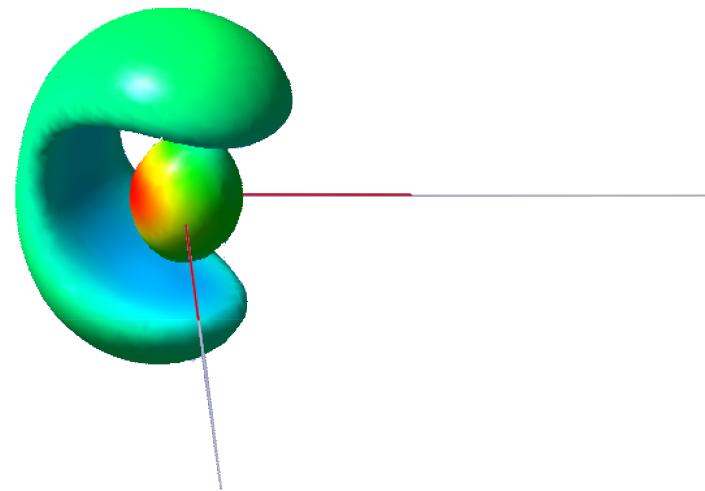
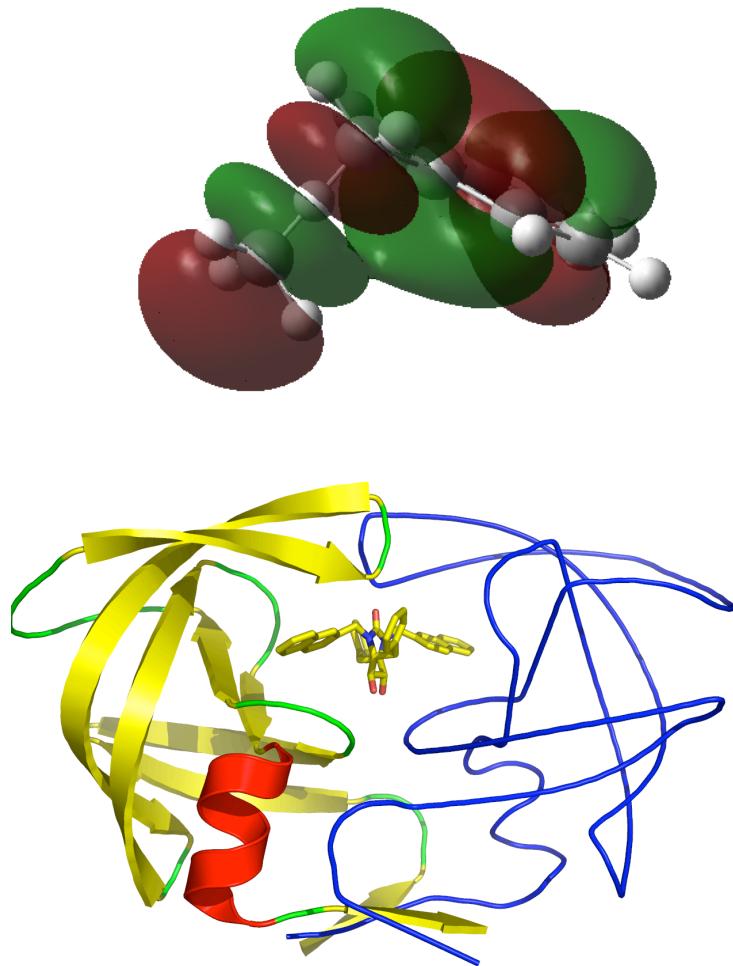


Introduction to Gaussian 09

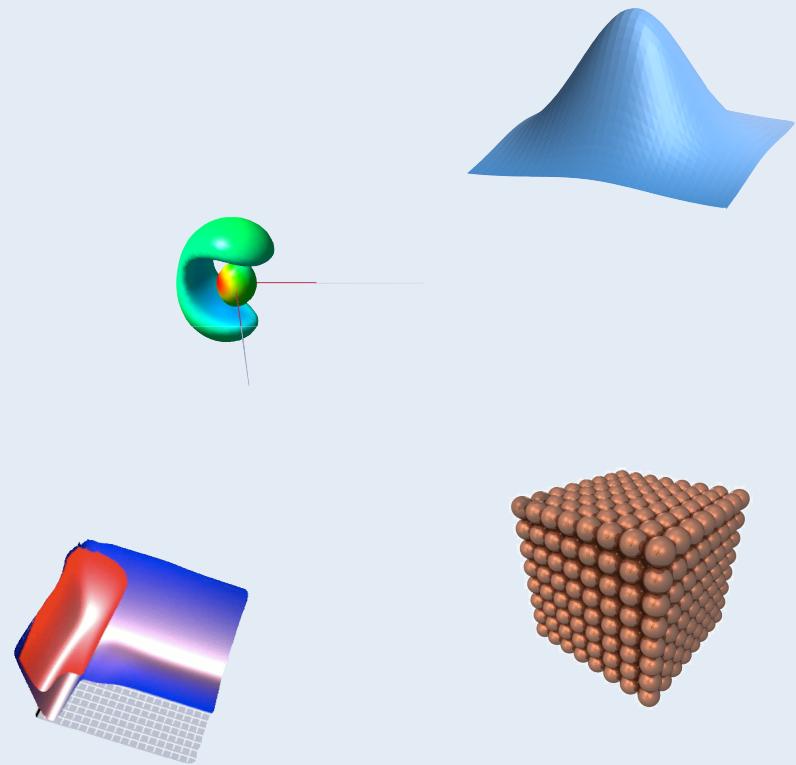


Benjamin Lynch
November 24, 2009

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Outline

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



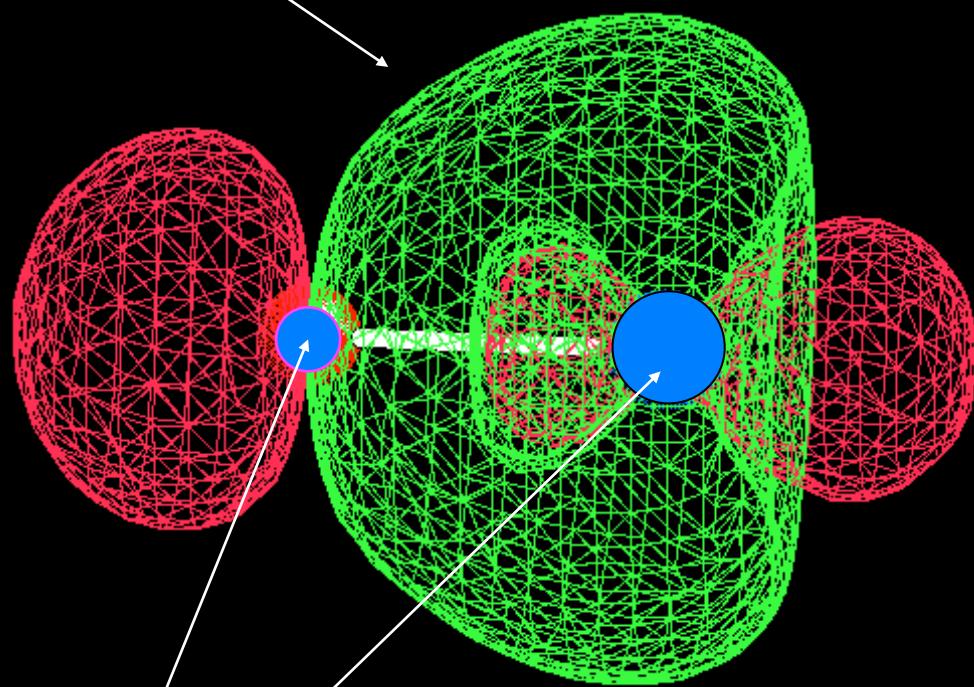
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Gaussian 09

- 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.

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Valence Electrons

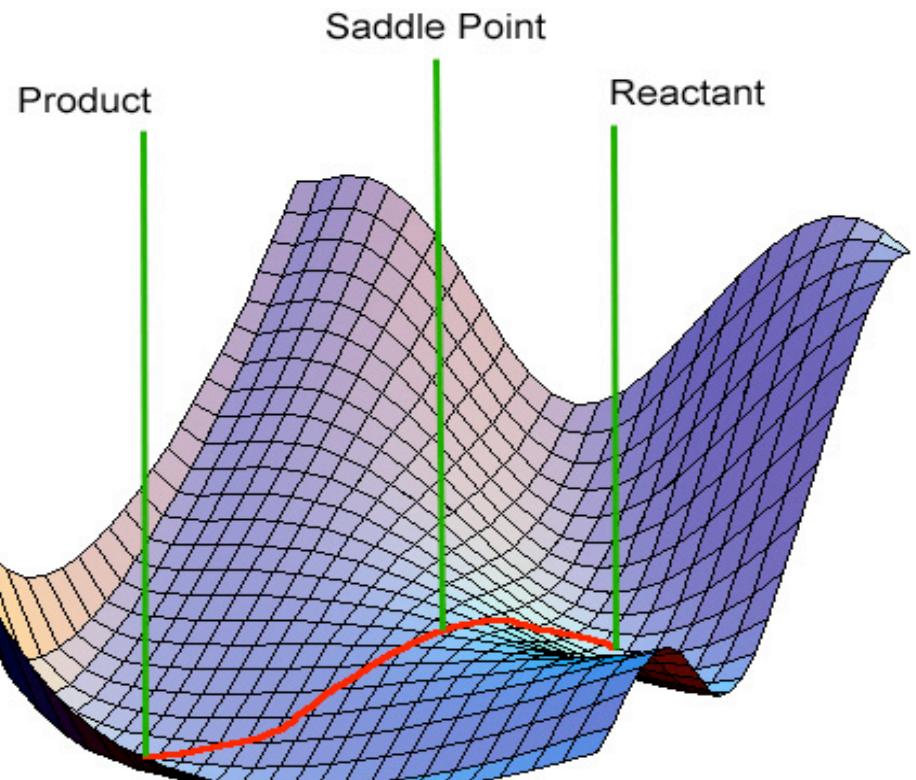
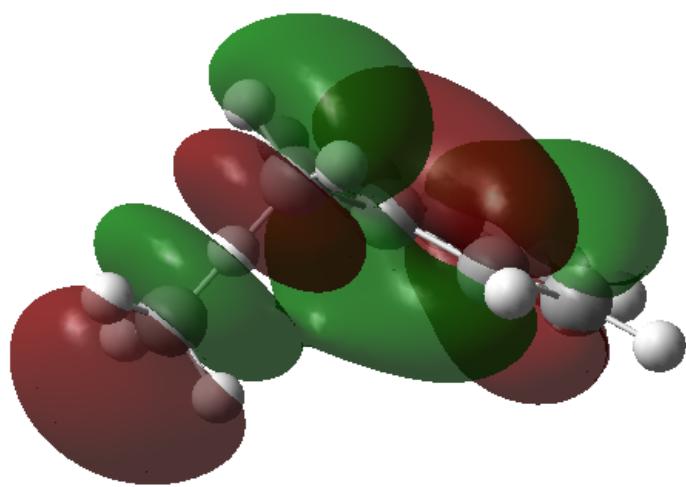


