

CP2K Exercises

Practical Exercises

- Exercises are all on the web

https://www.cp2k.org/events:2019_cp2k_workshop_ghent

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



For CP2K Beginners

- 'HowTo' exercises on various basic functions of CP2K:
Single-point energy & force calculation using DFT
`www.cp2k.org/howto:static_calculation`
- How to converge the total energy w.r.t. the CUTOFF and REL_CUTOFF
`www.cp2k.org/howto:converging_cutoff`
`www.cp2k.org/events:2018_summer_school:converging_cutoff`
- Experiment with SCF settings:
`www.cp2k.org/events:2018_summer_school:scf_setup`
- How to run geometry optimisation
`www.cp2k.org/howto:geometry_optimisation`



Intermediate Exercises

- Geometry and cell optimisation of NaCl clusters:
`www.cp2k.org/2016_summer_school:
geometry_and_cell_optimization`
- 'Surface Science' using DFT with local functionals:
`www.cp2k.org/exercises:2016_summer_school:gga`
- Running ab initio MD of liquid water:
`www.cp2k.org/exercises:2016_summer_school:aimd`
- Hybrid functional calculations and dispersion corrections:
`www.cp2k.org/exercises:2016_summer_school:hfx`

Intermediate Exercises

- **Linear Scaling DFT:**

`www.cp2k.org/exercises:2015_pitt:ls`

- **Electron correlation: MP2 and RPA:**

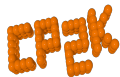
`www.cp2k.org/exercises:2015_pitt:mp2`

- **QM/MM using GEEP:**

`www.cp2k.org/exercises:2016_summer_school:qmmm`

- **Excited state calculations:**

`www.cp2k.org/exercises:2016_summer_school:excited`



Extended Exercises

- **Metadynamics calculations:**

www.cp2k.org/exercises:2015_cecam_tutorial:mtd1

- **QM/MM of Urea in water:**

www.cp2k.org/exercises:2015_cecam_tutorial:urea

- **Adsorption on metallic surfaces (Nudged Elastic Band):**

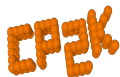
www.cp2k.org/exercises:2015_cecam_tutorial:neb

- **Force-field calculations on a protein:**

www.cp2k.org/exercises:2015_cecam_tutorial:forcefield

- **VIBRATIONAL_ANALYSIS, NMR, X-Ray, DFT+U:**

www.cp2k.org/



Scaling and Performance 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':
Consult with the experts for suggestions