Designing an Authentic and Interactive Tutorial on Quantum Chemistry for Undergraduate Researchers: An Apprenticeship Model

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Instructional Need

Situation:

• Research advisor that attracts undergraduates
• One graduate student in the lab (me)
• One semester with four undergraduate research students

Instructional Need:

A way to train students to do research while simultaneously starting them out on their research projects
Electronic Structure Tutorial – Version 1

• Interactive lecture
  • Students follow along while I explain electronic structure concepts and submit sample calculations to our cluster

• Homework
  • Exercises for students to practice skills learned in the tutorial

• Sample calculation files
  • Prepared input files for students to use during the tutorial

This worked, but perhaps not effectively as I hoped
STEM Studio

- **Third Century Initiative**: To stimulate creative thinking and intensify learning in and beyond the classroom

- **Cross-disciplinary researchers**:
  - Asst. Professor Leah Bricker (School of Ed.)
  - School of Education – Science Education
  - School of LSA – Chemistry, Ecology & Evolutionary Biology, Neuroscience

- **Studio workshop environment**: Individual research and design projects

- **Test and Improve STEM Studio environment**: Study the STEM Studio itself, including ways to include the broader community
Evidence-Based Design Principles

- Align materials and assessments with learning goals
- Contextualize the learning of key ideas in real-world problems
- Engage students in scientific practices that foster the use of key ideas
- Use technology as a tool to explore problems and to provide scaffolding
- Engage students and teachers in collaborative environments
- Support teachers in adopting and carrying out inquiry-based projects
Align materials and assessments with learning goals

Two-fold Learning Goals:

1) Students will be able to utilize Q-Chem during their undergraduate electronic structure research project

2) Students will transition between a novice and an expert chemist
Align materials and assessments with learning goals

• Align tutorial components with general characteristics of expertise outlined by Hatano and Oura (2003)
  • “Experts possess rich and well-structured domain knowledge...that can readily be used”
  • “The process of gaining expertise is assisted by other people and artifacts”
  • “Expertise occurs in socially significant contexts...expertise occurs in the process of producing the target outcomes of the activity”

• Begin to direct students away from the “school” mentality, where grades matter, towards the research mentality, where results and explanation matter

Engage students and teachers in collaborative environments

• Encourage social interactions that help the student become part of the community of practice – i.e. the research group (Brown, Collins, Duguid, 1989)

• Social interactions can aid in student transitions from peripheral to full participation in the research group (Lave, 1991)

• Interactive lecture

• **Follow-up Exercises**

• **Instructor Documentation**

• Sample calculation files
Tutorial Components – Interactive Lecture

• Interactive tutorial lecture provides students with the physics and math concepts required to understand basic electronic structure calculations
  
  • Current work to improve this section!!

• Example calculations guide students through sample files, allowing them to interact directly with the software
### Geometry Optimization

- **Molecule section:**
  - Reading an un-optimized coordinate file

- **Max number of cycles for geometry optimization**

- **Molecule section:**
  - Reading an optimized coordinate file

---

**Sample Code:**

```plaintext
$molecule
read methane.txt
$end

$rem
JOBTYPE opt
EXCHANGE B3LYP
CORRELATION none
BASIS 6-31G*
GEOM_OPT_MAXCYC 200
MAX_SCF_CYCLES 200
MEM_STATIC 500
MEM_TOTAL 8000
MOLDEN_FORMAT TRUE
$end

```

---

**Sample Code:**

```plaintext
$molecule
read
$end

$rem
JOBTYPE sp
EXCHANGE B3LYP
CORRELATION none
BASIS 6-31G*
GEOM_OPT_MAXCYC 200
MAX_SCF_CYCLES 200
SCF_GUESS READ
PRINT_GENERAL BASIS TRUE
PRINT_ORBITALS 10
MEM_STATIC 500
MEM_TOTAL 8000
MOLDEN_FORMAT TRUE
$end
```
Tutorial Components – Interactive Lecture

PBS File Structure

- Set the input filename: jobname will be changed to your input filename
- Set the coordinate filename: coordname will be changed to your coordinate filename
- Set up Qchem
- Set up your QC Scratch directory
- Print scratch location in your working directory
- Copy input files to running directory
- Run Qchem (parallel)
- Run Qchem (serial)
- Write job start/end time
- Copy output files to working directory

```
#PBS -S /bin/csh
#PBS -o jobname.err
#PBS -N jobname
#PBS -q geva
#PBS -j oe
#PBS -r n
#PBS -l nodes=1:ppn=4
#PBS -l walltime=6:00:00
#PBS -V

## SET JOBNAME TO YOUR INPUT FILE NAME (EXCLUDING THE .IN EXTENSION)
setenv job jobname
setenv coord coordname
setenv QC /export/geva/hlphil/Program/qchem-v4.1-Oct-13/qchem
setenv QCAUX $QC/aux
setenv QCMPI openmpi

cd $PBSREMTEDIR
mkdir $PBSREMTEDIR/scratch
## RUN FROM SCRATCH DIRECTORY
#cp -r $PBS_O_WORKDIR/$job $PBSREMTEDIR/scratch
setenv QSCRATCH $PBSREMTEDIR/scratch
pwd >> $PBS_O_WORKDIR/pbsdir_$job

## Copy $job.in

$QC/bin/qchem -save -pbs -np 4 $job.in $job.out $job
$QC/bin/qchem -save -pbs $job.in $job.out $job

echo '------------ Job started at: ------------'
date
echo
$QC/bin/qchem -save $job.in $job.out $job

echo

echo '------------ Job was done at: -------------'
date
cp $job.out $PBS_O_WORKDIR/
cp $job.in.fchk $PBS_O_WORKDIR/$job.fchk
```
Tutorial Components – Follow-up Exercises