Core Electrons

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

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How to Create Input Files

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Input File

% Resource management

Route card



blank line

Title section



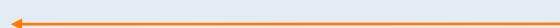
blank line

Molecular coordinates



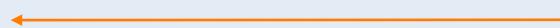
blank line

Geometric variables



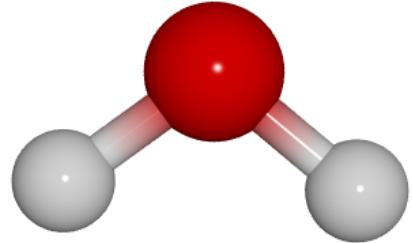
blank line

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



blank line

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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 r wf *file*
- %subst ln *dir* substitute link *n* with alternate executable found in *dir*

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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])]
```

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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

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Calculation Types:

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

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Levels of Theory:

- molecular mechanics
 - mm2, uff
- semi-empirical
 - AM1, PM3, PM6, MNDO, ...
- density functional theory
 - B3LYP, mPW91, M06, custom
- ...
- *ab initio*
 - HF, MP2, CCSD, QCISD, ...
- hybrid
 - G2, G3, oniom, ...

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Basis Set Types:

- all electron; Pople, Dunning, etc.
- effective core potential

User Supplied:

- use GEN keyword, #hf/gen

via input file:

C H O
6-31G(d,p)

F O
6-31G(d',p')

via external file:

@/home/blynch/basis/custom.gbs

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

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Spin multiplicity:

$$\text{multiplicity} = n + 1$$

where $n = \#$ of unpaired
electrons

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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

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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

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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.

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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`

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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**

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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
```

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New Features

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

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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.

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New Features

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

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New Features

- DFT
 - M06
 - M06L
 - wB97
 - HSE

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New Features

- Solvation
 - SCRF=SMD to calculate ΔG of solvation

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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

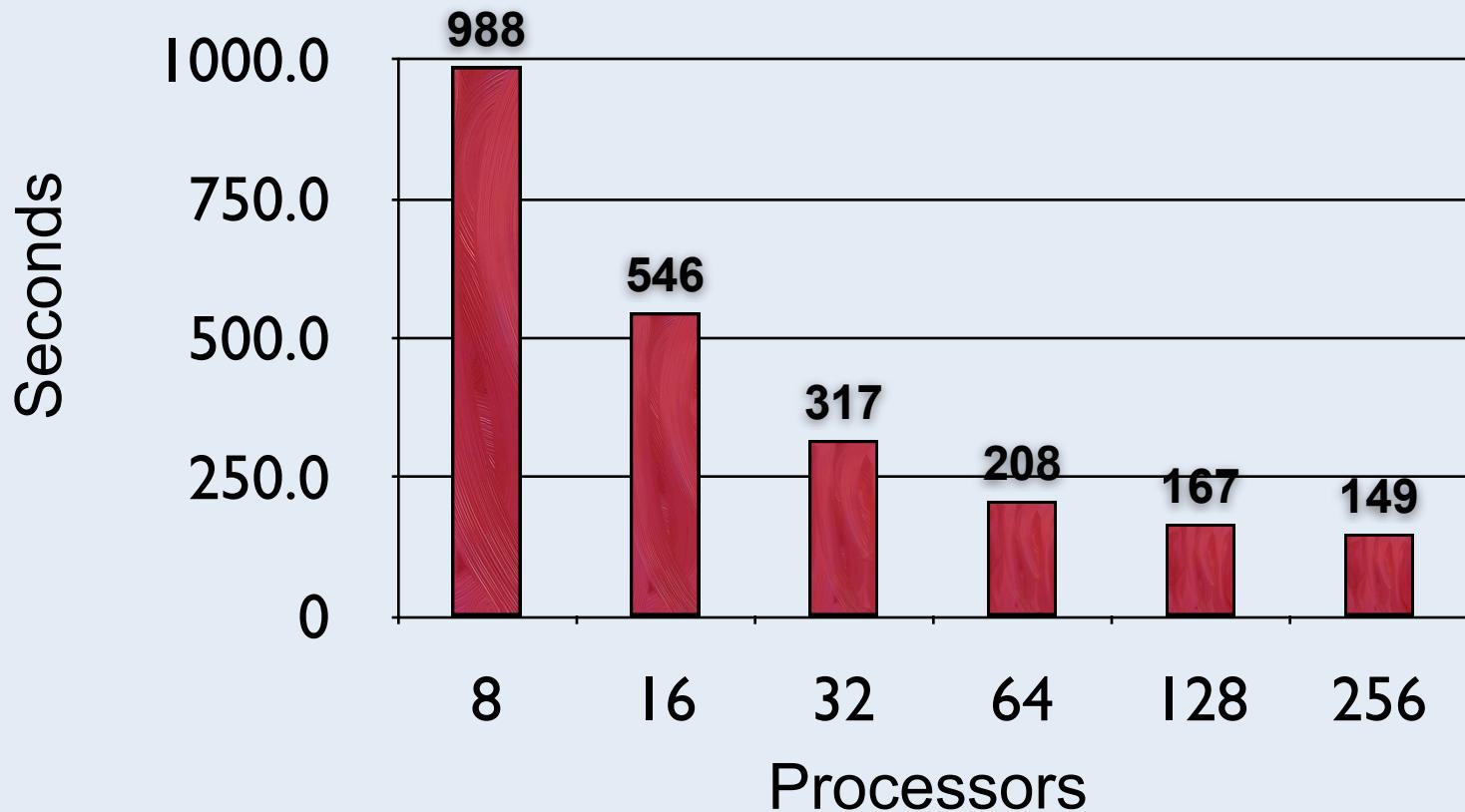
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Using Linda-Parallel Gaussian 09

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

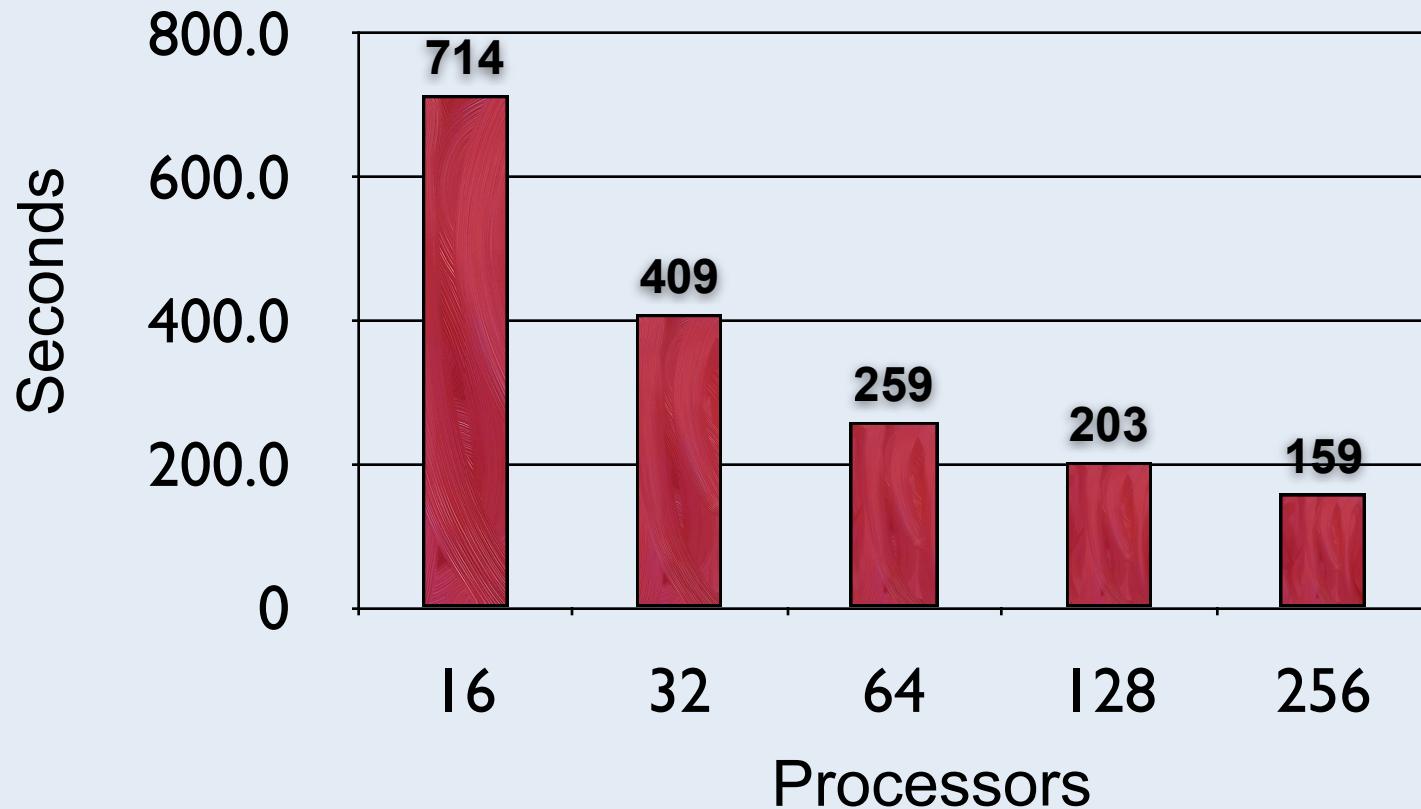
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Linda-Parallel M06/6-31G* on C₆₀



