

# User Manual

# CP2K

A program package to perform  
Molecular Dynamics Simulations

The CP2K developers group

CP2K program release 1.0

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## **Disclaimer**

Please note that this manual is not complete. Basically it refers to the CP2K program release 1.0, but the CP2K program package is continuously improved and extended. Therefore the ultimate reference is always the CP2K source code.

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# 1 Introduction

The CP2K project was started in 2000 at the Max-Planck institute for solid state research in Stuttgart. Now it is continued at the ETH Zurich (CSCS) and at the University Zurich. The current members of the CP2K developers group are

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## 2 Installation

You can download the current version of the CP2K code from [http://developer.berlios.de/project/?group\\_id=129](http://developer.berlios.de/project/?group_id=129) using CVS or FTP which also allow to update your current CP2K version. Alternatively, you can directly download the full CP2K tarball which you have to uncompress with

```
$ gunzip cp2k.tar.gz
```

Then extract the archive file with

```
$ tar -xvf cp2k.tar
```

In order to generate an executable change to the directory with the xvfto generate an e

### 3 Running CP2K

The CP2K program is started with the command

```
$ cp2k.sopt hinput filei >houtput filei
```

The start command for the parallel CP2K version depends on the parallel execution environment of the underlying architecture, e.g. with LINUX/MPICH you may start 4 processes with

```
$ mpirun -np 4 cp2k.popt hinput filei >houtput filei
```

## 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

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FFTLIB *FFTESSL, FFTSG, FFTSGI, FFTWg*

Defines the library which is used for the Fast Fourier Transformations (FFT). The

#### 4.4.2 Optional keywords

UNIT *f*ANGSTROM, BOHR, SCALED\_ANGSTROM, SCALED\_BOHR*g*

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

#### 4.6.2 Optional keywords

ELEMENT\_SYMBOL, ELEMENT *fstringig*

Defines the element to which the atomic kind belongs.

ATOMIC\_MASS, MASS *frealig*

MESH *fhintegeri hintegeri hintegerig*

Explicit definition of the grid size.

PLANE\_WAVES , PW

default

FORCES

The calculation of the forces is requested.

default: no force calculation

CHARGE *fhintegerig*

The total charge of the system.

default: 0

## 4.8 Section &QS ...&END

Program parameters QUICKSTEP

CUTOFF *fhrealig*

Plane waves cutoff of the largest grid in Rydberg.

default: 320

EPS\_DEFAULT *fhrealig*

Defines a default threshold v2 ETh

default: 3201.0E- ]TJ/F57.173 -23.398 Td[ (CHA) ]TJ6611.532.17 0.3-52.29587 0.

EPS\_RHO\_GSPACE *f<sub>hrealig</sub>*

Threshold value for the calculation of the electronic charge density in Fourier space.

default: 1.0E-8

EPS\_RHO\_RSPACE *f<sub>hrealig</sub>*

Threshold value for the calculation of the electronic charge density in real space.

default: 1.0E-8

PROGRESSION\_FACTOR,GREFAC *f<sub>hrealig</sub>*

Progression factor for the generation of the multi-grid levels.

default: 2.0

RELATIVE\_CUTOFF,REL\_CUTOFF *f<sub>hrealig</sub>*

Relative plane waves cutoff for each multi-grid level. Values less than 20.0 give

inaccurate results and values greater than 30.0 are used for reference e(ellw)10(a)20A1.2970.91

DENSITY\_GUESS, SCF\_GUESS, GUESS *f*ATOMIC, CORE, RESTART*g*

Defines the type of guess which is employed to generate the first density matrix. For RESTART a valid restart has to be supplied.

default: ATOMIC

\_MIXING, MIXING *f*<sub>real</sub>*i**g*

Factor for the mixing of the old and new density matrix during the wavefunction opti-

WORK\_SYEVX *frealig*

Defines the amount of additional work space for the PDSYEVX routine from the







**SCF\_ENERGIES**

Print all contributions to the total SCF energy.

**SET\_RADII**

Print the interaction radii of all Gaussian orbital sets.

**SPHERICAL\_HARMONICS**

Print the transformation matrices between Cartesian and spherical function.

**TIMING\_INFORMATION**

Print timing information depending on the IOLEVEL defined in the &CP2K section.

**TITLE**

Print the title.

**TOTAL\_**

## 5 Input examples

### 5.1 Argon atom

```

&CP2K
  PROGRAM      Quickstep
  IOLEVEL      10
  FFTLIB       FFTSG
&END

&DFT
  FUNCTIONAL    PADE
&END

&QS
  CUTOFF        300
  EPS_DEFAULT   1.0E-12
  EPS_RHO       1.0E-8
  EPS_GVG       1.0E-6
  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
  BASIS_SET     DZVP-GTH-PADE
  POTENTIAL     GTH
&END
&END

```

## 5.2 Water molecule

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

&DFT
  FUNCTIONAL    Pade
  FORCES
&END

&QS
  CUTOFF       200
&END

&SCF
  GUESS         ATOMIC
  MIXING        0.4
  EPS_SCF       1.0E-5
&END

&PRINT medium
&END

&KIND H
  BASIS_SET     DZV-GTH-PADE
  POTENTIAL     GTH
&END

&KIND O
  BASIS_SET     DZVP-GTH-PADE
  POTENTIAL     GTH
&END

&CELL
  UNIT          ANGSTROM
  ABC           10.0  10.0  10.0
&END

&COORD
  H   0.000000   -0.757136    0.520545
  O   0.000000    0.000000   -0.065587
  H   0.000000    0.757136    0.520545
&END
```



The GPW method works like pure plane waves methods with atomic pseudo potentials, since an expansion of Gaussian functions with large exponents is numerically not efficient or even not feasible. The current implementation of the GPW method uses only the pseudo potentials of Goedecker, Teter and Hutter (GTH) [1, 2] which consist of a local part  $V_{\text{loc}}^{\text{PP}}(r)$  and a non-local part  $V_{\text{nl}}^{\text{PP}}(\mathbf{r};\mathbf{r}')^{\dagger}$  as shown in Eq. 1.



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