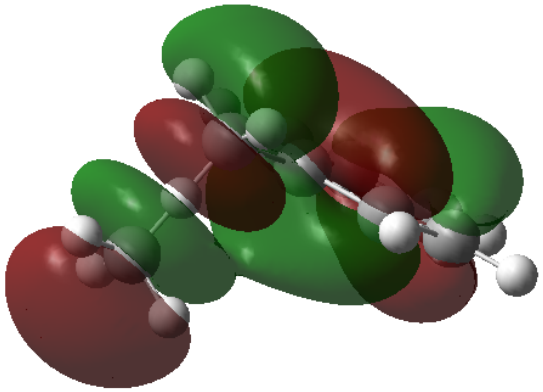
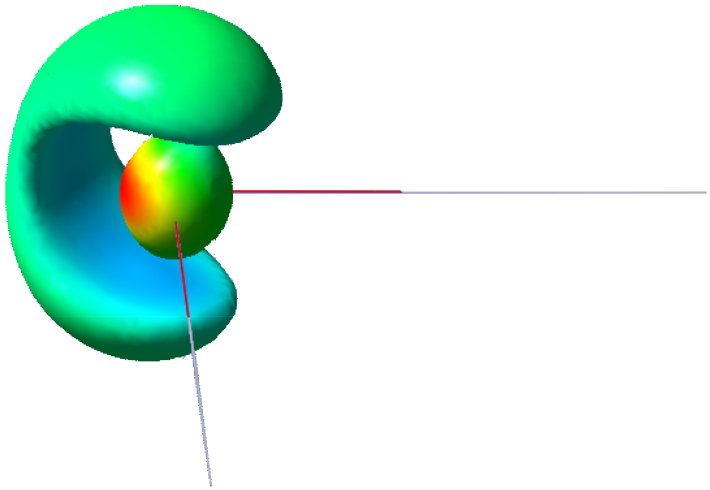
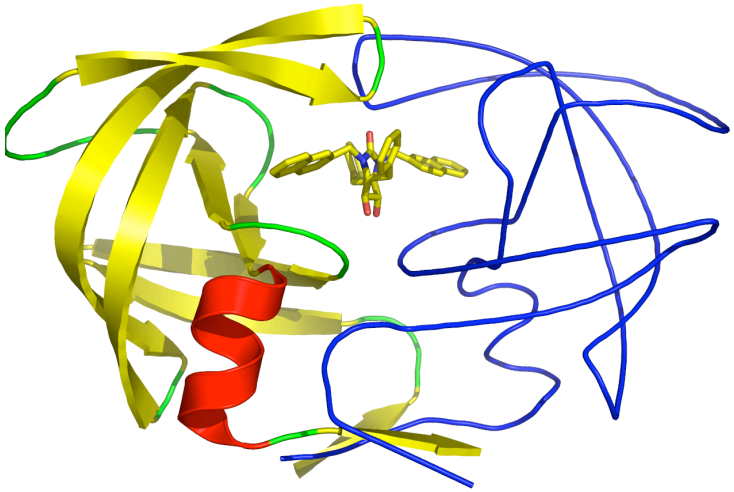
Introduction to Gaussian 09



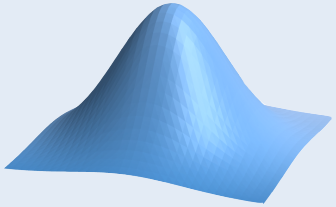


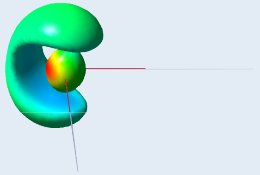


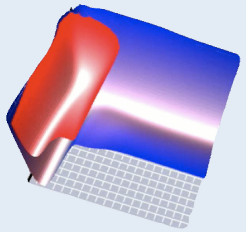
Benjamin Lynch
November 24, 2009

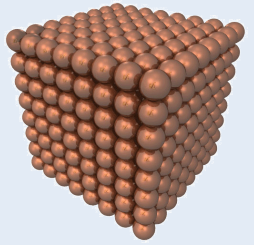
Outline

- Methods available
- Input files
  - Exercise 1
- New Features
- How to submit jobs
- Graphical Tools



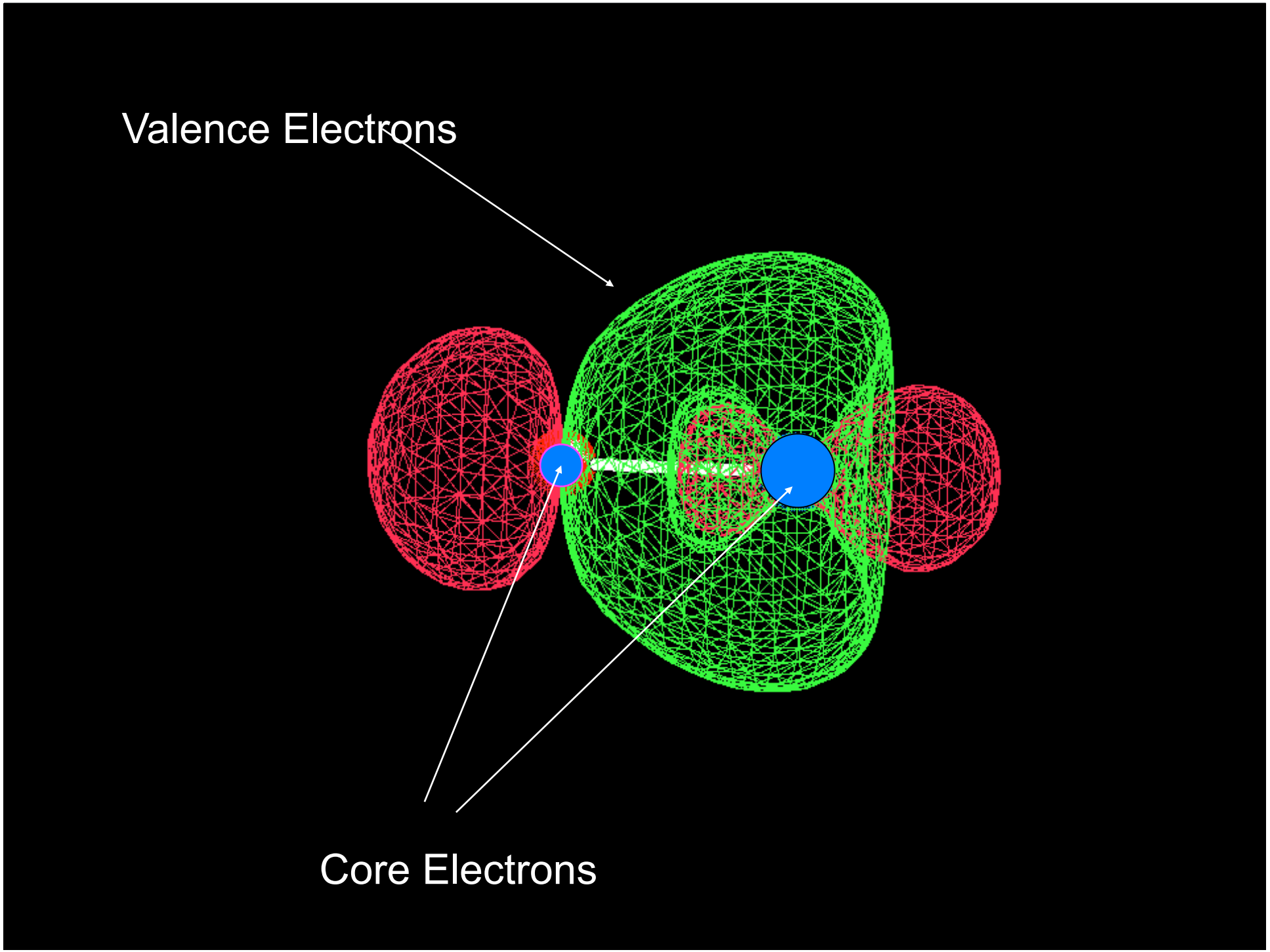






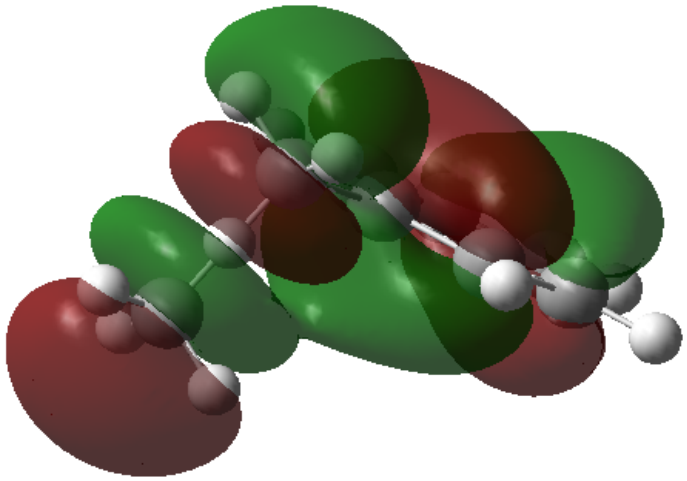
Gaussian 09

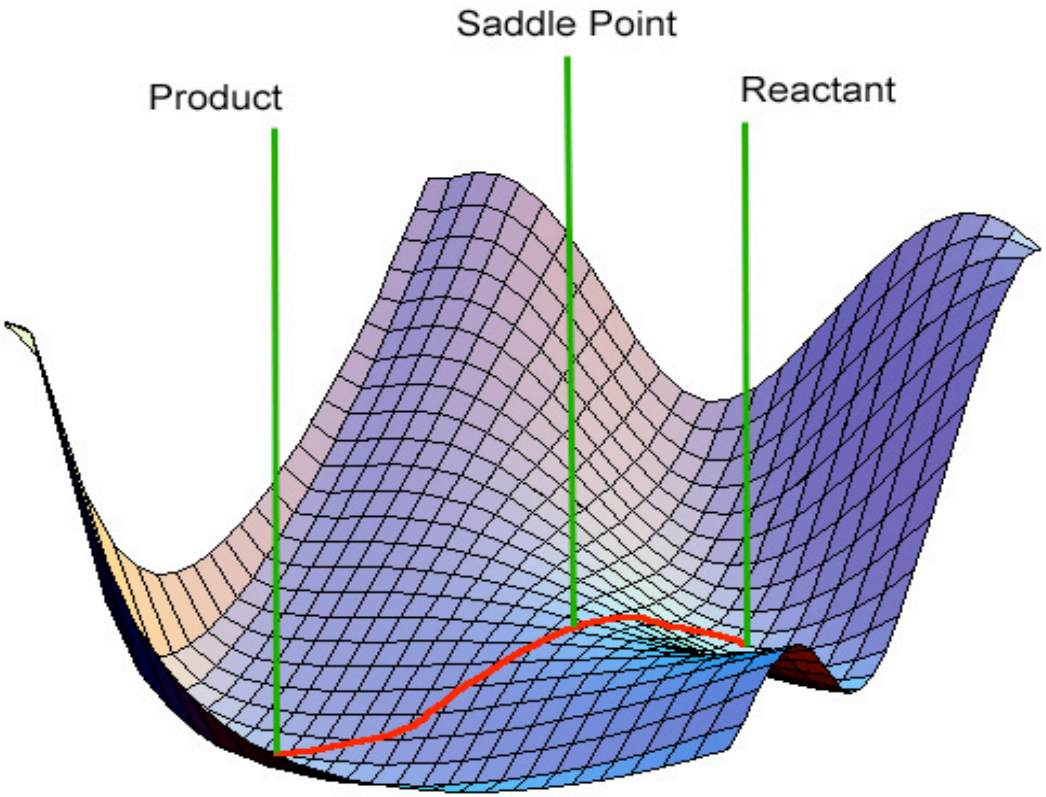
- an electronic structure package capable of predicting many properties of atoms, molecules, reactive systems, e.g.;
  - molecular energies
  - structures
  - vibrational frequencies
  - electron densities
  - utilizing ab initio, density functional theory, semi-empirical, molecular mechanics, and various hybrid methods.


