CP2K Exercises

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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
  https://www.cp2k.org/exercises:2016_summer_school:geometry_and_cell_optimization

- 'Surface Science' using local DFT
  https://www.cp2k.org/exercises:2016_summer_school:gga

- Running *ab initio* MD of liquid water
  https://www.cp2k.org/exercises:2016_summer_school:aimd

- Hybrid functional calculations and dispersion corrections
  https://www.cp2k.org/exercises:2016_summer_school:hfx

- Linear Scaling DFT
  https://www.cp2k.org/exercises:2015_pitt:ls

- Electron correlation: MP2 and RPA
  https://www.cp2k.org/exercises:2015_pitt:mp2

- QM/MM using GEEP
  https://www.cp2k.org/exercises:2016_summer_school:qmmm

- Excited state calculations
  https://www.cp2k.org/exercises:2016_summer_school:excited

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

- 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!