EMORY Emerson Center for Scientific Computation

Tentative Program

I. OVERVIEW

1. Modern methods of computational chemistry (MM, ab initio, DFT and Hybrid methods).
2. Introduction to the Emerson Center's facilities

II. Molecular mechanics and Molecular Dynamic

3. Molecular mechanics and Molecular Dynamic methods
4. Applications and Practical sessions on Problem solving.

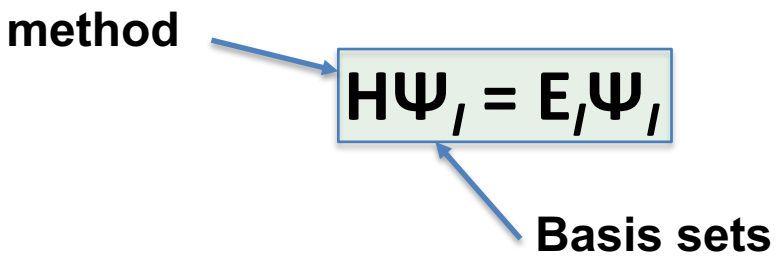
III. Transition Metal Chemistry and Catalysis

5. Computational approaches to the Transition Metal Chemistry
6. Computational Catalysis (including Organic, Inorganic and Enzymatic)
7. Practical sessions on Problem solving.

IV. Small Molecules and Excited State Studies

8. Overview Methodology
9. Application to Spectroscopy, problem solving.
10. Application to Radical Chemistry, problem solving.

Quantum Chemical Calculations: What is necessary ?



H Energy operator → Method

The Hamiltonian defines everything about the system

Results are:

E_I Total Energy for state *I*

Ψ_I Wavefunction for state *I* is a probabilistic description of electronic motion for a given geometry, charge and spin state

How to solve Hartee-Fock-Roothaan eq.?

- Use SCF approach:

1.Choose: Scientific Problem, basis set, Method
Provide infor. on spin state, charge and geometry

2. Calculate every integrals, V^{HF}
3. Calculate guess spin density matrix $\rho(r)$

4. Solve HFR equation and **get energy**

Determine whether procedure has converged
(for energy and density)

If NO $\Rightarrow$ go to step 4;

If NO

Repeat (4)
SCF cycle

If YES

If YES $\Rightarrow$ DONE , get final Energy, C and F and finish.

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What we can calculate ?

- Geometry
- Energy
- Vibrational Frequency
- EPR, NMR, Raman, and other physical properties
- Thermodynamic and kinetic parameters
- Reaction mechanisms
- Polizability and hyperpolyz.
- Spin-spin and spin-orbit interactions
- MORE

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You can do Computation @ the EMERSON CENTER

- **Computational Education;**
- **Expertize in Computation Based Res.**
- **Hardware & Software**

~3500 fast and parallel cores

Gaussian, MOLPRO, Gamess-US, VASP, AMBER TURBOMOLE, MOLCAS, Matlab, etc. (total of 33)

NSF

MRI-R2
CHE-0958205

EMERSON CENTER: HARDWARE

comp.chem.20

ssh –Y eclab@euch4e.chem.emory.edu
Passwd:

euch4e.chem.emory.edu
HOME=/home/chemistry/ch_res/eclab

cd spark

cd star

cd fire

$HOME/spark

mkdir USER
cd USER

Nodes = 36
Cores/node = 24
Speed = 2.6 GHz
Memory = 96 GB
Classes = spark24p
spark12p

spark (or spark.chem.emory.edu)

$HOME/star

mkdir USER
cd USER

Nodes = 36
Cores/node = 24, 16
Speed = 2.5 GHz
Memory = 80 GB
Classes = star24p
star16p
star8p
stars (1 core)

star (or star.chem.emory.edu)

$HOME/fire

mkdir USER
cd USER

Nodes = 16 + 1 GPU
Cores/node = 56 + 5000
Speed = 2.6 GHz
Memory = 196 GB
Classes = fire28p
fire-gpu

fire (or fire.chem.emory.edu)

Login the Emerson Center's Computers

From a Unix/MAC/iPad/iPhone terminal

ssh -Y eclab@euch4e.chem.emory.edu

From PC

1) Download and run PuTTY (www.putty.org)
2) Enable X-forwarding (Connection -> SSH -> Tunnels)
3) Under Session, choose SSH on port 22
4) Type **euch4e.chem.emory.edu** as host name
5) Click Open

A few UNIX commands and vi Editor

UNIX

Tree Structure: *Files and Directories*

cd - change directory: *cd directory_name*
rm - remove command: *rm file_name:* also: **rmdir, rm –I**
mv - move comman: *mv file_name*
mkdir - make directory: *mkdir directory_name*
cp - copy command: *cp file_name_1 file_name_2*
ls - list command

VI (View)

Command mode and **Insert mode**

vi *file_name*
Type **i** for insert command
Use backspace in order to correct mistake

:w **:w!** or **:wq** **:wq!** Write or write and quit
:q **:q!** quit
dd n delete
o Insert line

EMERSON CENTER:
Software (Selected List)

Electronic Structure

Gaussian-16, 09
Molpro-15.1
MOLCAS
GAMESS
TURBOMOLE
ORCA
VASP-5.2
DFTB+

MD Simulation & Modeling

GROMACS-19.1
NAMD-2.6
Rosetta
Amber-14

Graphics & Programming

MATLAB 2019
Mathematica 12.0
Gauss View 6

Command file (for LoadLeveler only):

```
#!/bin/ksh
#
###
# @ error = errcl.log
#
# @ initialdir = /star/chemistry/eclab/YOUR
# @ requirements = (Arch == "R6000") && (OpSys == "AIX53")
# @ notify_user = name@euch4e
# @ class = star16p
# @ group = ch_res
# @ queue
#
    INPF= test_inp
    OUTF= test_out

. /libs/scripts/g16/C01
chmod a+rw $OUTF
```

llsubmit xxxx.cmd

A Few LoadLeveler Commands

llq

```
Id                       Owner          Submitted   ST PRI Class        Running On
------------------------ ---------- ----------- -- --- ------------ -----------
euch4e.123949.0          nzhu        1/15 09:17   R  50  fire-gpu        euch7b
euch4e.123947.0          jamal       1/15 08:47   R  50  star24p         euch2c
euch4e.123944.0          zxk         1/14 11:48   R  50  spark24p        euch2d
euch4e.123950.0          jamal       1/15 11:17   R  50  spark24p        euch2d
euch4e.123929.0          zxk         1/13 09:49   R  50  spark24p        euch2d
euch4e.123926.0          zxk         1/13 09:46   R  50  spark24p        euch2d
euch4e.123928.0          zxk         1/13 09:48   R  50  spark24p        euch2d
euch4e.123927.0          zxk         1/13 09:46   R  50  spark24p        euch2d

8 job step(s) in queue, 0 waiting, 0 pending, 8 running, 0 held, 0 preempted
```

llcancel