Computers in Chemistry – Lecture II

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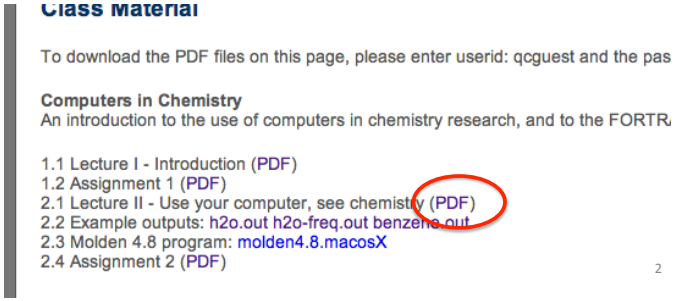
Get this lecture online

- Please go to: http://qc.chem.nagoya-u.ac.jp
- Click on “Teaching”
- Click on “PDF” link of “2.1 Lecture II - Use your computer, see chemistry”



High Performance Computing &

http://qc.chem.nagoya-u.ac.jp/hardware.html

HAWK (Irle Group)
412 CPU core Linux cluster + GPU test system
124 Opteron 2.4 GHz
288 Intel Xeon 3.0 GHz

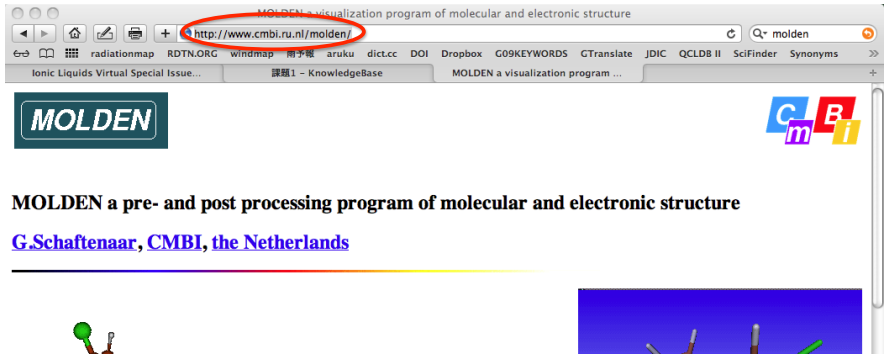
http://www.top500.org/
京 supercomputer
548,352 SPARC64 VIIIfx cores
Clockspeed: 2.0 GHz

Today’s Lecture

- Download a molecular visualization program (MOLDEN) to your Mac and run it under MacOS (=UNIX)
- Download GAUSSIAN output files to your Mac
- Molecular structure optimization (geometry optimization)
- Vibrational frequency calculations (IR, Raman spectra)
- Molecular orbital visualization

Download MOLDEN I

- In Safari or Firefox, open MOLDEN's website: http://www.cmbi.ru.nl/molden/



Download MOLDEN II

- Click on: "How to get a copy of Molden?"

module
molden4.7: partial optimisations are now possible (click here)
molden4.7: molden can now hold multiple structures in memory
molden4.6: features a forcefield optimisation program Ambfor (AMBER/GAFF forcefields)
molden4.6: now better supports Gaussian IRC optimisations and MP2 optimisations
molden4.6: Support for Orca.
molden4.6: Support for G functions with Gaussian.
molden4.6: features dynamic memory allocation for proteins and display of dipole moment.
full interactive opengl version of molden: gmolden

Molden topics:

- Register as a Molden User
- How to get a copy of Molden ?
- What are the latest changes/bugfixes to Molden ?
- The Z-Matrix Editor
- Using Molden with Gaussian outputs
- Using Molden with Mopac
- Using Molden with programs OTHER than Gamess/Gaussian/Mopac
- How to set up MOLDEN to use helper programs

Download MOLDEN III

- Click on: "How to get a copy of Molden?"

```
make

will make the executables molden, gmolden, ambfor and surf.

make gmolden

Will just make the interactive OpenGL version of Molden.

Click here to see the supported platforms.
Click here for pointers to compile molden from source on Linux.
Click here for information on the WindowsNT/95/98/XP/Vista version of molden.
Click here for Molden5.0,gmolden5.0, ambfor5.0, ambmd5.0 and surf executables for MacOSX, create
Click Here for instructions to compile the 64-bit version of molden5.0 for Mac OS X Lion, by Mas
```

- Actually, we are NOT going to do this! (since only 1 user from 1 university can download the program at the same time)

Download MOLDEN IV

- Instead: go back to: http://qc.chem.nagoya-u.ac.jp
- Click on "Teaching"
- Click on "molden4.8.macosX"

