

# CP2K EXERCISES

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Iain Bethune

[ibethune@epcc.ed.ac.uk](mailto:ibethune@epcc.ed.ac.uk)



# Practical Exercises

- Exercises are all on the web
- Larger data files available on ARCHER:
  - `/home/y14/shared/cp2k`
- Range of exercises depending on what you are interested in!



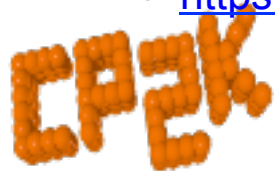
# For CP2K beginners

- Short 'HowTo' exercises on various basic functions of CP2K
- Single-point energy & force calculation using DFT
  - [https://www.cp2k.org/howto:static\\_calculation](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/howto:converging_cutoff)
- How to run geometry optimisation
  - [https://www.cp2k.org/howto: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](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](https://www.cp2k.org/exercises:2016_summer_school:gga)
- Running *ab initio* MD of liquied water
  - [https://www.cp2k.org/exercises:2016\\_summer\\_school:aimd](https://www.cp2k.org/exercises:2016_summer_school:aimd)
- Hybrid functional calculations and dispersion corrections
  - [https://www.cp2k.org/exercises:2016\\_summer\\_school:hfx](https://www.cp2k.org/exercises:2016_summer_school:hfx)
- Linear Scaling DFT
  - [https://www.cp2k.org/exercises:2015\\_pitt:ls](https://www.cp2k.org/exercises:2015_pitt:ls)
- Electron correlation: MP2 and RPA
  - [https://www.cp2k.org/exercises:2015\\_pitt:mp2](https://www.cp2k.org/exercises:2015_pitt:mp2)



# Extended Exercises

- Metadynamics calculations
  - [https://www.cp2k.org/exercises:2015\\_cecam\\_tutorial:mtd1](https://www.cp2k.org/exercises:2015_cecam_tutorial:mtd1)
- QM/MM of Urea in water
  - [https://www.cp2k.org/exercises:2015\\_cecam\\_tutorial:urea](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](https://www.cp2k.org/exercises:2015_cecam_tutorial:neb)
- Force-field calculations on a protein
  - [https://www.cp2k.org/exercises:2015\\_cecam\\_tutorial:forcefields](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 Friday)



# Bring-your-own system

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

