CPMD 3.13.2 Best Practices for Intel® Cluster Ready

HPC ADVISORY COUNCIL
NETWORK OF EXPERTISE
BEST PRACTICES

1. Introduction

The following best practices document is provided as courtesy of the HPC Advisory Council.

2. Application Description:

CPMD is a computational chemistry package that has been developed by the Molecular Sciences Software group of the Environmental Molecular Sciences Laboratory (EMSL) at the Pacific Northwest National Laboratory (PNNL). It provides many methods to compute the properties of molecular and periodic systems using standard quantum mechanical descriptions of the electronic wave function or density. It also has the capability to perform classical molecular dynamics and free energy simulations.

3. Version Information:

Download CPMD 3.13.2 at:

http://www.cpmd.org/

Also download the patch for 3.13.2_01 from the download page.

4. Prerequisites:

The instructions from this best practice have been tested with the following configuration:

4.1 Hardware Used:

The instructions from this best practice have been tested on the HPC Advisory Council, Dell PowerEdge M610 blade server based cluster.

- Dell PowerEdge M610 14-node cluster
- Intel Xeon X5670 CPUs @ 2.93 MHz
- Memory: 24GB per node @ 1333MHz
- Mellanox ConnectX-2 QDR InfiniBand Adapters
- Mellanox QDR InfiniBand Switch

4.2 Software Used:

- Intel® Cluster Ready running CentOS 5 Update 4
- Application: CPMD 3.13.2
- Compilers: Intel compilers, GNU compilers
- MPI: Intel MPI 4, Open MPI 1.5, Platform MPI 8.0.1
- Benchmark workload:
  - o Si512

5. Building CPMD

% . $HOME/OpenFOAM/OpenFOAM-1.7.1/etc/bashrc

Make sure that you use GNU compilers 4.4 version and not the version that comes with RHEL or CentOS by default.

6. Building OPENFOAM

Extract CPMD

% tar cpmd3.13_2.tar.gz

% cd ~/CPMD-3.13.2/SOURCE

Patch CPMD

% patch -p2 < 3.13.2_01.patch

Modify sysdepend.c

During the compile, you will run into this error:

mpicc -c -O -DPOINTER8 -DFFT_DEFAULT -DPARALLEL=parallel -DMAIA-x86_64-INTEL-IMPI -DINTEL_MKL -D__LINUX -c /home/demo/CPMD-3.13.2/SOURCE/sysdepend.c

<command line>:1:5: warning: missing whitespace after the macro name

/home/demo/CPMD-3.13.2/SOURCE/sysdepend.c: In function 'timef_':

/home/demo/CPMD-3.13.2/SOURCE/sysdepend.c:692: error: too few arguments to function 'gettimeofday'

make: *** [sysdepend.o] Error 1

You will need to modify the gettimeofday on line 692 with these 2 lines

struct timezone tz;

status=gettimeofday(&t,&tz);

Modify Makefile for Intel MPI (Intel Compilers and MKL)

MKLPATH=/opt/intel/mkl

FFLAGS = -I/opt/intel/impi/4.0.1.007/include64 -L/opt/intel/impi/4.0.1.007/lib64 -I${MKLPATH}/include/intel64

LFLAGS = -lm -lpthread -Wl,--start-group -L${MKLPATH}/lib/intel64 ${MKLPATH}/lib/intel64/libmkl_solver_lp64.a ${MKLPATH}/lib/intel64/libmkl_intel_thread.a ${MKLPATH}/lib/intel64/libmkl_core.a -lmkl_intel_lp64 -lmkl_intel_thread -lmkl_core -lmkl_blacs_intelmpi_lp64 -liomp5 -lpthread -Wl,--end-group

CFLAGS =

CPP = /lib/cpp -P -C -traditional

CPPFLAGS = -DPOINTER8 -DFFT_DEFAULT -DPARALLEL=parallel -DMAIA-x86_64-INTEL-IMPI -DINTEL_MKL -D__Linux

NOOPT_FLAG =

CC = mpicc -c –O

LD = mpiifort

SRC = /home/demo/CPMD-3.13.2/SOURCE

FC = mpiifort -fc=ifort -c -I. -I$(SRC)

Makefile changes for Open MPI 1.5 (Intel compilers and MKL)