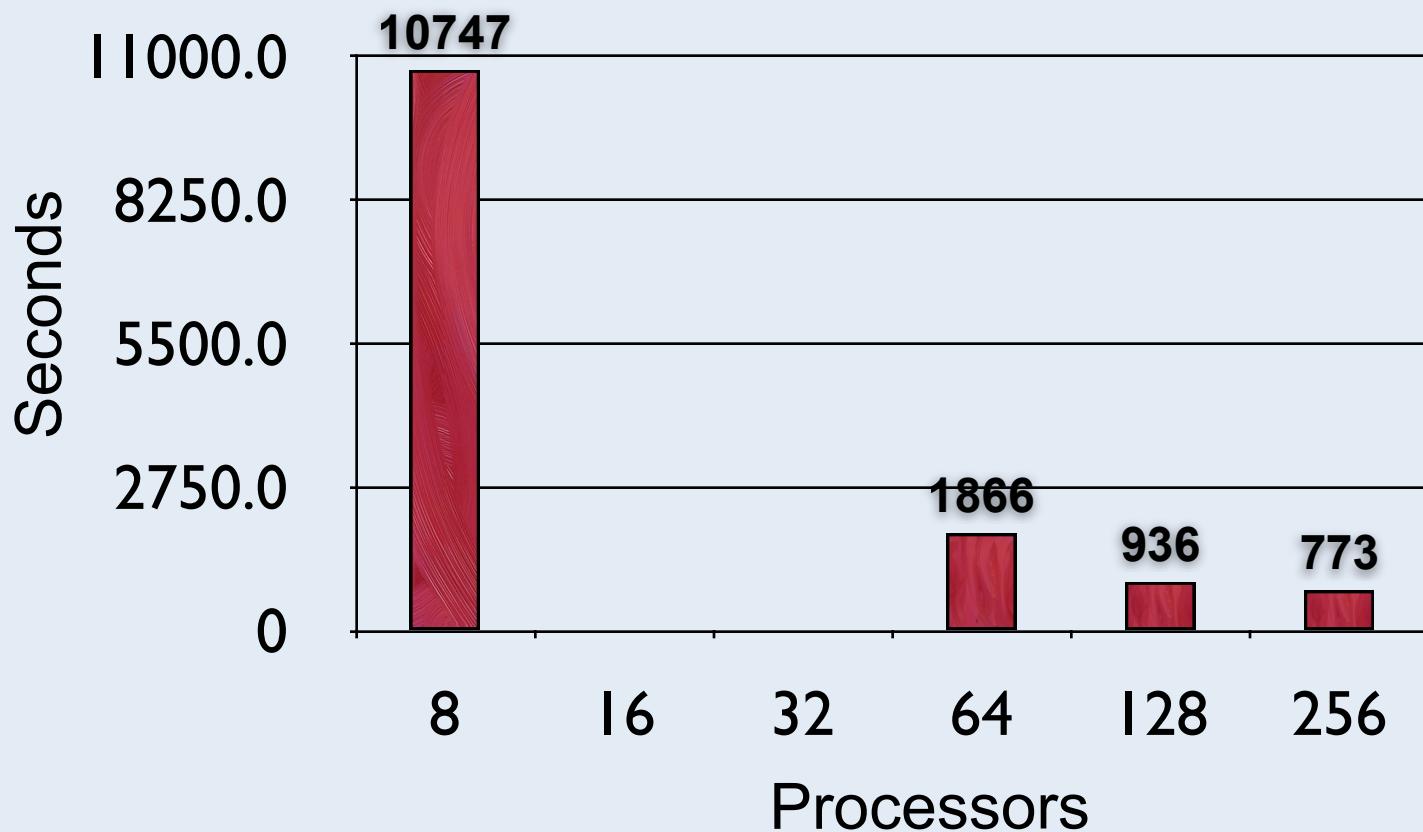
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Linda-Parallel M06/6-31G* Gradient on C₆₀



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Linda-Parallel MP2/6-31G* Energy on C₆₀



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Resource Considerations: %nprocshared

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

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Choosing %NProcShared:

Parallelized

- HF
- MCSCF
- DFT
- MP2
- CIS

Suggestion: 4-8 processors should be used

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Choosing the %NProcShared:

NOT- Parallelized much

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

Suggestion: 1-2 processors

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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

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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
```

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Building with Molden

- Login remotely
ssh -X blade.msi.umn.edu
- Load proper module
module load molden
- Launch Molden
molden

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Building with GaussView

- Login remotely

```
ssh -X calhoun.msi.umn.edu
```

```
ssh -X blade.msi.umn.edu
```

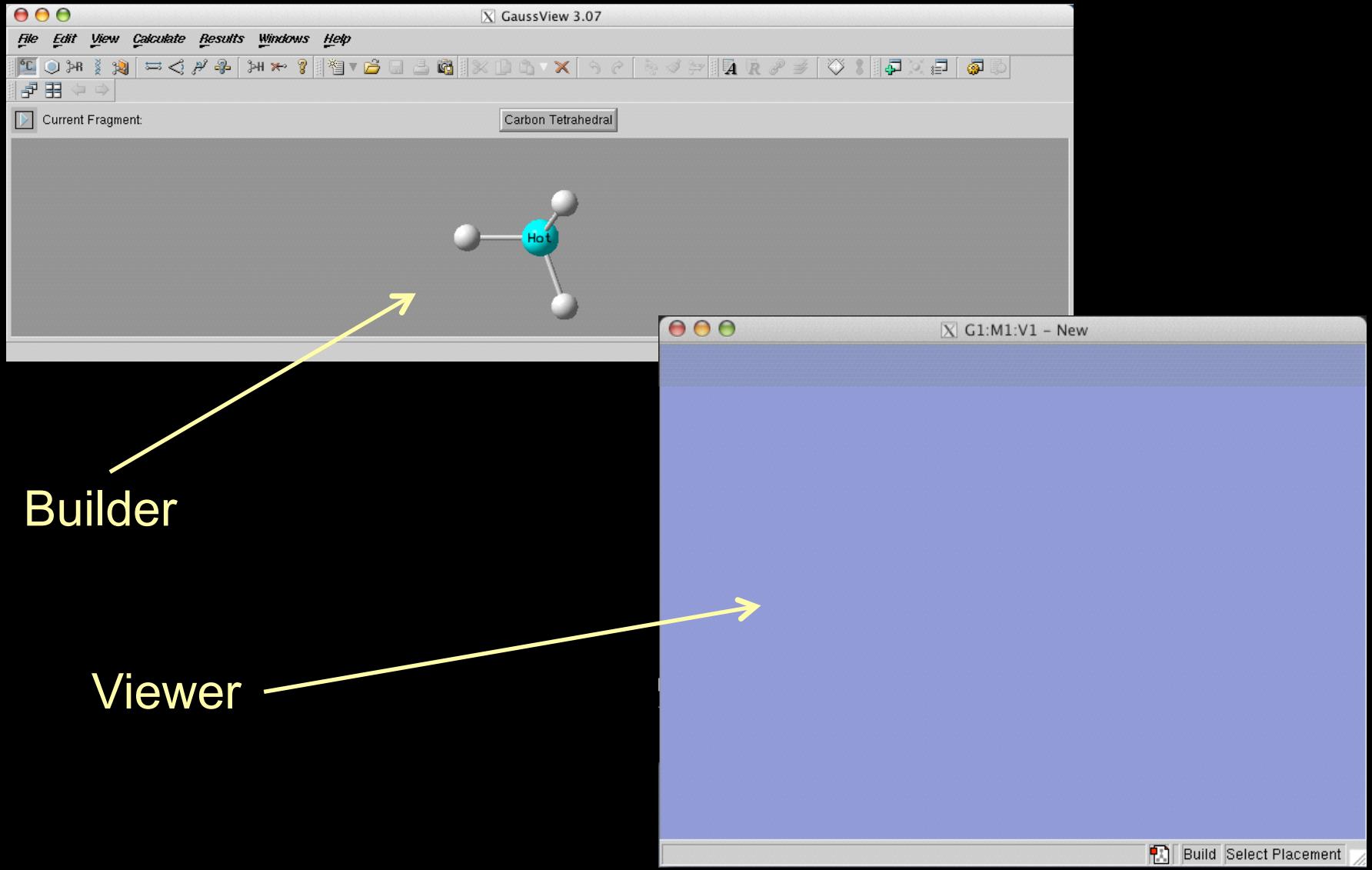
- Load proper module

