User Manual

CP2K

A program package to perform
Molecular Dynamics Simulations

The CP2K developers group

Disclaimer

2 Installation

You can download the current version of the CP2K code from

4 Input description

4.1 General rules

Warning: Do not expect the input to be logic. The programmers logic may be different from yours.

Warning: This input description may not refer to the actual version of the program you are using. Therefore the ultimate and authoritative input guide is the source code.

4.2.2 Optional keywords

FFTLIB *f*FFTESSL,FFTSG,FFTSGI,FFTW*g*

Defines the library which is used for the Fast Fourier Transformations (TJ/). The availability of the libraries depends on the archiiecture and/or installation, but at least the library is available which is included in the CP2K distribution.

default: FFTSG

IOLEVEL

4.4.2 Optional keywords

UNIT {ANGSTROM, BOHR, SCALED_ANGSTROM, SCALED_BOHR}
Defines the unit of length for the simulation cell and it also applies to the definition of the atomic coordinates in the input section &COORD. Moreover, all lengths and distances in the output are printed using this unit.
default: BOHR

4.5 Section &COORD

Each non-empty input line in this section defines an atom of the considered system. The first entry in each line has to correspond to an atomic kind name defined by a &KIND section which can be a *hstringi* or an *hintegeri* number. The kind name has to follow a set of three *hreali* numbers defining the *x*, *y*, and *z* coordinates of the atom.

4.6 Section &KIND

This section has to be defined for each atomic kind in a QUICKSTEP run. The name of the kind has to be defined right after the &KIND section keyword on the same input line. The kind name is referenced by the &COORD section. Alternatively, the atomic number of the kind can be defined as an integer number, e.g.

```
&KIND 6
```

for carbon which is equivalent to

```
&KIND C
```

In general, any *hstringi* can be defined for an atomic kind

```
&KIND hstringi
```

which allows to define different atomic kinds for the same element e.g. carbon with different orbital basis sets

```
&KIND C-DZVP
```

```
&KIND C-TZVP
```

One or more &KIND sections are required for a QUICKSTEP run.

4.6.1 Required keywords

ORBITAL_BASIS_SET, BASIS_SET, BAS {*hstringi*}
Name of the Gaussian orbital basis set which has to be read from the Gaussian basis set database file (see section &IO).

POTENTIAL, POT {*hstringi*}
Name of the atomic potential which has to be read from the potential database file (see section &IO).

4.6.2 Optional keywords

ELEMENT_SYMBOL,ELEMENT

`MESH` *{*`integer`*i* *h*`integer`*i* *h*`integer`*ig*
Explicit definition of the grid size.

`PLANE_WAVES,PW`
default

EPS_RHO *f*real*ig*
Threshold values for EPS_RHO_GSPACE and EPS_RHO_GSPACE.
default: 1.0E-8

EPS_RHO_GSPACE *f*real*ig*

`CHOLESKY_ON,CHOLESKY_OFF`
Decides whether the Cholesky decomposition is used in the eigensolver or not.
default: `CHOLESKY_ON`

`DENSITY_GUESS,SCF_GUESS,GUESS` *{*`ATOMIC,CORE`*}*
Defines the type of guess which is employed to generate the first density matrix.
default: `ATOMIC`

`DENSITY_MIXING,MIXING` *{*real*}*
Factor for the mixing of the old and new density matrix during the wavefunction optimization.
default: `0.4` (i.e. 40% of the new and 60% of the old density are used)

`EPS_DIIS` *{*real*}*
The DIIS procedure is switched on, if the maximum DIIS error vector element is below

INTERATOMIC_DISTANCES,DISTANCES
Print a matrix with the interatomic distances.
Warning: That is much output for largdistancsystems.

KIND_RADII
Print the maximum interaction radius of each atomic kind.

KINETIC_ENERGY_MATRIX,T_MATRIX
Print the kinetic energy integral matrix.

KOHN_SHAM_MATRIX
Print the Kohn-Sham matrix.

LUMO
Print the lowest unoccupied molecular orbital (LUMO) as a cube file.

MEMORY
Print informations about the memory usagdistancof the CP2K program.

MO_EIGENVALUES
Print the eigenvaluesistancof the molecular orbitals (MOs).

MO_EIGENVECTORS,MOS
Print the eigenvectors, eigenvalues, and the occupation numbers of the molecular orbitals (MOs).

MO_OCCUPATION_NUMBERS
Print the occupation numbers and the eigenvaluesistancof the molecular orbitals (MOs).

NEIGHBOR_LISTS
Print all neighbor lists.
Warning: That is much output for largdistancsystems.

ORTHO_MATRIX
Print the orthogonalisation matrix used to transform the Kohn-Sham matrix.

OVERLAP_MATRIX
Print the overlap matrix.

PGF_RADII
Print the interaction radiiistancof all primitive Gaussian-type functions.

PHYSICAL_CONSTANTS,PHYSCON
Print the valuesistancof all physical constants used in the program.

POTENTIALS

C6hhE 0 8aussian-rf 0 0 Tint the o4.406 cm 0l2P250(lists.)T

5 Input examples

5.1 Argon atom

```
&CP2K
 PROGRAM      Quickstep
 IOLEVEL      10
 FFTLIB       FFTSG
 RUN_TYPE     WFN_OPT
&END

&DFT
 FUNCTIONAL   PADE
&END

&QS
 CUTOFF       300
 REL_CUTOFF   30
&END

&SCF
 GUESS        ATOMIC
 EPS_DIIS     0.1
 MAX_DIIS     4
 EPS_SCF      1.0E-6
 MAX_SCF      30
 MIXING       0.4
&END

&PRINT medium
 NO_BLACS_INFO
&END

&KIND Ar
 BAS0S_SET    DZVP-GTH-PADE
 POTENTIAL    GTH
&END

&CELL
 UNIT         ANGSTROM
 ABC          12.0  12.0  12.0
&END

&COORD
 18     0.000000  0.000000  0.000000
&END
```

5.2 Water molecule

```
&CP2K
 PROGRAM      Quickstep
 IOLEVEL      10
```

6 Methods

6.1 GPW method

The electronic energy functional for a molecular or crystalline system in the framework of the Gaussian plane waves (GPW) method [4

[1] J. J. P. Stewart, P. Császár, and P. Pulay, J. Comput. Chem.