• Follow-up exercises guide students in practicing the skills and concepts learned in the tutorial

• Rationale helps students understand the practical relevance of each exercise to quantum chemistry research
Tutorial Components – Follow-up Exercises

• Exercise 1: Modify sample files – detailed instructions
  • Analyze the effect of basis set size

• Exercise 2: Modify sample files – no instructions
  • Analyze the effect of starting geometry/basis set
  • Double check your results for simple mistakes

• Exercise 3: Create and modify files
  • Analyze the effect of correlation treatment (HF/MP2/DFT)
  • Relate trends to key concepts in physical chemistry

• Exercise 4: Use molecule building software - iQmol
  • Relate to actual research done in the research group

• Exercise 5: Debugging sample files
Exercise 3 – Rationale:

Now that you are comfortable creating input files on your own, and you have considered some of the mathematical aspects that can cause differences in your calculation results, **you are ready to look into how different ways of treating electron interactions can affect your results.** There are two wavefunction based methods you will use: the Hartree-Fock method, which treats electron exchange and not correlation, and the Moller-Plesset perturbation theory (MP2) which extends the Hartree-Fock wavefunction to treat correlation using second order perturbation theory. You will also consider two levels of density functional theory, which consider electron exchange and correlation: the local density approximation (LDA) in which the electron density is treated as a uniform electron gas, and the generalized-gradient approximation (GGA) in which the variation of the LDA electron density is also considered. (See the tutorial or Q-Chem manual for more information on these methods).

This exercise will allow you to compare the ground state energies for all four methods. **You will begin to see the effect of including correlation as the number of electrons increases in a system.** You will also plot the orbital densities, which will allow you to see how hydrogen orbitals differ from multi-electron atomic orbitals (He), as well as how hydrogen atomic orbitals can combine to form molecular orbitals in a multi-atom system (the hydrogen molecule).
5. Compare the energies in table format as provided below: (Note: search for MP2 in the output file instead of Convergence in the MP2 calculations)

<table>
<thead>
<tr>
<th>System/Energy (au)</th>
<th>HF</th>
<th>MP2</th>
<th>LDA</th>
<th>GGA</th>
</tr>
</thead>
<tbody>
<tr>
<td>H-atom</td>
<td>-0.499948285</td>
<td>-0.499948285</td>
<td>-0.457031589</td>
<td>-0.494261345</td>
</tr>
<tr>
<td>He-atom</td>
<td>-2.861521996</td>
<td>-2.897246125</td>
<td>-2.723495094</td>
<td>-2.851878075</td>
</tr>
<tr>
<td>H₂-molecule</td>
<td>-1.102488041</td>
<td>-1.137331226</td>
<td>-1.027256147</td>
<td>-1.10099924</td>
</tr>
</tbody>
</table>

6. Compare the HF and MP2 H-atom energies. Is correlation important, and if so why? When does correlation begin to play an important role in your calculations?

7. Plot the occupied and first few virtual molecular orbitals for your calculations and provide them here. How do the hydrogen orbitals compare to those you have seen previously? How are the helium and fluorine orbitals similar or different? How do the hydrogen molecular orbitals compare to the atomic orbitals of hydrogen, helium, and fluorene?
• The documentation provides educative guidelines and design rationale for the instructor who implements the tutorial

*Rationale:*
Learning can occur differently in schools settings versus professional or apprentice settings (Lave, 1985; Brown, Collins, & Duguid, 1989). Chemistry research groups resemble apprentice environments, where novices learn from experts through participation in authentic activities (Stewart & Lagowski, 2003). Therefore, the instructor should focus on guiding the students as they have questions on the exercises, treating them as research apprentices.

Tutorial Components – Sample Files

• Sample files are used by the students during both the lecture and the exercises
  • Each exercise has specific sample files
• Instructors must modify the files to conform to their specific computational environment
Future Work

• **Research Question:** What is the effect of participation in the electronic structure tutorial on student performance on the CLASS-Chemistry attitude surveys?
  
  • Investigate this question by implementing the tutorial in a physical chemistry course (lab section)
  
  • *Quantitative Analysis* – CLASS-Chemistry scores
  
  • *Qualitative Analysis* – How do students approach problems during the tutorial?
  
    • Screen captures, interviews, focus groups, etc.
Conclusions

- Electronic Structure Tutorial designed from evidence-based principles

- Tutorial consists of
  - Interactive Lecture
  - Follow-up Exercises
  - Instructor Documentation
  - Sample Files

- STEM Studio provides an environment to revise and refine subsequent iterations of the tutorial design

- Future work involves studying the effect of participation in the tutorial on student learning outcomes
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