Hi , This is related to issues I have been facing with the setting up and running of Einstein toolkit on a cluster located at IUCAA, Pune, India.

The cluster is brand new and is based on a PBS job scheduler. Various modules on the cluster have to be loaded separately if required (using 'module load <package>' command) . There are two versions of HDF5 centrally available on the cluster: 1). hdf5-1.8.18 and 2). hdf5-1.10.4 as a part of the anaconda2 package (which also has to be loaded separately if required).

I am facing three issues which I will detail here. I will also mention some of the things I tried to fix them:

1. HDF5 version mismatch error:

      I have defined the directories of various packages required in the configuration script and pass it to sim for building (i.e. defined HDF5_DIR, HDF5_LIB_DIRS, HDF5_INC_DIRS , and simularly for hwloc, fftw3, MPI , etc) . Some packages were already centrally installed in the cluster and some I had to compile myself locally. I have supplied these paths to them (and added these package location to the environment variable $PATH and $LD_LIBRARY_PATH in $Home/.bashrc). I am using serial HDF5.

The issue I am facing is, whenever I compile with an HDF5 version other then 1.8.12, I get an error at runtime ' HDF5 version mismatch error' although compilation is successful. I have tried with: HDF5 1.10.5, 1.10.4, 1.8.21, 1.8.18 . According to the error message, the version mismatch is between hdf5-1.8.12 and the version I used to compile ETK(one of the above mentioned). Since the cluster / my user directory does not have hdf5 1.8.12, is it possible that some part of ETK is already compiled with 1.8.12 and that is leading to this error?

Here is an excerpt of the error:

Warning! ***HDF5 library version mismatched error***
The HDF5 header files used to compile this application do not match
the version used by the HDF5 library to which this application is linked.
Data corruption or segmentation faults may occur if the application continues.
This can happen when an application was compiled by one version of HDF5 but
linked with a different version of static or shared HDF5 library.
You should recompile the application or check your shared library related
settings such as 'LD_LIBRARY_PATH'.
'HDF5_DISABLE_VERSION_CHECK' environment variable is set to 1, application will
continue at your own risk.
Headers are 1.8.12, library is 1.10.4
      SUMMARY OF THE HDF5 CONFIGURATION
      ===============================

General Information:

      HDF5 Version: 1.10.4
      Configured on: Wed Dec 19 18:26:52 UTC 2018
      Configured by: root@3dad7c19-81ba-4672-4f33-547177f88490
      Host system: x86_64-conda_cos6-linux-gnu
      Uname information: Linux 3dad7c19-81ba-4672-4f33-547177f88490 4.4.0-62-generic #83-Ubuntu SMP Wed Jan 18 14:10:15 UTC 2017 x86_64 x86_64 x86_64 GNU/Linux
      Byte sex: little-endian

2. After this , What I then proceeded to do was to set the environment variable '
HDF5_DISABLE_VERSION_CHECK' to 1 or more as suggested by simfactory. In this case,
although the version mismatch error goes away, there are many HDF5 related warnings from
CARPETIOHDF5 from every process , everytime it attempts to open/write to an h5 file saying that
almost every hdf5 operation has failed because an attribute passed on to the hdf5 function was
invalid. I give here few examples :

HDF5-DIAG: Error detected in HDF5 (1.10.4) thread 140124312234880:
  #000: H5Tcompound.c line 344 in H5Tinsert(): not a compound datatype
    major: Invalid arguments to routine
    minor: Inappropriate type
  #000: H5Tcompound.c line 344 in H5Tinsert(): not a compound datatype
    major: Invalid arguments to routine
    minor: Inappropriate type

HDF5-DIAG: Error detected in HDF5 (1.10.4) thread 140198128102272:
  #000: H5P.c line 253 in H5Pcreate(): not a property list class
    major: Invalid arguments to routine
    minor: Inappropriate type

The simulation continues anyway.
Interestingly, both these errors (1 and 2) go away on compiling with hdf5-1.8.12.

