

High performance research computer in TAMU: Applications, Usage, and solutions to common questions

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1. Account

Home website of High-Performance Computing Center: <https://hprc.tamu.edu/>

Contact information of HPRC, you will need this many times and usually you will also need to make a phone call in case that your emails are not replied in time.

Hours: 9am-5pm

Location: 222 Jones St, Henderson Hall, Room 114A

Phone: 979-845-0219

Email: help@hprc.tamu.edu

Fax: 979-847-8643

HPRC in tamu provides three tiers of accounts, including **basic, startup, and research**, as below, and different account will be allocated with different amount of **Service Units (SUs)**. For detailed definition and calculation method of SU, please refer to the [official policy](#). Based on your identifies, you are eligible to apply for different accounts.

**Review table below for Service Units (SUs) of each allocation type in detail. 1 SU = 1 wallclock hour on 1 CPU.*

*** Basic allocations are 5000 SUs*

Type of Applicant	Need 5000 SUs?**	Need up to 100,000 SUs?	Need > 100,000 SUs?
Students	Basic		
Faculty	Basic	Startup	Research
Qualified Staff	Basic	Startup	Research
Post-Docs	Basic		
Research Associates	Basic	Startup	
Research Scientists	Basic	Startup	Research

1.1. Application form

To apply for an account, you will be asked to fill out an application form, which includes the following information. Take my application as an example.

1) Dr. O'Neill's personal information:

1. NetId: zoneill
2. 979-845-4931
3. zoneill@tamu.edu

2) Project description and software you need

We need to run a significant amount of building energy simulation cases to find the optimal scenarios. The software we will use include: EnergyPlus and GenOpt.

a. EnergyPlus is a whole building simulation program, and we will use version 9.3. Download link: <https://github.com/NREL/EnergyPlus/releases/tag/v9.3.0>

b. GenOpt, an optimization software which provides an easy-to-use interface with EnergyPlus. Download link: <https://simulationresearch.lbl.gov/GO/download.html>

3) Justification for using HPRC resources

Based on our estimation, the total execution time of our simulation experiment is more than 10,000 hours in our personal computer. Therefore, we think the high-performance computing system could help to resolve our execution time issues.

4) Justification for the number of hours requested..

Each of our simulation instance is involved with 6~24 parameters. To find the optimal scenarios, the number of required simulation instances with 6~24 parameters would be approximately 10,000 for this experiments. Besides, each instance takes approximately one cpu for 2 minutes. This process

need to be repeated for about 100~200 times for different experiment settings. Therefore, the total SUs need is $10,000 * 1/30 * 200 = 60,000$ SUs.

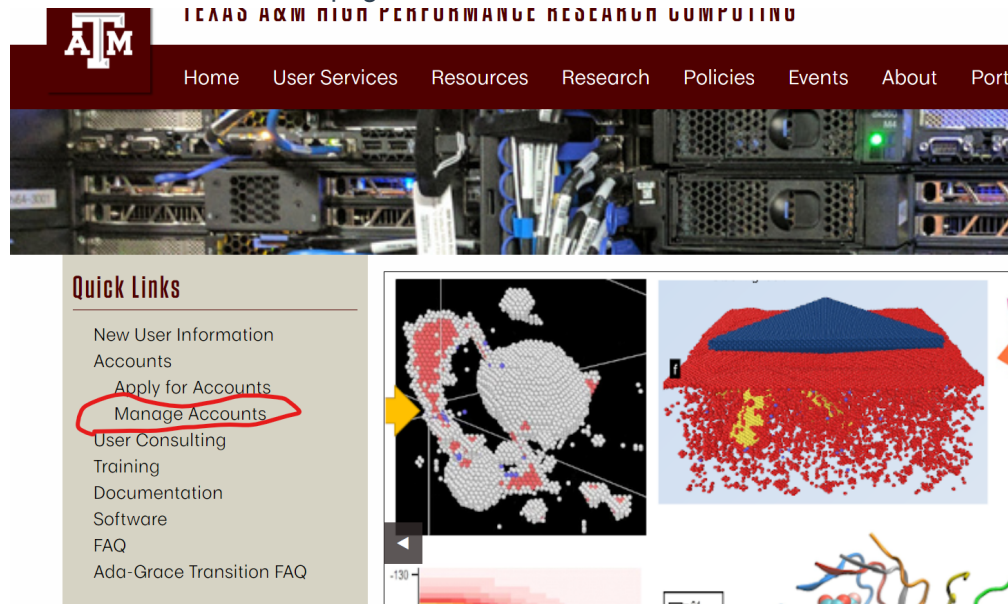
Other information

funding sources, researchers who will receive sub-allocations, etc.

1.2. Account manage

Usually after one or two office days, your application will be approved. However, as an student, we are only able to obtain less than 5,000 SUs and that is not enough for most cases. In this case, we could ask Dr. O'Neill (or your supervisor, research assistant in your group) to apply for a high tier account and then transfer their SUs to you.

After their applications completed, they could transfer their SUs in the [account management system](#). You are able to find this in the home page of HPRC.



