

DL-POLY 4 Installation Best Practices

1. Introduction:

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

2. Application Description:

DL_POLY is a general purpose classical molecular dynamics (MD) simulation software developed at Daresbury Laboratory by I.T. Todorov and W. Smith. The following instructions document the steps for running with the MPI libraries, Mellanox HPC-X

3. Version Information:

DL_POLY 4. More information about DL_POLY is available at <http://www.scd.stfc.ac.uk/SCD/44516.aspx>.

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 16-Core Intel E5-2697A v4 @ 2.60 GHz CPUs
- Mellanox ConnectX-4 EDR InfiniBand adapters
- Mellanox Switch-IB SB7700 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. Building DL_POLY

5.1 Makefile changes

Make the following changes to the Makefile for Mellanox HPC-X, or Intel MPI:

```
BDW.Intel.hpcx:
    $(MAKE) LD="mpif90 -o" \
    LDFLAGS="-O3 -xCORE-AVX2" \
    FC="mpif90 -c" \
    FCFLAGS="-O3 -xCORE-AVX2" \
    EX=$(EX) BINROOT=$(BINROOT) $(TYPE)

BDW.Intel.impi:
    $(MAKE) LD="mpiifort -o" \
    LDFLAGS="-O3 -xCORE-AVX2" \
    FC="mpiifort -c" \
    FCFLAGS="-O3 -xCORE-AVX2" \
    EX=$(EX) BINROOT=$(BINROOT) $(TYPE)
```

5.2 Building DL_POLY

Building DL_POLY for Mellanox HPC-X MPI Toolkit or Intel MPI

```

module load intel/compiler/2016.3.210
MPI=impi
MPI=hpcx

if [ "$MPI" == "hpcx" ]; then
    module load hpcx/icc-2016
elif [ "$MPI" == "impi" ]; then
    module load intel/impi/5.1.3.21
fi

make clean
make BDW.Intel$MPI

```

6. Running DL_POLY

6.1 Running DL_POLY with Mellanox HPC-X MPI Toolkit

```

module load intel/compiler/2016.3.210
module load hpcx/icc-2016
cp <input> $PWD

mpirun -np 1024 -bind-to core -mca btl_sm_use_knem 1 -mca coll_fca_enable 0 -mca
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 DLPOLY.Z

```

6.2 Running DL_POLY with Intel MPI

```

module load intel/compiler/2016.3.210
module load intel/impi/5.1.3.210
cp <input> $PWD

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 DLPOLY.Z

```