Class Material

To download the PDF files on this page, please enter userid: qcguest and the pas

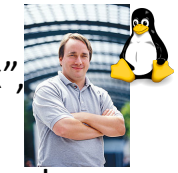
Computers in Chemistry
An introduction to the use of computers in chemistry research, and to the FORTR

1.1 Lecture I - Introduction (PDF)
1.2 Assignment 1 (PDF)
2.1 Lecture II - Use your computer, see chemistry (PDF)
2.2 Example outputs: h2o.out h2o-freq.out benzene.out
2.3 Molden 4.8 program: molden4.8.macosX
2.4 Assignment 2 (PDF)

- Save the file in your "Downloads" directory (in Japanese: ダウンロード). You may have to "<CTRL><click>": hold the "control" key, and click!

The Operating System of Your Mac

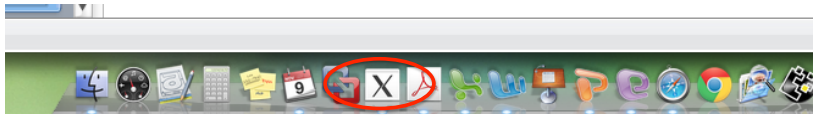
- Based on UNIX, and closely related to programming language “C”
- UNIX has a long history, was first developed in 1969 by AT&T/Bell Labs
- Became popular in in the ’90s as “Linux”, developed by “Linus Torvald”



- Linux and UNIX now base of operating systems such as Android, MacOS, etc. and used in webservers and data servers up to “K” Supercomputer in Kobe

Running programs under MacOS = UNIX I

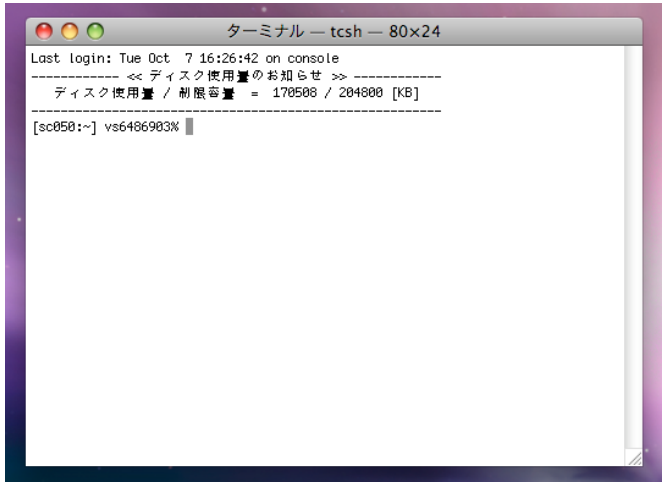
- Open X-Windows:



- X-Windows is the industry-standard graphical user interface for all Linux/UNIX/MacOS operating systems.
- Once you understand how to use X-Windows, you can use *graphics on most computer systems, from PC to Supercomputer*

Running programs under UNIX II

- X-Windows automatically opens a so-called “Terminal”



Running programs under UNIX III

- In a “Terminal”, you can move around in directories, and issue UNIX/Linux “commands”.
- Example of directory structure:

```
tree test
test                    directory of interest
|-- test1               subdirectory inside ‘test’ directory
|   `-- test1-file      file inside ‘test1’ subdirectory
|-- test2               another subdirectory inside ‘test’
|   |-- test2-file1     file inside ‘test2’ subdirectory
|   `-- test2-file2     another file inside ‘test2’ subdir.
`-- test3               another subdirectory inside ‘test’
                            empty
3 directories, 3 files
```

Running programs under UNIX IV

- After opening the terminal, you are always in your $HOME directory
- Useful commands to move around in your directory system:
- `pwd` – show current directory
- `cd <dir>` – change the current directory to <dir>
- `cd` – change current directory to "$HOME" directory
- `ls` – list contents inside current directory

Running programs under UNIX V

- After opening the terminal, you are always in your $HOME directory
- Useful commands to move around in your directory system:

1. `pwd` – show current directory
2. `ls` – list contents inside current directory
3. `cd <dir>` – change the current directory to <dir>
4. `cd` – change current directory back to "$HOME" directory

Running programs under UNIX VI

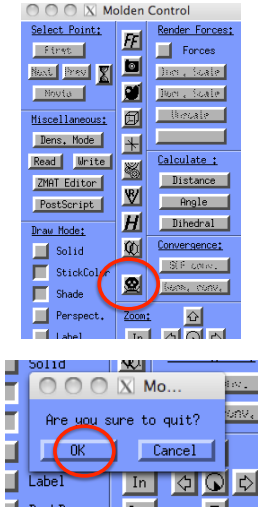
- `cd ..` – change current directory "up" on the directory tree
- `less <file>` – show the contents of a file (only works for text files, 'q' will exit)
- `mv <oldfile> <newfile>` – renames a file from <oldfile> to <newfile>
- `chmod a+rx <file>` – change mode of a file to "all users can read and execute"
- `./<file>` – execute (="run") a program contained in <file>

