



Hartree Centre

Science & Technology Facilities Council

<http://tinyurl.com/CP2KSchool2018>

[#CP2KSummerSchool](#)

# CP2K: Introduction and Overview

CP2K Summer School, 19-22 June 2018

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@iainbethune





# Health and Safety

On Wednesday mornings a fire alarm test of short duration is performed.

If the alarm does not stop, please leave your luggage and proceed through the nearest doors to outside the building

The map of the ground floor is attached to the entrance door of the lab.

Please do not take any liquids with you to your workplaces.

Please remember to wear your badges at all times while at the Daresbury site.





# Outline

- Summer School Intro
- CP2K Overview
  - Project History
- CP2K Features
- CP2K Information
- Obtaining CP2K





# Summer School Intro

- Welcome!
- 35 Participants
  - 26 Institutions
  - 54/46% UK/Overseas
- Aim to cover:
  - Practicalities of running calculations
  - Basics: DFT using Gaussian & Plane Waves, *ab initio* MD
  - Some specific topics: Hybrid Density Functionals ...





# Summer School Intro

- Agenda, slides, exercises on the web:
  - [https://www.cp2k.org/events:2018\\_summer\\_school:index](https://www.cp2k.org/events:2018_summer_school:index)
- Practicalities:
  - Coffee Breaks
  - Lunch (£6 voucher provided)
  - Dinner (Thursday night – make selection by 5pm today!)
    - <https://goo.gl/forms/kmvQRKOUzLHRosPi2>
  - Poster Session
  - Wifi
    - Eduroam
    - STFC-Guest (Host – iain.bethune@stfc.ac.uk)





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# Sponsors

**EPSRC**

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# Support for CP2K Users

- CP2K-UK: EPSRC Software for the Future
  - £500,000, 2013-2018
  - EPCC, UCL, Lincoln, KCL + 7 supporting groups
- Aims
  - Grow and develop existing CP2K community in UK
  - Lower barriers to *usage* and *development* of CP2K
  - Long-term sustainability of CP2K
  - Extend ability of CP2K to tackle challenging systems
- Annual user meetings & training
- Updates via mailing list





# Instructors

- Iain Bethune (School Organiser)
  - STFC Hartree Centre
- Matt Watkins & Sergey Chulkov
  - University of Lincoln
- Sanliang Ling
  - University of Nottingham
- Arno Proeme
  - ARCHER / EPCC, University of Edinburgh
- David Benoit (Thurs)
  - University of Hull



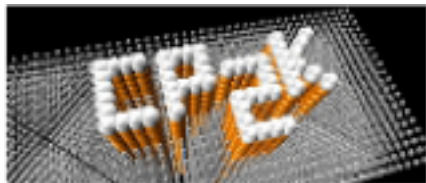




# CP2K Overview

“CP2K is a program to perform atomistic and molecular simulations of solid state, liquid, molecular, and biological systems. It provides a general framework for different methods such as e.g., density functional theory (DFT) using a mixed Gaussian and plane waves approach (GPW) and classical pair and many-body potentials.”

From [www.cp2k.org](http://www.cp2k.org) (and original home page from 2004!)



CP2K



# CP2K Overview

- Many force models:
  - Classical
  - DFT (GPW, GAPW + vDW)
  - LS-DFT
  - Hybrid Hartree-Fock
  - post-HF (MP2, RPA)
  - Combinations (QM/MM, mixed)
- Simulation tools:
  - MD (various ensembles)
  - Monte Carlo, Global Optimisation
  - Minimisation (GEO/CELL\_OPT)
  - Properties (Spectra, excitations ...)
- Open Source
  - GPL, [www.cp2k.org](http://www.cp2k.org)
  - 1m loc, ~2 commits per day
  - ~20 core developers



CP2K



# CP2K History

- 25<sup>th</sup> June 2001 – CP2K repository online at berliOS.de
  - Merger of Quickstep (DFT) + FIST (MD) codes
  - Jürg Hutter, Matthias Krack, Chris Mundy

- Oct 2011 – First ‘official’ release
  - CP2K 2.2
- 15 years on...
  - 1m lines of code, ~18.5k commits
  - 25 developers + many contributors
  - 1000s of users
  - Fully open-source (GPL)

