Sample Jobs

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Introduction

Sample input and jobscript are also available for each installed application. Those samples can also be used as a template file for your jobs. In this page, we will show you procedures how to run those sample jobs using GAMESS and Gromacs examples.

As for Gaussian and ORCA, please check g16sub/g09sub and osub special commands, respectively.
(NOTE: registration is required to use ORCA)

List of Installed Applications

There are several ways to know which applications are installed.

1. at web page

You can see the application list in this page.

2. module avail

"module avail" command will give you a (long) list of applications. Applications which should be submitted as jobs would be listed in "/apl/modules/apl" category, which is colored with red in the box below.

```
[user@ccfep3 ~]$ module avail
---------------------- /home/users/qf7/modules/defaults ----------------------
2022  2024  2025

----------------------------- /apl/modules/oneapi ------------------------------
compiler-rt/2022.0.2  intelmpi/2021.5.1     mkl/2022.2.1    tbb/2021.10.0
compiler-rt/2022.2.1  intelmpi/2021.7.1     mkl/2023.0.0    tbb/2021.11
...
(skipped)
...
------------------------------ /apl/modules/apl ------------------------------
abcluster/3.0        gromacs/2023.2-CUDA          nwchem/6.8
ABINIT-MP/v1r22      gromacs/2023.4               nwchem/7.0.2
ABINIT-MP/v2r4       gromacs/2023.4-CUDA          nwchem/7.2.2
ABINIT-MP/v2r8       gromacs/2023.5               nwchem/7.2.2-CUDA
amber/20u13          gromacs/2023.5-CUDA          nwchem/7.2.3
amber/22u1           gromacs/2024.2               nwchem/7.2.3-intel
amber/22u4           gromacs/2024.2-CUDA          openbabel/3.1.1
amber/24u1           gromacs/2024.4               openmolcas/v21.10
...
gromacs/2022.6       ntchem/2013.13.0.0/mpi       xtb/6.7.0
gromacs/2022.6-CUDA  ntchem/2013.13.0.0/mpiomp    xtb/6.7.1
gromacs/2023.2       ntchem/2013.13.0.0/serial

Key:
loaded  directory/  auto-loaded  default-version  modulepath
[user@ccfep3 ~]$
```

(Press "q" key or scroll to the bottom to quit "module avail" command.)

3. see /apl directly

Non-OS standard applications and libraries are installed under /apl. You can directly check the list there.

```
[user@ccfep3 /apl]$ ls
```

```
ABINIT-MP     autoconf      cudnn      gsl        namd       orca
GRRM          autodock      cudss      hpc-x      nbo        pbs
LigandMPNN    autodock-gpu  cusparselt i-pi       nciplot    plumed
ProteinMPNN   autodock-vina dalton     imolpro    ninja      psi4
RFDiffusionAA bio           dftb+      julia      ntchem     qe
RFdiffusion   boost         dftd4      lammps     nvhpc      reactionplus
RoseTTAFold-AA censo        dirac      libtorch   nwchem     scalapack
abcluster     cmake         eigen      luscus     omegafold  siesta
aiida         colabfold     elsi       lustre-dev oneapi     tcl
alphafold     conda         ffmpeg     magma      openbabel  togl
amber         cp2k          gamess     modules    openblas   turbomole
aocc          crest         gaussian   molden     openmm     vmd
aocl          crystal       genesis    molpro     openmolcas xcrysden
apptainer     cuda          gromacs    mvapich    openmpi    xtb
[user@ccfep3 /apl]$ ls /apl/amber
20u13  22u1  22u4  24u1  24u3
[user@ccfep3 /apl]$ ls /apl/amber/20u13
amber.csh   build          configure  lib64     README     test
amber.sh    cmake          dat        logs      recipe_at  update_amber
AmberTools  CMakeLists.txt doc        Makefile  samples    updateutils
benchmarks  cmake-packaging include    miniconda share      wget-log
bin         config.h       lib        miniforge src
[user@ccfep3 /apl]$
```

Location of Sample Files

Sample input for a certain application is generally available under /apl/(application name)/(version/revision)/samples directory.