Valence Electrons
Core Electrons

Visualization

- GaussView:
  - Graphical interface for Gaussian 09
  - sketch molecules
  - setup Gaussian 09 input files
  - graphically examine results
- Molden:
  - A graphical interface for Gaussian and other programs
  - setup Gaussian 09 input files
  - graphically examine results





How to Create Input Files

Input File

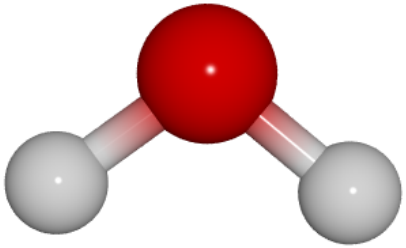
% Resource management
# Route card

Title section

Molecular coordinates

Geometric variables

Other input options (isotope masses, include files, …)



Water Optimization

```
%mem=32mb
#p hf/6-31g opt

hf/6-31g optimization of water

0  1
o
h  1  oh
h  1  oh  2  aoh

oh=0.9
aoh=104.0
```

system resources

computational model
type of calculation

title

charge & multiplicity

structure definition
(z-matrix)

variable values

Commands for Resource Management (link 0)

%mem=*n*	sets the amount of dynamic memory (*n*), default is 32MB. Units allowed, kb, mb, gb, kw, mw, or gw.
%nproc=*n*	sets the number of processors, *n*, to use
%chk=*file*	location and name of checkpoint *file*
%rwf=*file*	location and name of rwf *file*
%subst l*n dir*	substitute link *n* with alternate executable found in *dir*

Route Card Description:

- specifies keywords and options
- always begins with a # character
- keywords can be specified in any order
- options are grouped in parentheses, ()
- keywords should not be repeated
- route section can be up to 5 lines long
- ends with a blank line

Syntax:

#[p] method/basis [keyword=(opt1,opt2)] [keyword2=(opt1[,opt2])]

Example Routes:

hf/6-31g*

#p M06/cc-pvdz opt

#MP2/cc-pvtz maxdisk=12gb

HF/6-311g(d,p) freq scf=direct nosymm opt

#CCSD=(T,maxcyc=200)/6-31G* opt=ts

Calculation Types:

- single point energy and properties
- geometry optimization
- frequency
- reaction path following/searching

Levels of Theory:

- molecular mechanics
  - mm2, uff
- semi-empirical
  - AM1, PM3, PM6, MNDO, …
- density functional theory
  - B3LYP, mPWPW91, M06, custom

…

- *ab initio*
  - HF, MP2, CCSD, QCISD, …
- hybrid
  - G2, G3, oniom, …

Basis Set Types:

– all electron; Pople, Dunning, etc.

– effective core potential

User Supplied:

– use GEN keyword, #hf/gen

via input file:

```
C H 0
6-31G(d,p)
****
F 0
6-31G(d',p')
****
```

via external file:

```
@/home/blynch/basis/custom.gbs
```

http://www.emsl.pnl.gov/forms/basisform.html

Spin multiplicity:

multiplicity = *n* + 1

where *n* = # of unpaired electrons

Molecular Coordinate Types:

- Cartesian coordinates
- Z-matrix

Initial guess:

- where do you get initial geometric values?
  - experimental data
  - chemical intuition
  - previous calculation
- how do I generate the geometry?
  - by hand
  - graphical builder

Resource Considerations: %mem

%mem=200mb

200mb should be enough for all interactive jobs and many jobs that you submit to the queue.

Some jobs can take advantage of much more memory.

For large mp2 frequencies %mem=2gb can significantly increase the Speed of the calculation

Resource Considerations: %rwf

%rwf limit is obeyed by all HF, all DFT, MP2 energies, MP2 gradients

%rwf limit is ignored by QCISD, CCSD, CCSD(T), MP4, and

MP2 frequency calculations.

Resource Considerations: %chk

The checkpoint file contains a lot of information that does not Appear in the output file.

You can use this command to specify the location of the checkpoint file.

%chk=mychkfile

Interactive:

Command:

g09 < input_file > output_file

Notes:

1) **input and output files can use absolute or relative pathnames**
2) **Gaussian temporary files for can be redirected by setting the GAUSS_SCRDIR environment variable.**

   setenv GAUSS_SCRDIR /scratch2/blynch
3) **BE CAREFUL how long you run interactively**

Exercise 1

module load gaussian

Edit a file in pico, vi, or gedit

```
g09 < h2o.com
```

```
# M06   opt

water optimization

0 1
O
H  1  r1
H  1  r1  2  a1

r1=0.9
a1=120.0
```

New Features

- Linda 8.2
  - New version of tool that allows Gaussian jobs to run across nodes

New Features

- QCISD/CCSD restarts
  - CC amplitudes are saved in the checkpoint file
  - amplitudes from previous jobs can be read in to restart an unfinished calculation, or to use amplitudes from a smaller basis set as a guess for a larger calculation.

New Features

- Semi-empirical methods
  - New implementation of semi-empirical methods
  - PM6
  - DFTB

New Features

- DFT
  - M06
  - M06L
  - wB97
  - HSE

New Features

- Solvation
  - SCRF=SMD to calculate ΔG of solvation

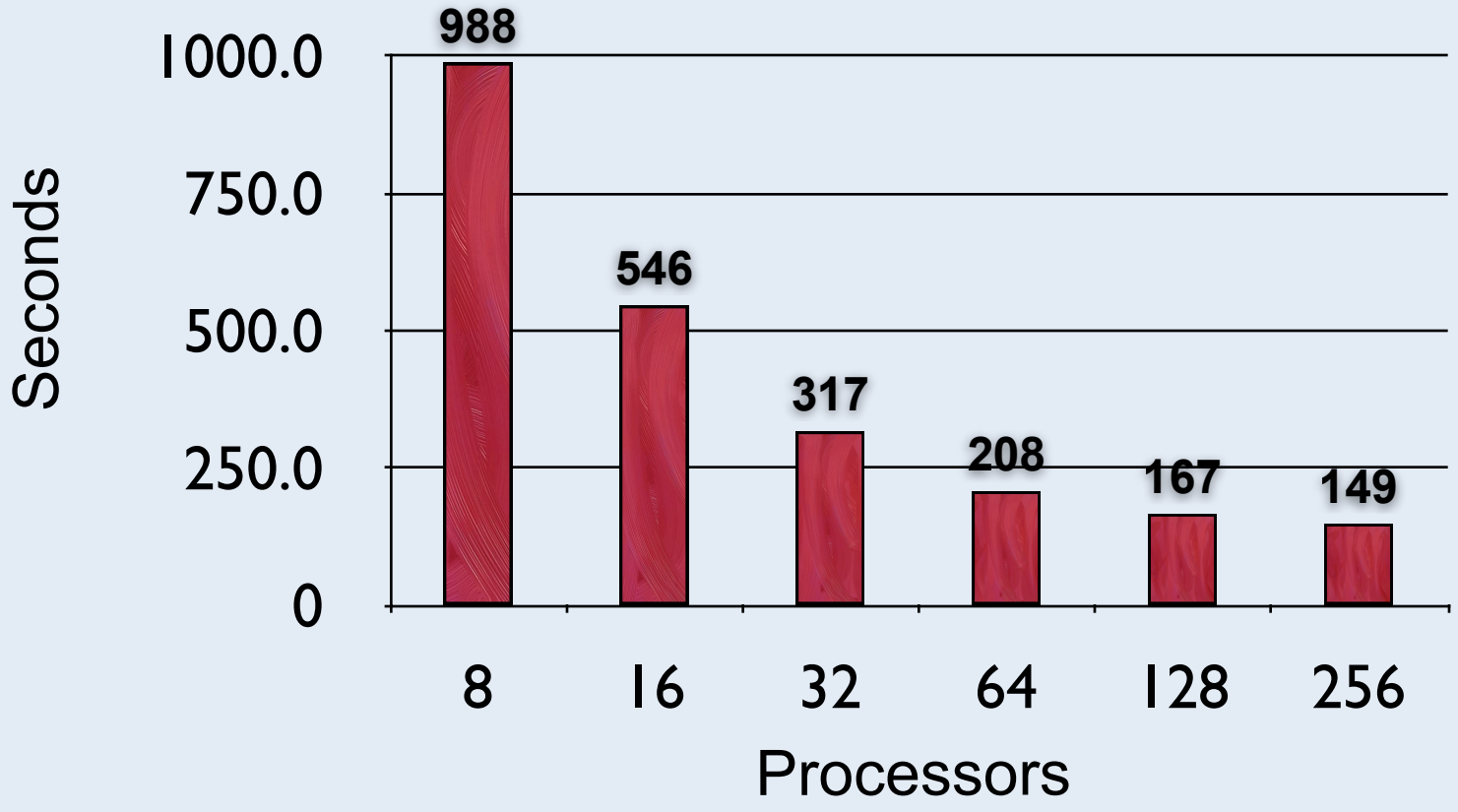
New Features

- Speed!
  - Linda enabled portions have been tested on up to 256 cores on Itasca
- New semi-empirical code
  - 5x speedup for AM1 over g03

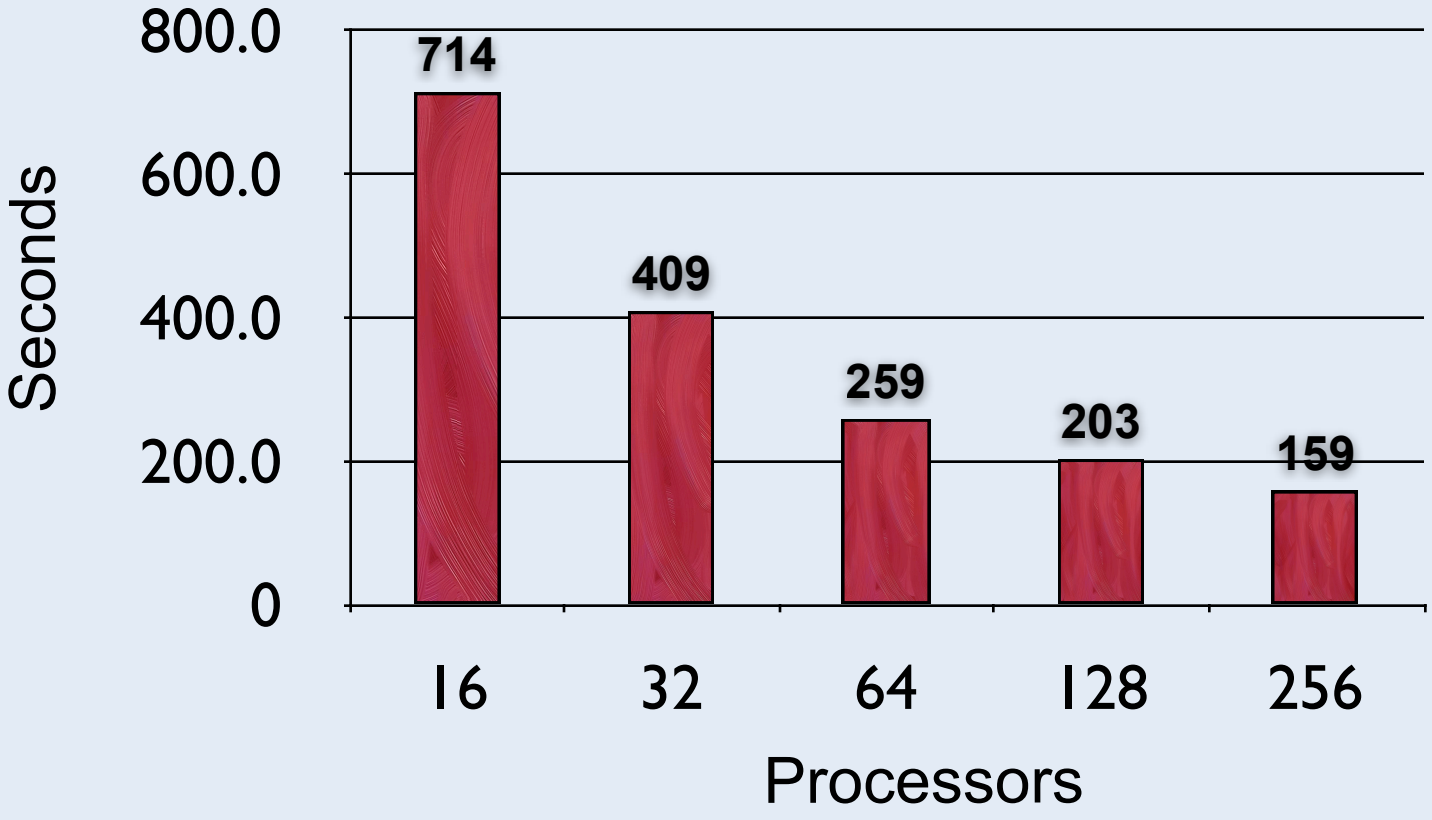
Using Linda-Parallel Gaussian 09

- HF, DFT, CIS=Direct
  - parallel energies, gradients, frequencies
- MP2, CCSD
  - limited portions