The account manage system is slightly different for basic accounts and startup/research accounts. That is, the manage system for startup/research accounts have a “transfer” page where SUs transfer requests could be submitted. You might need to ask help desk to add the billing account of a researcher who will receive sub-allocations.

Transfer Billing Units

Please complete this form to transfer billing units between your billing account and the project billing account of one of your researchers. This form will list only researchers with active billing accounts under your billing accounts. Please email help@hprc.tamu.edu to add, remove, or renew a project billing account for a researcher under your billing account. The transferred SUs will be available in about one hour for job submissions on clusters.

1

1 researchers found under selected PI account

Please select a system by clicking on one of the items below:

Terra / 1 billing account

Please select a billing account for the selected system:

(Fiscal Year / Account Number / Primary? / Account Description / Current Balance / PI)

FY2021 / 122773824548 / No / Startup / 200000.00 / O'Neill, Zheng Deng

Please select the billing account of a researcher under your selected billing account:

(Researcher Name / Account Number / Total Granted / Current Balance)

Feng, Feng / 122857130222 / 0.00 / 0.00

Billing accounts for inactive researchers will NOT be available for transfers. For adding or removing researchers from your billing account or any other assistance, please email help@hprc.tamu.edu with your billing account and the researcher's name. The transferred SUs will be available in about one hour for job submissions on clusters.

Please enter an amount for the transfer:

☒ Transfer to researcher

☐ Transfer from researcher

Submit

Reset

After the transfer is completed, you are supposed to have sufficient SUs in your account and next you will move forward to access and usage of the HPC.

2. HPRC usage tutorial

HPRC provides us detailed user guides, which basically covers every aspects you will need, including access the HPRC, file transfer, Job submission and etc. You could find these user guides [here](#).

HPRC is a Linux system with GUI, and if you are familiar with Linux commands you will feel comfortable with this system. If not, you might need to learn it from scratch. Good luck.

2.1. Access your account

On windows computers, you could use either [Putty](#) or [MobaXterm](#). Both these are SSH shells that allow you connect to HPRC remotely.

If you need to connect to HPR from outside of the campus, you will need to activate TAMU VPN first.

Then, after you log into HPC, you could use the following command to check your account balance..

```
myproject -l
```

```
(base) [ffeng@terra2 ~]$ myproject -l
```

List of ffeng's Project Accounts							
Account	FY	Default	Allocation	Used & Pending SUs	Balance	PI	
122774970664	2021	N	150000.00	0.00	150000.00	O'Neill, Zheng Deng	
122774975429	2021	Y	5000.00	-1.22	4998.78	O'Neill, Zheng Deng	

2.2. file transfer

To transfer file into/from the HPC, you could use [WinSCP](#). You could find the detailed user guides [here](#).

Besides, you could also use GIT to download files from the online Repositories.

2.3. Software

HPRC has many pre-installed software, including python, cmake, and etc. You could search this by keywords using the following command, taking python as an example..

```
m1a python
```

You will get a list of python modules in the server. Then, you could select one of them by loading it to your account using the following command.

```
m1 Python/3.8.6-GCCcore-10.2.0
```

Generally, you need to load these software every time when you start a new HPR connection. So it is highly recommended to write all commands in a bash file.

2.3.1. Installing new software

Installing new software is the most tricky me for me.. Theoretically, you could ask the help desk to install software for you. However, after several request emails, the reply I got from the help desk is to install the software by myself, and here is the instructions they sent me.

```
export INSTALL_LOC=$SCRATCH/programs/EnergyPlus-9-5-0 # you can edit
mkdir -p $INSTALL_LOC
ml CMake/3.18.4-GCCcore-10.2.0
cd $SCRATCH
wget url(for your package)
tar -xzf v9-5-0.tar.gz
cd EnergyPlus-9.5.0
cmake -DCMAKE_INSTALL_PREFIX=$INSTALL_LOC

make -j4 install
echo "Program located at $INSTALL_LOC"
```

Basically, this instruction is correct. However, you will get some error when you follow this.

First, this cmake version might not work for you case. You could check the building instruction for you software which will give the cmake version requirements and etc.

The problem I got is

“CMake: The C Compiler is not able to compile a simple test program”

There are several solutions for this problem.

1) You could add an option to cmake command to walk around this problem as below.

```
cmake -CMAKE_TRY_COMPILE_TARGET_TYPE=STATIC_LIBRARY -
DCMAKE_INSTALL_PREFIX=$INSTALL_LOC
However, this doesn't work for my case.
```

2) Use a different cmake version, here is the version that I used.

```
ml CMake/3.16.4-GCCcore-9.3.0
```

Second, some software have some dependencies that is not installed or inconsistent with the existing software in the system. For example. EnergyPlus v9.3. require at least python 3, and if you have python 2 as default python version this installation process will raise a problem. So load python 3 to your system.

```
ml Anaconda3/2020.11
```

Lastly, after installation is completed, you need to add the installation path to you system path as below.

```
export PATH= $SCRATCH/programs/EnergyPlus-9-4-0:$PATH
```

2.4. Job submission, monitor, and etc.

Then, you could submit your Job and carry out your simulation. For this part, refer to the official guide for instructions.