```
module load gaussian
```

- Launch GaussView

```
gv
```

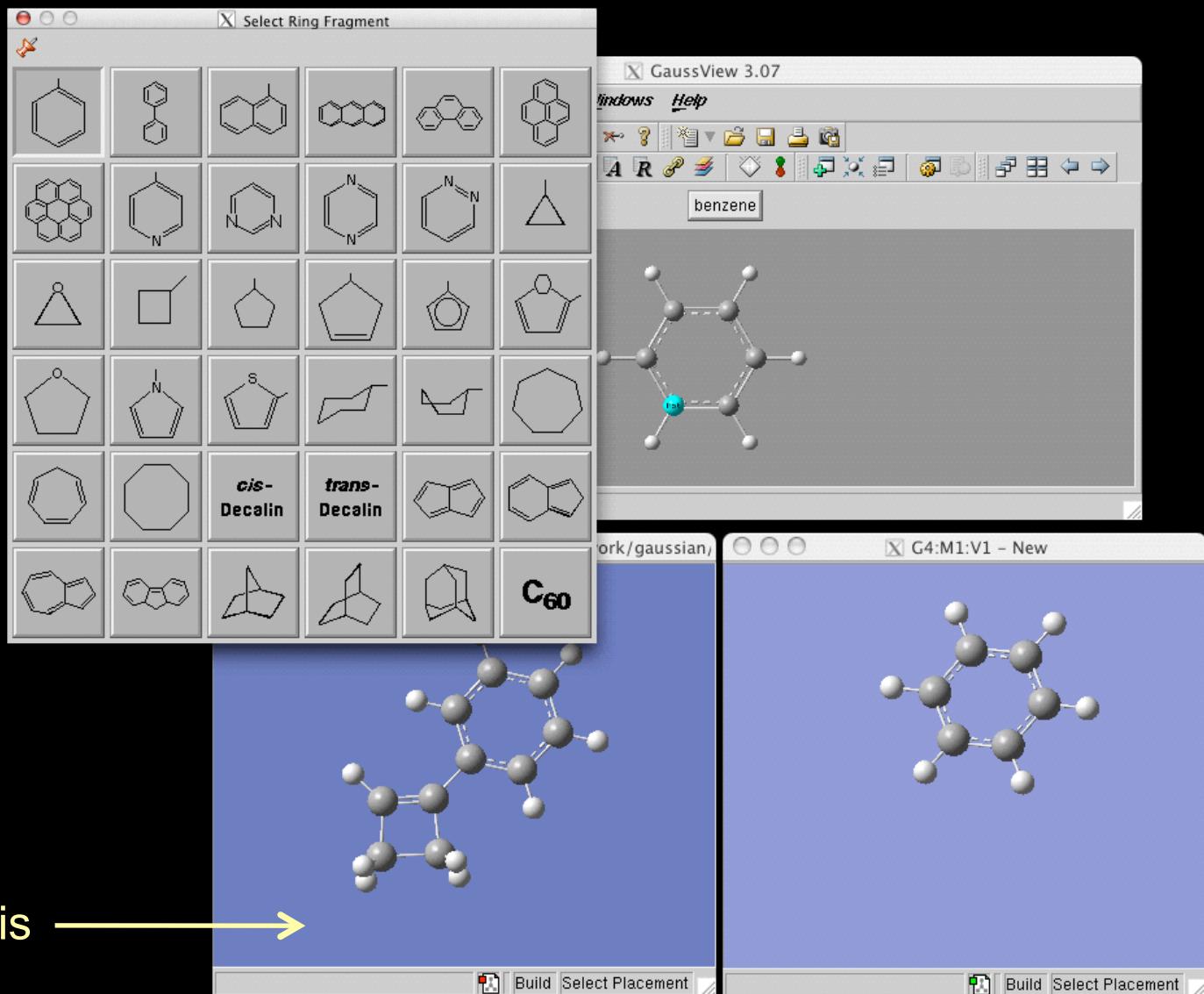
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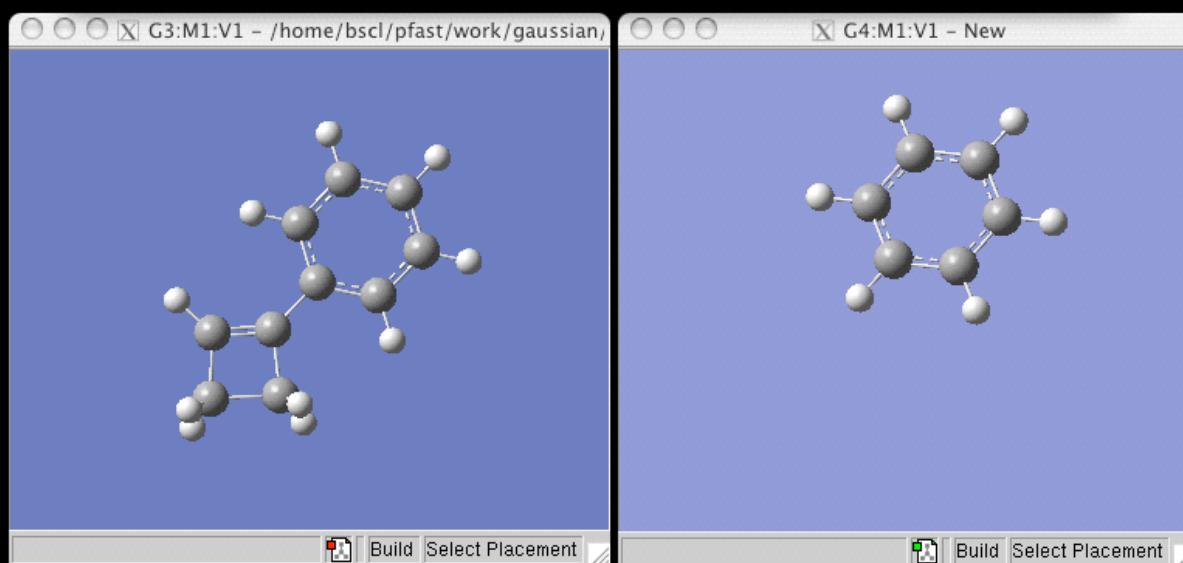
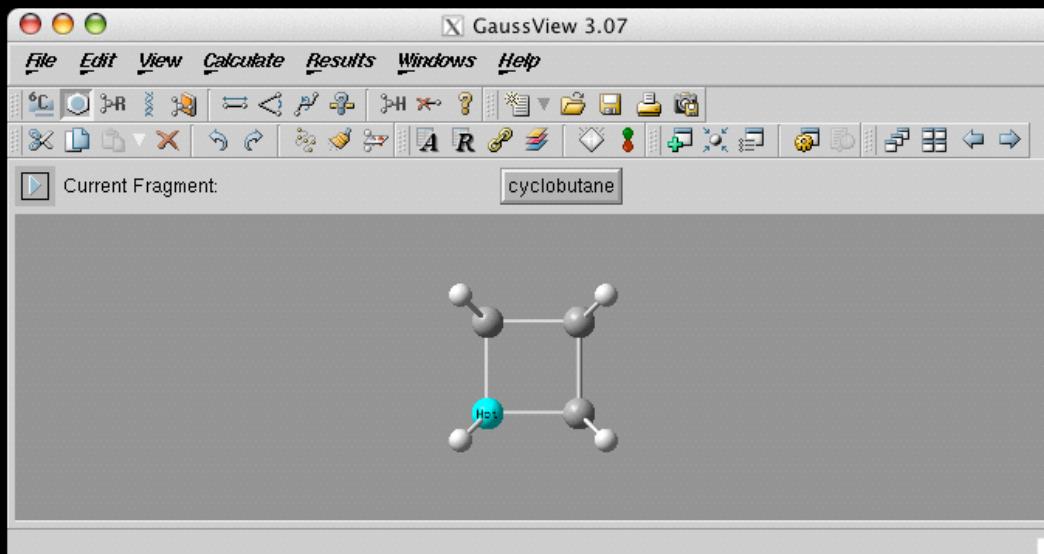
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Molecule Building



Molecule Building



X Select Element

Result:

H		X	Bq										He				
Li	Be																
Na	Mg																
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				