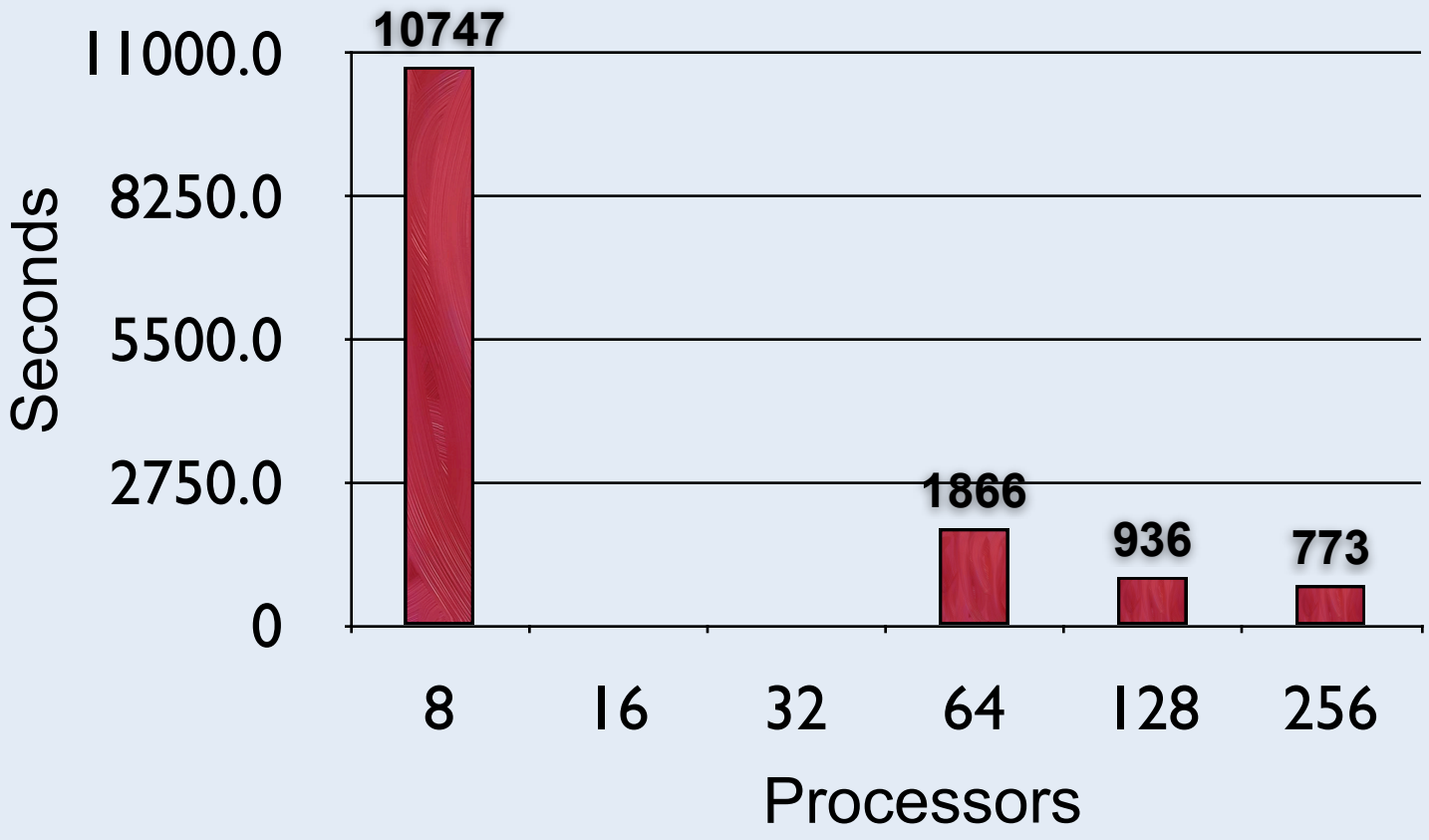
Linda-Parallel M06/6-31G* on C_{60}



Linda-Parallel M06/6-31G* Gradient on C_{60}



Linda-Parallel MP2/6-31G* Energy on C_{60}



Resource Considerations: %nprocshared

This will set the number of processors used on each node for the calculation.

Choosing %NProcShared:

Parallelized

- HF
- MCSCF
- DFT
- MP2
- CIS

Suggestion: 4-8 processors should be used

Choosing the %NProcShared:

NOT- Parallelized much

- CCSD
- CCSD(T)
- Almost everything not listed on the previous slide

Suggestion: 1-2 processors

Recommended Number of Processors

Method	Energy	Gradient / Opt	Freq / Hessian
HF	**8**	**8**	**8**
HDFT	**8**	**8**	**8**
Pure DFT	**8**	**8**	**8**
MP2	**8**	**8**	**8**
MP4	**2**	1	1
MP5	2	1	1
CCSD	2	1	1
CCSD(T)	2	1	1
CIS	**8**	**8**	**8**
CISD	2	1	1

Recommended Number of Nodes for HF, DFT, HDFT, MP2 (Energy + Gradient)

Machine	Nodes	Total Cores
Altix	**1**	**16**
Elmo	**1**	**16**
Blade	**8**	**32**
Calhoun	**8**	**64**
Itasca	**16**	**128**

```
ssh -X blade.msi.umn.edu
module load gaussian
qg09 -n 8 myjob.com
```

