How to use YZ-HPC

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1 Getting started with the HPC

1.1 How do I get access to the HPC

Fill out the appropriate tab of the HPC Access Request Form. Access is typically granted within few business days.

1.2 How do I login in the system

Only SSH access is available to login in the system. Any SSH client from various Operating System can be used. Additionally a web browser can be used to get login (firefox, google-chrome, Internet Explorer and Microsft edges were tested).

1.2.1 From web browser

url https://10.100.11.71:443

Permission Accept the secure access

localhost 10.100.11.71

Port 22

username USERNAME

password PASSWORD

1.3 How do I run my jobs on the HPC

See the documents below sections for basic examples of several types of jobs on the HPC system.

- HPC Sample Job: OpenMPI
- HPC Sample Job: LAMMPS
- HPC Sample Job: Gaussian

1.4 How many jobs can I run?

1.5 Why are some of my jobs stuck in the queue?

2 HPC Sample Job: OpenMPI

2.1 Overview

This document shows a very simple ”Hello, World!” type program using OpenMPI libraries, adapted from MPI Tutorial: MPI Hello World.

mpi_hw.c

```
#include <mpi.h>
#include <stdio.h>

int main(int argc, char** argv) {
  MPI_Init(NULL, NULL);
  int world_size;
  MPI_Comm_size(MPI_COMM_WORLD, &world_size);
  int world_rank;
  MPI_Comm_rank(MPI_COMM_WORLD, &world_rank);
  char processor_name[MPI_MAX_PROCESSOR_NAME];
  int name_len;
  MPI_Get_processor_name(processor_name, &name_len);
  printf("Hello world from processor %s, rank %d"
     " out of %d processors\n",
     processor_name, world_rank, world_size);
  MPI_Finalize();
}
```

2.2 Loading OpenMPI

There are two different version of openMPI available for computing. They are version 2.1.3 and 3.0.0. Use module tools to load the appropriate version of the MPI.

```
$ module load openMPI
```

2.3 Compiling

On the login node or a compute node, the source can be compiled after the module loaded as:

```
$ mpicc -o mpi_hw mpi_hw.c
```

2.4 Running the compiled code

No one should run an MPI code directly in the HPC. Use batch script to submit as a job on the system.

2.5 Running MPI in batch

Make a Slurm job script named mpi_hw.sh with the following contents.

mpi_hw.sh

```
#!/bin/bash
$SBATCH --node=2
$SBATCH --job-name=mpi_hw
$SBATCH --output=mpi_hw

module load openMPI

mpicc -o mpi_hw mpi_hw.c

mpirun ./mpi_hw
```

2.6 Submitting job in Queue

```
$ sbatch mpi_hw.sh
```