2. Submission related warning:

I have tweaked the machine file in /simfactory/mdb/machines , the runscript and the submit script
with my knowledge to suit the cluster and then compiling the application. I am attaching them here.
On submitting a simulation using the 'sim create-submit' command, I always get the following
warning message:

Executing submit command: qsub -k oe /mnt/home/visitor/cvaishak/simulations/qc0-111/output-
0000/SIMFACTORY/SubmitScript
Warning: submit either failed or could not determine job id, output:
Warning: 4839.hn1

The job gets submitted and runs , but I would like to fix this warning message. I think I am not
setting some of the variables right in the machine file (like submit pattern, exechost etc) .

3. Submit /Run errors:

I have taken the pbs-normal submit script and removed some lines that were not necessary to make
a submitscript for our cluster (see in attachments) .

On submitting a simulation that requires more than one node, I get the following error in the corresponding .err file:

+ set -e
+ cd /mnt/home/visitor/cvaishak/simulations/qc0-13/output-0000-active
+ echo Checking:
+ pwd
+ hostname
+ date
+ echo Environment:
+ export CACTUS_NUM_PROCS=64
+ CACTUS_NUM_PROCS=64
+ export CACTUS_NUM_THREADS=1
+ CACTUS_NUM_THREADS=1
+ export GMON_OUT_PREFIX=gmon.out
+ GMON_OUT_PREFIX=gmon.out
+ export OMP_NUM_THREADS=1
+ OMP_NUM_THREADS=1
+ echo Starting:
++ date +%s
+ export CACTUS_STARTTIME=1568286980
+ CACTUS_STARTTIME=1568286980
+ '[' 64 = 1 ']'
+ mpirun -np 64 /mnt/home/visitor/cvaishak/simulations/qc0-13/SIMFACTORY/exe/cactus_sim -L
3 /mnt/home/visitor/cvaishak/simulations/qc0-13/output-0000/qc0-mclachlan.par
Warning: Permanently added 'hpc008,10.1.3.8' (ECDSA) to the list of known hosts.^M
ssh_askpass: exec(/usr/libexec/openssh/ssh-askpass): No such file or directory^M
Permission denied, please try again.^M
ssh_askpass: exec(/usr/libexec/openssh/ssh-askpass): No such file or directory^M
Permission denied, please try again.^M
ssh_askpass: exec(/usr/libexec/openssh/ssh-askpass): No such file or directory^M
Permission denied (publickey,gssapi-keyex,gssapi-with-mic,password).^M
[mpiexec@hpc006] HYDU_sock_write (utils/sock/sock.c:289): write error (Bad file descriptor)
[mpiexec@hpc006] HYD_pmcd_pmiserv_send_signal (pm/pmiserv/pmiserv_cb.c:178): unable to
write data to proxy
[mpiexec@hpc006] ui_cmd_cb (pm/pmiserv/pmiserv_pmci.c:77): unable to send signal
downstream
[mpiexec@hpc006] HYDT_dmxu_poll_wait_for_event (tools/demux/demux_poll.c:77): callback
returned error status
[mpiexec@hpc006] HYD_pmci_wait_for_completion (pm/pmiserv/pmiserv_pmci.c:196): error
waiting for event
[mpiexec@hpc006] main (ui/mpich/mpiexec.c:336): process manager error waiting for completion

This does not happen with other MPI programs that I run on the cluster, when I use more than one node to run (like a python MPI code I submit as 'qsub script' using a PBS script similar and simpler to the one I used as a submitscript for ETK). The stdout corresponding to this is:

Simulation name: qc0-13
Running simulation qc0-13
Preparing:
Checking:

The run never starts.

Firstly, I believe I should'nt be getting this error as I do not on other MPI jobs that use more than one node. I tried to fix this error by locally compiling the program 'openssh' and 'ssh-askpass' since I do not have access to the central system directories (/usr/libexec) . The latter is stored in a 'libexec' directory in my user directory and I can't get simfactory or my profle to recognize its location. I have tried exporting this to $PATH and $LD_LIBRARY_PATH but this is probably not the right way.

I get the same error when I try to use more than a few nodes in an interactive session. An interactive session is launched by:

qsub -I -l select=n

and I use 'sim create-run ' to run the simulation on the selected compute nodes.

Thankyou in advance!