CP2K SOURCE CODE DEVELOPMENT

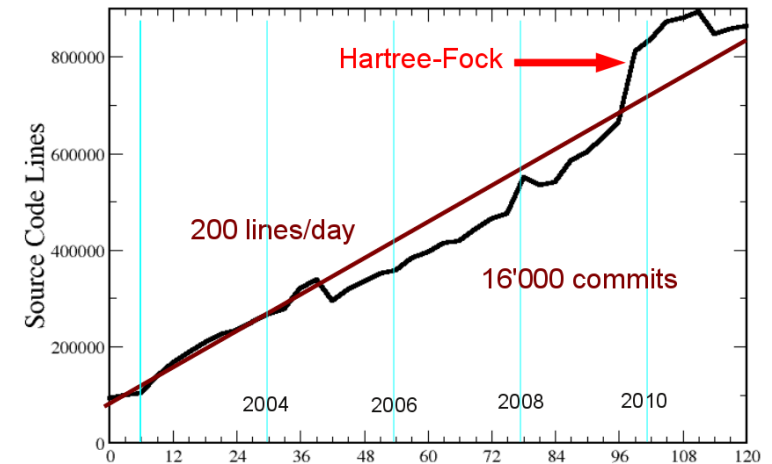


Image from Jürg Hutter

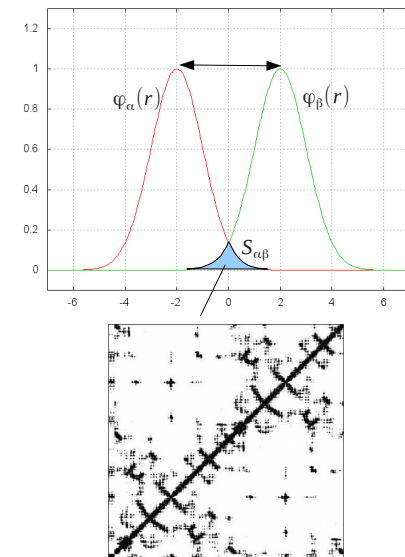
New release!  
CP2K 6.1 (June 2018)





# CP2K Features

- QUICKSTEP DFT: Gaussian and Plane Waves Method (VandeVondele *et al*, Comp. Phys. Comm., 2005)
  - Advantages of atom-centred basis (primary)
    - Density, KS matrices are sparse
    - Advantages of plane-wave basis (auxiliary)
      - Efficient computation of Hartree potential
      - Efficient mapping between basis sets
      - -> Construction of the KS Matrix is  $\sim O(n)$
- Orbital Transformation Method (VandeVondele & Hutter, J. Chem. Phys., 2003)
  - Replacement for traditional diagonalisation to orthogonalise wave functions (non-metallic systems only)
    - Cubic scaling but  $\sim 10\%$  cost



CP2K



# CP2K Features

- QM/MM (Laino *et al*, JCTC, 2005, 2006)
  - Fully periodic, linear scaling electrostatic coupling
- Gaussian and Augmented Plane Waves (Iannuzzi *et al*, CHIMIA, 2005)
  - Partitioning the electronic density -> all-electron calculations
- Hartree-Fock Exchange (Guidon *et al*, JCP, 2008)
  - Beyond local DFT (later MP2, RPA...)
  - Auxiliary Density Matrix Method (Guidon *et al*, JCTC, 2010)
- Linear Scaling DFT (VandeVondele, Borstnik & Hutter, JCTC, 2012)
  - Fully linear scaling condensed-phase DFT, up to ~1m atoms





# CP2K Features

- Many XC functionals
  - 100s via `libxc`, dispersion (pair-potential and non-local)
- Excited States
  - Realtime and Linear Response TD-DFT
    - With Hybrid functionals since 2017
  - Ehrenfest Dynamics (Andermatt *et al*, JCTC, 2016)
- Classical Potentials (FIST)
  - CHARMM/AMBER, pair-potentials, core-shell model, any analytic potential...
- Semi-empirical and DFTB
  - MNDO, AM1, PM6, PNNL ...





# CP2K Features

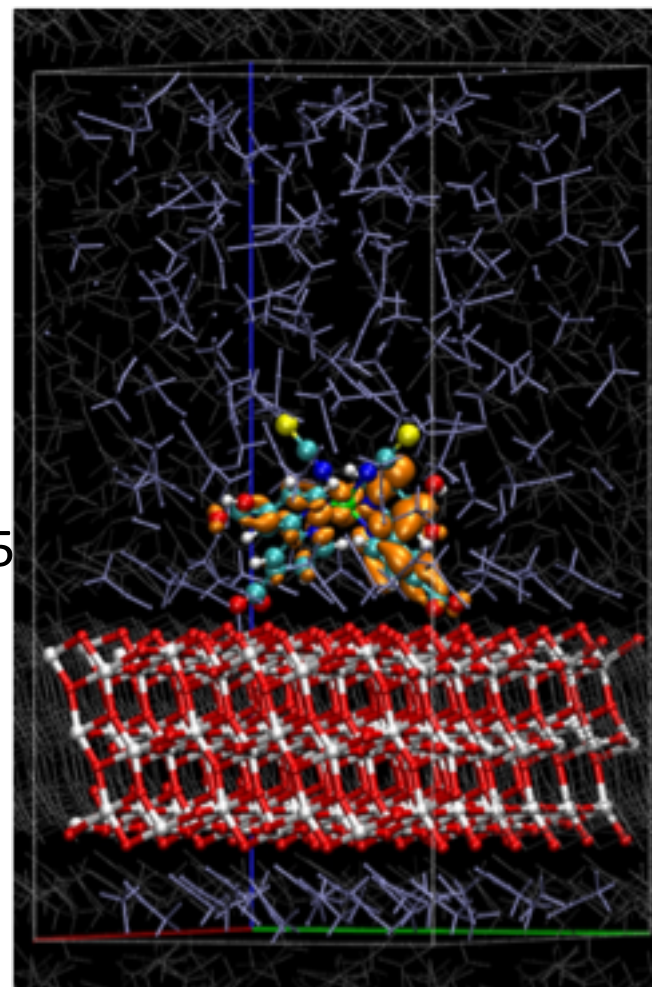
- Molecular Dynamics
  - Born-Oppenheimer MD in various ensembles
- Metadynamics
  - Free energy calculations - inbuilt module or use PLUMED
- Optimisation
  - Geometry/cell optimisation (local minimisation)
  - Global optimisation (Schütt Diploma thesis 2014)
  - Nudged elastic band
- Properties calculation
  - Atomic charges (Mulliken ...)
  - Spectra (EPR, NMR, NQR, IR, XAS ...)