Example: check sample directory of gromacs 2024.5.

```
[user@ccfep3 /apl]$ ls /apl
ABINIT-MP     autoconf      cudnn      gsl        namd       orca
GRRM          autodock      cudss      hpc-x      nbo        pbs
LigandMPNN    autodock-gpu  cusparselt i-pi       nciplot    plumed
ProteinMPNN   autodock-vina dalton     imolpro    ninja      psi4
RFDiffusionAA bio           dftb+      julia      ntchem     qe
RFdiffusion   boost         dftd4      lammps     nvhpc      reactionplus
RoseTTAFold-AA censo        dirac      libtorch   nwchem     scalapack
abcluster     cmake         eigen      luscus     omegafold  siesta
aiida         colabfold     elsi       lustre-dev oneapi     tcl
alphafold     conda         ffmpeg     magma      openbabel  togl
amber         cp2k          gamess     modules    openblas   turbomole
aocc          crest         gaussian   molden     openmm     vmd
aocl          crystal       genesis    molpro     openmolcas xcrysden
apptainer     cuda          gromacs    mvapich    openmpi    xtb
[user@ccfep3 /apl]$ ls /apl/gromacs/
2016.5       2021.6       2022.4      2023.2-CUDA  2024.2      2024.5-CUDA
2016.6       2021.6-CUDA  2022.4-CUDA 2023.4       2024.2-CUDA 2025.2
2020.6       2021.7       2022.6      2023.4-CUDA  2024.4      2025.2-CUDA
2021.4       2021.7-CUDA  2022.6-CUDA 2023.5       2024.4-CUDA
2021.4-CUDA  2021.7-mdtest 2023.2      2023.5-CUDA  2024.5
[user@ccfep3 /apl]$ ls /apl/gromacs/2024.5
bin  include  lib64  samples  share
[user@ccfep3 /apl]$ ls /apl/gromacs/2024.5/samples/
conf.gro  grompp.mdp     sample-mpi.sh       sample-threadmpi.sh
cp2k      sample-mpi.csh sample-threadmpi.csh topol.top
```

(package name with "-CUDA" is GPU-enabled version.)

Files in Sample Directory

In a sample directory, there is only one input data set in principle.However, there can be several job scripts in a sample directory (same input but using different shell, hardware, setting method).

Examples:

- sample.sh => /bin/sh sample script
- sample.csh => /bin/csh sample script
- sample-gpu.sh => /bin/sh sample script using GPU

Reading and comparing those files might be helpful to you.

Example: gamess 2022R2

There are three scripts (sample.csh, sample-module.sh, sample.sh) for GAMESS 2022R2.

```
[user@ccfep4 ~]$ ls /apl/gamess/2022R2/samples/
exam01.inp  sample.csh  sample-module.sh  sample.sh
```

Example: gromacs 2024.5

There are four different scripts for Gromacs 2024.5.

```
[user@ccfep4 samples]$ ls
conf.gro  grompp.mdp      sample-mpi.sh       sample-threadmpi.sh
cp2k      sample-mpi.csh  sample-threadmpi.csh topol.top
```

- -mpi => parallel version with Open MPI (HPC-X); multinode parallel possible.
- -threadmpi => thread MPI parallel version; multinode parallel not available.
- (cp2k directory contains sample of QM/MM calculation using gromacs (double precision) and cp2k)

Run Sample: Basics

- copy files to your directory.
- "cd" to the directory, where the copied files exist
- submit a job (e.g. jsub sample.sh)
- Optional: usually, you can run samples on the login servers (e.g. sh ./sample.sh)
    - The way of # of CPUs specification might be different between "jsub" and "sh" cases.
    - GPU runs are not possible on ccfep. Please login to ccgpu from ccfep ("ssh ccgpu" command).
    - ccgpu is equipped with two GPU cards. MPI-parallel tests are also possible.

Example 1: gamess2022R2

We here assume your test directory is ~/gamess2022R2_test.

```
[user@ccfep4 ~]$ mkdir -p ~/gamess2022R2_test
[user@ccfep4 ~]$ cd ~/gamess2022R2_test
[user@ccfep4 gamess2022R2_test]$ cp /apl/gamess2022R2/samples/* .
[user@ccfep4 gamess2022R2_test]$ ls
exam01.inp  sample-module.sh  sample.csh  sample.sh
[user@ccfep4 gamess2022R2_test]$ jsub sample.sh
4008689.cccms1
```

Status of submitted job can be checked with "jobinfo -c".

```
[user@ccfep4 gamess2022R2_test]$ jobinfo -c
--------------------------------------------------------------------------------
Queue   Job ID Name            Status CPUs User/Grp       Elaps Node/(Reason)
--------------------------------------------------------------------------------
H       4008689 sample.sh      Run       4  user/---         -- ccc001
--------------------------------------------------------------------------------
[user@ccfep4 gamess2022R2_test]$
```

