

# 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

9

FFTLIB *FFTESSL, FFTSG, FFTSGI, FFTWg*

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

#### 4.4.2 Optional keywords

SUBCELLS *f<sub>hrealig</sub>*

The simulation cell is divided into subcells for the generation of the neighbor lists. The specified value defines the size of the subcells. Values between 1 . 0 and 2 . 0 show a good performance.

default: 1 . 5

UNIT

POTENTIAL, POT *fstringig*

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 *fstringig*

Defines the element to which the atomic kind belongs.

ATOMIC\_MASS, MASS *frealig*

Defines an atomic mass different from the default atomic mass, e.g. for the definition of isotopes.

PAO\_MIN\_BAS *f*list of *hintegerig*





**ARPACK ON**

The ARPACK eigensolver is used in a parallel run which requires a proper installation of the ARPACK library.

default: no ARPACK usage

**CHOLSKY ON , CHOLSKY OFF**

Decides whether the Cholesky decomposition is used in the eigensolver or not.

default: CHOLSKY ON

**DENSITY GUESS , SCF GUESS , GUESS**

NREBUILD *fhintegerig*

Number of SCF steps between two full calculations of the electronic charge density.  
default: 1

SMEAR *fhrealig*

Window size in atomic units with respect to the eigenvalue of the highest occupied molecular orbital (HOMO) for the smearing of the occupation numbers.  
default: 0.0

WORK\_SYEVX *fhrealig*

Defines the amount of additional work space for the PDSYEVX routine from the SCALAPACK library. A value between 0.0 and 1.0 is accepted. (only for parallel runs using SCALAPACK and an eigensolver with diagonalization).  
default: 0.0

## 4.10 Section &PRINT ...&END

This sections allows for detailed output control when running QUICKSTEP. There are 5 predefined print levels: 0, 1, 2, 3, and 4 which correspond to the keywords

**BLACS\_INFO**

Print the process grid information of BLACS (Balic linear algebra subprograms)

**CARTESIAN\_MATRICES**

Print all operator matrices in the Cartesian instead of the spherical representation.

**CELL\_PARAMETERS , CELL**

Print the simulation cell data like the cell vectors, cell volume etc.

**CORE\_**







## 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.



## Index

ARPACK, 14

files

    basis set, 7



EPS\_RHO\_RSPACE, 13

EPS\_