CP2K: INTRODUCTION AND OVERVIEW

CP2K Summer School, 23-26 Aug 2016

Iain Bethune

ibethune@epcc.ed.ac.uk

http://tinyurl.com/CP2K2016

Outline

- Summer School Intro

- CP2K Overview
  - Project History

- CP2K Features

- CP2K Information

- Obtaining CP2K

Summer School Intro

- Welcome!

- 52 Participants
  - 33 Institutions
  - 42/58% UK/Overseas
  - 50% have used CP2K before

- Aim to cover:
  - Practicalities of running calculations
  - Basics: common Hamiltonians, Ab Initio MD
  - Some specific topics: QM/MM, Excited States, WF Correlation

Sponsors

Support for CP2K Users

- CP2K-UK: EPSRC Software for the Future
  - £500,000, 2013-2018
  - EPCC, UCL, 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

EPSRC

Pioneering research
and skills

Instructors

- Iain Bethune (School Organiser)
  - EPCC, University of Edinburgh

- Matt Watkins & Sergey Chulkov
  - University of Lincoln

- Lev Kantorovich & Lianheng Tong
  - King's College London

- Sanliang Ling (Tues – Weds)
  - University College London

- Jan Wilhelm
  - University of Zurich

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 (and original home page from 2004!)
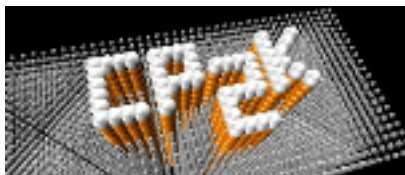
CP2K Overview

- 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
  - 1m loc, ~2 commits per day
  - ~20 core developers

CP2K History

- 25th 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, ~16k commits
  - 25 developers + many contributors
  - 1000s of users
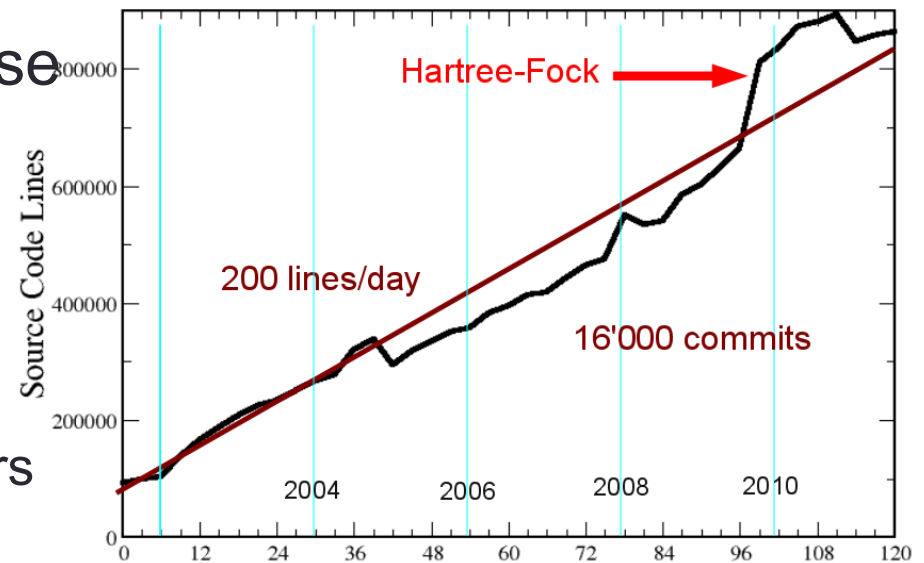 - Fully open-source (GPL)

CP2K SOURCE CODE DEVELOPMENT
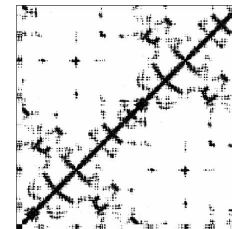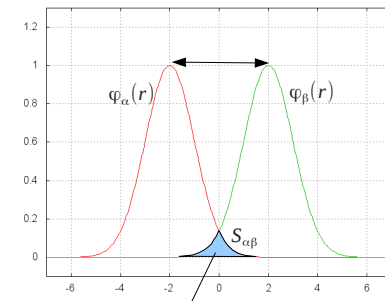

