Introduction to GaussView and Gaussian

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• Description of Both Programs
• How to Create Input Files (with GaussView)
• How to Submit Calculations
• How to Visualize Output
Gaussian 03:

an electronic structure package capable of predicting many properties of atoms, molecules, and reactive systems

e.g.

• Energies
• Structures
• Vibrational frequencies

utilizing *ab initio*, density functional theory, semi-empirical, molecular mechanics, and hybrid methods.
GaussView:

graphical interface for Gaussian 03

- build molecules or reactive systems
- setup Gaussian 03 input files
- graphically examine results
Description
• Input
• Submit
• Visualize
Calculations with Gaussian
Types of Calculations

- single point energy and properties (electron density, dipole moment, …)
- geometry optimization
- frequency
- reaction path following
Levels of Theory Available:

– semi-empirical
  AM1, PM3, MNDO, …

– density functional theory
  B3LYP, MPW1PW91, …

– ab initio
  HF, MP2, CCSD, CCSD(T), …

– hybrid
  G2, G3, …

The level of theory is the set of underlying approximations used to describe the chemical system. Higher levels of theory are often more accurate however they come at much greater computational cost.
Basis Sets Available:

– Pople-type
  3-21G, 6-31G, 6-311G(d,p), ...
– Dunning
  cc-pVDZ, aug-cc-pVTZ, ...
– Huzinaga and Others
  MIDIX, ...
– User-defined

Basis sets are used for most calculations in Gaussian. They are a set of functions that are used to describe electronic wavefunctions.
Creating Input Files for Gaussian
Water Optimization Input File

%mem=32mb

#p hf/6-31g opt

hf/6-31g optimization of water

0 1
0
h 1 oh
h 1 oh 2 ahol

oh=0.9
ahoh=104.0

system resources
computational model
type of calculation
title
charge & multiplicity
structure definition (z-matrix)
variable values
Spin multiplicity:

\[ \text{multiplicity} = n + 1 \]

where \( n \) = \# of unpaired electrons
Building with GaussView:

• Instead of typing all the coordinates, theory, basis set, etc., we can use GaussView.

• The calculation is specified by pointing and clicking to build the molecule, and using pull-down menus to select the calculation type, level of theory and basis set.

• GaussView generates the Gaussian input file, and can run Gaussian without ever returning to the Unix prompt.

• GaussView can also be used to read Gaussian output files and visualize the results.
Getting Started with GaussView:

• Login remotely
  ssh -X sp.msi.umn.edu

• Load Gaussian/GaussView module
  module add g03

• Launch GaussView
  gv
Description • Input • Submit • Visualize
<table>
<thead>
<tr>
<th>Mouse Button</th>
<th>Action</th>
<th>Function</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Left</strong></td>
<td>Click</td>
<td>Selects or inserts item</td>
</tr>
<tr>
<td></td>
<td>Drag Left/Right</td>
<td>Rotates about Y-axis</td>
</tr>
<tr>
<td></td>
<td>Drag Up/Down</td>
<td>Rotates about X-axis</td>
</tr>
<tr>
<td><strong>Center/Left-Right</strong></td>
<td>Drag</td>
<td>Translation of molecule</td>
</tr>
<tr>
<td><strong>Right</strong></td>
<td>Drag Left/Right</td>
<td>Rotates about Z-axis</td>
</tr>
<tr>
<td></td>
<td>Drag Up/Down</td>
<td>Zooms in and out</td>
</tr>
</tbody>
</table>

*Note: Holding down the Tab key limits mouse action to the closest distinct fragment.*
Molecule Building

Fragments are Selected

Selected fragments Are previewed here

Molecule is put together Here

Description • Input • Submit • Visualize
The atom labeled “Hot” is where the fragment will attach to the system you are building.
Steps to Building

• Choose an atom or fragment
• Choose the location of the fragment that will attach to your molecule in the builder window
• Select/add the fragment to your molecule in the viewer window
• repeat
Elements:
Ring Fragments:

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R-Group Fragments:
Biological Fragments:
Molecule Building

clean up

This option will use a MM calculation to optimize the geometry (very fast).
Submitting Calculations
Interactive:

Command:

```
g03 < input_file > output_file
```

Notes:

1) input and output files can use absolute or relative pathnames

2) Gaussian temporary files can be redirected by setting the GAUSS_SCRDIR environment variable.

```
setenv GAUSS_SCRDIR /scratch/pfast
```

3) BE CAREFUL how long you run interactively
Batch:

Command:

    qg03 [-options] input_file

Options:

- **h**: help, display a usage list and the defaults
- **e**: email notification
- **m**: total amount of memory
- **n**: node, choose the particular processor
- **p**: number of processors
- **r**: run?
- **s**: scratch space
- **t**: amount of wallclock time
Submitting jobs through GaussView:

Select **Gaussian**
Choose Job Type

Description • Input • Submit • Visualize
Method & Basis Set

Description • Input • Submit • Visualize
Save Input File
Description • **Input** • Submit • Visualize

[Image of a GaussView 3.07 software window with a Save Input File dialog box open. The dialog box shows a file path `/home/bsci/pfast/work/gaussian/kass/` and options for file name `test.com`, file type `Gaussian Input Files (*.gif, *.com)`, and save options `Write Cartesians`, `Append Extra Input`, `New Molecule Group`.]
The submission dialogue box will appear a little different depending on which machine you are running GaussView on.
Submitting your Gaussian job

If you haven’t saved your input file yet, Gaussview will prompt you to save your input file.

You will name the input file, and then submit the calculation.

When Gaussian is finished running, you will receive a message in Gaussview.
How to Visualize
Visualization Features

Description • Input • Submit • Visualize
How to view your output

• Your submitted calculation will run in the background.
• When it is complete, Gaussview will inform you and ask you if you wish to view an output file.
• From the list of files, you can pick your output (something.chk)
How to view your output

• If you ever want to open an output file again, you can go to:

  File → Open

In the GaussView menus to open any output file.
Output that can be visualized

- Geometry
- Vibrations
- Orbitals
- Electron density
- Electrostatic potential
Main results menu
Frequencies

Description • Input • Submit • Visualize
Spectra

Description • Input • Submit • Visualize
A cube file is a format of 3-D data that can be plotted.

You can generate a cube file to display orbitals, electron densities, electrostatic potentials, etc.
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Questions?

http://www.gaussian.com

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