Guide to running GAMESS-US

What is GAMESS-US?

GAMESS (US) is a program for ab initio molecular quantum chemistry. Briefly, GAMESS can compute SCF wavefunctions ranging from RHF, ROHF, UHF, GVB, and MCSCF. Correlation corrections to these SCF wavefunctions include configuration interaction, second order perturbation theory and coupled-cluster approaches, as well as the density functional theory approximation. Excited states can be computed by CI, EOM, or TD-DFT procedures. Nuclear gradients are available for automatic geometry optimisation, transition state searches, or reaction path following.

Computation of the energy Hessian permits prediction of vibrational frequencies, with IR or Raman intensities. Solvent effects may be modelled by the discrete effective fragment potentials, or continuum models such as the Polarizable Continuum Model. Numerous relativistic computations are available, including infinite order two component scalar relativity corrections, with various spin-orbit coupling options. The Fragment Molecular Orbital method permits use of many of these sophisticated treatments to be used on very large systems, by dividing the computation into small fragments. Nuclear wavefunctions can also be computed, in VSCF, or with explicit treatment of nuclear orbitals by the NEO code.

Step 1 - Log in

The example used in this guide is configured to run on the Swansea Sandy Bridge cluster. Connect to *login.hpcwales.co.uk* with your HPC Wales user credentials using your preferred method (e.g. PuTTY from a Windows machine or ssh from any Linux terminal), then **`ssh sw-sb-log-001`** to connect to the Swansea system.

The steps below involve typing commands (**`in bold font`**) in the terminal window.

Step 2 - Load a GAMESS-US module

A number of GAMESS-US binary packages are available. Note that in common with most other software packages on the system, these are built with the Intel compiler.

- List pre-installed GAMESS_US versions:
  ```
  module avail gamess
  ```
- Load the preferred version (20131206):
  ```
  module load gamess
  ```
- Confirm the loaded modules. Note that this is currently the latest version of the code. All dependencies are handled automatically via the module file:
  ```
  module list
  ```

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Step 3 - Create a directory

From your home directory, create a directory to hold the GAMESS-US data:

```
cd ~
mkdir GAMESS
```

Step 4 - Obtain a test case

A number of test cases are provided with the installation at:

```
/app/chemistry/gamess/20131206/sb/intel-13.0/intel-4.1/example
```

and

```
/app/chemistry/gamess/20131206/sb/intel-13.0/intel-4.1/example/all
```

These directories contains the required GAMESS input files, as well as SLURM job scripts. Focusing on the first directory, copy the input file and job script to your user space:

```
cd ~/GAMESS
cp /app/chemistry/gamess/20131206/sb/intel-13.0/intel-4.1/example/example.inp .
cp /app/chemistry/gamess/20131206/sb/intel-13.0/intel-4.1/example/gamessexample.SLURM.q .
```

This 64-core example performs an MP2 optimisation on the molecular species $C_2H_2S_2$ in a CCQ basis set.

The other test cases may be copied to your user space as follows:

```
cp /app/chemistry/gamess/20131206/sb/intel-13.0/intel-4.1/example/all/*.inp .
cp /app/chemistry/gamess/20131206/sb/intel-13.0/intel-4.1/example/all/*.q .
```

There are three simple test cases, with input files exam01.inp (methylene, $^1A_1$ state, RHF/STO-2G), exam08.inp ($^1A_1$ H_2O RHF + MP2 gradient calculation) and exam15.inp (C_2 diatom, in the electronic state $^2\Pi_u$).

Step 5 - Submit a parallel job

You are now ready to run this test case with the supplied job script *gamessexample.SLURM.q*

- From your working directory, submit the job using: `sbatch gamessexample.SLURM.q`
- Check the job queue using: `squeue`
- Note that the example is executed under control of the `rungms` script,

  /app/chemistry/gamess/20131206/sb/intel-13.0/intel-4.1/bin/rungms

  with four parameters to be specified, as shown in the example. Note also that the majority of the files created during the job are routed to the user's scratch directory,

/scratch/$USER/GAMESS.<JobID>, and may be deleted on job termination. The 64-core job should complete in ca. seven minutes.

- If the case runs successfully, the log file - *example.sb.out.64.<JobID>* - routed to the GAMESS directory should contain all the output and the message “EXECUTION OF GAMESS TERMINATED NORMALLY”. Inspect the log files for more information.
- Compare your job output with the reference output file:

/app/chemistry/gamess/20131206/sb/intel-13.0/intel-4.1/example/example.sb.out.64

Step 6 - More Test Cases

More test cases are distributed with GAMESS. They can be found at

```
/app/chemistry/gamess/20131206/sb/intel-13.0/intel-4.1/tests/standard
```

and http://www.msg.ameslab.gov/gamess/GAMESS_Manual/tests.pdf

Adapt the job script above to run these cases.

To create a new case, refer to the section on Input Examples of the GAMESS Manual, which is widely available online: http://www.msg.ameslab.gov/gamess/GAMESS_Manual/tests.pdf

A PDF version of all sections of the documentation is also available at: http://www.msg.ameslab.gov/gamess/documentation.html

References

- Official GAMESS website: http://www.msg.ameslab.gov/gamess/
- GAMESS Update Paper: http://www.msg.ameslab.gov/advances/advances.html
- “General atomic and molecular electronic structure system”, Schmidt, M.W., Baldridge, K.K., Boatz, J.A., Elbert, S.T., Gordon, M.S., Jensen, J., Koseki, S., Matsunaga, N., Nguyen, K. A., Su, S., Windus, T.L., Dupuis, M., Montgomery, J.A.:J. Comput. Chem. 14, 1347-1363 (1993).
- GAMESS User Documentation: http://www.msg.ameslab.gov/gamess/documentation.html