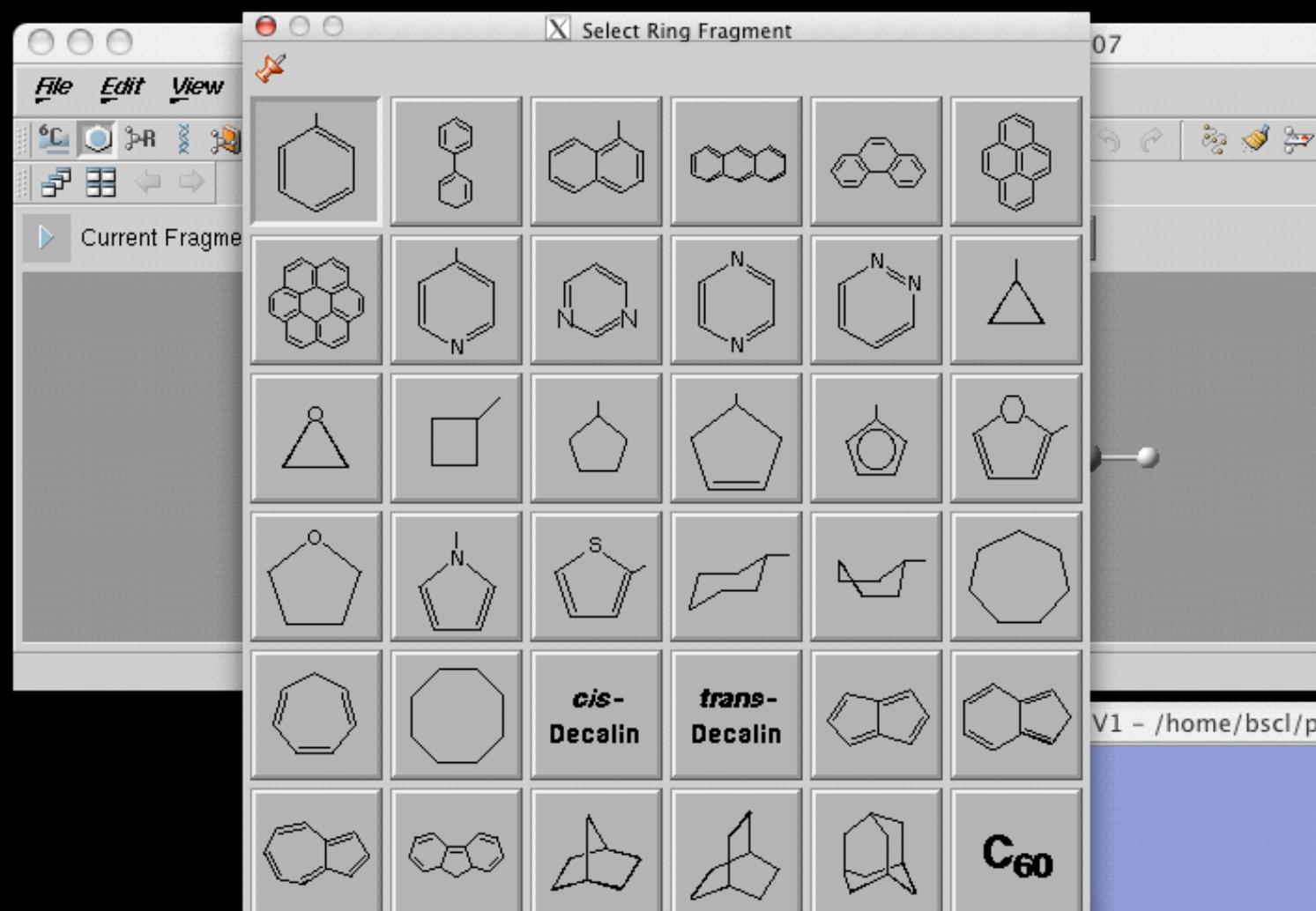
Select Carbon Fragment:

Elements:

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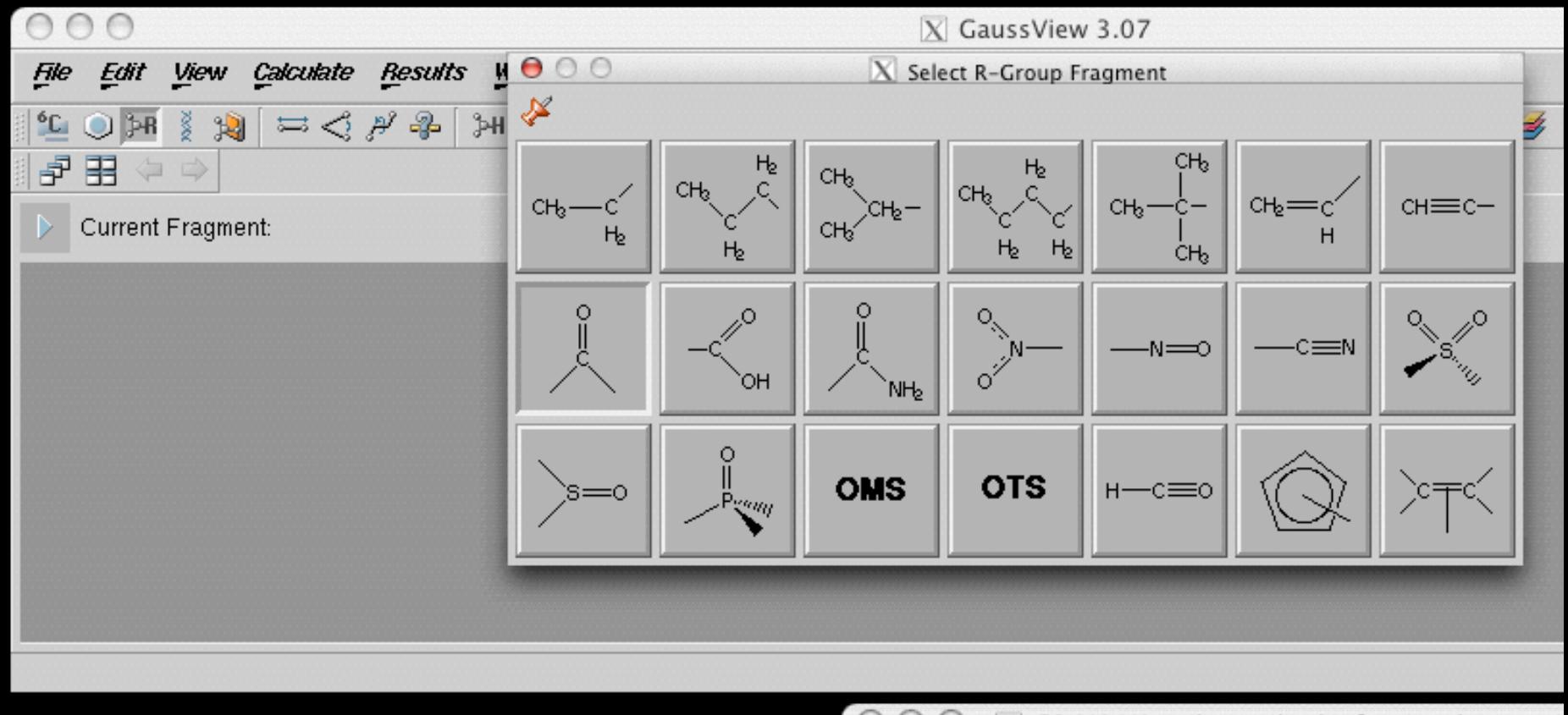


Ring Fragments:

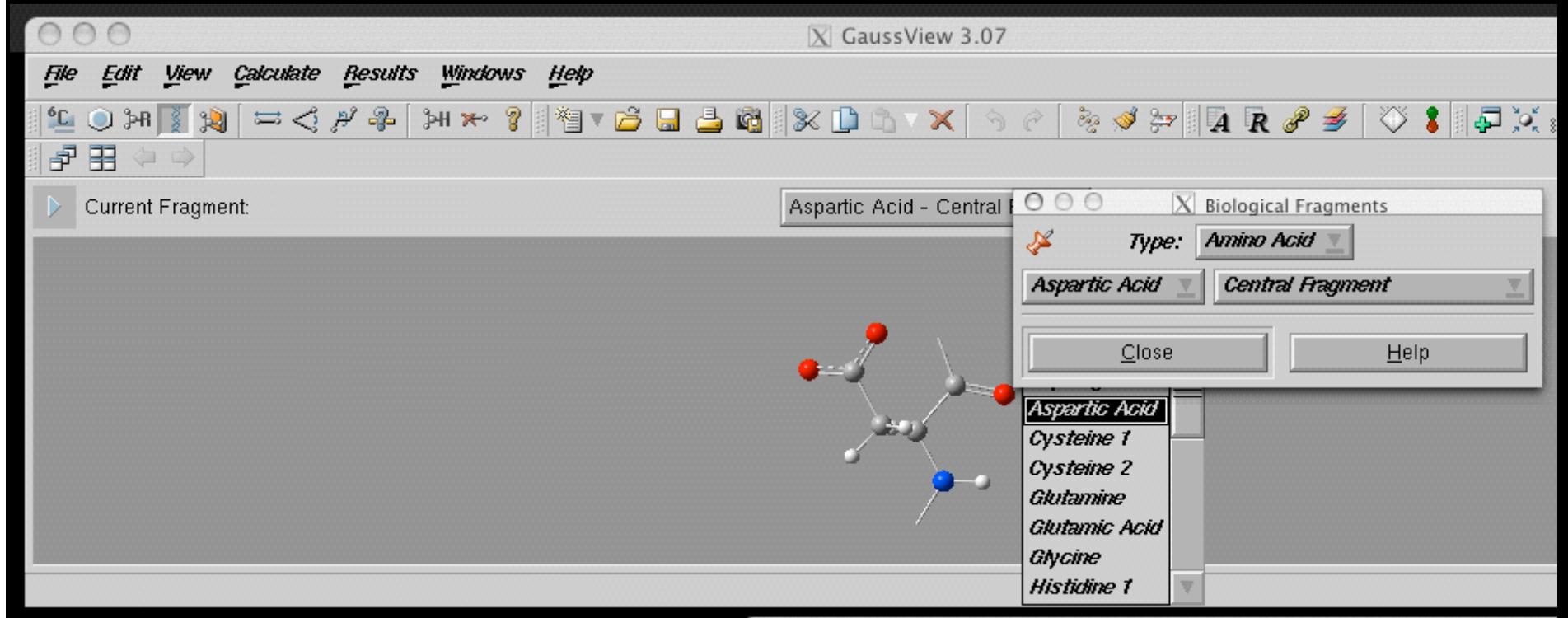
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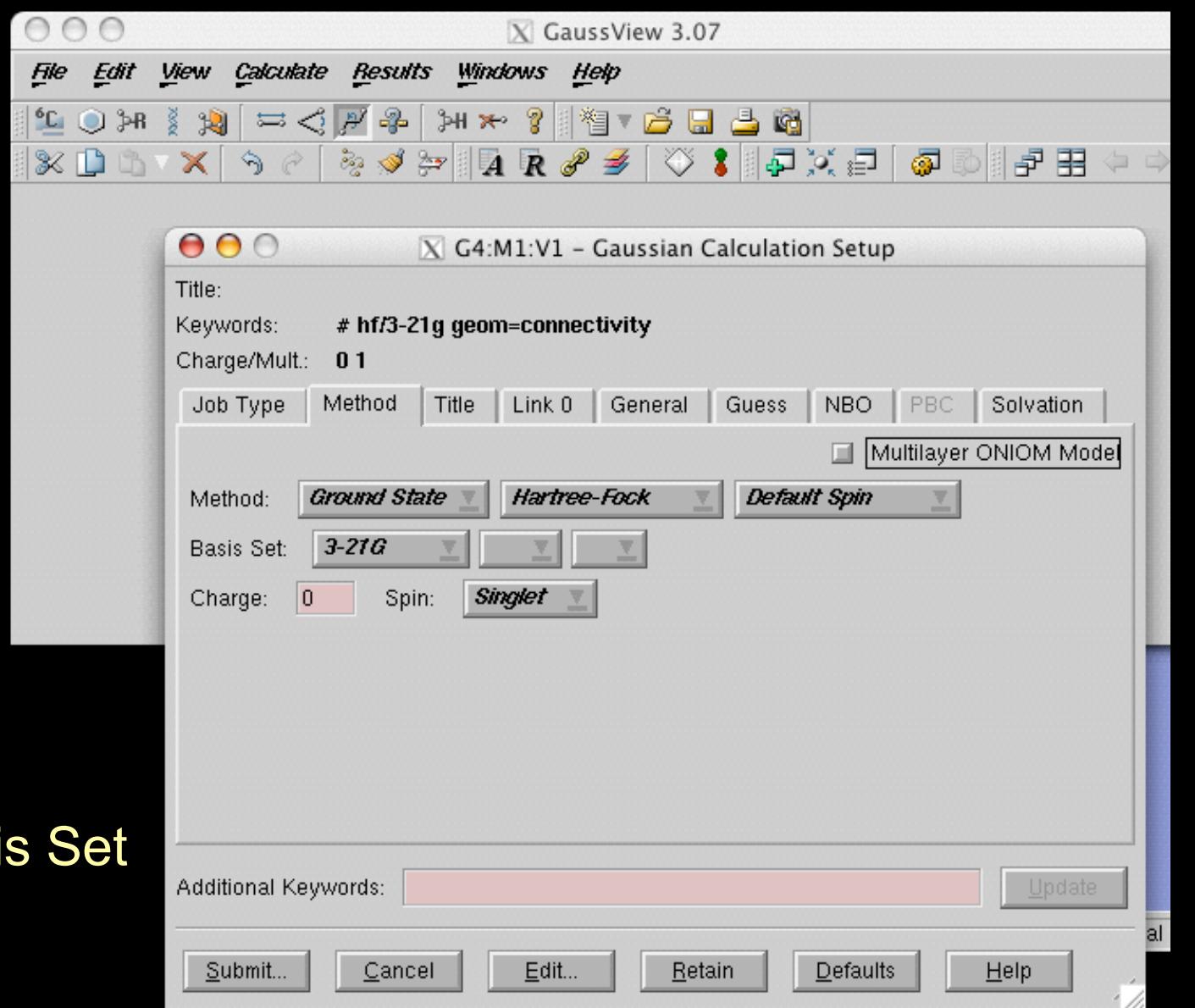
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R-Group Fragments:



Biological Fragments:





Method & Basis Set

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Sample Input File

