Machine-dependent Information

ISSP System B: Ohtaka

1. Append the following to the end of `~/.bashrc`:

```
ulimit -s unlimited
export PATH=$HOME/bin:$PATH
module purge
module load openmpi/4.1.5-oneapi-2023.0.0-classic
```

ISSP System C: Kugui

1. Append the following to the end of `~/.bashrc`:

```
ulimit -s unlimited
export PATH=$HOME/bin:$PATH
module purge
module load nvhpc-nompi/24.7 openmpi_nvhpc compiler-rt tbb mkl
if which nvidia-cuda-mps-control > /dev/null 2>&1 ; then
  export CUDA_MPS_PIPE_DIRECTORY=$(pwd)/nvidia-mps-$(hostname)
  export CUDA_MPS_LOG_DIRECTORY=$(pwd)/nvidia-log-$(hostname)
  echo "start nvidia-cuda-mps-control at" $(hostname)
  nvidia-cuda-mps-control -d
fi
```

> [!TIP]
> Script for loading the required `modules` and starting MPS.

PROF

about warning output

> [!INFO]
> The following messages may appear on the log file of the calculation, but you can ignore them.
>
> ```
> [cpu121:54969] 7 more processes have sent help message help-mpi-
> common-cuda.txt / dlopen failed
> [cpu121:54969] Set MCA parameter "orte_base_help_aggregate" to 0 to
> see all help / error messages
> ----------------------------------------------------------------------
> -------
> The library attempted to open the following supporting CUDA
> libraries,
> but each of them failed.  CUDA-aware support is disabled.
> libcuda.so.1: cannot open shared object file: No such file or
> ```

```
directory
libcuda.dylib: cannot open shared object file: No such file or
directory
/usr/lib64/libcuda.so.1: cannot open shared object file: No such
file or directory
/usr/lib64/libcuda.dylib: cannot open shared object file: No such
file or directory
If you are not interested in CUDA-aware support, then run with
--mca opal_warn_on_missing_libcuda 0 to suppress this message.  If
you are interested
in CUDA-aware support, then try setting LD_LIBRARY_PATH to the
location
of libcuda.so.1 to get passed this issue.
```