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:**

4. **Prerequisites:**
The instructions from this best practice have been tested on the following configuration:

   **Hardware:**
   - 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
   --with-fca=${HPCX_HOME}/fca --with-mxm=${HPCX_HOME}/mxm \
   --with-hcoll=${HPCX_HOME}/hcoll \n   --with-platform=contrib/platform/mellanox/optimized \n   --with-slm --with-pmi \n   --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_64/modulefiles
module load hpcx.i2016
/opt/VPSolution-2015.01_Linux-em64t/vpsolver/2015.01/pamworld \n   -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-icc-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/libcoremt.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_THRESH=0 -x mca coll_fca_enable 0 -x mca coll_hcoll_enable 0 -x mca pml_yalla -x mca mtl_mxm_np 0 -x MXM_TLS=ud,shm,sel_f -x MXM_SHM_RNDV_THRESH=32768 -x KMP_BLOCKTIME=0 -x mca btl_openib,sm.sel_f -x mca btl_openib_if_include mlx5_0:1 -x MXM_RDMA_PORTS=mlx5_0:1 -x mca rmaps_base_dist_hca mlx5_0:1 -x fca_ib_dev_name=mlx5_0 -x HCOLL_MAIN_IB=mlx5_0:1 -x HCOLL_IB_IF_INCLUDE=mlx5_0:1 -x mca rmaps_base_mapping_policy=slot' \
-mpirad /opt/hpcx-v1.6.392-icc-MLNX_OFED_LINUX-3.3-1.0.0.0-redhat7.2-x86_64/omp\n-i-v1.10.i2016 \n-mpiexe /opt/hpcx-v1.6.392-icc-MLNX_OFED_LINUX-3.3-1.0.0.0-redhat7.2-x86_64/omp\n-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