RUNNING CP2K CALCULATIONS

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Overview

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- CP2K Input file
  - The Basics
  - The How – FORCE_EVAL
  - The What – MOTION
- Basis Sets and Pseudopotential libraries
- CP2K Output
  - Controlling what gets written
  - Overview of an output file
- Restarting a calculation

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How to run CP2K

- CP2K binaries:
  - `cp2k.version` where `version` is usually one of:
    - `sopt` – Serial, optimised
    - `ssmp` – Single process + symmetric multiprocessor (OpenMP)
    - `popt` – Parallel (MPI), optimised
    - `psmp` – Parallel (MPI) + symmetric multiprocessor (OpenMP)
- Available from http://www.cp2k.org/download
  - Linux binaries (released versions)
  - Also in Linux package managers
  - Source code (released versions and latest trunk), GPL
  - May be pre-installed, e.g. NSCCS, ARCHER …

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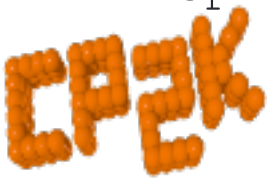
How to run CP2K

- Basic command line options:
  - `cp2k.sopt -i input_file -o output_file`
    - By default, output goes to the standard output
    - Output to file appends (beware!)
    - Input file is the last argument if not otherwise specified
- Other useful options:
  - `cp2k.sopt --version`
  - `cp2k.sopt --check input_file`
  - `cp2k.sopt --html-manual`
  - `cp2k.sopt --help`



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How to run CP2K

- Typical files associated with a CP2K run:
  - Input (required):
    - e.g. `H2O-32.inp` (main input file, name and extension are arbitrary)
  - Optional inputs:
    - `POTENTIAL` (psuedopotential library)
    - `BASIS_SET` (basis set library)
    - Structure file (e.g. psf, xyz, crd …)
    - …
  - Outputs:
    - `PROJECT-1.restart` (input file to restart calculation)
    - `PROJECT-pos-1.xyz` (trajectory for MD or GEO_OPT)
    - `PROJECT-1.ener` (MD energies, temperature, cons. Q …)
    - `PROJECT-1.cell` (cell parameters for NPT MD or CELL_OPT)
    - `PROJECT-RESTART.wfn` (orbitals for restart)

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CP2K Input file: The Basics

- Full documentation available online:
  - http://manual.cp2k.org
  - Or generate with `--html-manual`
- Sections – 13 (optional) top level sections

```
&BEGIN section_name [params]
…
&END [section_name]
```

- Keywords

```
KEYWORD value
KEYWORD [ON|OFF] [YES|NO] [TRUE|FALSE] …
KEYWORD
```

- Nesting
  - Sections may others sections and keywords

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CP2K Input file: The Basics

- Basic pre-processing syntax
  - `@INCLUDE 'filename'` – copy in text from file
  - `@SET VAR value` – define a variable
  - `$VAR` – replaced with variable value
  - `@IF / @ENDIF` – simple logic
  - `!` or `#` – comments
- Units
  - Numerical entries have a default unit (see manual)
  - Specify other units by hand e.g.

    `ABC [nm] 100 100 100` (or `bohr`, default is `angstrom`)

    `EMAX_SPLINE [eV] 50` (or `Ry`, `joule`, default is `hartree`)
  - Also combinations e.g. `[hartree*bohr^-2]`

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CP2K Input file: The Basics

- `GLOBAL` section (required)

```
&GLOBAL
  PROJECT H2O-32
  RUN_TYPE MD
  PRINT_LEVEL HIGH
  &TIMINGS
     THRESHOLD 0.000001
  &END
  WALLTIME 3600
&END GLOBAL
```

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CP2K Input file: The How

- FORCE_EVAL section (required)

```
&FORCE_EVAL
  METHOD QS   (or FIST, QMMM ...)
  &DFT
  …
  &END DFT
  &SUBSYS
  …
  &END SUBSYS
&END FORCE_EVAL
```

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CP2K Input file: The How

```
&DFT
  BASIS_SET_FILE_NAME GTH_BASIS_SETS
  POTENTIAL_FILE_NAME POTENTIAL
  &MGRID
    CUTOFF 280
    REL_CUTOFF 30
  &END MGRID
  &QS
    EPS_DEFAULT 1.0E-12
    WF_INTERPOLATION PS
    EXTRAPOLATION_ORDER 3
  &END QS
  &SCF
    SCF_GUESS ATOMIC
    &OT ON
      MINIMIZER DIIS
    &END OT
    &PRINT
      &RESTART OFF
      &END
    &END
  &END SCF
  &XC
    &XC_FUNCTIONAL Pade
    &END XC_FUNCTIONAL
  &END XC
&END DFT
```

