Setting RHEL 7 for scientific research (ML, Statistics, Genomics, IoT)

Gcc 4.8.5 (Default)

# Install Intel parallel XE

For one month, it is free

2019 version has compatibility with CUDA 10.1

MKL

Install C, C++, Fortran

CC=”icc”

CXX=”icpc”

F77=”ifort”

FC=”ifort”

AR=”xiar”

LD=”xild”

“-fPIC -qopenmp -O3 -ipo -xHost”

./configure CC=icc AR=xiar CFLAGS="-fwrapv" –enable-optimizations

# Install another GCC 8.2.0

GCC 8.2.0 has compatibility with CUDA 10.1

Install C, C++, Fortan

CC=$HOME/toolchains/bin/gcc CXX=$HOME/toolchains/bin/g++ **\**

cmake .. -DCMAKE\_CXX\_LINK\_FLAGS="-Wl,-rpath,$HOME/toolchains/lib64 -L$HOME/toolchains/lib64"

$ clang++ -std=c++11 -stdlib=libc++ -nostdinc++ **\**

-I<libcxx-install-prefix>/include/c++/v1 **\**

-L<libcxx-install-prefix>/lib **\**

-Wl,-rpath,<libcxx-install-prefix>/lib **\**

test.cpp

# install clang

Check libstdc++, libc

# Install CUDA

10.2 – 2020/05/06 most updated one

10.1 – Good for compatibility

10.0 – keep for safety

CuDNN 7.6.5

GTX 750 Ti – cuda capability 5.0

# Install R

Compile with Intel cc has better performance

MKL

# Install python

Using pyenv, install multiple versions

Using jupyter notebook, keep isolated environment

Install cupy, numpy, scipy, cuda

# Install openmpi

4.0.2 (2019/10) – prefix=$HOME/local

Mpicc

Mpic++

Mpifort

# Install tensorflow

Bazel

R2.0 – this version is working with Bazel

R2.1 – most updated version (5/6/2020)

# Install pytorch

Packaged version with cuda 10.1 does not work!

# Tip

Ldd -> show related library (to check underneath library)

Strace -> show error

# RHEL

Make account – ibm-cloud-faith

# Jupyter setting

Python virtualenv

> pyenv virtualenv 3.3.3 pytorch

> pyenv activate pytorch

> pyenv virtualenvs

> pyenv deactivate