HOOMD Blue Install 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:

HOOMD-blue stands for "Highly Optimized Object-oriented Many-particle Dynamics - Blue Edition". It performs general purpose particle dynamics simulations. It takes advantage of NVIDIA GPUs. It is a free, open source software. The HOOMD-blue simulations are configured and run using simple python scripts. The development effort is led by Glotzer group at University of Michigan. Many groups from different universities have contributed code to HOOMD-blue.

3. Version Information:

HOOMD-blue (git master 28Jan14)

4. Prerequisites:

4.1 Hardware:

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

Dell™ PowerEdge™ R720xd 32 - node (640-core) "Jupiter" cluster

- Dual-Socket Hexa Core Intel E5-2680 V2 @ 2.80 GHz CPUs (Turbo mode enabled Unless otherwise stated)
- Memory: 64GB memory, DDR3 1600 MHz
- OS: RHEL 6.2, OFED 2.3-1.0.1 InfiniBand SW stack
- Hard Drives: 24x 250GB 7.2 RPM SATA 2.5" on RAID 0
- Intel Cluster Ready certified cluster
- Mellanox Connect-IB FDR InfiniBand adapters
- Mellanox ConnectX-3 QDR InfiniBand and Ethernet VPI adapters
- Mellanox SwitchX SX6036 VPI InfiniBand and Ethernet switches
- CUDA 5.5
- MPI

o Open MPI 1.8.4rc3

- Application: HOOMD-blue (git master 28Jan14)
- Benchmarks

o Lennard-Jones Liquid Benchmarks (16K, 64K Particles)

5. Installation Instructions

To compile HOOMD-blue, you would first need to install the dependencies for HOOMD-blue:

boost_1_55_0

cmake-2.8.12.1

6. Compiling HOOMD-blue

Follow the step to download the HOOMD-blue source code:

http://codeblue.umich.edu/hoomd-blue/doc/page_compile_guide_linux_generic.html

$ git clone https://bitbucket.org/glotzer/hoomd-blue

To compile HOOMD-blue with cmake (for MVAPICH2-GDR):

```
$ mkdir hoomd-build
$ cd hoomd-build
$ cmake -DPYTHON_EXECUTABLE=/usr/bin/python
-DCMAKE_INSTALL_PREFIX=/home/hoomd/hoomd-blue-
mvapich2gdr ../hoomd-blue/ -DCUDA_TOOLKIT_ROOT_DIR=/
usr/local/cuda-5.5 -DTHRUST_INCLUDE_DIR=/usr/local/cuda-
5.5/include
$ make -j 10 install
```

7. Running HOOMD-blue

Making sure nv_peer_mem is loaded for GPUDirect RDMA from the Mellanox web page:
http://www.mellanox.com/page/products_dyn?product_family=116

Compile and install the kernel module (nv_peer_mem.ko) according to its README file. Check the nv_peer_mem kernel module is loaded:

```
# lsmod|grep nv_peer_mem
nv_peer_mem          3750  0
ib_core            117605  12
nv_peer_mem,rdma_ucm,ib_ucm,rdma_cm,iw_cm,ib_
ipoib,ib_cm,ib_uverb
s,ib_umad,mlx5_ib,ib_sa,ib_mad
nvidia            8356269  2 nvidia_uvm,nv_peer_mem
```

8. Running the Benchmarks

For instance, the benchmark file contains the following settings:

$ cd hoomd-blue-ompi/share/hoomd/benchmarks

$ vim lj_liquid_bmark_8000.hoomd

```
#! /usr/bin/env python


from hoomd_script import *

init.create_random(N=8000, phi_p=0.2)
lj = pair.lj(r_cut=3.0)
lj.pair_coeff.set('A', 'A', epsilon=1.0, sigma=1.0)

all = group.all()
integrate.mode_standard(dt=0.005)
integrate.nvt(group=all, T=1.2, tau=0.5)


# warm up run
run(2000)


nlist.set_params(r_buff=0.4, check_period=5)
# these paramters ^^^       ^^^         are determined
automatically by running with the next line uncommented
# tune.r_buff(set_max_check_period=True)


# quick benchmark run
run(2000, profile=True)

# full benchmark
run(50000, limit_hours = 5.0 / 60.0)


#raw_input("Benchmark complete: press enter to exit");
```

For MVAPICH2-GDR:

```
$ mpirun_rsh -np 2 -hostfile
/home/hoomd/hostfile/hostfile.mvapich.4
MV2_USE_CUDA=1 MV2_USE_GPUDIRECT=1 /home/hoomd/
hoomd
-blue-mvapich2gdr/bin/hoomd /home/hoomd/hoomd-
blue-mvapich2gdr/share/hoomd/benchmarks/lj_liquid_
bmark_8000.hoomd
```

For Open MPI:

```
$ mpirun -x LD_LIBRARY_PATH –hostfile ~/hostfile -np 4 -mca
btl_openib_if_include mlx5_0:1 -mca
btl_openib_want_cuda_gdr 1
/home/hoomd/hoomd-blue-ompi/bin/hoomd /home/
hoomd/hoomd-blue-
ompi/share/hoomd/benchmarks/lj_liquid_bmark_8000.
hoomd
```

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