Basis and PP library files

Parameters for the realspace multi-grids

Quickstep options

Control of SCF procedure, including minimisation scheme

Exchange-Correlation Functional (LDA)

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CP2K Input file: The How

```
&SUBSYS
 &CELL
   ABC 9.8528 9.8528 9.8528
 &END CELL
 # 32 H2O (TIP5P,1bar,300K) a = 9.8528
 &COORD
O       2.280398       9.146539       5.088696
O       1.251703       2.406261       7.769908
O       1.596302       6.920128       0.656695
...
H       0.837635       8.186808       8.987268
H       8.314696      10.115534       2.212519
H       8.687134       8.667252       2.448452
 &END COORD
 &KIND H
   BASIS_SET TZV2P-GTH
   POTENTIAL GTH-PADE-q1
 &END KIND
 &KIND O
   BASIS_SET TZV2P-GTH
   POTENTIAL GTH-PADE-q6
 &END KIND
&END SUBSYS
```

Cell definition

Particle coordinates

Could also @include an external file or parse other formats via

```
&TOPOLOGY
   COORD_FILE_NAME
&END TOPOLOGY
```

Definitions of atomic kinds

Could specify charge, mass …

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CP2K Input file: The What

- `MOTION` section

```
&MOTION
  &MD
    ENSEMBLE NVE
    STEPS 10
    TIMESTEP 0.5
    TEMPERATURE 300.0
  &END MD
&END MOTION
```

- Also used to control Geometry Optimisation, NEB, Monte Carlo, …

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Basis Sets and PP libraries

- CP2K uses Goedecker-Teter-Hutter, seperable Pseudopotentials
  - Several sets of PPs and corresponding optimised basis sets are available
  - See `cp2k/data` or online: http://sourceforge.net/p/cp2k/code/HEAD/tree/trunk/cp2k/data
  - POTENTIAL, GTH_POTENTIALS
    - Wide range of PPs for at many elements - LDA (PADE), PBE, BLYP …
  - BASIS_SET, GTH_BASIS_SET, BASIS_MOLOPT
    - Various qualities / size of basis
    - Make sure Basis and PP match (functional and number of electrons)
    - Some documentation and references at head of each file

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CP2K Output: Controlling what gets written

- The `PRINT_LEVEL` keyword in `&GLOBAL`
  - `SILENT`, `LOW`, `MEDIUM` (default), `HIGH`, `DEBUG`
  - `HIGH` can give more information if you are interested
    - Also gives some per-process logging in parallel jobs
  - For long MD runs (e.g. classical), recommend using `LOW`
- Fine grained control is available via print-keys
  - Most input sections contain a `&PRINT` sub-section
  - Each `&PRINT` sub-section has further subsections for each quantity that may be printed

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CP2K Output: Controlling what gets written

- For example, the `&PRINT` section in `&MOTION` contains

  `&CELL`

  `&FORCES`

  `&TRAJECTORY`

  `&VELOCITIES`

  ...

- Each section has parameters (and defaults) for which print level it is output
  - `&TRAJECTORY` defaults to `LOW`
  - `&VELOCITIES` defaults to `HIGH`

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CP2K Output: Controlling what gets written

- Can also specify frequency of printing via `&EACH` sub-section e.g.

```
&PRINT
  &CELL
     &EACH
        MD 100
     &END EACH
  &END CELL
&END PRINT
```

- Control over filenames, file formats etc. at each `&PRINT` section

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CP2K Output: Overview of an output file

…

Restarting a calculation

- If you need to restart your job…
  - Hardware failure
  - Batch system time limit
  - Need more MD sampling
  - …

- CP2K dumps a restart input file which can be directly re-run
  - `cp2k.sopt -i PROJECT-1.restart`
  - Continuous numbering of MD steps
  - Stores all state variables (incl. extended system)
  - Use `SCF_GUESS RESTART`