If the system is not terribly crowded, the job will soon finish and you can get the result.

```
[user@ccfep4 gamess2022R2_test]$ ls ~/gamess2022R2_test
exam01.dat  exam01.log  sample-module.sh  sample.sh.e4008689
exam01.inp  sample.csh  sample.sh         sample.sh.o4008689
[user@ccfep4 gamess2022R2_test]$
```

Reference: sample.csh (Explanations colored with blue do not exist in the original file)

```
#!/bin/sh
#PBS -l select=1:ncpus=4:mpiprocs=4:ompthreads=1  # <= 4-core job (in a vnode)
#PBS -l walltime=24:00:00  # <= time limit of this jobs is 24 hours

if [ ! -z "${PBS_O_WORKDIR}" ]; then
  cd ${PBS_O_WORKDIR}  # <= cd to directory where you submit job (standard action for PBS jobs)
  NCPUS=$(wc -l < ${PBS_NODEFILE})
else
  NCPUS=4  # <= these two lines are setting for non-queuing system run
  export OMP_NUM_THREADS=1
fi

module -s purge
module -s load intelmpi/2021.7.1     #  <= load required packages; depend on application
module -s load compiler-rt/2022.2.1

# processes per node; equal to mpiprocs value
PPN=4  # <= PPN = process per node; set to the mpiprocs value defined in the beginning

VERSION=2022R2
RUNGMS=/apl/gamess/${VERSION}/rungms
INPUT=exam01.inp

${RUNGMS} ${INPUT:r} 00 $NCPUS $PPN >& ${INPUT%.*}.log # <= run GAMESS here
```

Example 2: gromacs 2024.5

We here assume your test directory is ~/gromacs2024.5_test.

```
[user@ccfep4 ~]$ mkdir -p ~/gromacs2024.5_test
[user@ccfep4 ~]$ cd ~/gromacs2024.5_test
[user@ccfep4 gromacs2024.5_test]$ cp /apl/gromacs/2024.5/samples/* .
[user@ccfep4 gromacs2024.5_test]$ ls
conf.gro  grompp.mdp      sample-mpi.sh       sample-threadmpi.sh
cp2k      sample-mpi.csh  sample-threadmpi.csh topol.top
[user@ccfep4 gromacs2024.5_test]$ jsub sample-mpi.sh
4008695.ccpbs1
```

Status of submitted job can be checked with "jobinfo -c".

```
[user@ccfep3 gromacs2024.5_test]$ jobinfo -c
--------------------------------------------------------------------------------
Queue   Job ID Name           Status CPUs User/Grp       Elaps Node/(Reason)
--------------------------------------------------------------------------------
H       4008695 sample-mpi.sh  Run       6  user/---          -- ccc001
--------------------------------------------------------------------------------
```

If the system is not terribly crowded, the job will soon finish and you can get the result.

```
[user@ccfep4 gromacs2024.5_test]$ ls ~/gromacs2024.5_test
conf.gro     grompp.out       sample-mpi.sh          state.cpt
confout.gro  md.logmdout.mdp  sample-mpi.sh.e4008695  topol.top
cp2k         mdout.mdp        sample-mpi.sh.o4008695  topol.tpr
ener.edr     mdrun.out        sample-threadmpi.csh
grompp.mdp   sample-mpi.csh   sample-threadmpi.sh
[user@ccfep4 gromacs2024.5_test]$
```

Reference: sample-mpi.sh (Explanation colored with blue do not exist in the original file)

```
#!/bin/sh
#PBS -l select=1:ncpus=6:mpiprocs=6:ompthreads=1 # <= 6 core jobs (6 MPI processes)
```

```
#PBS -l walltime=00:30:00  # <= time limit is 30 minutes

if [ ! -z "${PBS_O_WORKDIR}" ]; then
 cd "${PBS_O_WORKDIR}" # <= chdir to job submission directory
 NPROCS=$(wc -l < "${PBS_NODEFILE}")
else
 # when jsub is NOT used # <= if jsub is not employed
 NPROCS=6
 export OMP_NUM_THREADS=1
fi

module -s purge
module -s load gromacs/2024.5 # <= environment vars etc. are read from module

###############################################################################

N_MPI=$NPROCS
N_OMP=$OMP_NUM_THREADS

gmx grompp -f grompp.mdp >& grompp.out
mpirun -n ${N_MPI} gmx_mpi mdrun -ntomp ${N_OMP} -s topol >& mdrun.out
```

Tips about job scripts

You can found some examples of job header lines in this page.