NWChem 6.0 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:

NWChem 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 wavefunction or density. It also has the capability to perform classical molecular dynamics and free energy simulations.

3. Version Information:

Download NWChem 6.0 at:

http://www.nwchem-sw.org

4. Prerequisites:

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

4.1 Hardware:

- 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:

- OS: Intel® Cluster Ready Platform, using CentOS 5 Update 4
- Application: NWChem 6.0
- Compilers: Intel compilers, GNU compilers
- MPI: Intel MPI 4, Open MPI 1.5, MVAPICH2-1.5.1p1, Platform MPI 7.1
- Benchmark workload:
  - o siosi6: LDA calculations of 3 zeolite fragments (347,1687,3554) (Si28O67H30)
  - o h2o7: MP2 gradient calculation of molecule (H2O7)

5. Building NWChem

Extract NWChem

```
% tar xvfz Nwchem-6.0.tar.gz
```

Environment Variables for using Intel compilers

Prior to compiling the NWChem software, some of the environmental variables are needed to be set first.

```
export NWCHEM_TOP=~/nwchem/nwchem-6.0
export LARGE_FILES=TRUE
export ENABLE_COMPONENT=yes
export TCGRSH=/usr/bin/ssh
export NWCHEM_TARGET=LINUX64
export USE_MPI=y
export USE_MPIF=y
export IB_HOME=/usr
export IB_INCLUDE=$IB_HOME/include
export IB_LIB=$IB_HOME/lib64
export IB_LIB_NAME="-libumad -libverbs -lp-
  thread"
export ARMCI_NETWORK=OPENIB
export LD_LIBRARY_PATH=${LD_LIBRARY_
  PATH}:/application/intel/impi/lib64
export NWCHEM_MODULES=all
export FOPTIMIZE="-O3
  -xSSE2,SSE3,SSSE3,SSE4.1,SSE4.2 -no-prec-div
  -funroll-loops -unroll-aggressive"
export COPTIMIZE="-O3
  -xSSE2,SSE3,SSSE3,SSE4.1,SSE4.2 -no-prec-div
  -funroll-loops"
```

For more information on building NWChem with different compilers, you can visit this this Argonne wiki page:

https://wiki.alcf.anl.gov/index.php/NWChem

Environment variables for using Intel MPI 4

```
export MPI_HOME=/application/intel/impi
export MPI_LOC=$MPI_HOME
export MPI_LIB=$MPI_LOC/lib64
export MPI_INCLUDE=$MPI_LOC/include64
```

export LIBMPI='-lmpigf -lmpigi -lmpi_ilp64 -lmpi'

Environment variables for using MVAPICH2-1.5

export MPI_HOME=/application/mvapich2-1.5.1p1-intel

export MPI_LOC=$MPI_HOME

export MPI_LIB=$MPI_LOC/lib

export MPI_INCLUDE=$MPI_LOC/include

export LIBMPI='-lmpich -lrdmacm -libverbs'

Environment variables for using Platform MPI 7.1

export MPI_HOME=/opt/platform_mpi

export MPI_LOC=$MPI_HOME

export MPI_LIB=$MPI_LOC/lib/linux_amd64

export MPI_INCLUDE=$MPI_LOC/include/64

export LIBMPI='-lmpi'

Compiling NWChem using Intel Compilers

% cd $NWCHEM_TOP/src

% make nwchem_config

% make CC=/opt/intel/Compiler/11.1/073/bin/intel64/icc

FC=/opt/intel/Compiler/11.1/073/bin/intel64/ifort

6. Running NWChem

Running with Intel MPI

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

% mpiexec -np 168 -IB path_to/nwchem path_to/siosi6.nw

%mpdallexit

Running with MVAPICH2 MPI

%mpdboot -r ssh -n $host -f ~/hostfile-node14

%mpiexec -machinefile ~/machinefile.14 -np 168 path_to/nwchem path_to/siosi6.nw

% mpdallexit

Running with Platform MPI

% mpirun -np 168 -IBV -cpu_bind -prot -hostfile ~ / hostfile-ib14 path_to/siosi6.nw

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