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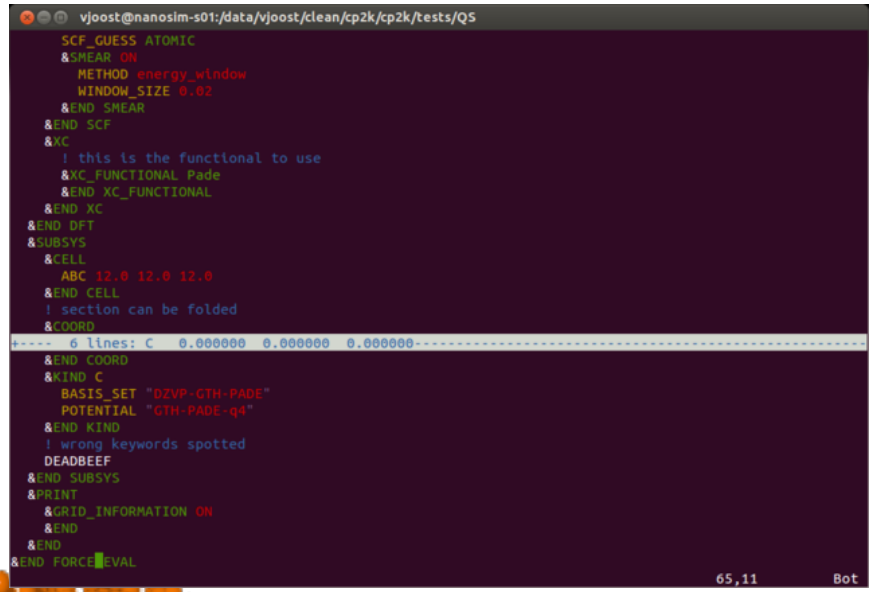
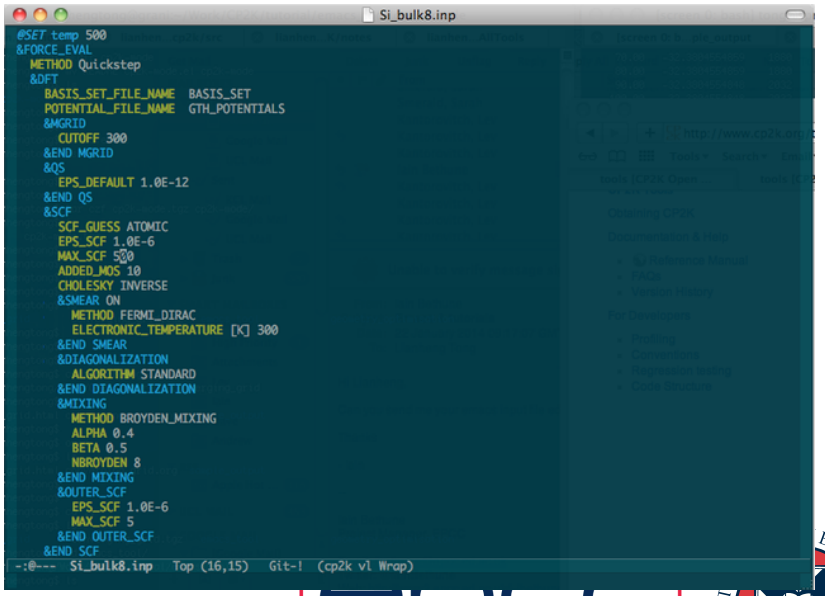
Tools for building CP2K input

- Plugins are available for your favourite(!) text editors:
  - https://www.cp2k.org/tools:vim
  - https://www.cp2k.org/tools:emacs
  - Syntax highlighting, indentation, show/hide sections, keywords





Tools for building CP2K input

- Python interfaces
  - Atomic Simulation Environment (ASE) – see tomorrow
  - PyCP2K (https://github.com/SINGROUP/pycp2k)
    - Object-oriented wrapper following the CP2K input format
    - Auto-completion (for e.g. Spyder IDE)
    - E.g. GLOBAL%RUN_TYPE is GLOBAL.Run_type
    - May use ASE for execution

```
23
24 #=====================  Write the simulation input  ==========================
25 GLOBAL.Run_type = "ENERGY_FORCE"
26 GLOBAL.Print_level = "LOW"
27 FORCE_EVAL.Method = "Quickstep"
28 FORCE_EVAL.PRINT.FORCES.Section_parameters = "ON"
29 DFT.Basis_set_file_name = "BASIS_SET"
30 DFT.Potential_file_name = "POTENTIAL"
31 DFT.QS.Eps_default = 1.0E-10
32 SCF.Scf_guess = "ATOMIC"
33 SCF.Eps_scf = 1.0E-7
34 SCF.Max_scf = 300
35 SCF.DIAGONALIZATION.Section_parameters = "ON"
36 SCF.DIAGONALIZATION.Algorithm = "STANDARD"
37 SCF.MIXING.Section_parameters = "T"
38 SCF.MIXING.Method = "BROYDEN_MIXING"
39 SCF.MIXING.Alpha = 0.4
40 SCF.MIXING.Nbroyden = 8
41 KIND = SUBSYS.KIND_add("Si")  # Section_parameters can be provided as argument.
42 KIND.Basis_set = "DZVP-GTH-PADE"
43 KIND.Potential = "GTH-PADE-q4"
44 calc.create_cell(SUBSYS, lattice)
45 calc.create_coord(SUBSYS, lattice)
46
47 #=====================  Run the simulation  ==========================
48 calc.run()
~
~
3 fewer lines                                                  31,1          Bot
```

Tools for building CP2K input

- CP2K Input Editor
  - Browser-based:
    - http://cp2k-www.epcc.ed.ac.uk/cp2k-input-editor
  - Show/hide sections
  - Dropdowns for option selection
  - Tooltip help on every keyword
  - Basic input validation
  - Library of example input template files
  - Supports CP2K releases 2.5-2.7, 3.0, 4.0

