VASP Benchmark

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2023-03-14

Contents

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 (Infiband over GbE). A free software stack (Open64/MVAPICH2/ACML/ScaLAPACK) performs well, comparable to the Intel stack. For now, however, the examples given here are done with proprietary software.

1 VASP on Bright Cluster Manager

1.1 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
```

The `speedup` script sets the frequency of all CPU cores on each cluster node.

1.2 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
```

1.3 Build The Benchmark

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

1.4 Run The Benchmark

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

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

1.5 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
```

2 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` does not exist. This is announced like this:

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

2.1 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
```

If this does not work, which is probably the case, 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 another error may occur

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

This files can be found at:

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

And they should be replaced inside the `makefile`.

```
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
```

3 Warnings

3.1 ifort - manual

Suppressing warning and remarks:

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

4 Links

4.1 VASP Analysis and Profiling

The original link to a PDF https://www.hpcadvisorycouncil.com/pdf/VASP_Analysis_and_Profiling_AMD.pdf with slides from 2013 should be available. However, sometimes (2020-10-21) the PDF is not available. In that case, the PDF is available via archive.org https://web.archive.org/web/20190419065437/http://hpcadvisorycouncil.com/pdf/VASP_Analysis_and_Profiling_AMD.pdf.

4.2 Installation, Compiling

- VASP 5.3.5
- VASP 5.x.x
- VASp 6.x.x
- with Intel Composer XE 12.1.3 and OpenMP

4.3 Intel MKL link advisor

- Advisor v6.13

4.4 Performance Optimisation

- Hardware optimization Softpanorama
- GCC and profiling ivofilot.nl
- vasp.at backup at archive.org

5 History

Version	Date	Notes
0.1.4	2023-03-14	Improve writing, minor changes
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

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