Helium Cluster new user instructions (07/09/2020)

**1. Basic information**

-Operating system: openSusi

-Access: you can only edit files under your home directory. So you have to Install new program and tools in your home directory (/home/your\_name).

-Python environment: Conda is available, however, user cannot modify the base environment, to configure python environment, so it is recommended to create your own env if needed:

**2. Common programs**

-To enable a program in your environment, you need to include it in your .bashrc file. Here are the path for different program:

Basic python env:

export PATH=/opt/intel/intelpython3/bin:$PATH

Python version: 3.6.10

PSI4:

export PATH=/opt/software/psi4/psi4-github-bin-icpc-2020.2-opt-c++14/bin:$PATH

export LD\_LIBRARY\_PATH=/opt/software/gcc-7.2.0-install/lib:/opt/software/gcc-7.2.0-install/lib64:$LD\_LIBRARY\_PATH

export PYTHONPATH=/opt/software/psi4/psi4-github-bin-icpc-2020.2-opt-c++14/lib:$PYTHONPATH

Orca:

export PATH=/opt/software/orca\_4\_2\_1\_linux\_x86-64:$PATH

Molpro and several other programs are available on Emerson center clusters, ask if needed.

It is not necessary to install your own PSI4, unless you need to modify some psi4 functionality. If you want to install your own, follow <https://admiring-tesla-08529a.netlify.app/installs/v132/>

Forte:

a) Go to forte github page, <https://github.com/evangelistalab/forte>, clone the url. Then   
git clone “forte url”   
at the place where you want to install forte

b) Download and install ambit: <https://github.com/jturney/ambit>

Same with Forte, clone the url, git clone to the place you want.

c) Install ambit:

In the ambit folder you downloaded, write the cmake command, here is one example

cmake -H. -B~/source/ambit\_obj \

-DCMAKE\_INSTALL\_PREFIX=~/source/ambit\_install \

-DCMAKE\_C\_COMPILER=icc \

-DCMAKE\_CXX\_COMPILER=icpc \

-DCMAKE\_BUILD\_TYPE=Release

Then run this command.

After cmake, go to ambit\_obj directory, run

make

After make. Run

make install

Then ambit is ready to use. There should be an ambit\_install folder.

d) In the Forte folder you downloaded, run

psi4 –plugin-compile

This command should display a cmake command.

Then same as ambit, we write the cmake command, adding the ambit path.

Here is my example:

cmake -C \

/opt/software/psi4/psi4-github-bin-g++-7.2.0-opt-c++17/share/cmake/psi4/psi4PluginCache.cmake \ -DCMAKE\_PREFIX\_PATH=/opt/software/psi4/psi4-github-bin-g++-7.2.0-opt-c++17/bin/psi4 \ -Dambit\_DIR=/home/nan/source/ambit\_install/share/cmake/ambit \ -DCMAKE\_BUILD\_TYPE=Debug .

Then when cmake is done, run

make

Forte is now ready.

Remember to include forte install directory into your pythonpath, this is my example:

export PYTHONPATH=/home/nan/source/:$PYTHONPATH

Generally, it is good to keep a source folder under your home directory, then install everything there, this makes the path management easier.

**3. Job submission**

We are currently using Torque PBS for job management.

A general job submission script:

#!/bin/sh

# **Job configuration**

### Job name

#PBS -N test\_job

### Declare job non-rerunable

#PBS -r n

### Output files

#PBS -e test.err

#PBS -o test.log

### Number of nodes

#PBS -l nodes=1:ppn=1

# This job's working directory

echo Working directory is $PBS\_O\_WORKDIR

cd $PBS\_O\_WORKDIR

echo Running on host `hostname`

echo Time is `date`

echo Directory is `pwd`

echo This jobs runs on the following processors:

echo `cat $PBS\_NODEFILE`

# Define number of processors

NPROCS=`wc -l < $PBS\_NODEFILE`

echo This job has allocated $NPROCS nodes

# **Script Body**

# Run psi4 with scratch in a temporary directory

PSI4\_SCRATCH=`mktemp -d /tmp/psi4\_\_XXXXXX`

echo The psi4 scratch dir is $PSI4\_SCRATCH

function finish {

rm -rf "$PSI4\_SCRATCH"

}

trap finish EXIT

export OMP\_NUM\_THREADS=$NPROCS

export MKL\_NUM\_THREADS=$NPROCS

# Run psi4

psi4 -s "$PSI4\_SCRATCH" -n $NPROCS

We currently have 20 nodes (19 available for PBS) and 16 ppn each. PSI4 can take advantage of the parallelization, so to accelerate your job, you can use ppn=16 at max.

In your psi4 input file, you can specify how much memory you use:

memory 8 GB

Each node have a maximum 128 GB memory. For jobs with ppn=n, it is suggested to use a maximum memory of 8\*n GB, for example, ppn=8, memory use should be less than 64 GB.

The script body can be modified to run other jobs like Orca, qforte, PySCF or other python script, if interested.