CP2K PRACTICALS

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CP2K Exercises

- Various exercises are available from:
  - http://www.cp2k.org/exercises
  - Most recent: “CECAM 4th CP2K Tutorial” Also older exercises
  - Mostly ‘worked examples’ from system setup and calculations to analysis / visualisation of results

- For specific ‘HowTo’ guides see:
  - http://www.cp2k.org/tutorials
  - Guides to basic (and some advanced!) CP2K skills e.g.
    - converging `CUTOFF` for QS calculations
    - how to run geometry optimisations…

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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
- How to run geometry optimisation
  - https://www.cp2k.org/howto:geometry_optimisation

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Intermediate Exercises

- ‘Surface Science’ using local DFT
  - https://www.cp2k.org/exercises:2015_pitt:gga
- Running *ab initio* MD of liquid water
  - https://www.cp2k.org/exercises:2015_pitt:aimd
- Hybrid functional calculations and dispersion corrections
  - https://www.cp2k.org/exercises:2015_pitt: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

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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
- http://www.epcc.ed.ac.uk/~ibethune/files/CP2K_CECAM.tar.gz (1.8 GB!!!)

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CP2K Exercises

- The CP2K `tests` directory
  - Great source for example input files for all kinds of calculations
  - Grouped (mostly) logically:
    - `QS/regtest-gpw-1` – Quickstep GPW calculations
    - `QS/regtest-dm-ls-scf` – Quickstep using linear scaling SCF
    - `Fist/regtest-opt` – Geometry and Cell optimisations using classical potentials
    - `SE/regtest-*` - various semi-empirical calculations
  - WARNING:
    - Tests are designed to run quickly so may not produce converged or accurate outputs! Check parameters for your system…

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Scaling Tests

- Several benchmark systems are provided at:
  - https://www.cp2k.org/performance

- Suggested experiments:
  - Explore the effects of simulation size, accuracy parameters on performance

  - Try out performance ‘tweaks’

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Bring-your-own system

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

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