel.a%~/bm/build/intel/fftw3xf/\
libfftw3xf_intel.a%' src/vasp.5.2.12/makefile
diff src/vasp.5.2.12/makefile.original src/vasp.5.2.12/makefile
73c73
< FFT3D = fftmpi.o fftmpi_map.o fftw3d.o fft3dlib.o
↳ $(MKL_PATH)/libfftw3xf_intel.a
---
> FFT3D = fftmpi.o fftmpi_map.o fftw3d.o fft3dlib.o
↳ ~/bm/build/intel/fftw3xf/libfftw3xf_intel.a
```

Then an other error occurs

```
1 ifort: error #10236: File not found: '/opt/intel/mkl/lib/intel64/
libmkl_scalapack_lp64.a'
2 ifort: error #10236: File not found: '/opt/intel/mkl/lib/intel64/
libmkl_blacs_intelmpi_lp64.a'
```

They can be found at:

```
/prod/compilers/intel/cs-xe-2013/binary/composer_xe_2013.1.117/mkl/lib/intel64/
```

```
sed -i -e
↳ 's%/opt/intel/mkl/lib/intel64/libmkl_blacs_intelmpi_lp64.a%/prod/\
compilers/intel/cs-xe-
↳ 2013/binary/composer_xe_2013.1.117/mkl/lib/intel64/\
libmkl_blacs_intelmpi_lp64.a%' src/vasp.5.2.12/makefile

sed -i -e
↳ 's%/opt/intel/mkl/lib/intel64/libmkl_scalapack_lp64.a%/eurora_old/\
```

```
prod/compilers/intel/cs-xe-  
↳ 2013/binary/composer_xe_2013.1.117/mkl/lib/intel64/  
libmkl_scalapack_lp64.a%' src/vasp.5.2.12/makefile
```

4 Warnings

4.1 ifort - manual

Suppressing warning and remarks:

Option `-diag-disable warn` (Linux and Mac OS X) and `/Qdiag-disable:warn` (Windows) disable all Source Checker diagnostics except those that have an “error” severity level. They suppress all Source Checker warnings, cautions, and remarks.

5 Links

5.1 VASP Analysis and Profiling

The original link to a [PDF](#) from slides of 2013 should be available. However sometimes (2020-10-21) are not. In this case the document is available via [archive.org](#)

5.2 Installation, Compiling

- [VASP 5.3.5](#)
- [VASP 5.x.x](#)
- [VASp 6.x.x](#)
- [with Intel Composer XE 12.1.3 and OpenMP](#)

5.3 Intel MKL link advisor

- [Advisor v6.13](#)

5.4 Performance Optimisation

- Hardware optimization [Softpanorama](#)
- GCC and profiling [ivofilot.nl](#)
- [vasp.at](#) backup at [archive.org](#)

6 Disclaimer of Warranty

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