Introduction to Computational Quantum Chemistry

Practical Lesson 1: Molecular Builders & Single Point Calculations

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Builders and SPs

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Available builders on Wolf cluster

- Avogadro
 - + fast
 - + free
 - + forcefield preoptimization
- Gabedit
 - + aligning structures in coordinate system
 - relatively slow
- Gaussview
 - + generating specific distances/angles/dihedrals
 - + aligning molecules
 - commercial
- Nemesis
 - No idea

- The most widely used in QM are XYZ and Z-matrices
- Cube files:
 - Grid of points with specific values of a given quality
 - Electron density, Electrostatic potential, Laplacian of el. density...
 - Generated from Gaussian wavefunction
- Wavefunction files:
 - Gaussian: (Formatted) checkpoint
 - ADF: TAPEs
 - Turbomole: mos

Practical task I: Gaussian

• Prepare input file for calculations:

- Most builders can generate the file for you (usually has to be edited)
- You can write it yourself from scratch
- General suffix is either ".com" or ".gjf"
- Use:
 - 2 cores
 - 3 GB of memory
- Save the wavefunction
- Gaussian manual:

http://www.gaussian.com/g_tech/g09ur.htm

- Add gaussian module
- g09 input.com

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- Read the logfile, see the structure, extract information
- *qmutil*: nifty module to extract data from gaussian output:
 - extract-gopt-ene logfile
 - extract-gopt-xyz logfile
 - extract-gdrv-ene logfile
 - extract-gdrv-xyz logfile
 - extract-xyz-str xyzfile framenumber
 - extract-xyz-numstr xyzfile

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- Stores wavefunction in binary
- Convert into ASCII file:
 - formchk -3 file.chk
- Can be read by gaussview ¹
- Analysis of orbitals, electron density
- Export into cubefiles (ASCII grid files)

 ¹ A bug in Gaussview: Change word "independent" to "independent".
 Image: Change word "independent" to "independent".

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- Turbomole is probably the fastest code available here (for Gaussian-type basis functions)
- Tmolex as GUI (licence not available)
- RI-J approximation of coulombic term extremely fast (meta)GGA SCF convergence
- Interactive preparation of the input using define
- Turbomole manual: http:

//www.turbomole-gmbh.com/turbomole-manuals.html

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Preparing the job: Define

- First two items can be skipped
- Molecular geometry:
 - a coord Reads in the geometry
 - ired Generates internal coordinates
 - Proceed to next stage
- Basis set:
 - b all def2-SVP Assign this basis set to all atoms
 - * Proceed to next stage
- Method
 - eht Perform initial guess from Extended Hückel Theory
 - Accept all defaults

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define - cont.

- Method
 - dft Enter the DFT submenu
 - on Use DFT
 - func b-lyp Select the functional
 - grid m5 Increase the gridsize to m5
 - * Exit the submenu
 - ri Enter the RI submenu
 - m Assign memory for RI
 - 2000 As much as possible
 - on Use RI
 - Exit the submenu
 - dsp Use dispersion correction
 - on Use Grimme D3 correction
 - Exit the submenu
 - marij Multipole-Accelerated RI-J
- * End the define session

- For running TM in parallel mode use the parallel build
- module add turbomole:7.00:x86_64:para
- Infinity selects it by default if ncpu > 1

mnovak@wolf

#!/bin/bash
module add turbomole:7.00
jobex -ri -c 1024 > dft.out

File	Contens
dft.out	Optimization procedure
energy	Energies of steps
gradient	Gradients of steps
mos	Molecular orbitals
freq.out	Output from aoforce program

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- Only software using Slater-type orbitals
- Up to 2-component relativistic effects (ZORA+SpinOrbit)
- Awful output file structure
- Extremely fast and efficient
- ADF GUI: adfview
- Very bad memory handling

Preparing ADF input

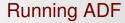
- Using GUI (the easiest way)
- Write from scratch
- Keywords in blocks:

ATOMS*	definition of geometry in xyz	
SYMMETRY NOSYMM	Switch off all symmetry	
XC*	DFT functional	
BASIS*	Basis set	
SAVE TAPE21	Save wavefunction	
NOPRINT LOGFILE	Do not print input into logfile	
* Section terminated by END keyword		

• Manual pages: http://www.scm.com/Doc/Doc2014/ADF/ ADFUsersGuide/page1.html

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• *adf* < input.adf > output.out

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