```
chk=test.chk
mem=6MW
nproc=1
# hf/6-31g

Title Card Required

0 1
C
C          1      B1
C          2      B2  1      A1
C          3      B3  2      A2  1      D1
C          4      B4  3      A3  2      D2
C          1      B5  2      A4  3      D3
H          2      B6  1      A5  6      D4
H          3      B7  2      A6  1      D5
H          4      B8  3      A7  2      D6
H          5      B9  4      A8  3      D7
H          6      B10 1      A9  2      D8
C          1      B11 6      A10 5      D9
C          12     B12 1      A11 6      D10
C          12     B13 1      A12 6      D11
C          13     B14 12     A13 1      D12
H          13     B15 12     A14 1      D13
H          14     B16 12     A15 1      D14
H          14     B17 12     A16 1      D15
H          15     B18 13     A17 12     D16
H          15     B19 13     A18 12     D17

B1      1.40140000
B2      1.40140000
B3      1.40140000
B4      1.40140000
B5      1.40140000
B6      1.07000000
B7      1.07000000
B8      1.07000000
B9      1.07000000
B10     1.07000000
B11     1.54000000
B12     1.39937109
B13     1.53787622
B14     1.53786963
B15     1.07000000
B16     1.07000000
```

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

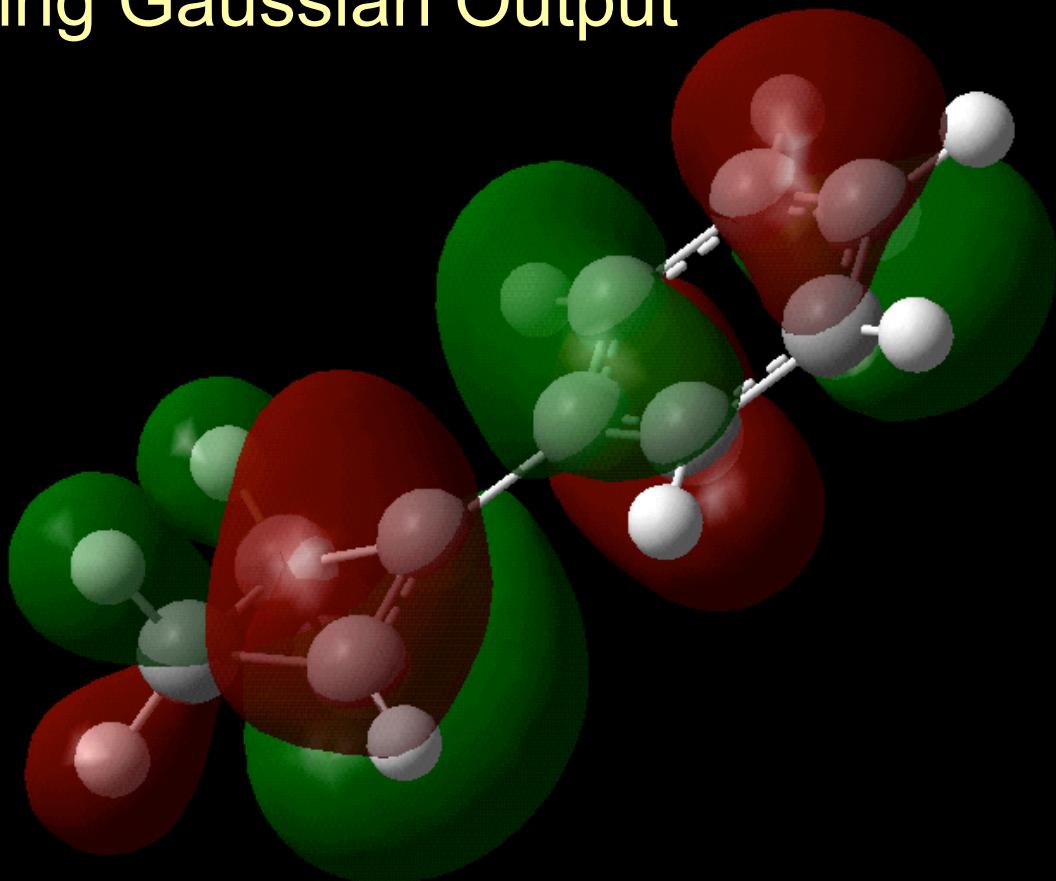
Open the file created called XXXX.out

(where XXXX was the input file name)

It's all text

It gives an outline of the calculation performed

Visualizing Gaussian Output



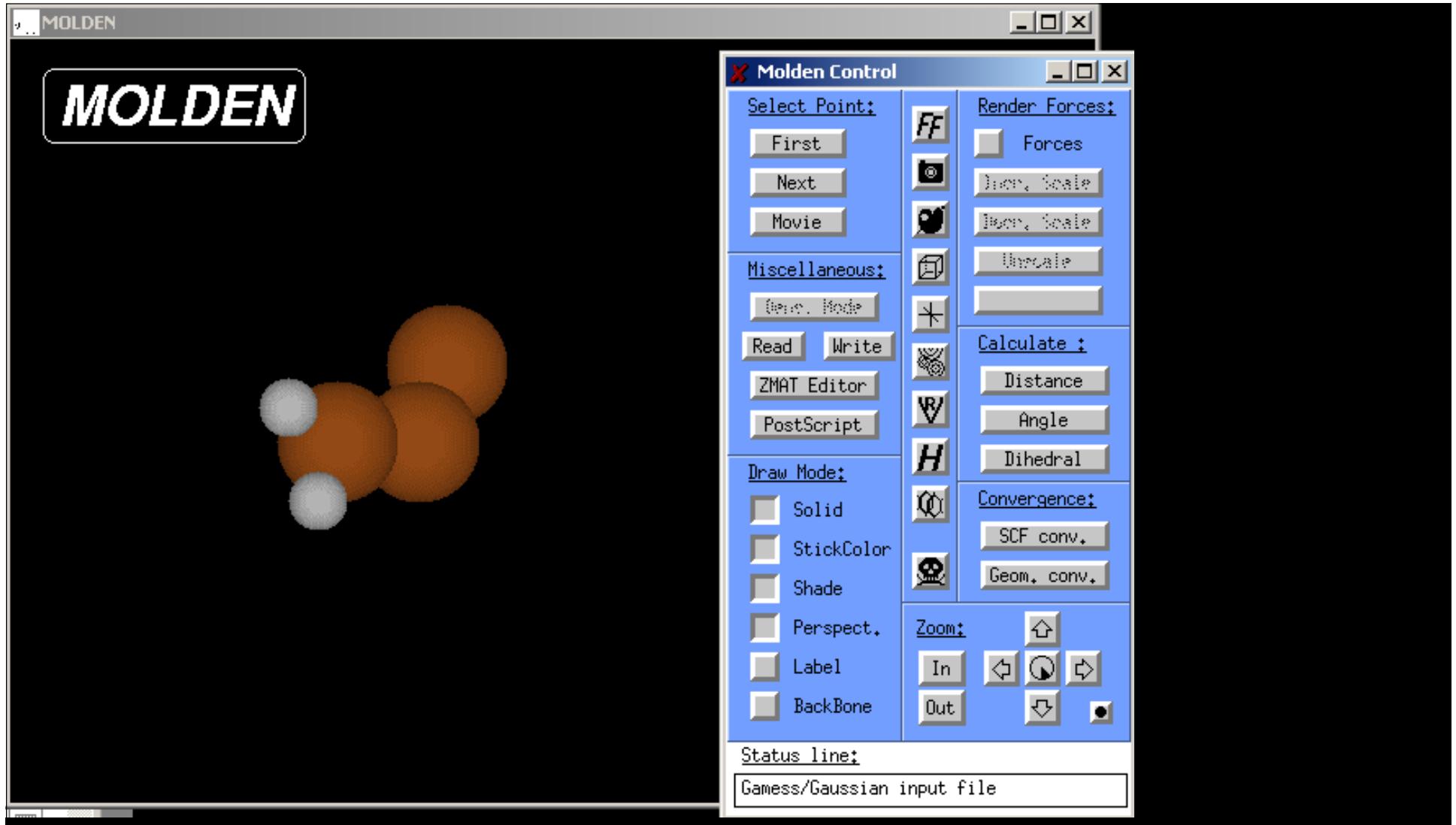
How to View Output Visually

