How to use YZ-HPC

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Contents

1 Getting started with the HPC

The configuration of YZ-HPC is described below:

- Hardware
  - Compute Node: 05
    - CPU: Intel Xeon 4-core 2.1 GHz
    - RAM: 8 GB 800 MHz
  - Compute Node: 16
    - CPU: Intel Core 2 Duo 2.6 GHz
    - RAM: 4 GB 800 MHz
  - Total Core: 52 Compute Core
  - Total RAM: 104 GB
- Software
  - OS: Telisc OS
  - Module Environment: lmod
  - Task/Job Management and Schedular: SLURM
- Computation Software: OpenMPI (Version 2.1.3 and 3.0.0)
- Molecuar Dynamics: LAMMPS
- Computational Chemistry: Gaussian (g09)

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. Before requesting access, a minimum experience with the followings are expected:

- How to work on Linux Terminal
- How to write within Linux Terminal (with vim/nano)
- Basics of OpenMPI
- File transfer tools (rsync, FileZilla, WinSCP etc.)

1.2 YZ-HPC Documentation

All the documentation are described brifely at http://yz-hpc.phy.edu. An HPC Access Request Form or Registration form is available for registering into YZ-HPC. A username with password will be sent to the user after the registration completion. Those username and password is very important for login.

NOTE: DO NOT CHANGE THE PASSWORD.

1.3 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).

1.3.1 From web browser

url http://yz-hpc.phy.edu

CLI Click **Go to Command Line Interface**

Permission Accept the secure access

localhost 10.100.11.71

Port 22

username USERNAME

password PASSWORD

A login shell will be available if everything goes fine.

1.4 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

1.5 How many jobs can I run?

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

2 How do I use TextEditor

By default vim and nano text editor is provided in the YZ-HPC because of their simplicity.

2.1 Documentation on TextEditor

- Vim (An online tutorial is available at here)
- Nano (A simple tutorial is available at here)

3 How do I transfer file into/from YZ-HPC

Any standard SSH tool can be used to transfer files between HPC and client computer. The rsync, WinSCP are Filezilla very useful tools.

3.1 Documentation on File Transfer

4 HPC Sample Job: OpenMPI

4.1 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();
}
```

4.2 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
```

4.3 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
```

4.4 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.

4.5 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
```

4.6 Submitting job in Queue

```
$ sbatch mpi_hw.sh
```

4.7 Useful Links for openMPI

- MPI tutorial
- MPI tutorial

5 Script for Slurm Job Submission

The job flags are used with SBATCH command. The syntax for the SLURM directive in a script is ”#SBATCH ¡flag¿”. Some of the flags are used with the srun and salloc commands, as well as the fisbatch wrapper script for interactive jobs.

Table 1: My caption

Resource	Flag Syntax	Description	Notes
partition	–partition=general-compute	Partition is a queue for jobs.	default on ub-hpc is general-compute
qos	–qos=general-compute	QOS is quality of service value (limits or priority boost)	default on ub-hpc is general-compute
time	–time=01:00:00	Time limit for the job.	1 hour; default is 72 hours
nodes	–nodes=2	Number of compute nodes for the job.	default is 1; compute nodes
cpus/cores	–ntasks-per-node=8	Corresponds to number of cores on the compute node.	default is 1
node type	–constraint=IB or –constraint=IB&CPU-E564	Node type feature. IB requests nodes with InfiniBand	default is no node type specified; compute nodes
resource feature	–gres=gpu:2	Request use of GPUs on compute nodes	default is no feature specified;
memory	–mem=24000	Memory limit per compute node for the job. Do not use with mem-per-cpu flag.	memory in MB; default limit is 3000MB per core
memory	–mem-per-cpu=4000	Per core memory limit. Do not use the mem flag,	memory in MB; default limit is 3000MB per core
account	–account=group-slurm-account	Users may belong to groups or accounts.	default is the user's primary group.
job name	–job-name="hello_test"	Name of job.	default is the JobID
output file	–output=test.out	Name of file for stdout.	default is the JobID
email address	–mail-user=usernamebuffalo.edu	User's email address	required
email notification	–mail-type=ALL –mail-type=END	When email is sent to user.	omit for no email
access	–exclusive	Exclusive acccess to compute nodes.	default is sharing nodes