Image from Jürg Hutter

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 ~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 ~10% cost

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
  - 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 …)
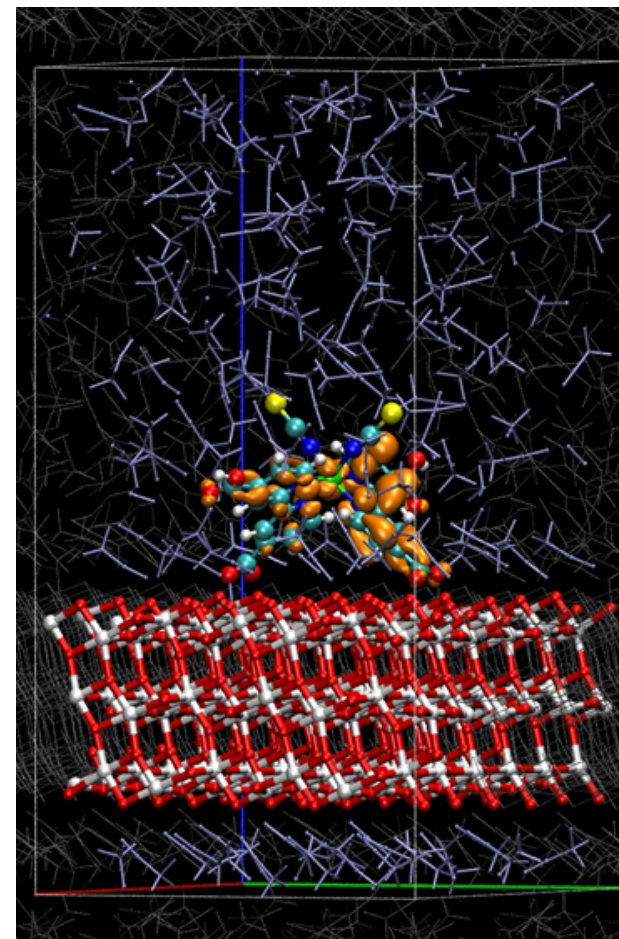 - Spectra (EPR, NMR, NQR, IR, XAS ...)

CP2K Features

- And LOTS more…
  - https://www.cp2k.org/features
  - Recent review paper:

  Hutter *et al*, *WIREs Comput Mol Sci* 2014, 4:15–25http://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

CP2K Information

- CP2K Website (http://www.cp2k.org)
  - Everything else is linked from here
  - Now a 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
  - Bug reporting
  - Source tarball / binary downloads
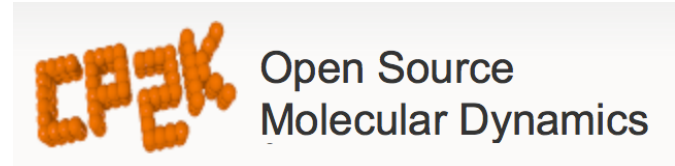
CP2K Information

- 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?
  - Current release 3.0 (Dec 2015)

  Default version on ARCHER!

  + stable, major bug-fixes are back-ported
  + source and binaries available from http://www.cp2k.org/download
  + available for Ubuntu / Debian / Fedora via package managers
  - missing latest features, minor bugs are not always fixed

  http://www.cp2k.org/version_history

  - Current release 2.6 (Sep 2015)
  + available for Ubuntu / Debian / Fedora via package managers

  - SVN trunk version 4.0
  + latest features, fixes, performance improvements
  + actively developed
  - bugs may exist (see http://dashboard.cp2k.org)
  - must be obtained from SVN and compiled from source

Obtaining CP2K

- CP2K download contents:
  - `README, COPYRIGHT, INSTALL`
  - `src` – source code (mostly Fortran 03, a little C++)
  - `makefiles` – To build CP2K
  - `arch` – machine-specific options files
  - `data` – standard data files (basis sets, PPs …)
  - `tests` – over 2700 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 "CP2K Summer School 2016" 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…

CP2K: Introduction and Overview

Questions?