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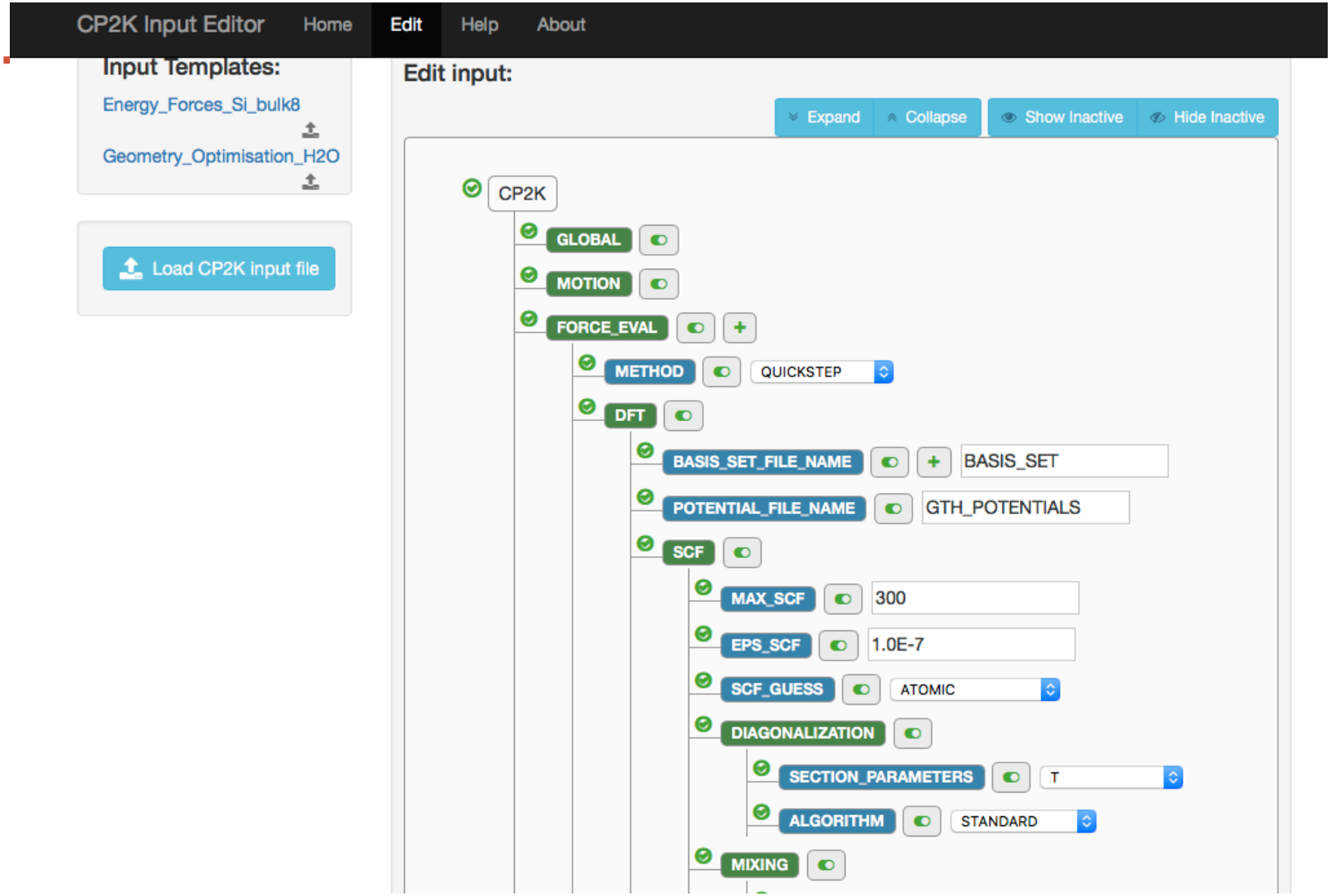
CP2K Input Editor
Home
Edit
Help
About
Input Templates:
Energy_Forces_Si_bulk8
Geometry_Optimisation_H2O
Load CP2K input file
Edit input:
Expand
Collapse
Show Inactive
Hide Inactive
CP2K
GLOBAL
MOTION
FORCE_EVAL
METHOD
QUICKSTEP
DFT
BASIS_SET_FILE_NAME
BASIS_SET
POTENTIAL_FILE_NAME
GTH_POTENTIALS
SCF
MAX_SCF
300
EPS_SCF
1.0E-7
SCF_GUESS
ATOMIC
DIAGONALIZATION
SECTION_PARAMETERS
T
ALGORITHM
STANDARD
MIXING

Running a CP2K Calculation

Questions?