1. Introduction

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

2. Application Description:

Virtual Performance Solutions (VPS) is a software package developed by the ESI Group. The product is originated from the well-known CAE modeling application PAM-CRASH. The application of VPS is primarily used in the automotive industry, which the application is used for crash simulation and designing of occupant safety systems. It simulates the performance of a proposed vehicle design and evaluate the potential for injury to occupants in multiple crash scenarios

The following instructions document the steps for running ESI-PAMCRASH with the MPI library called Mellanox HPC-X

3. Version Information:

VPS Solutions Version 2013.1

4. Prerequisites:

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

4.1 Hardware:

The instructions from this best practice have been tested on the Dell PowerEdge R720xd 32-node cluster at the HPC Advisory Council.

- Intel® Xeon® 10-core CPUs E5-2680 V2 @ 2.80 GHz
- Mellanox ConnectX®-3 VPI 56Gb/s FDR InfiniBand HCA (Driver: MLNX_OFED 2.3-2.0.1)
- Mellanox SwitchX SX6036 36-Port 56Gb/s FDR InfiniBand switch

4.2 Software:

a) OS: Red Hat Enterprise Linux 6.2

b) Intel Compilers: composer_xe_2015.1.133

c) MPI Libraries: HPC-X version 1.2.0 (based on Open MPI 1.8.4)

5. Setting up PAM-CRASH (VPS) For running HPC-X:

The following details the changes needed to make newer HPC-X to work on PAM-CRASH. In order to take advantage of HPC-X, there are some changes needed to make, due to the fact that HPC-X is based on the more recent version of OMPI versions than the version of OMPI 1.4 that is supported in PAM-CRASH.

5.1 To load HPC-X library for Intel Compilers:

module use /opt/hpcx-v1.2.0-267-icc-MLNX_OFED_
LINUX-2.3-2.0.1-
redhat6.2/modulefiles
module load hpcx

5.2 Soft links to redirect old libraries

Need to create soft links for libmpi_f77.so.0, libmpi.so.0 and others. Otherwise you will see this:

[MPM] dlopen mpif_openmpi-1.4.o failed: libmpi_f77.so.0: cannot open shared object file: No such file or directory
[MPM] dlopen mpif_openmpi-1.4.o failed: libmpi_f77.so.0: cannot open shared object file: No such file or directory
[MPM] dlopen mpif_openmpi-1.4.o failed: libmpi_f77.so.0: cannot open shared object file: No such file or directory

You would need to add these soft links (needed by PAM-CRASH) to redirect the new libraries available in HPC-X:

[root@jupiter000 lib]# pwd
/application/hpcx-v1.2.0-267-icc-MLNX_OFED_LINUX-2.3-
2.0.1-redhat6.2/ompi-mellanox-v1.8/lib
[root@jupiter000 lib]# ln -s libopen-rte.so.7 libopen-rte.so.0
[root@jupiter000 lib]# ln -s libopen-pal.so.6 libopen-pal.so.0
[root@jupiter000 lib]# ln -s libmpi.so.1 libmpi.so.0
[root@jupiter000 lib]# ln -s libmpi_mpifh.so libmpi_f77.so.0

5.3 Include HPC-X path when running pamworld

Need to LD_PRELOAD libmpi.so because Open MPI has an issue with dlopen and python.

LD_PRELOAD=/application/hpcx-v1.2.0-267-icc-MLNX_OFED_
LINUX-2.3-2.0.1-redhat6.2/ompi-mellanox-v1.8/lib/libmpi.so.0
/path_to/VPS_2013.01_UNIX/vpsolver/2013.01/pamworld <…
rest of arguments>…

Otherwise you will see this error:

[jupiter032:38863] MCW rank 9 bound to socket 1[core 18[hwt 0]], socket 1[core 19[hwt 0]]: [./././././././././.][./././././././/B/B]
[warn] Epoll ADD(1) on fd 0 failed. Old events were 0; read change was 1 (add); write change was 0 (none): Operation not permitted

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It looks like opal_init failed for some reason; your parallel process is likely to abort. There are many reasons that a parallel process can fail during opal_init; some of which are due to configuration or environment problems. This failure appears to be an internal failure; here's some additional information (which may only be relevant to an Open MPI developer):

opal_shmem_base_select failed
 --> Returned value -1 instead of OPAL_SUCCESS

5.4 Command to run:

Please note that "-mpi openmpi-1.4" is specified so that the HPC-X can be used. And you could include the options for HPC-X in the -mpiext argument

LD_PRELOAD=/opt/hpcx-v1.2.0-268-icc-MLNX_OFED_LINUX-2.3-2.0.2-redhat6.5/ompi-mellanox-v1.8/lib/libmpi.so.0 pamworld -mpidir /opt/hpcx-v1.2.0-268-icc-MLNX_OFED_LINUX-2.3-2.0.2-redhat6.5/ompi-mellanox-v1.8/bin -mpi openmpi-1.4 -mpiext "-mca btl openib,sm,self -mca btl_openib_if_include mlx5_0:1 --map-by node -mca mtl ^mxm -mca coll_fca_enable 1 -x fca_mpi_slow_num_polls=100000000 -x fca_mpi_slow_sleep=0 --report-bindings -x OMP_NUM_THREADS=1" -prod pamcrash_safe -lic CRASH-SAF -cf hosts.list -fp 1 -vers 2012.3 SIDE.pc