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:
ESI PAM-CRASH 2015.1. For more information about ESI PAM-CRASH (VPS), please visit:
https://www.esi-group.com/software-solutions/virtual-performance/virtual-performance-solution

4. Prerequisites:
The instructions from this best practice have been tested on the following configuration:
Hardware:
- Dell PowerEdge R730 32-node (896-core) "Thor" cluster.
- Dual-Socket 14-Core Intel E5-2697Av4 @ 2.60 GHz CPUs
- Mellanox ConnectX-4 EDR InfiniBand adapters
- Mellanox Switch-IB 2 VPI InfiniBand switch

OS and software:
- RHEL 7.2, MLNX_OFED_LINUX-3.3-1.0.4.0 InfiniBand SW stack
- MPI: Mellanox HPC-X v1.6.392
- Compilers: Intel Composer 2016.3.210
- Application: ESI PAM-CRASH

5. Installation

It is assumed that PAM-CRASH has been installed on /opt/VPSolution-2015.01_Linux-em64t.

For the installation, this version of HPC-X was compiled and built using Intel Compilers 2015, it is necessary to compile HPC-X using the Intel Compilers 2016 to ensure the same version of Intel compiler runtimes are used across our software stack to guarantee stability of the software.

5.1 Compile HPC-X using Intel Compilers 2016
We use a script below to simply the compilation of HPC-X.

```
$ module load intel/compiler/2016.3.210
$ pwd
/opt/hpcx-v1.6.392-icc-MLNX_OFED_LINUX-3.3-1.0.0.0-redhat7.2-x86_64/sources
```

```
$ cat rebuild-ompi-i2016.sh
#!/bin/bash
module purge
module load intel/compiler/2016.3.210
export CC=icc
export CXX=icpc
export FC=ifort
export F77=ifort
rm -rf openmpi-gitclone
tar xfp openmpi-gitclone.tar.gz -C /dev/shm
cd /dev/shm/openmpi-gitclone

module use /opt/hpcx-v1.6.392-icc-MLNX_OFED_LINUX-3.3-1.0.0.0-redhat7.2-x86_64/
modulefiles
module load hpcx

./configure --prefix=${HPCX_HOME}/ompi-v1.10.i2016 --with-knem=${HPCX_HOME}/kne
m \
             --with-fca=${HPCX_HOME}/fca --with-mxm=${HPCX_HOME}/mxm \
             --with-hcoll=${HPCX_HOME}/hcoll \
             --with-platform=contrib/platform/mellanox/optimized \
             --with-slurm --with-pmi \
             --enable-mpi-thread-multiple --with-verbs 2>&1 | tee config-output.
log

make -j32 all 2>&1 |tee build.log
make -j24 install 2>&1| tee install.log
$ ./rebuild-ompi-i2016.sh
```

6. Running ESI PAM-CRASH using HPC-X

This is an example to run PAM-CRASH using HPC-X. The specification of the flags are described below:
- mpiext: The would include all the options for HPC-X. In the list of options specified, we specified mlx5_0:1 as the InfiniBand interface to be used.
- mpidir: To specify the HPC-X installation that we built using Intel Compilers 2016
- mpiexe: The HPC-X mpirun executable.

```
$ module load intel/compiler/2016.3.210
$ module use /opt/hpcx-v1.6.392-icc-MLNX_OFED_LINUX-3.3-1.0.0.0-redhat7.2-x86_6
4/modulefiles
module load hpcx.i2016
/opt/VPSolution-2015.01_Linux-em64t/vpsolver/2015.01/pamworld \
-mpiext '--display-map --report-bindings -x LD_PRELOAD=/opt/intel/compilers_and
_libraries_2016.3.210/linux/compiler/lib/intel64/libirc.so:/opt/hpcx-v1.6.392-i
cc-MLNX_OFED_LINUX-3.3-1.0.0.0-redhat7.2-x86_64/ompi-v1.10.i2016/lib/libmpi.so:
```

```
/home/esi/VPSolution-2015.01_Linux-em64t/vpsolver/2015.01/Linux/em64t/Shared/li
bifcoremt.so.5: -x HCOLL_ML_DISABLE_ALLGATHERV=1 --bind-to core -mca btl_sm_use
_knem 1 -x MXM_SHM_KCOPY_MODE=knem -x MALLOC_MMAP_MAX_=0 -x MALLOC_TRIM_THRESHO
LD_=-1 -mca coll_fca_enable 0 -mca coll_hcoll_enable 0 -mca pml yalla -mca mtl_
mxm_np 0 -x MXM_TLS=ud,shm,self -x MXM_SHM_RNDV_THRESH=32768 -x KMP_BLOCKTIME=0
 -mca btl openib,sm,self -mca btl_openib_if_include mlx5_0:1 -x MXM_RDMA_PORTS=
mlx5_0:1 -mca rmaps_base_dist_hca mlx5_0:1 -x fca_ib_dev_name=mlx5_0 -x HCOLL_M
AIN_IB=mlx5_0:1 -x HCOLL_IB_IF_INCLUDE=mlx5_0:1 -mca rmaps_base_mapping_policy
slot' \
-mpidir /opt/hpcx-v1.6.392-icc-MLNX_OFED_LINUX-3.3-1.0.0.0-redhat7.2-x86_64/omp
i-v1.10.i2016 \
-mpiexe /opt/hpcx-v1.6.392-icc-MLNX_OFED_LINUX-3.3-1.0.0.0-redhat7.2-x86_64/omp
i-v1.10.i2016/bin/mpirun \
-mpi openmpi-1.8.2 \
-prod pamcrash_safe -cf /home/esi/hostfile/hostfile.pmpi.124 -wd /tmp/esi/test
-fp 1 -nt 1  /tmp/esi/test/test_noFPM_75.pc
```