MKLPATH=/application/intel/mkl

FFLAGS = -I/application/openmpi-1.4.2-intel/include -L/application/openmpi-1.4.2-intel/lib -I${MKLPATH}/include/intel64

LFLAGS = -lm -lpthread -Wl,--start-group -L${MKLPATH}/lib/intel64 ${MKLPATH}/lib/intel64/libmkl_solver_lp64.a ${MKLPATH}/lib/intel64/libmkl_intel_thread.a ${MKLPATH}/lib/intel64/libmkl_core.a -lmkl_intel_lp64 -lmkl_intel_thread -lmkl_core -lmkl_blacs_openmpi_ilp64 -liomp5 -lpthread -Wl,--end-group

CFLAGS =

CPP = /lib/cpp -P -C –traditional

CPPFLAGS = -DPOINTER8 -DFFT_DEFAULT -DPARALLEL=parallel -DMAIA-x86_64-INTEL-IMPI -DINTEL_MKL -D__Linux

NOOPT_FLAG =

CC = icc -c –O

LD = mpif90

AR = /usr/bin/ar –r

SRC = /home/demo /CPMD-3.13.2/SOURCE

FC = ifort -c -I. -I$(SRC)

Makefile changes for Open MPI 1.5 (GNU compilers and ATLAS+LAPACK)

CFLAGS=-c -O2 –Wall

CPP=/lib/cpp -P -C –traditional

CPPFLAGS=-D__Linux -D__GNU -DFFT_FFTW -DPARALLEL -DPOINTER8 -D__Linux

FFLAGS=-c -O2 -fcray-pointer

LFLAGS=-L/usr/lib64/atlas -latlas -L/application/fftw-2.1.5-gnu/lib -lfftw –llapack

FFLAGS_GROMOS=' $(FFLAGS)'

FC=mpif77

CC=mpicc

LD=mpif77

SRC = /home/demo/CPMD-3.13.2/SOURCE

FC = mpif90 -c -I. -I$(SRC)

Makefile changes for Platform MPI (GNU compilers and ATLAS+LAPACK)

CPP=/lib/cpp -P -C –traditional

CPPFLAGS=-D__Linux -D__GNU -DFFT_FFTW -DPARALLEL -DPOINTER8 -D__Linux

FFLAGS=-c -O2 -I/application/fftw-2.1.5-gnu -fcray-pointer -I/opt/platform_mpi/include

LFLAGS=-L/opt/platform_mpi/lib/linux_amd64 -L/application/fftw-2.1.5-gnu/lib -L/usr/lib64/atlas -latlas -llapack -lfftw –lmpi

FFLAGS_GROMOS=' $(FFLAGS)'

FC=mpif77

CC=mpicc

LD=mpif77

7. Running CPMD

These are the examples of running CPMD, you may need to modify the file paths for your environment

Running with Intel MPI

% mpdboot -r ssh -f ~/mpd.hosts.ib.14 -n 14

% mpiexec -np 168 -IB /home/demo/CPMD-3.13.2/gnu-platformmpi/cpmd.x /home/demo/CPMD-test/std/Si512/inp-1

%mpdallexit

Running with Open MPI with Tuned Collectives

%mpirun -np 168 -mca btl self,sm,openib -hostfile \

/home/demo/hostfile-ompi.14 -mca mpi_paffinity_alone 1 \

-mca coll_base_verbose 1 -mca coll_tuned_use_dynamic_rules 1 \

-mca coll_tuned_alltoall_algorithm 3 -mca coll_tuned_allreduce_algorithm 4 \

/home/demo/CPMD-3.13.2/intel-ompi/cpmd.x /home/demo/CPMD-test/std/Si512/inp-1

Running with Platform MPI

% mpirun -np 168 -IBV -cpu_bind -prot -hostfile ~ /hostfile-ib14 /home/demo/CPMD-3.13.2/gnu-platformmpi/cpmd.x /home/demo/CPMD-test/std/Si512/inp-1

HPC ADVISORY COUNCIL
NETWORK OF EXPERTISE

350 Oakmead Pkwy, Sunnyvale, CA 94085
Tel: 408-970-3400 • Fax: 408-970-3403
www.hpcadvisorycouncil.com