Building with Molden

- Login remotely

  ssh -X blade.msi.umn.edu

- Load proper module

  module load molden

- Launch Molden

  molden

Building with GaussView

- Login remotely

  ssh -X calhoun.msi.umn.edu

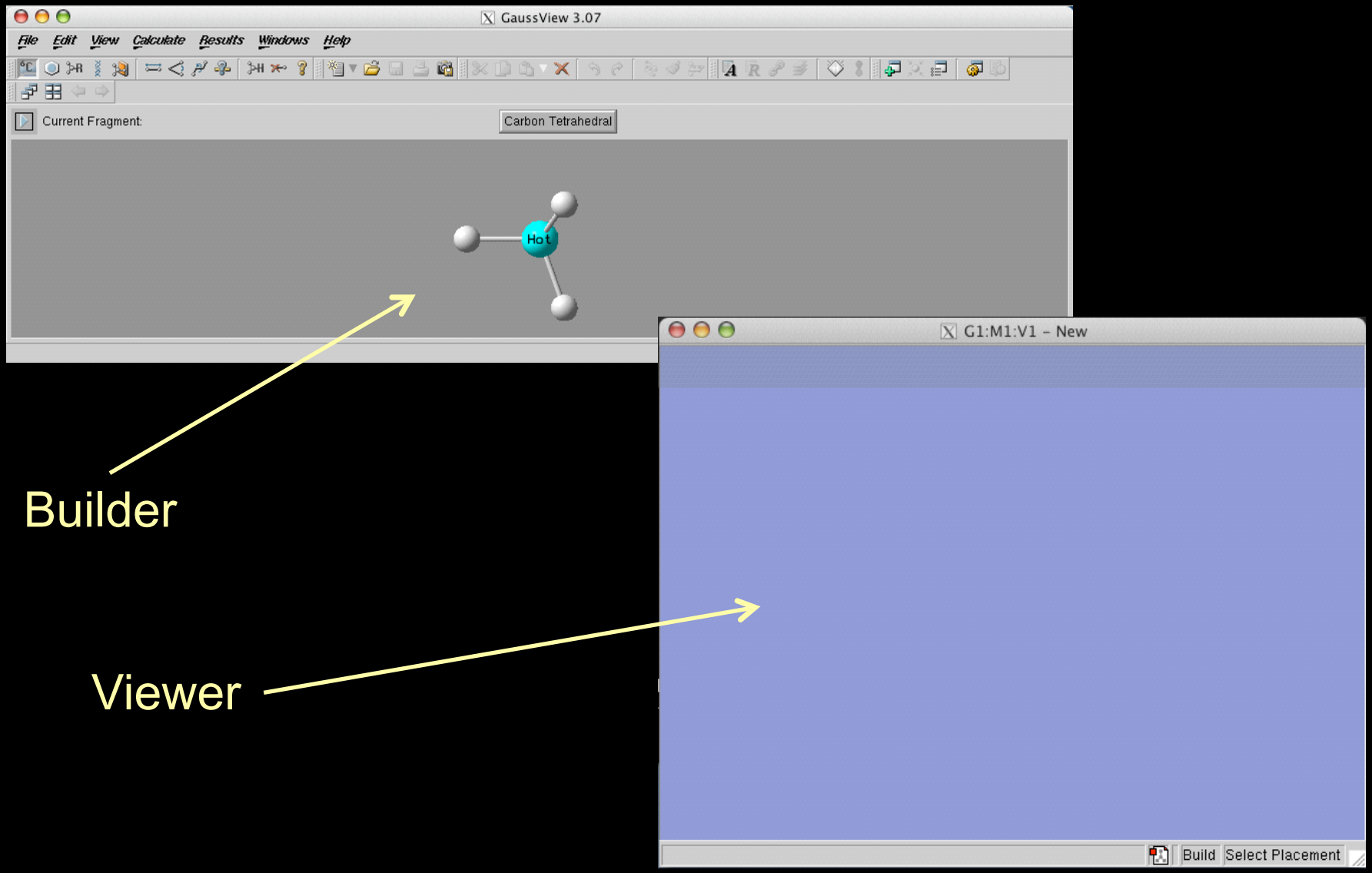
  ssh -X blade.msi.umn.edu

- Load proper module

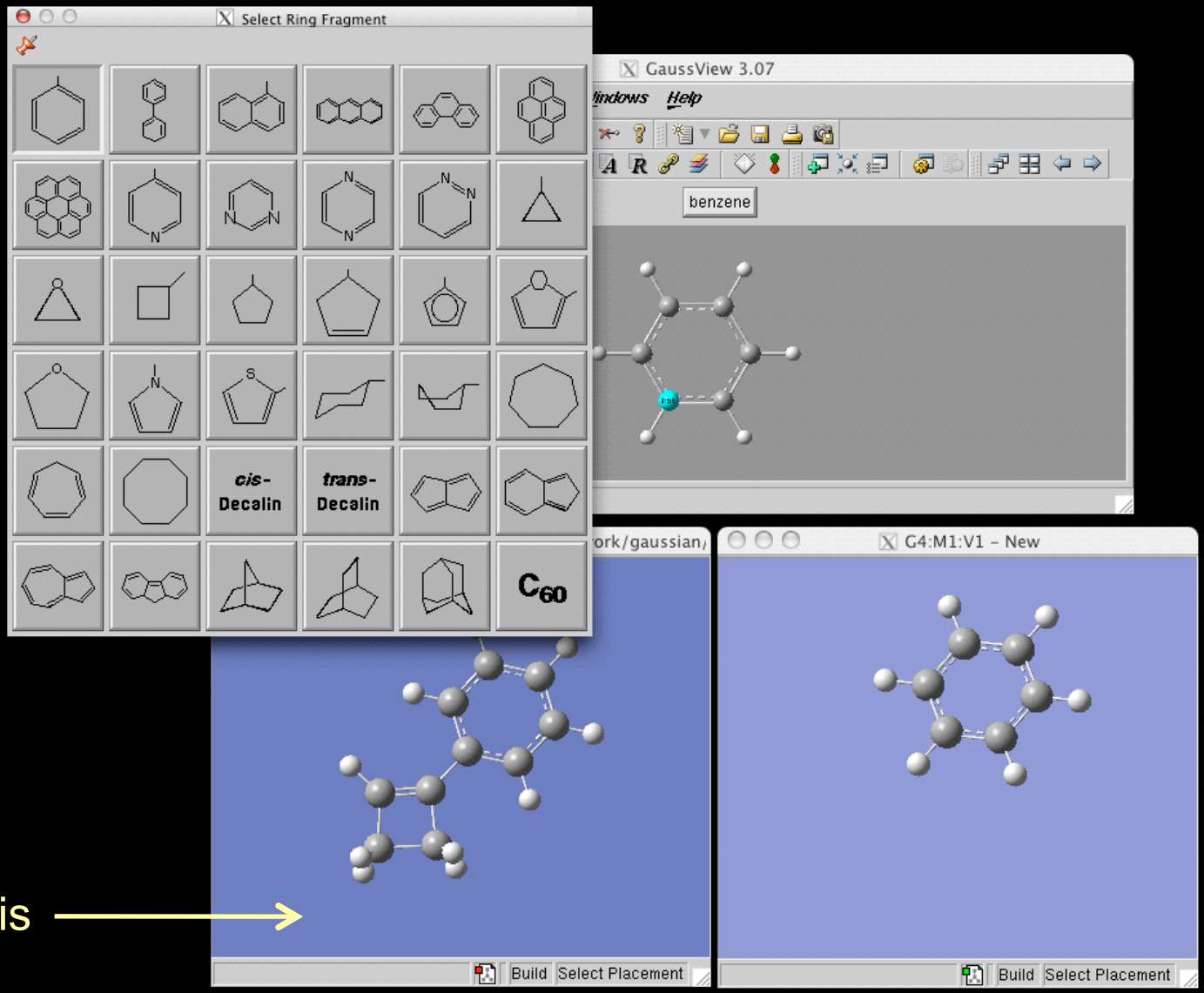
  module load gaussian

- Launch GaussView

  gv

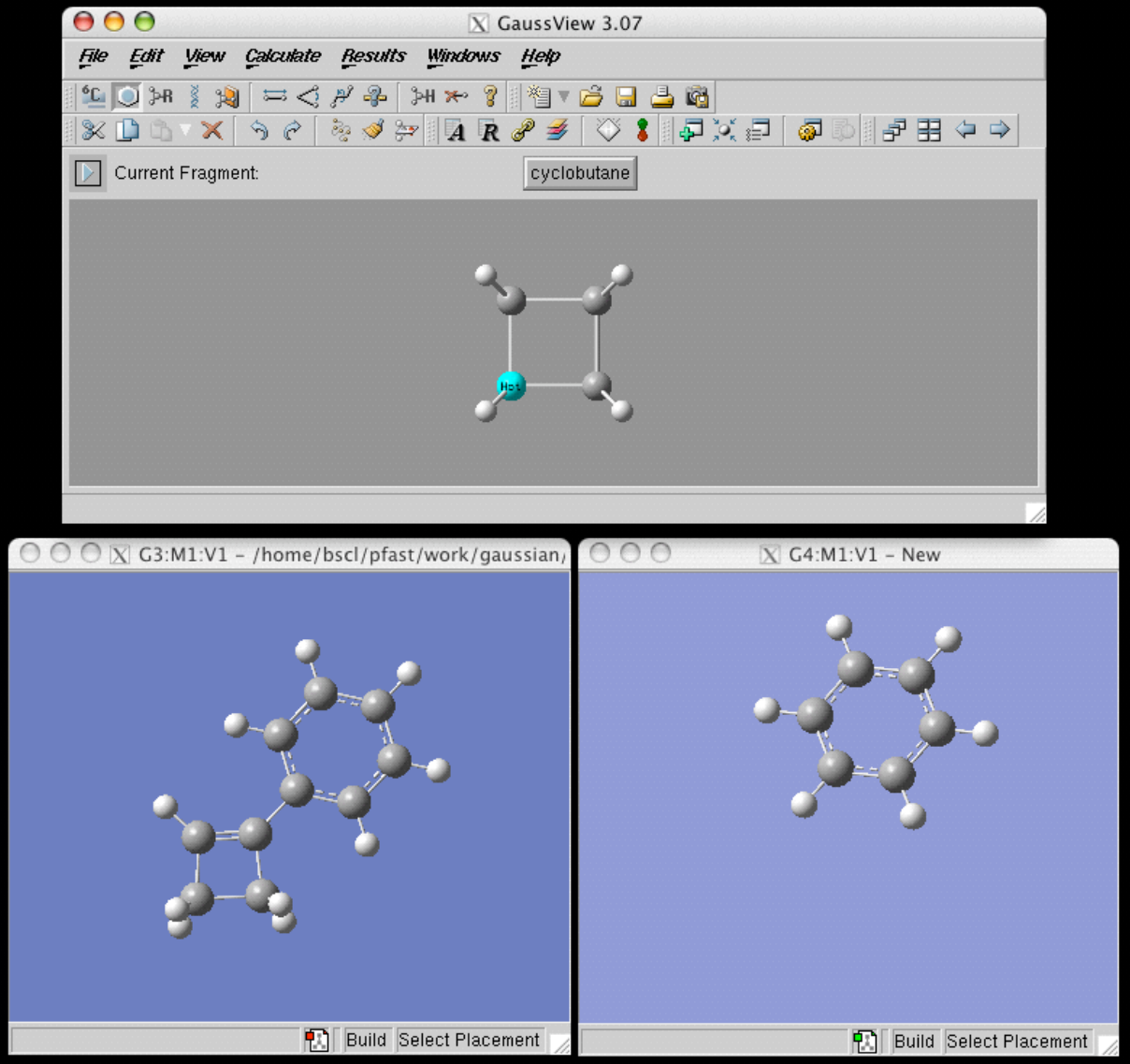

GaussView 3.07
File Edit View Calculate Results Windows Help
Current Fragment:
Carbon Tetrahedral
Hot
G1:M1:V1 - New
Build
Select Placement
Builder
Viewer