Running MOLDEN I

- `cd Downloads`
- `chmod a+rx molden4.8.macosX` – change mode of this file to "all users can read and execute"
- `./molden4.8.macosX` – execute (="run") MOLDEN
- You should see two windows like this:

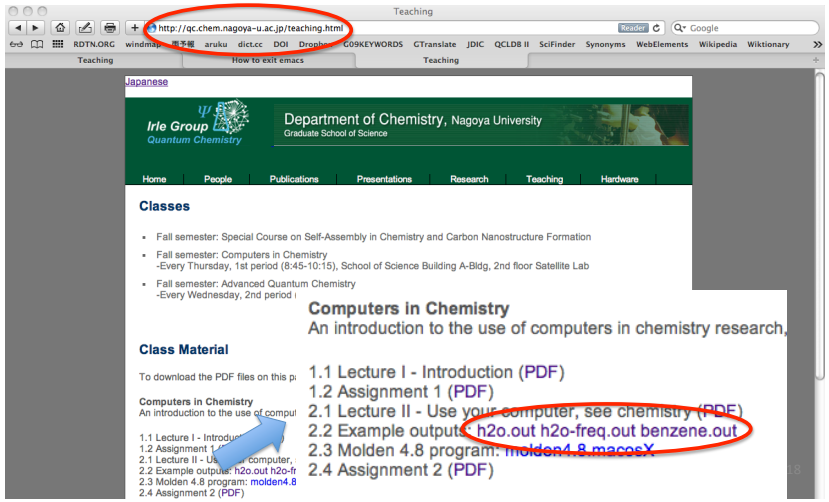
Running MOLDEN II

- Quit MOLDEN:



Running MOLDEN III

- Download example GAUSSIAN output files:



Running MOLDEN IV

- <Ctrl>Click (press “control key” while you click”)
  → Save linked file to “Downloads”
- Do this for all three files:
- h2o.out (water geometry optimization)
- h2o-freq.out (water IR and Raman calculation
- benzene.out (benzene molecular orbitals)

In your terminal, type:

```
cd
cd Downloads
ls
```

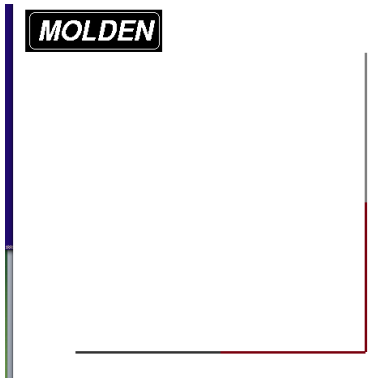
(you should see: h2o.out.txt, h2o-freq.out.txt, benzene.out.txt)

Running MOLDEN V

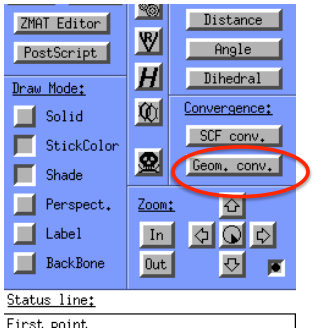
- Rename the files from “*.out.txt” to “*.out”
- `mv h2o.out.txt h2o.out`
- `mv h2o-freq.out.txt h2o-freq.out`
- `mv benzene.out.txt benzene.out`
- Let’s start with the H2O geometry optimization:
- `./molden4.8.macosX h2o.out`

Running MOLDEN VI

- You should see rectactangular water, after you rotate the molecule:

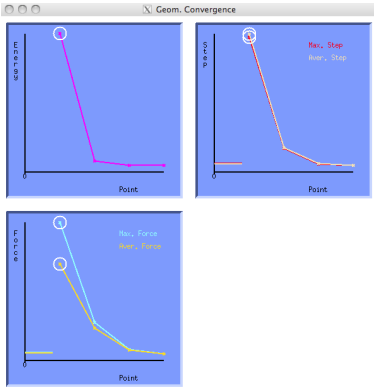


Click on “Geom. conv.”



