NWChem 6.5
Installation Best Practices

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 aims to provide its users with computational chemistry tools that are scalable both in their ability to treat large scientific computational chemistry problems efficiently, and in their use of available parallel computing resources from high-performance parallel supercomputers to conventional workstation clusters.

3. Version Information:
NWChem 6.5. More information about NWChem is available at http://www.nwchem-sw.org.

4. Prerequisites:
The instructions from this best practice have been tested on the following configuration:
Hardware:

- Dell PowerEdge R730 32-node (1024-core) "Thor" cluster.
- Dual-Socket 14-Core Intel E5-2697Av4 @ 2.60 GHz CPUs
- Mellanox ConnectX-4 EDR InfiniBand adapters
- Mellanox Switch-IB 2 VPI InfiniBand switch

OS and software:

- RHEL 7.2
- MLNX_OFED_LINUX-3.3-1.0.4.0 InfiniBand SW stack
- MPI: Mellanox HPC-X v1.6.392 and Intel MPI 5.1.3

5. Building NWChem

5.1 HPC-X
The following shows the steps to compile NWChem using Mellanox HPC-X MPI toolkit:

```
module load intel/compiler/2016.3.210
module load hpcx/icc-2016
export LARGE_FILES=1
export USE_NOFSCHECK=1
export LIB_DEFINES="-DDFLT_TOT_MEM=1051477248"
export TCGRSH="/usr/bin/ssh"
export NWCHEM_TARGET=LINUX64
export ARMCI_NETWORK=OPENIB
export USE_MPI=y
export USE_MPIF=y
export MPI_LOC=$OMPI_HOME
export MPI_INCLUDE="-I$MPI_LOC/include -I$MPI_LOC/lib"
export MPI_LIB="-L$MPI_LOC/lib"
export LIBMPI="-lmpi_usempif08 -lmpi_usempi_ignore_tkr -lmpi_mpifh -lmpi"
```

```
export SCALAPACK="-L$MKLROOT/lib/intel64 -lmkl_scalapack_ilp64 -lmkl_intel_ilp6
4 -lmkl_core -lmkl_sequential -lmkl_blacs_intelmpi_ilp64 -lpthread -lm"
export SCALAPACK_SIZE=8
export BLASOPT="-L$MKLROOT/lib/intel64 -lmkl_intel_ilp64 -lmkl_core -lmkl_seque
ntial -lpthread -lm"
export BLAS_SIZE=8
export NWCHEM_TOP=$PWD


cd $NWCHEM_TOP/src
sed "s/-xW -tpp7/-xCORE-AVX2/g" -i $NWCHEM_TOP/src/tools/ga-5-3/configure

make clean
make nwchem_config NWCHEM_MODULES=all
make CC=icc FC=ifort
```

5.2 Intel MPI

The following shows the steps to compile NWChem using Intel MPI:

```
module load intel/compiler/2016.3.210
module load intel/impi/5.1.3.210
export LARGE_FILES=1
export USE_NOFSCHECK=1
export LIB_DEFINES="-DDFLT_TOT_MEM=1051477248"
export TCGRSH="/usr/bin/ssh"
export NWCHEM_TARGET=LINUX64
export ARMCI_NETWORK=OPENIB
export USE_MPI=y
export USE_MPIF=y
export MPI_LOC=$I_MPI_ROOT
export MPI_INCLUDE=$MPI_LOC/include64
export MPI_LIB=$MPI_LOC/lib64
export LIBMPI="-lmpifort -lmpi"
export SCALAPACK="-L$MKLROOT/lib/intel64 -lmkl_scalapack_ilp64 -lmkl_intel_ilp6
4 -lmkl_core -lmkl_sequential -lmkl_blacs_intelmpi_ilp64 -lpthread -lm"
export SCALAPACK_SIZE=8
export BLASOPT="-L$MKLROOT/lib/intel64 -lmkl_intel_ilp64 -lmkl_core -lmkl_seque
ntial -lpthread -lm"
export BLAS_SIZE=8
export NWCHEM_TOP=$PWD


cd $NWCHEM_TOP/src
sed "s/-xW -tpp7/-xCORE-AVX2/g" -i $NWCHEM_TOP/src/tools/ga-5-3/configure
```

```
make clean
make nwchem_config NWCHEM_MODULES=all
make CC=icc FC=ifort
```

6. Running NWChem using HPC-X

6.1 HPC-X

The following shows the runtime parameter used for running NWChem using Mellanox HPC-X:

```
module load intel/compiler/2016.3.210
module load hpcx/icc-2016
mpirun -np 1024 -bind-to core -mca btl_sm_use_knem 1 -mca coll_fca_enable 0 -mc
a coll_hcoll_enable 1 -mca coll_hcoll_np 0 -x HCOLL_ENABLE_MCAST_ALL=0 -x HCOLL
_CONTEXT_CACHE_ENABLE=1 -mca pml yalla -mca mtl_mxm_np 0 -x MXM_TLS=ud,shm,self
 -x MXM_RDMA_PORTS=mlx5_0:1 -mca btl_openib_if_include mlx5_0:1 -x MALLOC_MMAP_
MAX_=0 -x MALLOC_TRIM_THRESHOLD_=-1 <Executable> <INPUT>
```

6.2 Intel MPI

The following shows the runtime parameter used for running NWChem using Intel MPI:

```
module load intel/compiler/2016.3.210
module load intel/impi/5.1.3.210
mpirun -np 1024 -genv I_MPI_PIN on -genv I_MPI_DEBUG 4 -genv DAT_OVERRIDE /etc/
dat.conf -genv I_MPI_DAT_LIBRARY /usr/lib64/libdat2.so -IB -genv MV2_USE_APM 0
-genv I_MPI_FABRICS shm:ofa -genv I_MPI_OFA_USE_XRC 1 -genv I_MPI_OFA_NUM_ADAPT
ERS 1 -genv I_MPI_OFA_ADAPTER_NAME mlx5_0 -genv I_MPI_OFA_NUM_PORTS 1 -genv MAL
LOC_MMAP_MAX_=0 -genv MALLOC_TRIM_THRESHOLD_=-1 <Executable> <INPUT>
```