Tackling real problems with Quantum Mechanics

Chris J. Pickard

Lecture Five

What are you trying to prove?

- What system are you studying?
- What do you want to know about it?
- Can you express your question clearly?
- Is the question of the form: is it A, B or C?
- Are you trying to understand an experiment?
- Are you trying to make a prediction?

What level of theory do you need?

- Can your question be answered using a simple model?
- Can you get away with a classical picture?
- Can you use empirical methods?
- If you need to use Quantum Mechanics, is density functional theory going to be good enough?
- Are you interested in structures, or energy differences, and barriers?
- Are you interested in experimental observables?

Will your calculations ever finish?

- How big a system do you need to exhibit the phenomena of interest?
- Can your chosen level of theory handle a system of this size?
- Can you model the system as a cluster, or are periodic boundary conditions required?
- You must gain lots of experience with small, quick to run, calculations first

Before starting the main calculations

- Validate your chosen method
  - can it reproduce known results (ideally from different methods)
  - are the results consistent with phyisical intuition
- Does everything work well on your computing platform?
- How does the method scale with system size?

Will your computational results be reliable

- Check all your convergence parameters on small systems first
- Check the convergence with the integration grids
- Check the convergence with the k-point mesh
- Check your pseudopotentials and/or basis sets
- How certain can you be of your results? You must estimate this to make sense of your final results

Doing the main calculations

- You are armed with your tested set of parameters, pseudopotentials and basis sets, and an estimate of the size of the calculation
- Find the appropriate computing resources
- If you need to use a new computer architecture, try out a few small jobs to get some experience
- You may need to learn about the machine's queuing system
- Run your big jobs, and monitor their progress (to check your timing estimates are on track)
- When you get your results, save them, back them up, guard them!!

Understanding the results

- Check the simple things first
  - Did you find the ground state electronic structure?
  - Did you find the relaxed atomic structure?
  - Does anything look "strange"?
  - Do the total energies look correct? the forces?
- The rest is dependent on the particular problem, and should follow from the design of your calculations
- Are your results reasonable?
- Are the conclusive?
- Take into account your error estimates

What could be learnt in the future

- If your results weren't conclusive, what went wrong?
  - a problem with the theory?
  - a problem with the implementation?
  - or too computationally demanding
- Can you try to calculate the same thing, using a different tactic?

- If your results were sucessful, how far can you take them?
- Can you apply the same approach to other similar situations?
- Can you apply the method to fields that initially look very different?