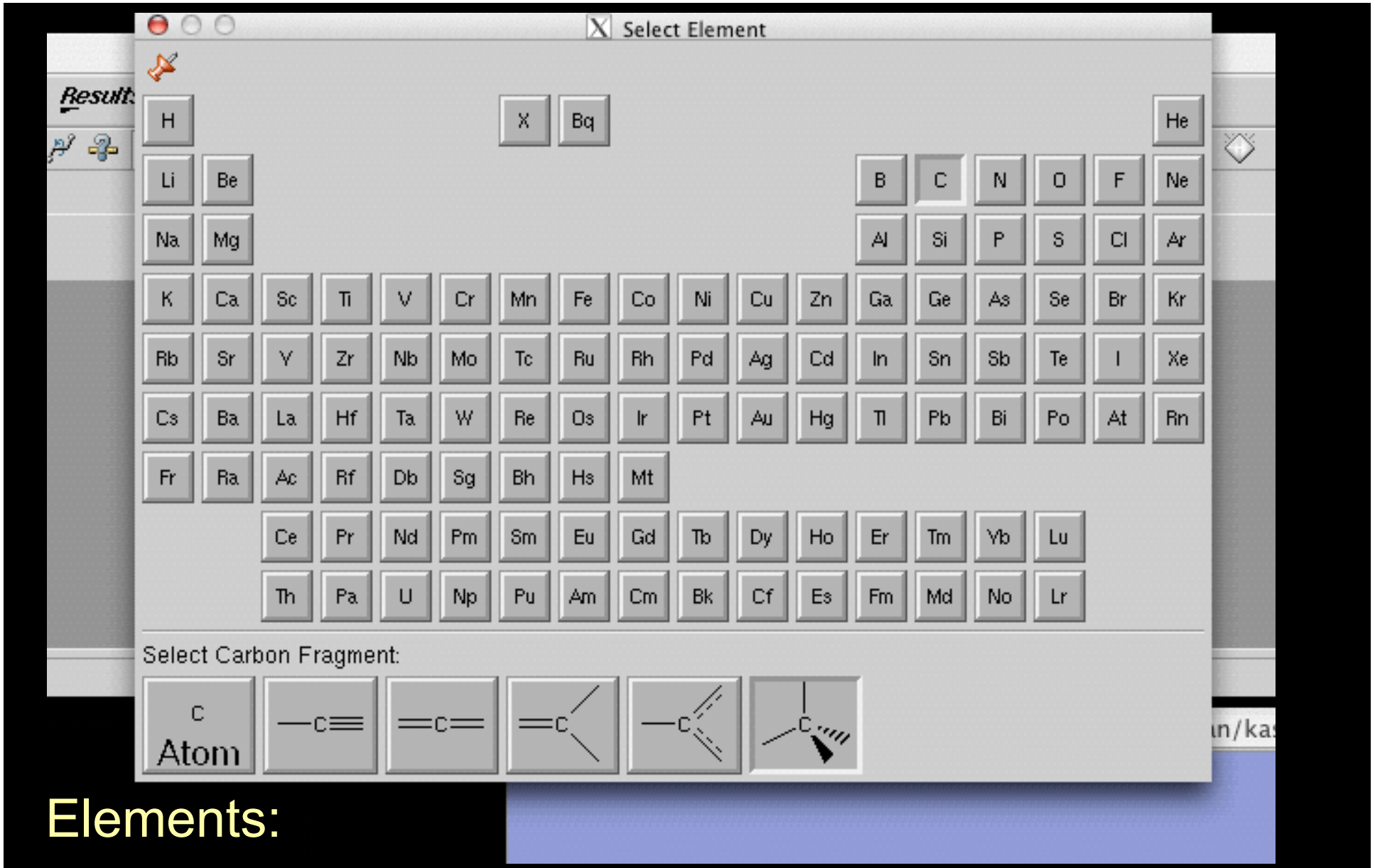
Molecule Building



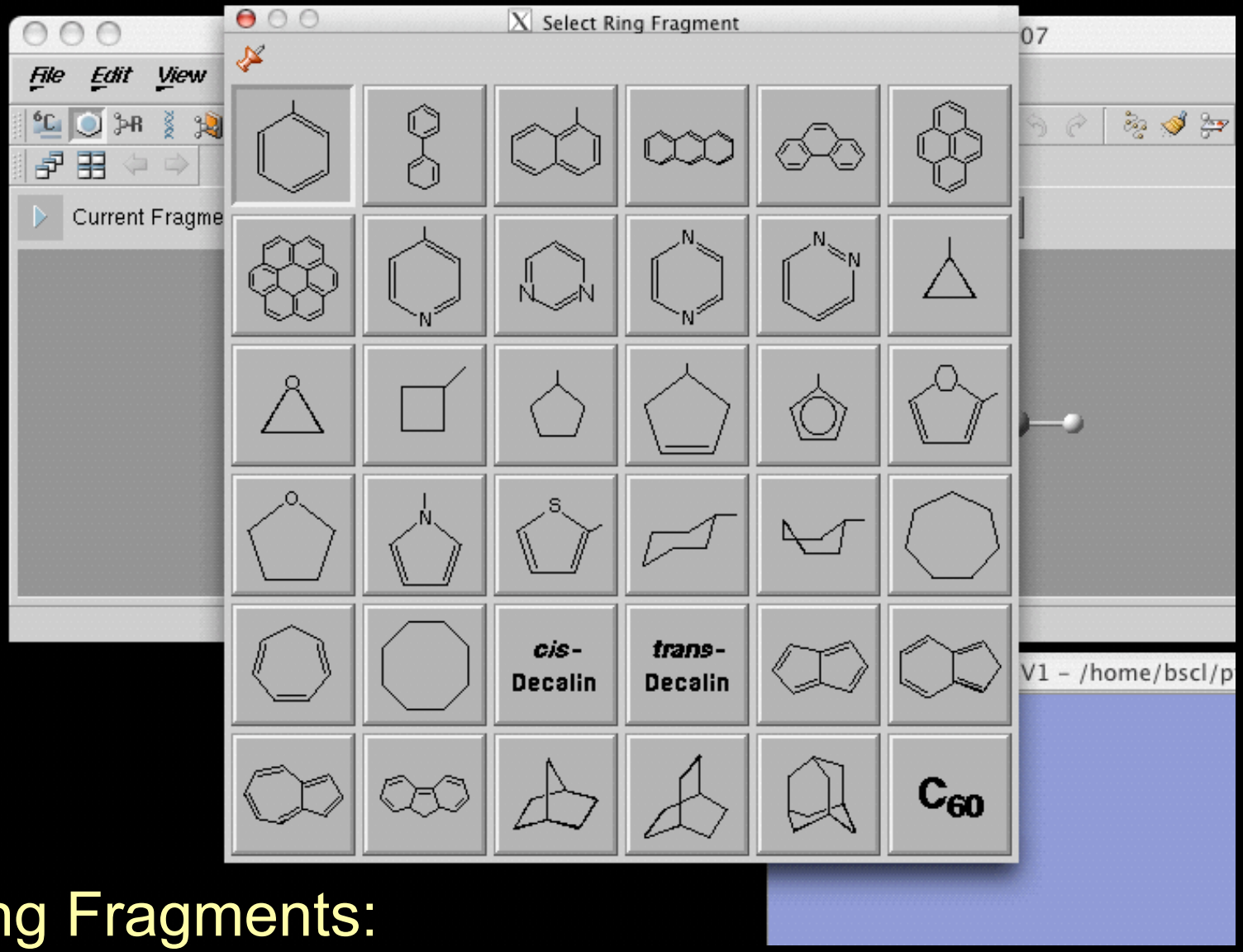
making this →

Molecule Building



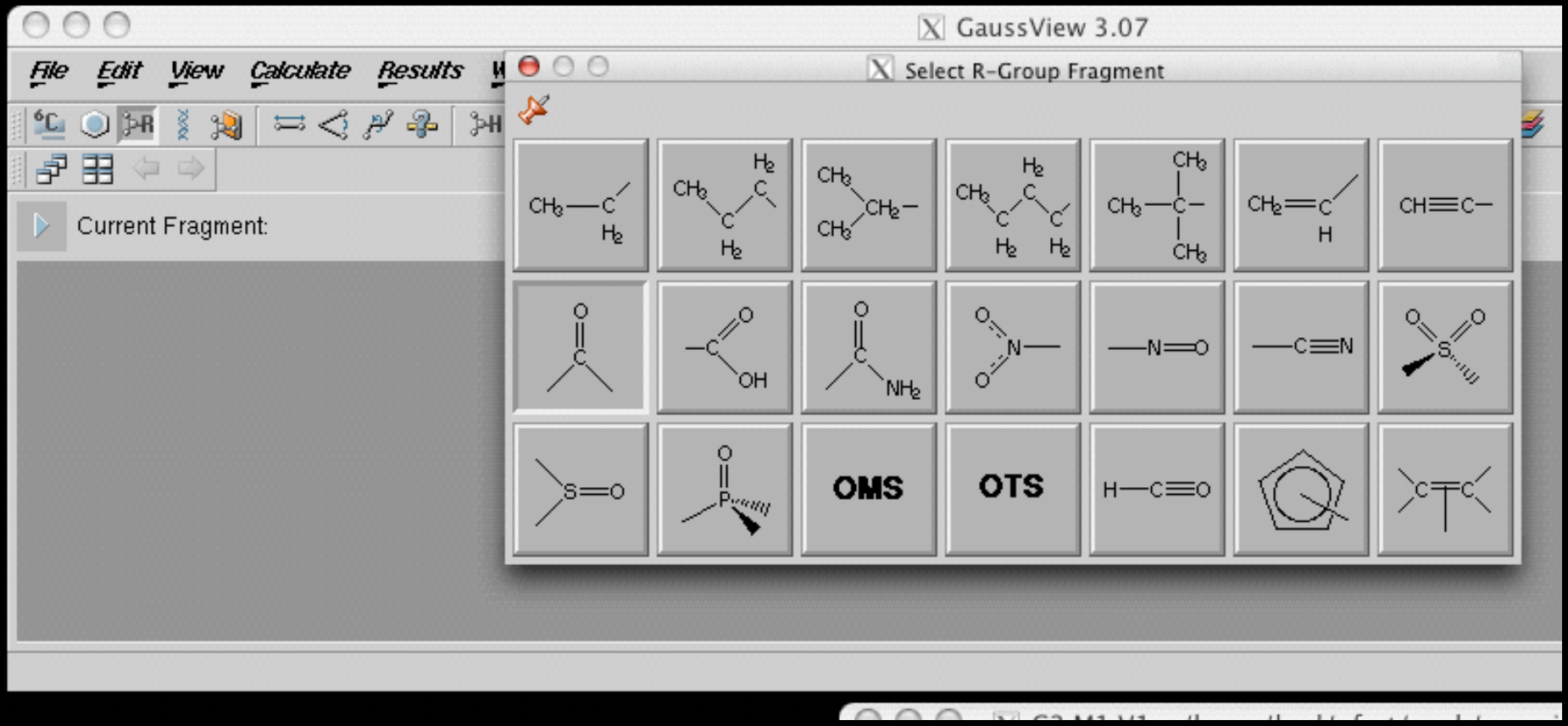

Select Element
H
X
Bq
He
Li
Be
B
C
N
O
F
Ne
Na
Mg
Al
Si
P
S
Cl
Ar
K
Ca
Sc
Ti
V
Cr
Mn
Fe
Co
Ni
Cu
Zn
Ga
Ge
As
Se
Br
Kr
Rb
Sr
Y
Zr
Nb
Mo
Tc
Ru
Rh
Pd
Ag
Cd
In
Sn
Sb
Te
I
Xe
Cs
Ba
La
Hf
Ta
W
Re
Os
Ir
Pt
Au
Hg
Tl
Pb
Bi
Po
At
Rn
Fr
Ra
Ac
Rf
Db
Sg
Bh
Hs
Mt
Ce
Pr
Nd
Pm
Sm
Eu
Gd
Tb
Dy
Ho
Er
Tm
Yb
Lu
Th
Pa
U
Np
Pu
Am
Cm
Bk
Cf
Es
Fm
Md
No
Lr
Select Carbon Fragment:
C
Atom

Elements:

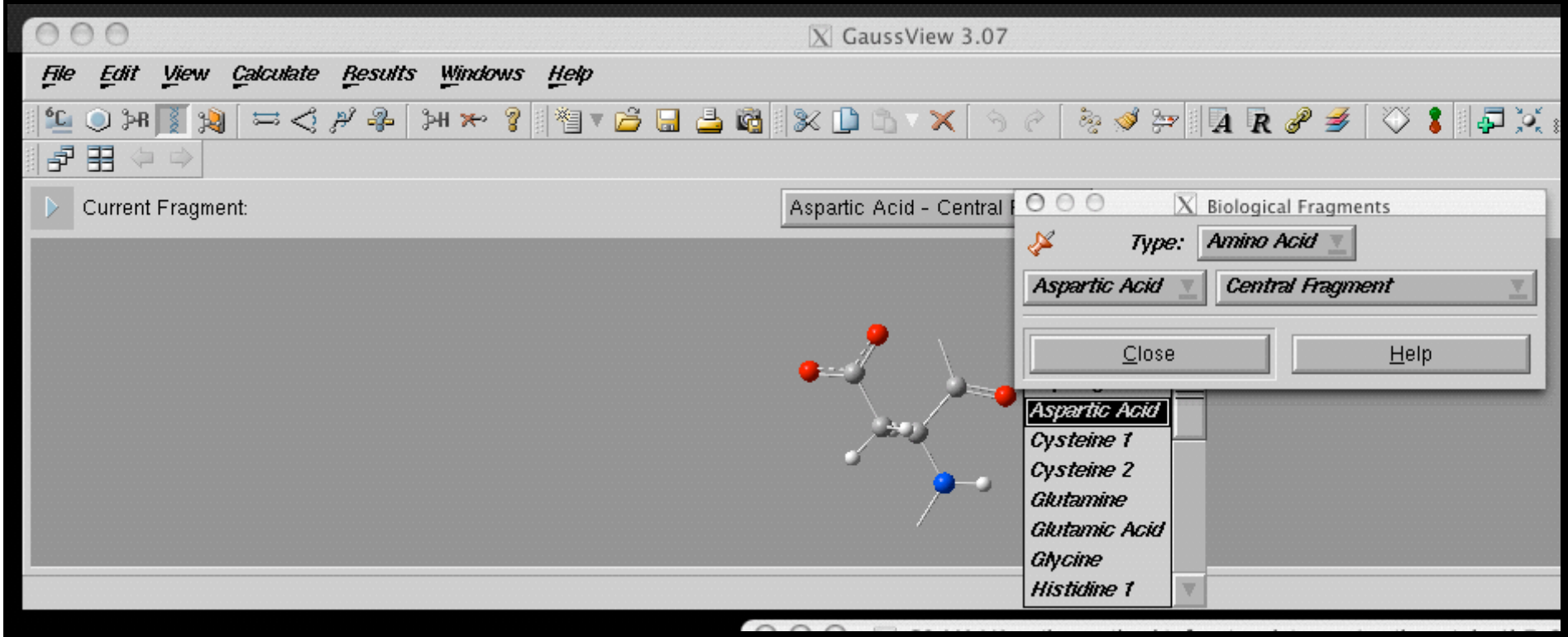


Ring Fragments:

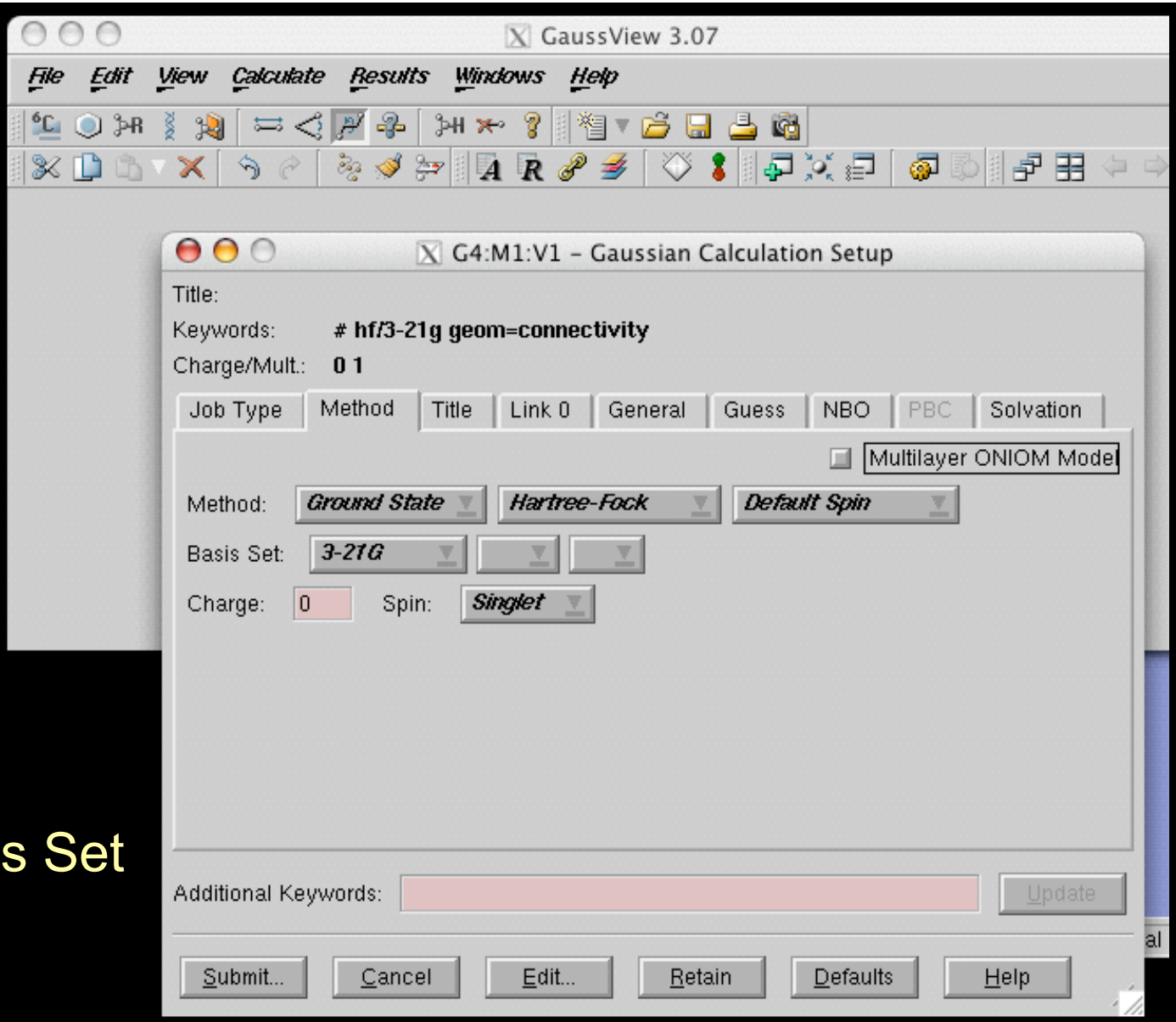
R-Group Fragments:

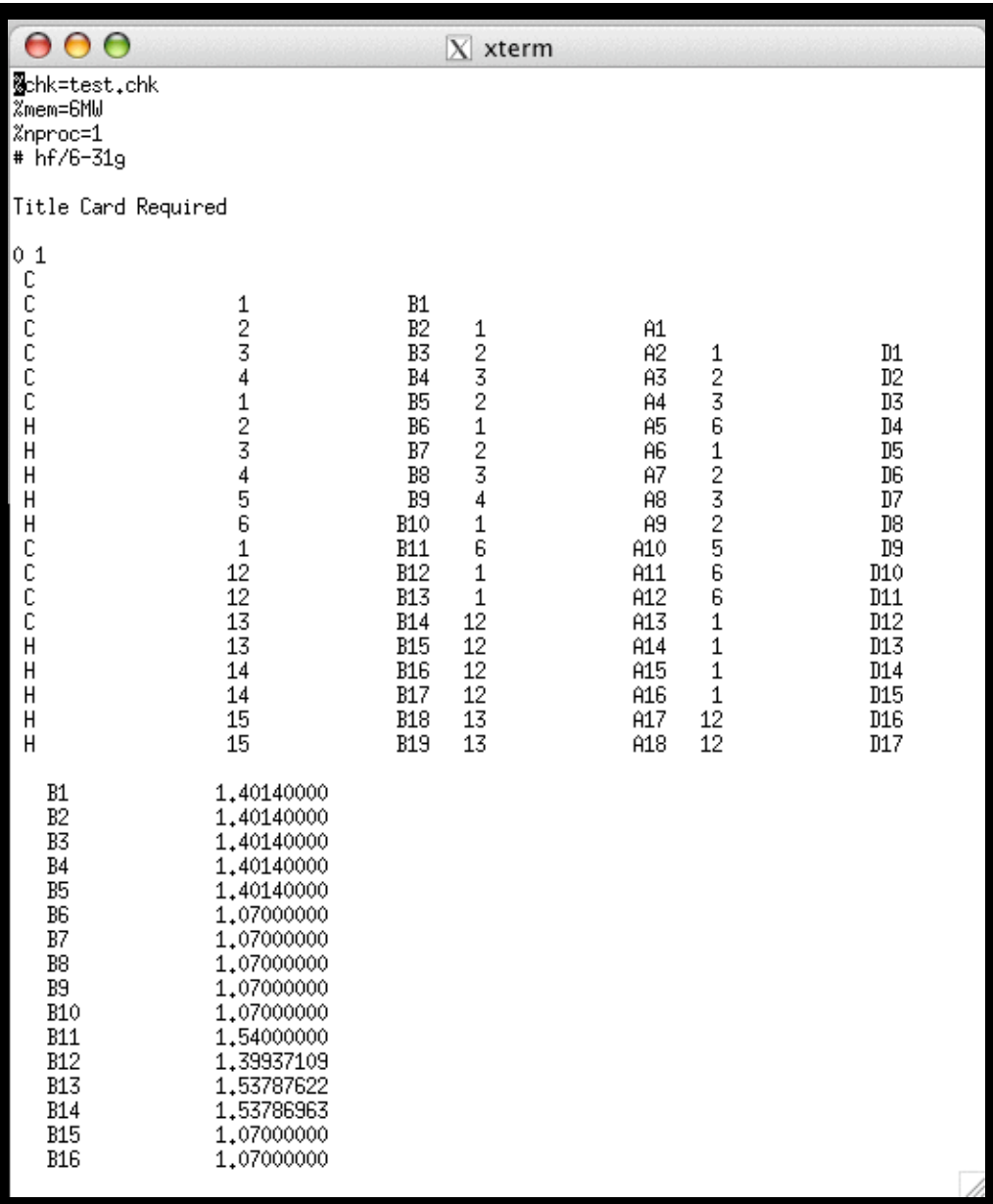


Biological Fragments:



Method & Basis Set





Sample
Input File

Exercise 2

- Create CH_3CHO in Gaussview
- Exit GaussView and edit input file with text editor to perform M05/3-21G energy calculation
- open .chk file in Gaussview and plot HOMO

Submitting Calculations

Submitting your calculation on core systems:

Command:

module load <*version*>

Available versions:

g03	available to academic researchers
gaussian/g09.a02	Gaussian09 Revision A.02 (available to researchers at Twin Cities Campus)

Systems:

Altix, Blade, Calhoun, Elmo, Itasca, BSCL, SDVL, BMSDL

Batch:

Command:

qg09 [-options] input_file

Options:

-h	help, display a usage list and the defaults
-e	email notification
-m	total amount of memory
-n	number of nodes
-p	number of processors per node
-r	immediately run job?
-s	scratch space
-t	amount of wallclock time

Specific queue options

Queue Commands:

PBS:

qsub *job.pbs*	submit *job.pbs*
qstat [options]	check the queue
qdel *jobid*	cancel job in the queue

less

vi

pico

emacs

Gaussview

Molden

tail

How to View Output

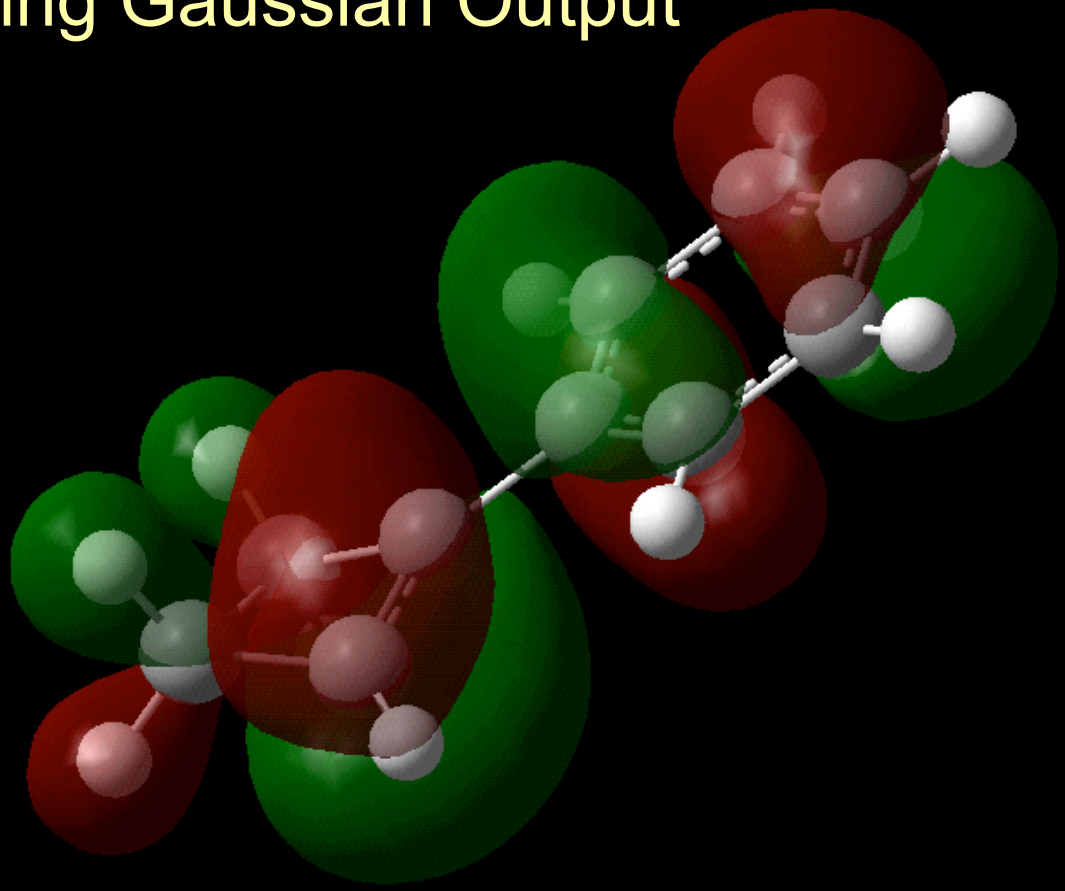
Open the file created called XXXX.out

(where XXXX was the input file name)