Running MOLDEN VII

- You should see the “geometry optimization history:

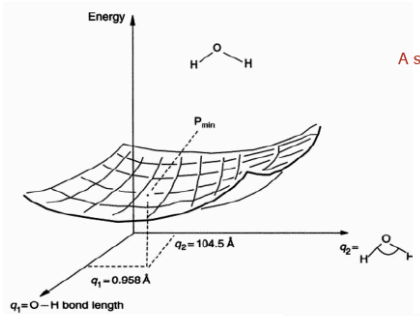


Click on “each point and see how the structure and energy changes

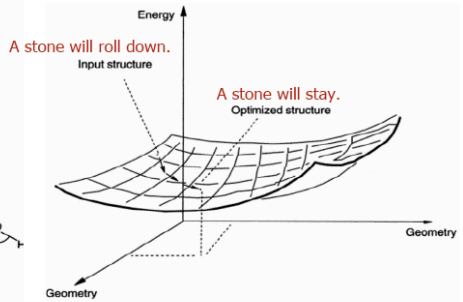
This was calculated using B3LYP/6-31G*

Molecular structure optimization

Energy minimum (Equilibrium structure)



Energy minimization Geometry optimization

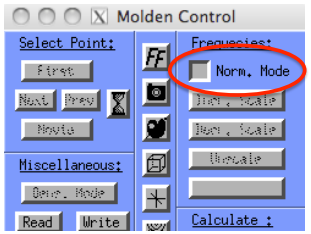


$$\frac{\partial E}{\partial q_1} = \frac{\partial E}{\partial q_2} = \cdots = 0 \quad \text{for all q}$$

$$\frac{\partial^2 E}{\partial q^2} > 0 \quad \text{for all q}$$

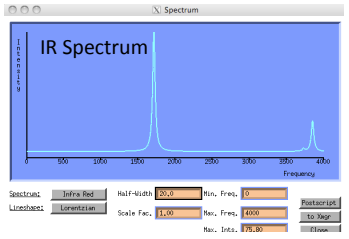
Running MOLDEN VIII

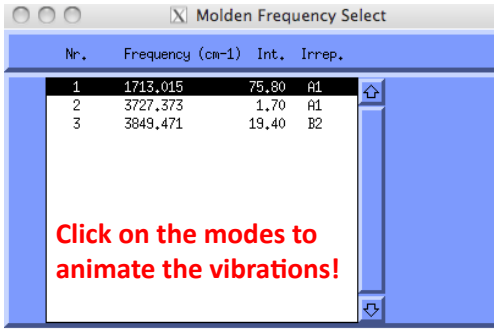
- exit Molden
- Now let’s see IR and Raman spectra of H_2O
- `./molden4.8.macosX h2o-freq.out`
- You should see: H_2O at equilibrium (=optimized) geometry
- Click on: “Norm. Mode”

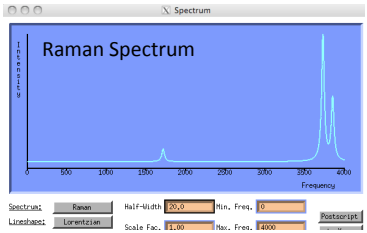


Running MOLDEN IX

- You should see:

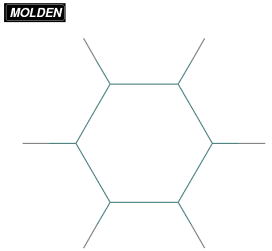






Running MOLDEN X

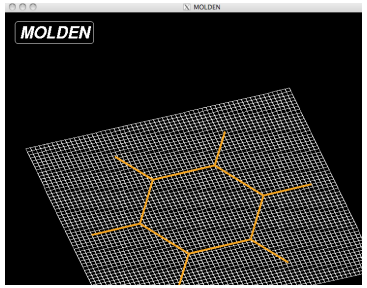
- exit Molden
- Let's see the some molecular orbitals (MOs) now
- `./molden4.8.macosX benzene.out`
- You should see: benzene at optimized geometry, B3LYP/6-31G* level of theory



Running MOLDEN XI

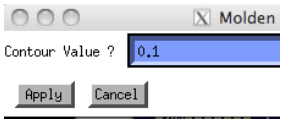
- Click on "Dens. mode"

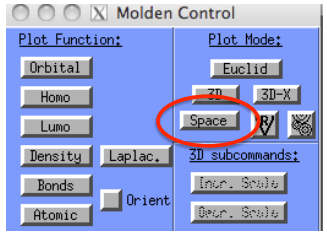
- You should see:



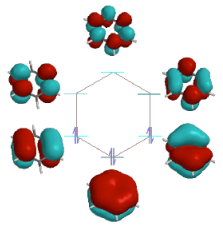
Running MOLDEN XII

- Now visualize the π–MOs
- Click on "Space"
- Enter value "0.1"





Click on "Orbital", and select any orbital you wish to see.



Task: find the 6 familiar π orbitals and record the orbital energies