CP2K Exercises

Iain Bethune

iain.bethune@stfc.ac.uk

@iainbethune
Practical Exercises

- Exercises are all on the web:
  https://www.cp2k.org/events:2018_summer_school:index

- Larger data files available on ARCHER:
  /home/y14/shared/cp2k

- Range of exercises depending on what you are interested in!
For CP2K Beginners

• Short ‘HowTo’ exercises on various basic functions of CP2K:
  • Single-point energy & force calculation using DFT
    https://www.cp2k.org/howto:static_calculation

• How to converge the total energy w.r.t. the CUTOFF and REL_CUTOFF
  https://www.cp2k.org/howto:converging_cutoff
  https://www.cp2k.org/events:2018_summer_school:converging_cutoff

• Experiment with SCF settings:
  https://www.cp2k.org/events:2018_summer_school:scf_setup

• How to run geometry optimisation
  https://www.cp2k.org/howto:geometry_optimisation
Intermediate Exercises

- Geometry and cell optimisation of NaCl clusters
- ‘Surface Science’ using local DFT
- Running *ab initio* MD of liquid water
- Hybrid functional calculations and dispersion corrections
- Linear Scaling DFT
- Electron correlation: MP2 and RPA
- QM/MM using GEEP
- Excited state calculations
Extended Exercises

• Metadynamics calculations
  https://www.cp2k.org/exercises:2015_cecam_tutorial:mtd1
• QM/MM of Urea in water
  https://www.cp2k.org/exercises:2015_cecam_tutorial:urea
• Adsorption on metallic surfaces (Nudged Elastic Band)
  https://www.cp2k.org/exercises:2015_cecam_tutorial:neb
• Force-field calculations on a protein
  https://www.cp2k.org/exercises:2015_cecam_tutorial:forcefields
• Also VIBRATIONAL_ANALYSIS, NMR, X-Ray, DFT+U
  • In /home/y14/shared/cp2k
Scaling Tests

• Several benchmark systems are provided at:
  • [https://www.cp2k.org/performance](https://www.cp2k.org/performance)

• Suggested experiments:
  • Explore the effects of simulation size, accuracy parameters etc. on performance
  • Try out performance ‘tweaks’ (see talk on Thurs)
Bring-your-own system

• Convert a simulation from another code to CP2K
• Compare accuracy and performance
• Ask us for help!