It's all text

It gives an outline of the calculation performed

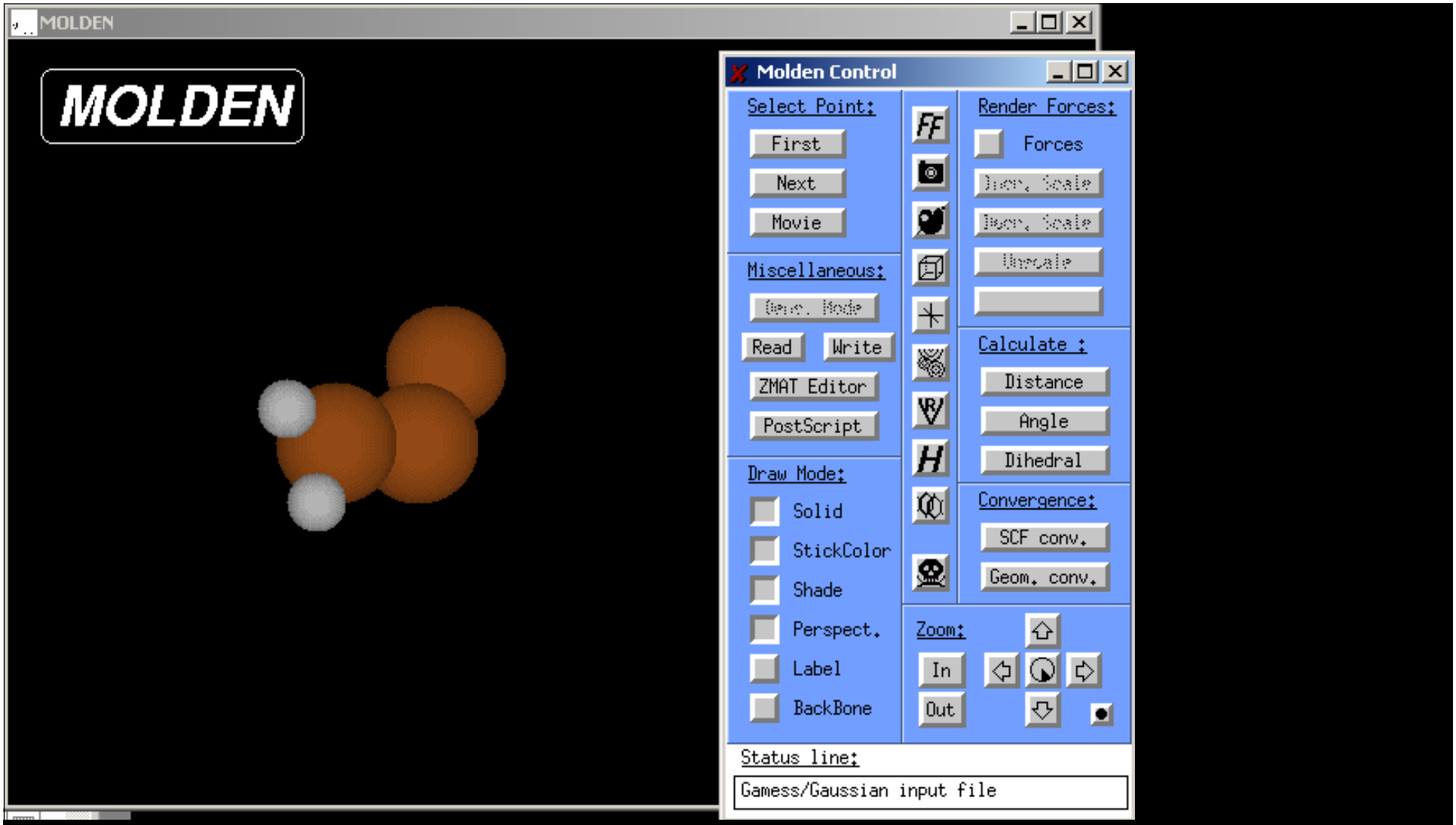
Visualizing Gaussian Output



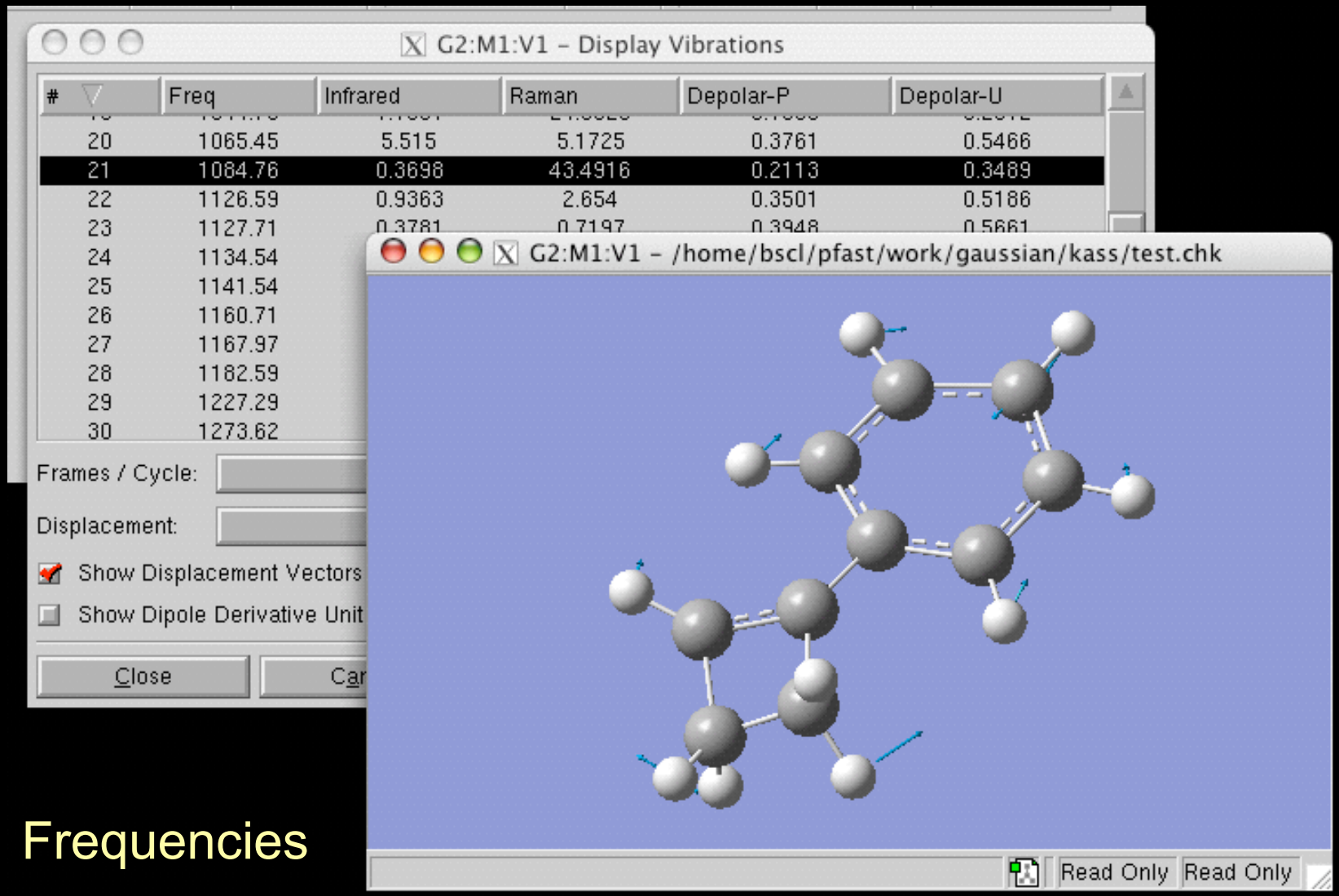
How to View Output Visually

```
module load gaussian

gv myoutput.out
```

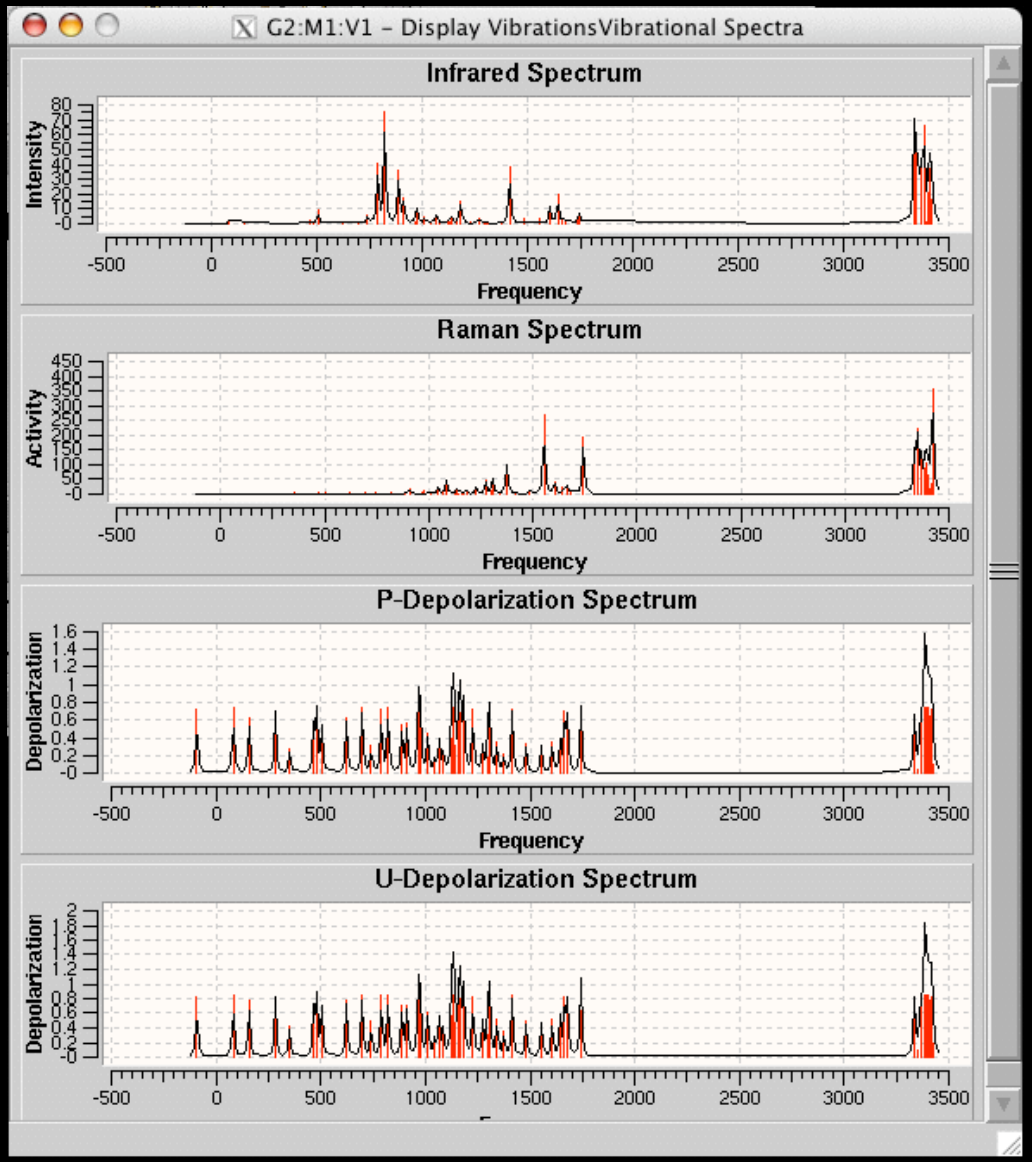
```
module load molden

gmolden myoutput.out
```


MOLDEN
MOLDEN
Molden Control
Select Point:
First
Next
Movie
Miscellaneous:
Read
Write
ZMAT Editor
PostScript
Draw Mode:
Solid
StickColor
Shade
Perspect.
Label
BackBone
Render Forces:
Forces
Calculate :
Distance
Angle
Dihedral
Convergence:
SCF conv.
Geom. conv.
Zoom:
In
Out
Status line:
Gamess/Gaussian input file

