CP2K

Authors

CP2K developers group (as stated in GitHub repository) including Joost VandeVondele, Tiziano Müller, Ole Schütt, Matthias Krack, Jürg Hutter and many others
https://github.com/cp2k/cp2k/blob/master/COPYRIGHT

Homepage

The project homepage provides complete documentation concerning the source code, precompiled binaries, manual, tutorials, examples, FAQ and many useful links.
https://www.cp2k.org/about

Source

Source code is available in the official GitHub repository. All the resulting releases can be downloaded from the project homepage. Useful comments on compilation in the Cygwin environment as well as the corresponding binaries are presented by Aoyama Iwao in his Github repository.
https://github.com/cp2k/cp2k/releases/
https://www.cp2k.org/download
https://github.com/brhr-iwao/CP2K_for_Windows

Reference

CP2K, A. General Program to Perform Molecular Dynamics Simulations. *CP2k developers group under the terms of the GNU General Public License*.

Description & Use

CP2K is an universal quantum chemistry and solid state physics computational package capable of preforming calculations on all states of matter. The utilized theory levels include DFTB, LDA, GGA, MP2, RPA, semi-empirical methods (AM1, PM3, PM6, RM1, MNDO) and classical force fields (AMBER, CHARMM). Moreover, CP2K can do simulations of molecular dynamics, metadynamics, Monte Carlo, Ehrenfest dynamics, vibrational analysis, core level spectroscopy, energy minimization, and transition state optimization using NEB or dimer method. (Detailed overview of features is available in the homepage.)
https://www.cp2k.org/about

Quick start

Use in command line / shell:

```
cp2k -i [name of input file] -o [name of the output file]
```
(in Windows command line)

or

```
./cp2k -i [name of input file] -o [name of the output file]
```
(in Android shell).

The result will appear in the same location.

Program status

The current package contains CP2K binaries of version 4.0 (Development Version) with the minimal requirements compiled for x86 based Windows operating system.

License

CP2K

The distribution of CP2K binaries is published for free (under GPL v.3) at Mobile Chemistry Portal and Google Play Store with kind permission of Tiziano Müller. Both the slightly modified source codes for generic Android binaries as well as for the binaries adapted to running in a standard Android filesystem (with defined hardlinks to each used file) are available for download below. The included data files (basis sets, manual, examples and tests) were taken from the official source code distribution.

MinGW

The Windows version contains few essential dynamic link libraries which are part of MinGW runtime.
http://www.mingw.org/

```
Copyright (c) 2012 MinGW.org project

Permission is hereby granted, free of charge, to any person
obtaining a copy of this software and associated documentation files
(the Software"), to deal in the Software without restriction,
including without limitation the rights to use, copy, modify, merge,
publish, distribute, sublicense, and/or sell copies of the Software,
and to permit persons to whom the Software is furnished to do so,
subject to the following conditions:

The above copyright notice, this permission notice and the below
disclaimer shall be included in all copies or substantial portions
of the Software.

THE SOFTWARE IS PROVIDED "AS IS", WITHOUT WARRANTY OF ANY KIND,
EXPRESS OR IMPLIED, INCLUDING BUT NOT LIMITED TO THE WARRANTIES OF
```

MERCHANTABILITY, FITNESS FOR A PARTICULAR PURPOSE AND NONINFRINGEMENT. IN NO EVENT SHALL THE AUTHORS OR COPYRIGHT HOLDERS BE LIABLE FOR ANY CLAIM, DAMAGES OR OTHER LIABILITY, WHETHER IN AN ACTION OF CONTRACT, TORT OR OTHERWISE, ARISING FROM, OUT OF OR IN CONNECTION WITH THE SOFTWARE OR THE USE OR OTHER DEALINGS IN THE SOFTWARE.

BLAS

CP2K binaries for Android offered by us were statically linked to BLAS library (freely-available software package, available in the homepage). The Windows package contains the corresponding dynamic library.
http://www.netlib.org/blas/

LAPACK

CP2K binaries for Android offered by us were statically linked to LAPACK library (released under modified BSD license, check the homepage for details). The Windows package contains the corresponding dynamic library.
http://www.netlib.org/lapack/

X11-Basic

GUI of the Windows version was built using X11-Basic (by Markus Hoffmann) framework (GPL v.2). For correct functionality, SDL library (available under GNU LGPL license) is included in package.
http://x11-basic.sourceforge.net/
https://www.libsdl.org/

Advanced Installer

The MSI installer for Windows was created using the Advanced Installer (Freeware edition).
https://www.advancedinstaller.com/
https://www.advancedinstaller.com/top-freeware-features.html

Contact

Compilation of the source code for Android/Windows as well as the Android/Windows app development was done by Alan Liška (alan.liska@jh-inst.cas.cz) and Veronika Růžičková (sucha.ver@gmail.com), J. Heyrovský Institute of Physical Chemistry of the CAS, v.v.i., Dolejškova 3/2155, 182 23 Praha 8, Czech Republic.
Website: http://www.jh-inst.cas.cz/~liska/MobileChemistry.htm