```
module load gaussian
```

```
gv myoutput.out
```

```
module load molden
```

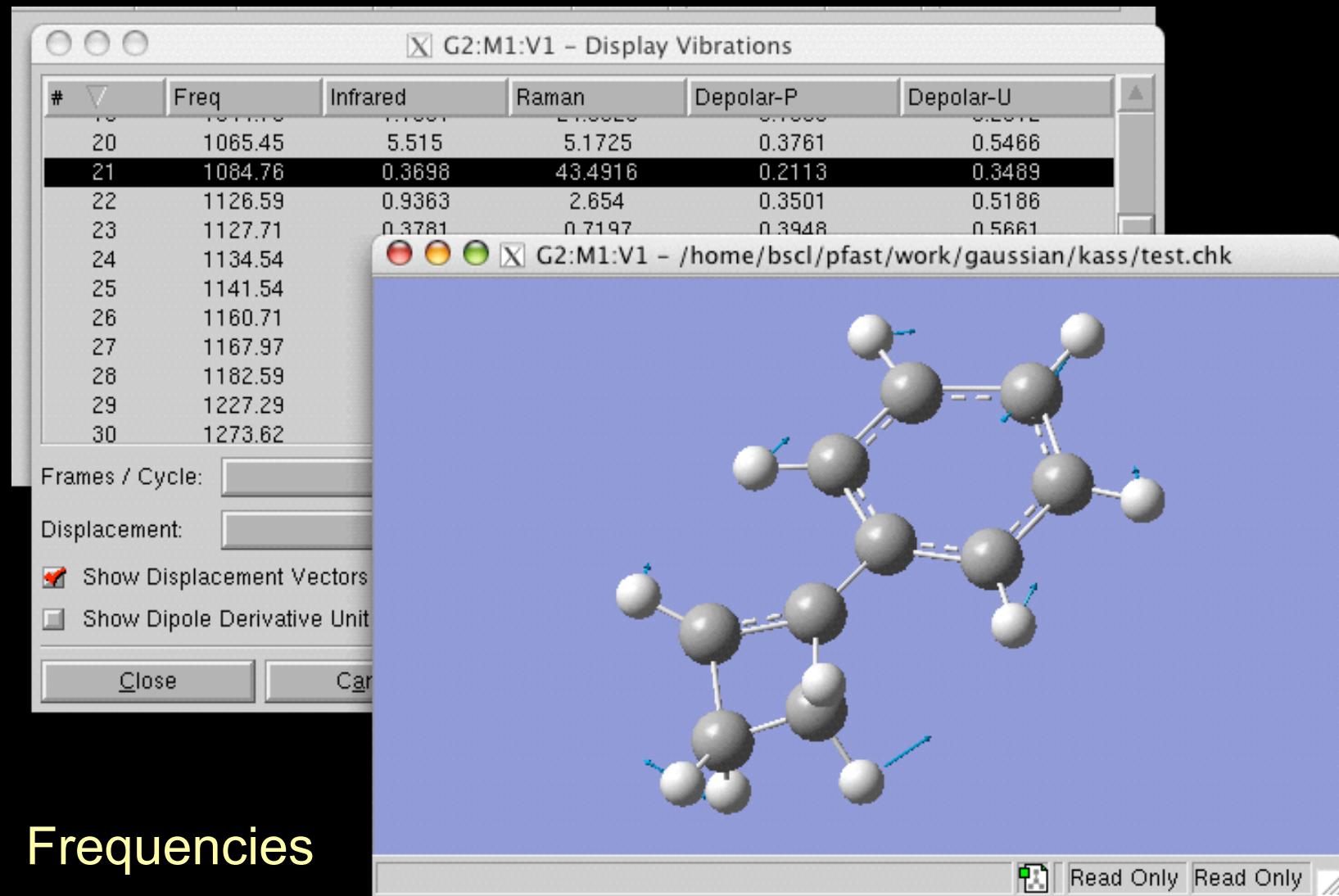
```
gmolden myoutput.out
```



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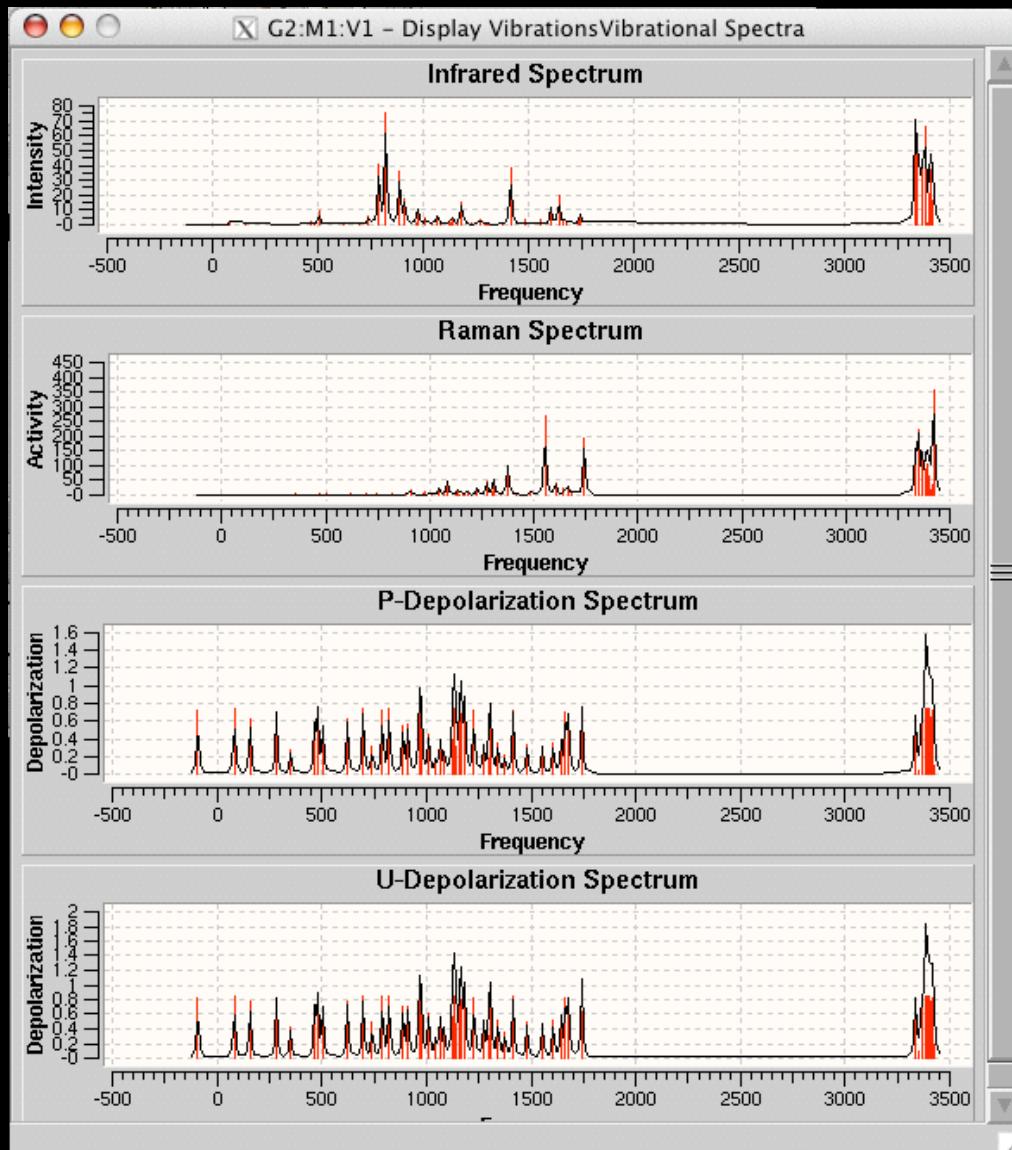
Visualization using Gaussview



Frequencies

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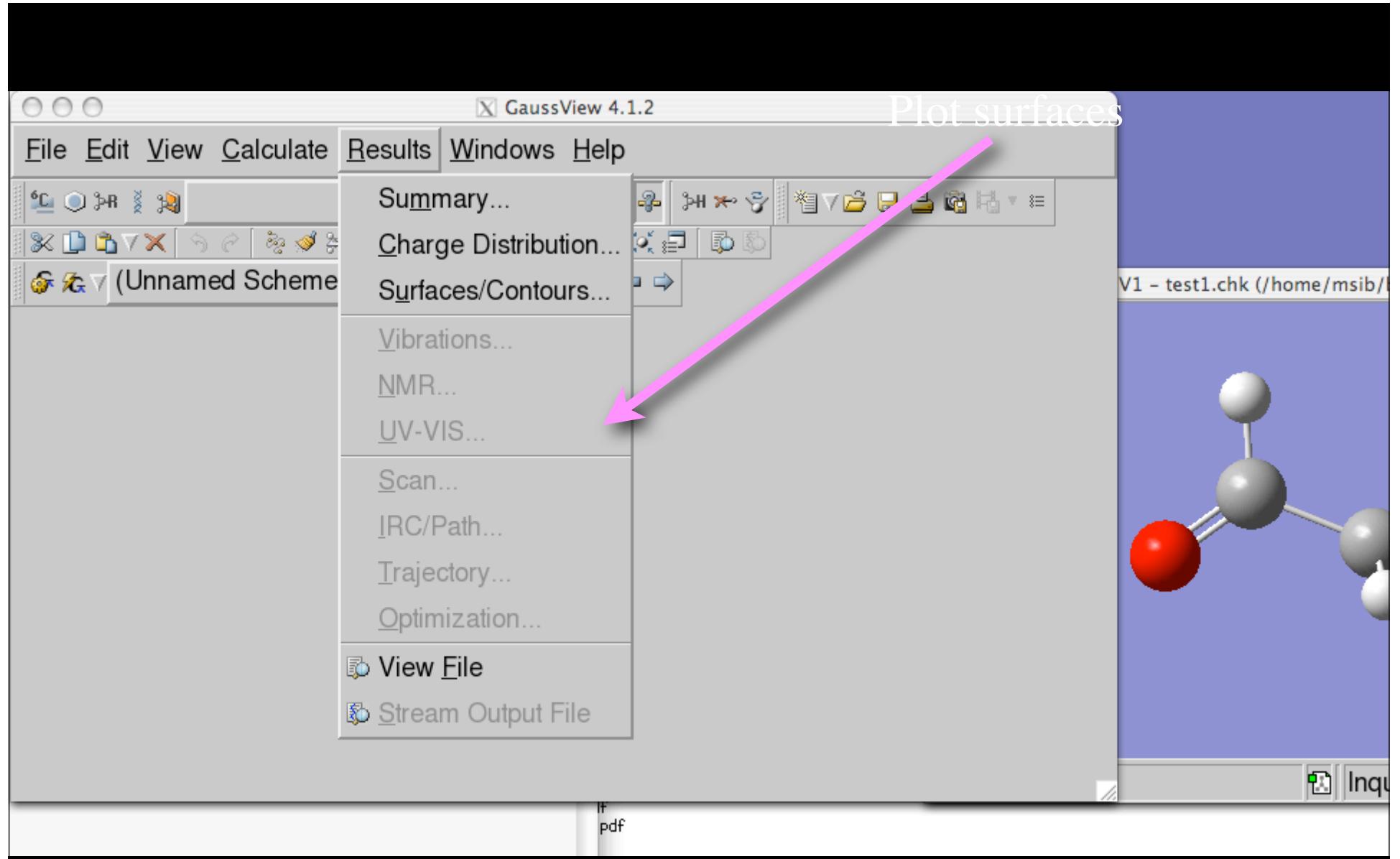


Spectra

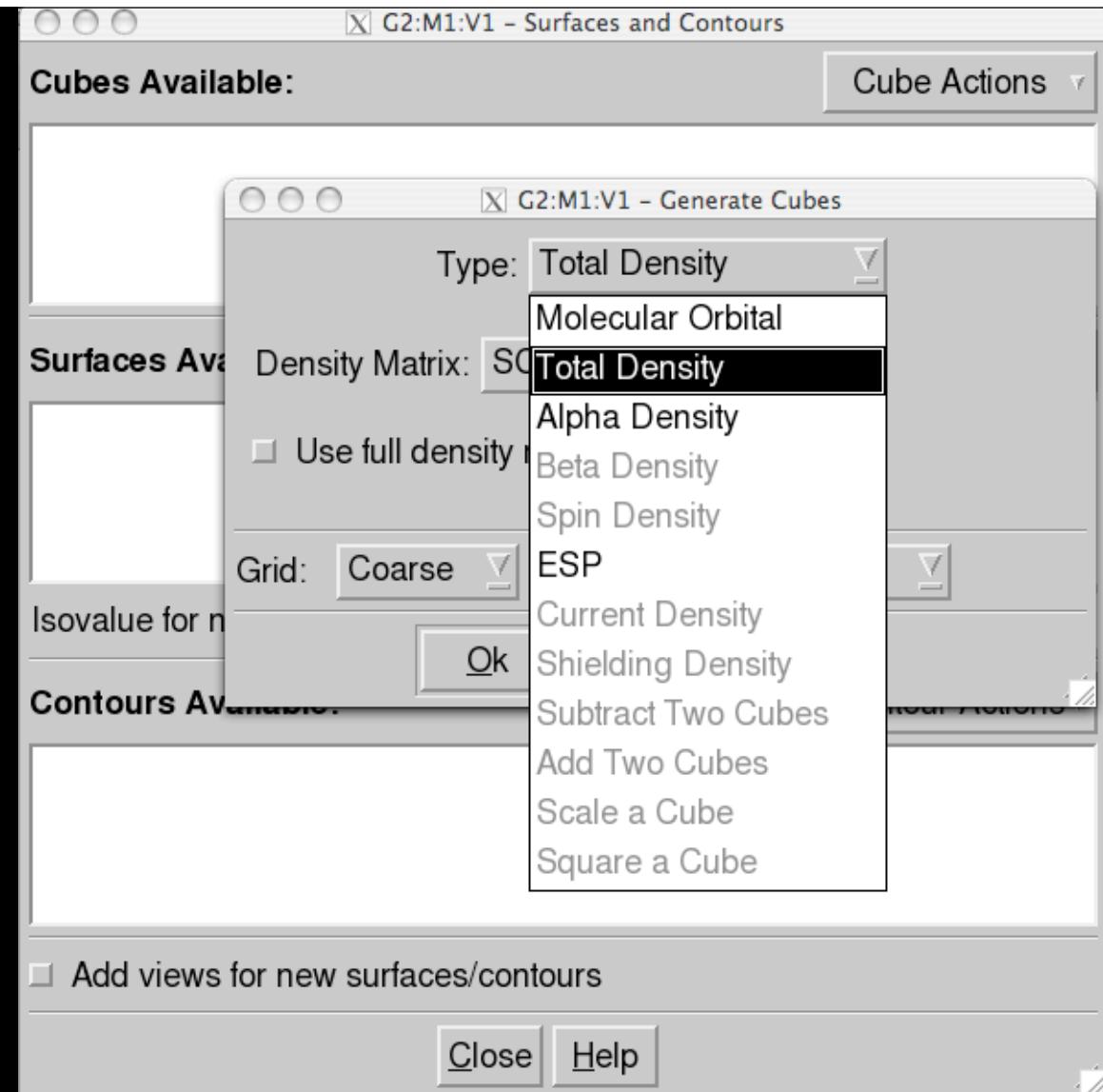
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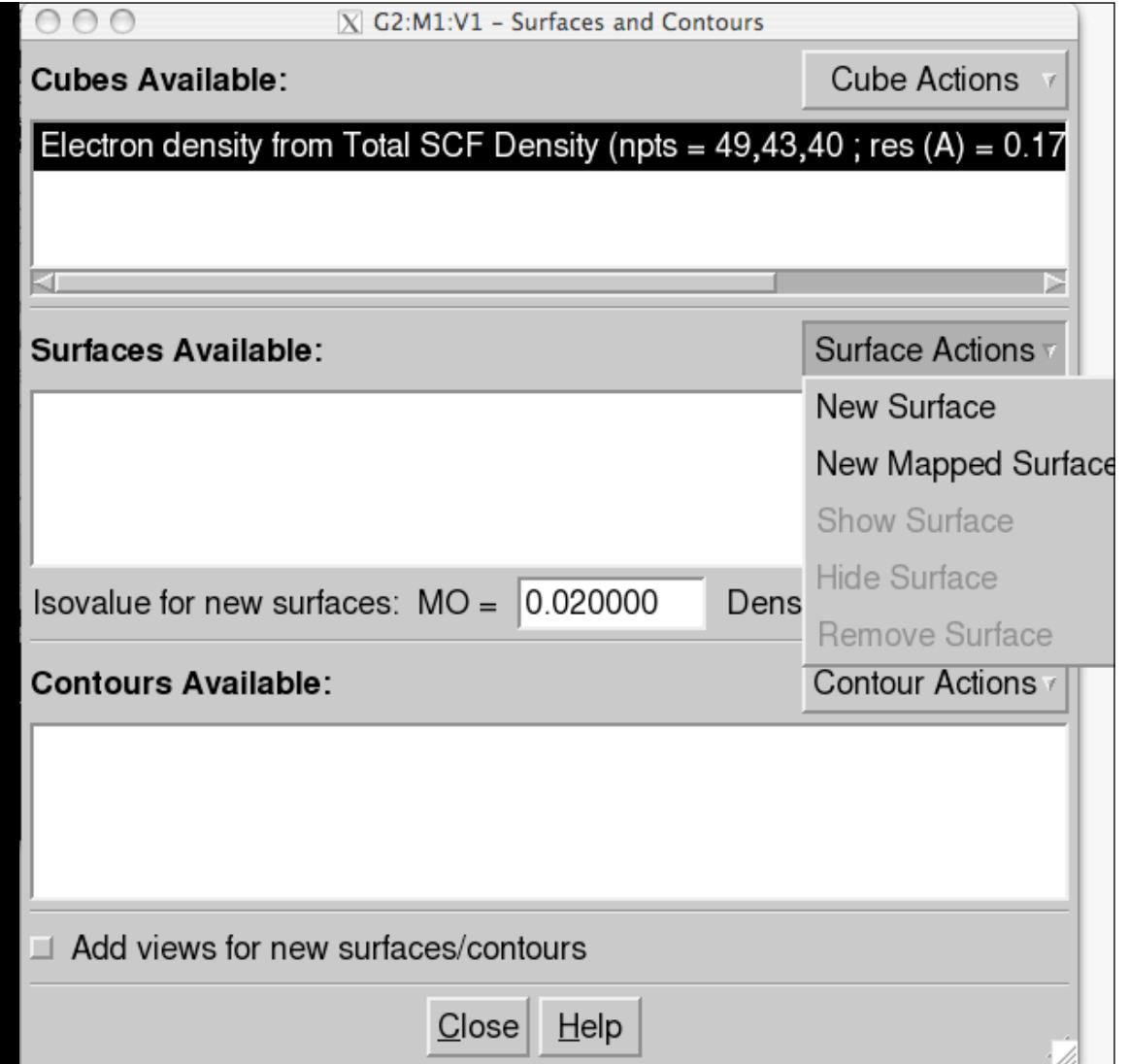
