Getting GAMESS Graphical

Jerry T. Godbout, Department of Chemistry, St. Bonaventure University
jtgodbou@sbu.edu

Disclaimer: This, like most free advice, is overpriced. The author has no formal involvement with any software package mentioned, but is at least a user of most .

This is basically a three-step process:

1. Input generation
    a. Generation of input geometry
    b. Specification of job parameters (basis set, optimization, etc)
2. GAMESS calculation
3. Converting text output to something humans can comprehend

Step 1 is split up since many packages can take care of step 1a, but not 1b. This isn't such a big deal though, since generating the input geometry is by far the most challenging part of the whole process. Adding a line or two of keywords afterwards is not a big deal

Option 1 – All in one package

WebMO (www.webmo.net)

This is a web-based interface that takes care of steps one and three. It has a point and click molecule builder similar to Spartan. You can also supply some of the more common parameter choices (job type, basis set) using drop down menus. Once the job is completed, WebMO condenses highlights of the job output into a web page (you can also access the complete raw output). Along with the final numbers, you get

- A dynamic ball and stick picture of the resulting structure
- Vector representations of normal modes and dipole moments

It can also use a few other types of structure files (such a set of xyz coordinates) as an input geometry. It is also possible to use the final geometry of one job as the starting point of another.

This package makes the whole process quite simple and works nicely for teaching environments. Its main weakness is that running non-standard jobs is awkward, but is possible to hack the scripts to make it quite easy again. There is a Pro version that isn't free, but does add some nice features. WebMO has a demo system on their web site you can play around with. The other requirement that may be problematic is that is must be run on a Linux system that will run GAMESS and act as the web server for WebMO as well. Overall, this system is quite nice for step 1, but leaves something to be desired for step 3.

Option 2 – As Many Packages As Necessary (Three, not counting GAMESS itself)

If you want the best of both worlds, you may want to use separate tools for handling the input and output. There are many packages available to handle either the input or output processing. Here is the general process.

1. Generating input geometry

   Many packages can generate some type of molecular geometry file from a point and click builder like Spartan's. One of these is ChemSketch from ACD labs. Although it's not free, the near ubiquitous Chem 3D also does this nicely. Generally these programs can't create a true GAMESS input file, but will give you the atomic coordinates in a few common formats such as xyz coordinates, or a .pdb or .mol format.

2. Babel, or WinBabel (http://www.eyesopen.com/products/applications/babel.html) is a program that can translate chemical data files. It can generate the initial geometry portion of the GAMESS input file, but you will have to supply the other keywords. Babel will even tell you where these lines are supposed to go.

3. Let GAMESS do its thing.

4. Process the output.

   There are many, many choices here. Two of the most powerful are Molekel (http://www.cscs.ch/molekel/ my current favorite) and Molden (http://www.cmbi.ru.nl/molden/). Both are available on both Windows and Unix/Linux platforms. Both however, do seem to run better under Unix/Linux. Both versions of Molden require X-Windows, which can be a little awkward to set up on Windows. Both of these programs:

   - Produce the requisite pretty molecule picture
   - Report structural parameters (bond lengths, angles, etc.)
   - Animate vibrations
   - Generate surfaces such as molecular orbitals and electrostatic potentials. (both programs can make some pretty sweet pictures)