# CP2K Features

- And LOTS more...
  - <https://www.cp2k.org/features>
  - Recent review paper:
  - Hutter *et al*, *WIREs Comput Mol Sci* 2014, 4:15–25  
<http://dx.doi.org/10.1002/wcms.1159>
- Some highlight applications:
  - <http://www.cp2k.org/science>
- All for free!
  - Please cite the references
  - Please give feedback / patches / feature requests
  - Please spread the word about CP2K!



DSSC: see Shiffmann *et al*, PNAS, 2010

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# CP2K Information

- CP2K Website (<http://www.cp2k.org>)
  - Everything else is linked from here
  - Community wiki – so feel free to contribute!
- CP2K Sourceforge site (<http://sf.net/p/cp2k>) :
  - Contains source code repository (SVN)
    - public read-only, read-write access to developers
    - Mirrored to github (<https://github.com/cp2k>)
  - Bug reporting
  - Source tarball / binary downloads



Open Source  
Molecular Dynamics





# CP2K Information

- CP2K Discussion Group (<http://groups.google.com/group/cp2k>)
  - Email / web forum
  - Users and developers
  - Searchable history
- CP2K Input reference manual (<http://manual.cp2k.org>)
  - Documents *every* possible CP2K input keyword
  - Mostly with helpful descriptions
  - More later...
- 





# Obtaining CP2K

- Which version?
  - Development version 5.0 (Jan 2017) **Default version on ARCHER!**
    - + stable, well tested on ARCHER
    - missing latest features
  - Current release 6.1 (Jun 2018)
    - + stable, major bug-fixes are back-ported
    - + source and binaries available from <http://www.cp2k.org/download>
  - SVN trunk version 7.0
    - + latest features, fixes, performance improvements
    - + actively developed **[http://www.cp2k.org/version\\_history](http://www.cp2k.org/version_history)**
    - bugs may exist (see <http://dashboard.cp2k.org> )
    - must be obtained from SVN and compiled from source
  - Previous releases 2.6, 4.1 ...
    - + available for Ubuntu / Debian / Fedora via package managers





# Obtaining CP2K

- CP2K download contents:
  - `README`, `COPYRIGHT`, `INSTALL`
  - `src` – source code (mostly Fortran 03, a little C++)
  - `makefiles` – To build CP2K (Thursday!)
  - `arch` – machine-specific options files
  - `data` – standard data files (basis sets, PPs ...)
  - `tests` – over 3000 input files!
  - `tools` – mostly for developers + cubecruncher
- After building:
  - `lib` – CP2K internal libraries
  - `obj` – compiled object files
  - `exe` – CP2K binaries





# CP2K Exercises

- Various exercises are available from:
  - <http://www.cp2k.org/exercises>
  - See “2018 > CP2K-UK Summer School” for this week
  - Also older exercises
  - Mostly ‘worked examples’ from system setup and calculations to analysis / visualisation of results
- For specific ‘HowTo’ guides see:
  - <http://www.cp2k.org/tutorials>
  - Guides to basic (and some advanced!) CP2K skills
    - e.g. converging CUTOFF for QS calculations





# CP2K Exercises

- The CP2K tests directory
  - Great source for example input files for all kinds of calculations
  - Grouped (mostly) logically:
    - `QS/regtest-gpw-1` – Quickstep GPW calculations
    - `QS/regtest-dm-ls-scf` – Quickstep using linear scaling SCF
    - `Fist/regtest-opt` – Geometry and Cell optimisations using classical potentials
    - `SE/regtest-*` - various semi-empirical calculations
- **WARNING:**
  - Tests are designed to run quickly so may not produce converged or accurate outputs! Check parameters for your system...

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Questions?

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