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A cube file is a 3-D array of the values of some property.

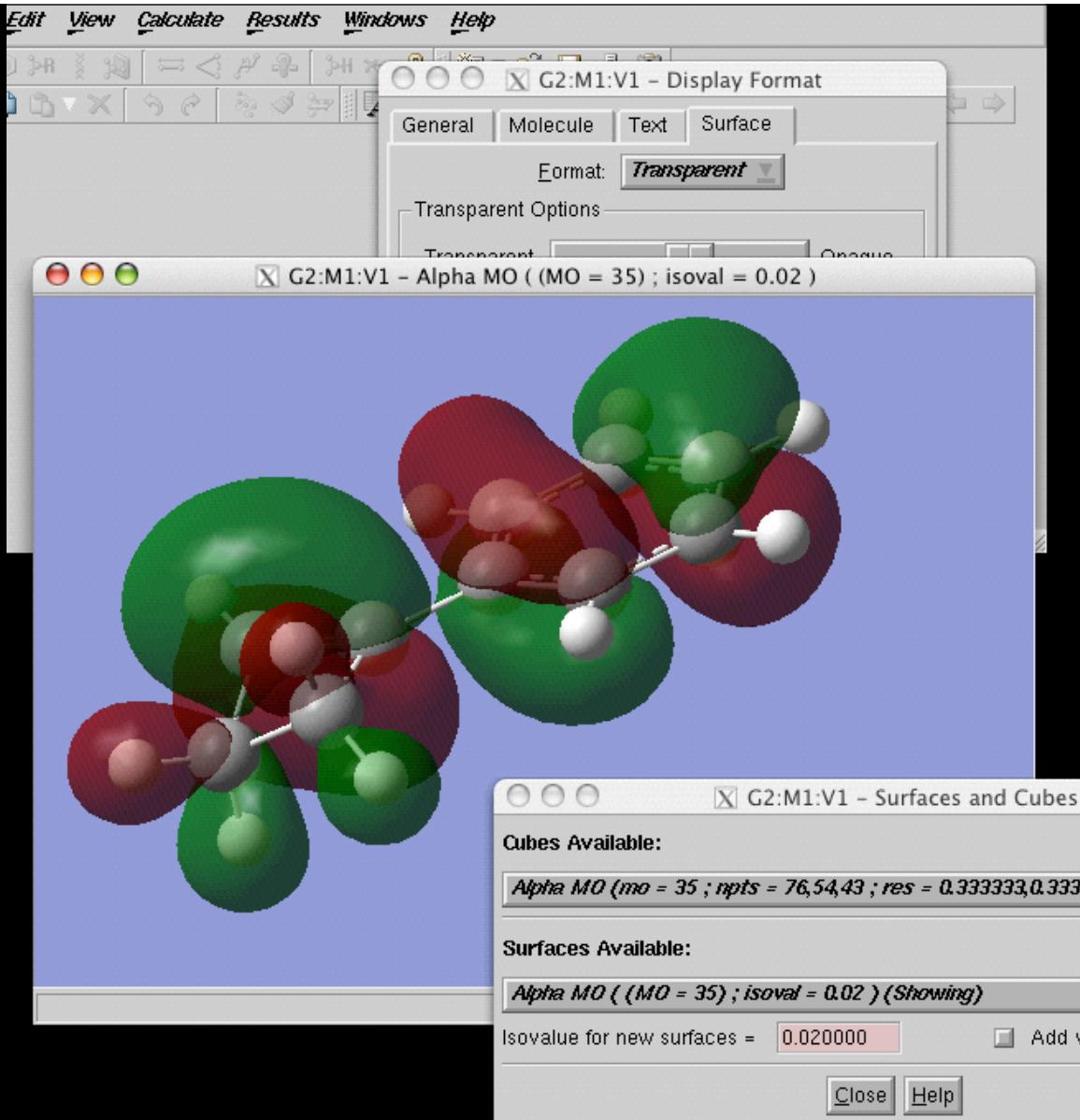


A New Mapped Surface
can map properties onto an
isosurface from an existing
cube file.



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



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?

email: blynch@msi.umn.edu
help@msi.umn.edu

phone: 612-624-4122
612-626-0802 (helpline)

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