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
10. Application to Radical Chemistry, problem solving.
Quantum Chemical Calculations: What is necessary?

H Energy operator $\rightarrow$ Method
The Hamiltonian defines everything about the system

$H\Psi_i = E_i\Psi_i$

Basis sets

Results are:

$E_i$, Total Energy for state $i$

$\Psi_i$, 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, $V_{\text{HF}}$
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 YES $\Rightarrow$ DONE, get final Energy, C and F and finish.
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
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)
ssh -Y eclab@euch4e.chem.emory.edu
Passwd:

emerson centered: hardware

- spark (or spark.chem.emory.edu)
  - $HOME/spark
    - mkdir USER
    - cd USER
    - # Nodes = 36
    - # Cores/node = 24
    - # Speed = 2.6 GHz
    - # Memory = 96 GB
    - # Classes = spark24p, spark12p

- star (or star.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)

- fire (or fire.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
Login the Emerson Center’s Computers

From a Unix/MAC/iPad/iPhone terminal
ssh -Y e克拉@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 command: `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` or `:w!` Write or write and quit
- `:q` or `: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 xxxxx.cmd
A Few LoadLeveler Commands

**llq**

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<thead>
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<th>Id</th>
<th>Owner</th>
<th>Submitted</th>
<th>ST</th>
<th>PRI</th>
<th>Class</th>
<th>Running On</th>
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<td>fire-gpu</td>
<td>euch7b</td>
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</tr>
</tbody>
</table>

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

**llcancel**