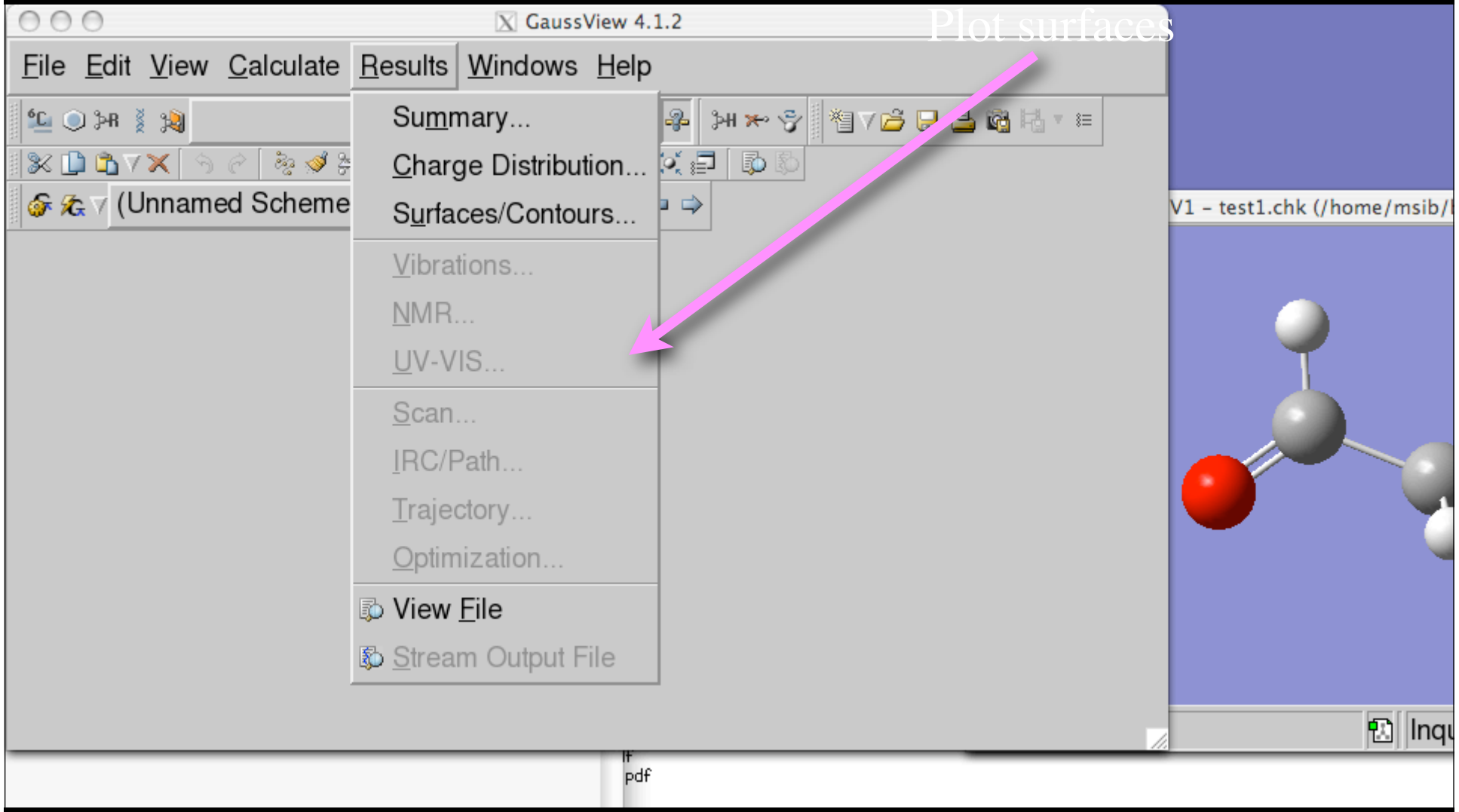
Visualization using Gaussview



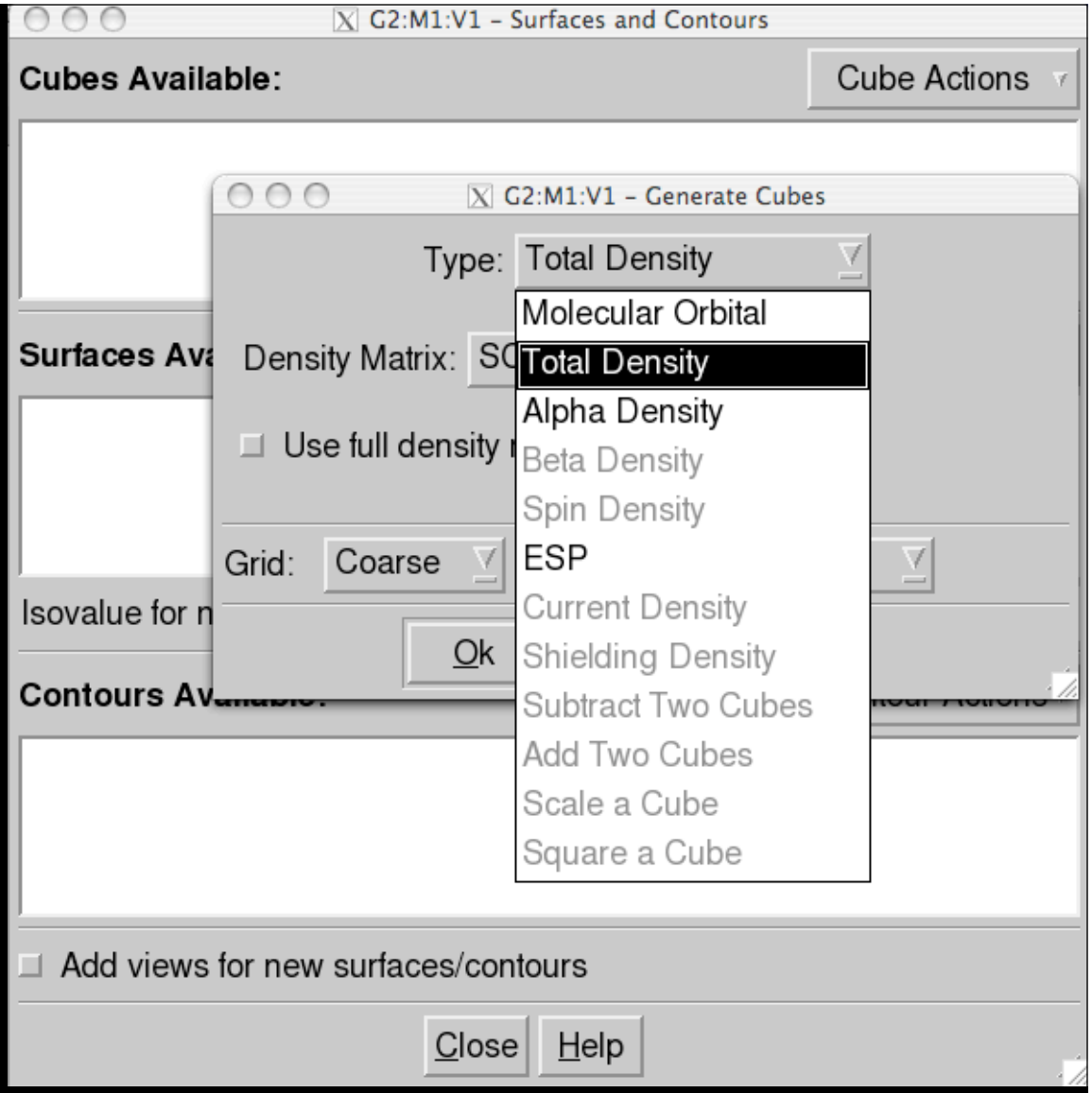
Frequencies


G2:M1:V1 - Display VibrationsVibrational Spectra
Infrared Spectrum
Intensity
Frequency
Raman Spectrum
Activity
Frequency
P-Depolarization Spectrum
Depolarization
Frequency
U-Depolarization Spectrum
Depolarization

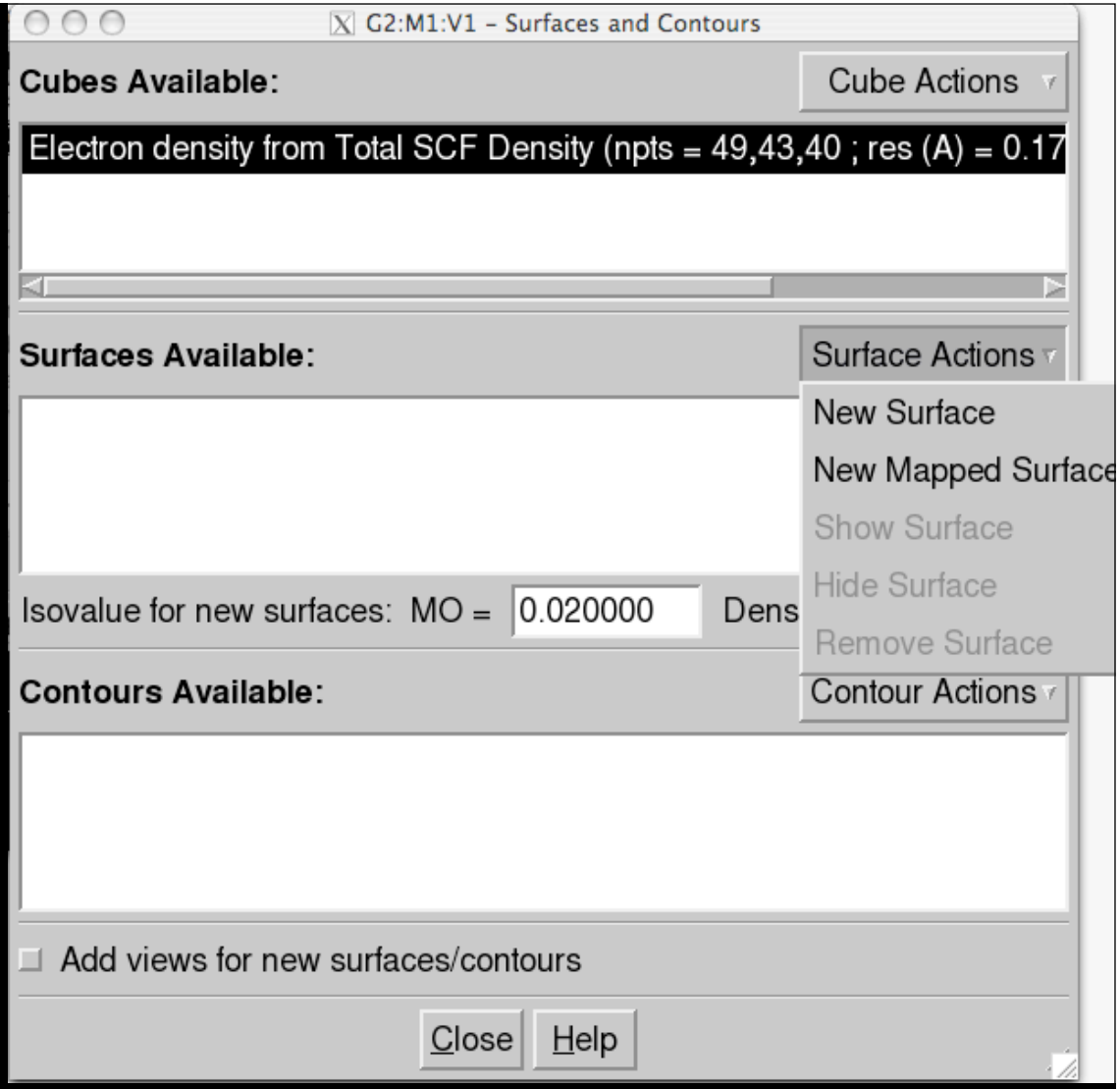
Spectra


GaussView 4.1.2
Plot surfaces
File Edit View Calculate Results Windows Help
Summary...
Charge Distribution...
Surfaces/Contours...
Vibrations...
NMR...
UV-VIS...
Scan...
IRC/Path...
Trajectory...
Optimization...
View File
Stream Output File
(Unnamed Scheme
V1 - test1.chk (/home/msib/
pdf

A cube file is a 3-D array of the values of some property.



A New Mapped Surface can map properties onto an isosurface from an existing cube file.

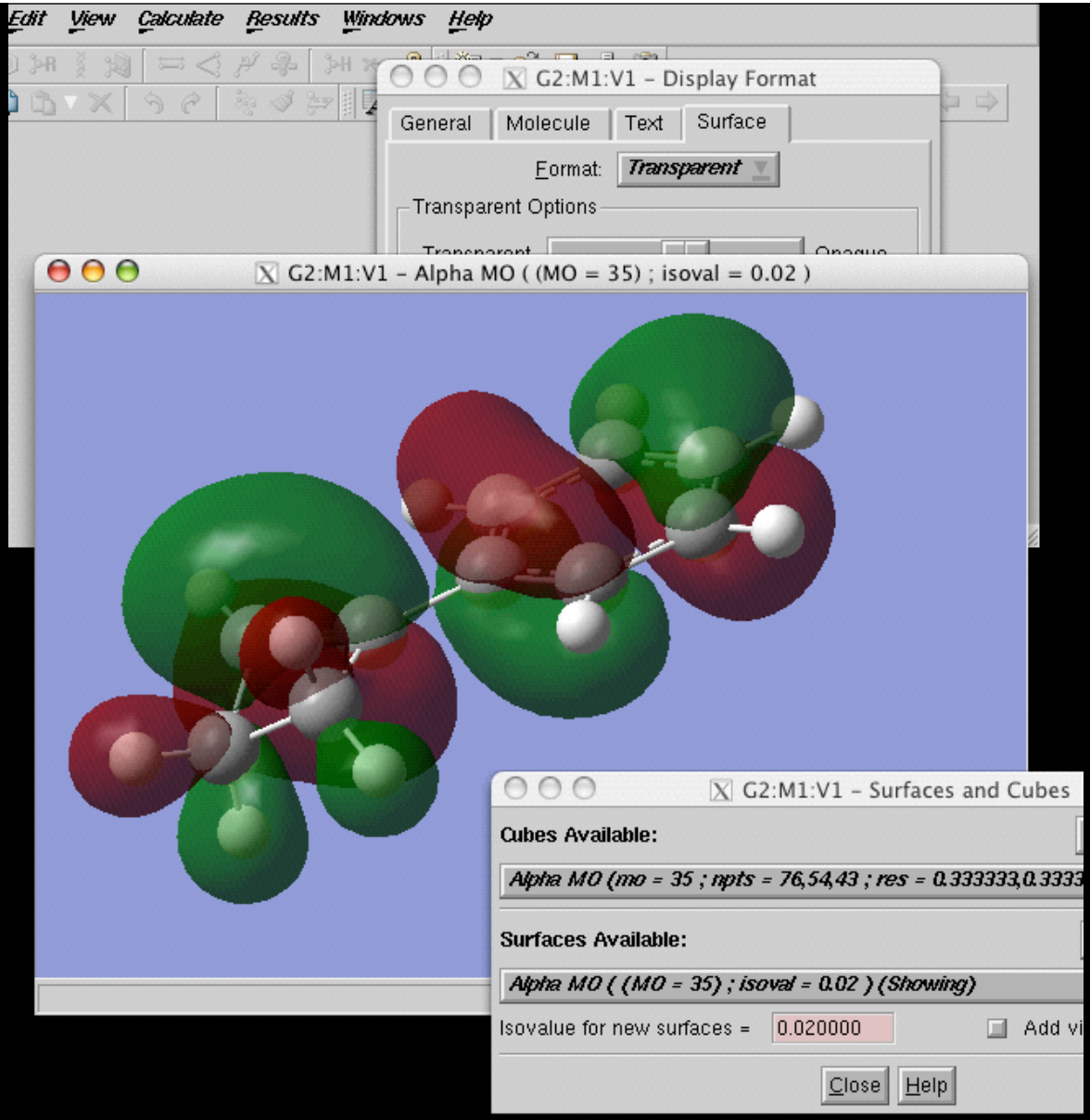


Exercise 3

1. open .chk from CH_3CHO calculation in Gaussview and plot HOMO

2. Plot an electron density isosurface

3. Plot the electrostatic potential mapped onto the electron density isosurface


Edit View Calculate Results Windows Help
G2:M1:V1 – Display Format
General Molecule Text Surface
Format: Transparent
Transparent Options
G2:M1:V1 – Alpha MO ((MO = 35) ; isoval = 0.02)
G2:M1:V1 – Surfaces and Cubes
Cubes Available:
Alpha MO (mo = 35 ; npts = 76,54,43 ; res = 0.333333,0.3333
Surfaces Available:
Alpha MO ((MO = 35) ; isoval = 0.02) (Showing)
Isovalue for new surfaces = 0.020000
Add vi
Close Help

Common Errors

Memory Errors

Not enough memory to run at all: LenERI 3000000

Increase memory by 87346382 words

Error termination via Lnk1e in /usr/local/g03/g03.b01/g03/l906.exe

Solution: Increase %mem

Disk Errors

No file to extend for IUnit=1 –

Out of disk space

Error termination in NtrErr

Solutions: make more space available

check disk quotas

maxdisk=1gb

SCF Failure

What to do?

Possible keywords that may help:

scf=xqc

scf=(maxcyc=500)

scf=…

guess=read (read in a converged guess from a different theory)

Coupled cluster iteration failure

CCSD(maxcyc=200)

Not many options currently available

Re-consider your choice of basis set

Check the orbitals

Re-consider the applicability of CCSD to The system you are studying.

Optimization failures

What to do?

Restart the calculation from the last geometry and continue

Look at the structure, adjust it manually, and continue.

For difficult saddle-point searches: opt=(TS,CalcAll)

Think about how the program works

First, Gaussian needs to read your input file (does file exist?)

Make sense of geometry (do atoms overlap?)

Make sense of keywords (do keywords define an ambiguous calculation?)

Make sense of electronic state (do charge and multiplicity make sense?)

Solve HF equations, converge CC iterations, converge geometry, calculate frequencies, …

Questions?

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