PyFR 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:

PyFR is an open-source Python based framework for solving advection-diffusion type problems on streaming architectures using the Flux Reconstruction approach of Huynh. The framework is designed to solve a range of governing systems on mixed unstructured grids containing various element types. It is also designed to target a range of hardware platforms via use of an in-built domain specific language derived from the Mako templating engine. For further information, see http://www.pyfr.org.

3. Version Information:

PyFR Version 1.0.0

Download from:

http://www.pyfr.org/download/PyFR-1.0.0.zip

4. Prerequisites:

4.1 Hardware:

The instructions from this best practice have been tested on the HPC Advisory Council, Dell™ PowerEdge™ R730 32-node cluster.

- Dual Socket Intel® Xeon® 14-core CPUs E5-2697 V3 @ 2.60 GHz
- Mellanox ConnectX-4 EDR 100Gb/s InfiniBand adapters
- Mellanox Switch-IB SB7700 36-Port 100Gb/s EDR InfiniBand switches

4.2 Software:

a. OS: Red Hat Enterprise Linux 6.5

b. GNU Compiler for Linux; 4.8.2

c. Other:

- Python-3.4.3
- mvapich2-2.1
- hdf5-1.8.15
- binutils-2.25
- Cmake-2.8
- OpenBlas-0.2.14
- CUDA-6.5

5. Installation

5.1 Building mvapich2 with CUDA support

Download mvapch2 from http://mvapich.cse.ohio-state.edu/download/mvapich/mv2/mvapich2-2.1.tar.gz.

```
export PATH=/usr/local/cuda-6.5/bin:$PATH

export LD_LIBRARY_PATH=/usr/local/cuda-6.5/lib64:$LD_LIBRARY_PATH

FLAGS="--enable-cuda "

FLAGS+="--with-libcuda=/usr/lib64 "

FLAGS+="--with-libcudart=/usr/local/cuda-6.5/lib64 "

FLAGS+="--with-cuda=/usr/local/cuda-6.5 "

FLAGS+="--prefix=<PATH>/mvapich2-2.1_cuda "

FLAGS+="--enable-f77 --enable-fc --enable-cxx "

FLAGS+="--with-pmi --with-slurm "

FLAGS+="--with-device=ch3:mrail --with-rdma=gen2 "

./configure $FLAGS

make -j 24

make install
```

5.2 Building Python3

Download python3 from https://www.python.org/ftp/python/3.4.3/Python-3.4.3.tgz.

```
./configure --prefix=$PWD/install

make

make test

make install
```

5.3 Installing Python packages for PyFR

```
export PYTHONHOME=<Path to Python3>

export PATH=$PYTHONHOME/bin:$PATH

pip3 install --upgrade pip
```

a. h5py

```
# Uncomment below two lines if h5py installation fails.
#export CFLAGS="-I${HDF5_DIR}/include"
#export LDFLAGS="-L${HDF5_DIR}/lib"

pip3 install h5py
```

b. mpi4py

```
export PATH=<PATH>/mvapich2-2.1_cuda/bin:$PATH
pip3 install mpi4py
```

c. pycuda

```
export CFLAGS="-I/usr/local/cuda-6.5/include"
export LDFLAGS="-L/usr/local/cuda-6.5/lib64"
pip3 install pycuda
```

d. Other packages

```
pip3 install mako
pip3 install mpmath
pip3 install numpy
pip3 install pytools
```

5.4 Building metis-5.1.0

Download metis from http://glaros.dtc.umn.edu/gkhome/fetch/sw/metis/metis-5.1.0.tar.gz.

```
export PATH=<Path to CMake>/bin:$PATH
make config shared=1 cc=gcc prefix=$PWD/install

make
make install
```

5.5 Building OpenBLAS

Download OpenBlas from http://github.com/xianyi/OpenBLAS/archive/v0.2.14.tar.gz.

```
make
make PREFIX=$PWD/install install
```

5.6 Building PyFR

```
export PATH=<Path to CMake>/bin:<Path to metis-5.1.0>/bin:$PATH
cd PyFR-1.0.0
export PYTHONPATH=.:$PYTHONPATH

python3 setup.py build
python3 setup.py install

# pyfr should be installed under $PYTHONHOME/bin.
```

6. Running PyFR using Taylor_Green dataset

```
export LD_LIBRARY_PATH=<Path to metis-5.1.0>/lib:$LD_LIBRARY_PATH
export PYTHONHOME=<Path to Python3>
export PATH=$PYTHONHOME/bin:<Path to metis-5.1.0>/bin:<PATH>/mvapich2-2.1_cuda/bin:$PATH

# For openmp backend, add following lines to taylor_green.ini:
[backend-openmp]
cblas = <PATH to OpenBLAS>/lib/libopenblas.so

# For cuda backend, add following lines to taylor_green.ini:
backend-cuda]
device-id = round-robin

# To execute PyFR using 8 nodes with 28 cores per node and CUDA.
NP=$((28*8))
pyfr partition $NP taylor_green.pyfrm taylor_green-1-84.515.pyfrs .
mpirun -n $NP pyfr restart taylor_green.pyfrm taylor_green-1-84.515.pyfrs taylor_green.ini -p -b cuda
```

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