CP2K: HIGH PERFORMANCE ATOMISTIC SIMULATION

Iain Bethune
ibethune@epcc.ed.ac.uk

http://tinyurl.com/CP2K-QUB

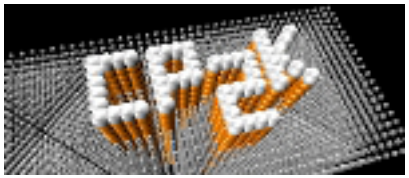
epcc

THE UNIVERSITY OF EDINBURGH

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 (2004!)



epcc

THE UNIVERSITY OF EDINBURGH

CP2K Overview

- Many force models:
  - Classical
  - DFT (GPW, GAPW + vDW)
  - Hybrid Hartree-Fock
  - LS-DFT
  - post-HF (MP2, RPA)
  - Combinations (QM/MM, mixed)
- Simulation tools
  - MD (various ensembles)
  - Monte Carlo
  - Minimisation (GEO/CELL_OPT)
  - Properties (Spectra, excitations …)
- Open Source
  - GPL, www.cp2k.org
  - 1m loc, ~2 commits per day
  - ~10 core developers

cp2k

epcc

THE UNIVERSITY OF EDINBURGH

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, ~16.5k commits
  - 25 developers + many contributors
  - 100s (1000s?) of users
  - Fully open-source (GPL)

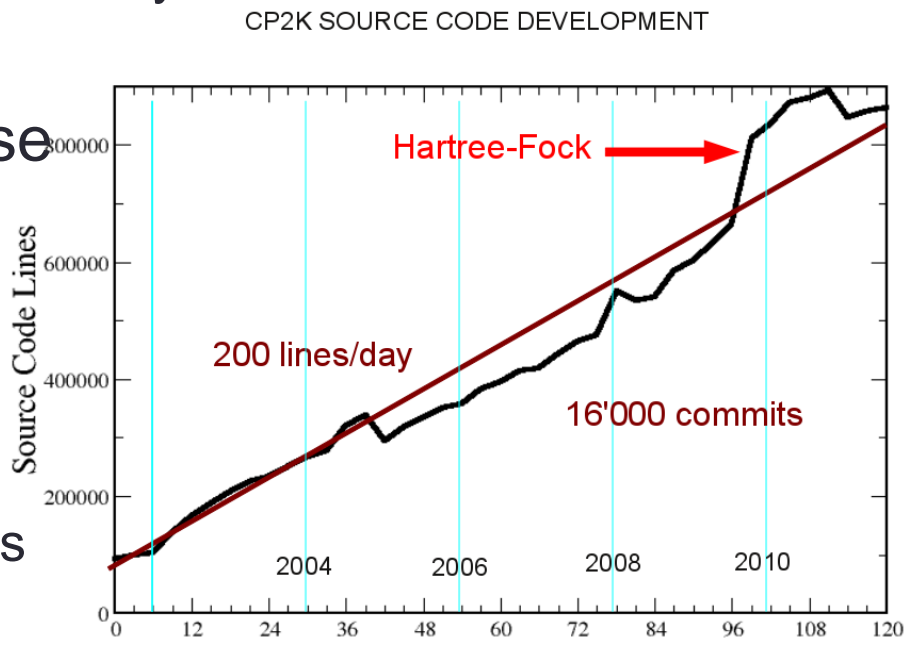


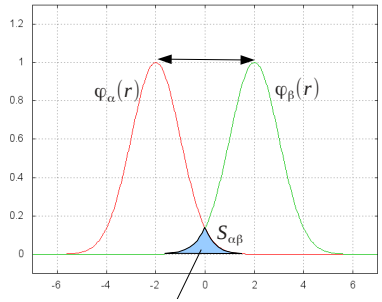
Image from Jürg Hutter

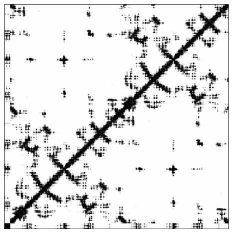
epcc

THE UNIVERSITY OF EDINBURGH

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 optimise molecular orbital coefficients (non-metallic systems only)
    - Cubic scaling but ~10% cost

cp2k

epcc

THE UNIVERSITY OF EDINBURGH

CP2K Features

$$
\begin{aligned}
E^{\mathrm{el}}[n] &= \sum_{\mu\nu} P_{\mu\nu} \left\langle \varphi_\mu \left| -\frac{1}{2}\nabla^2 + V_{\mathrm{loc}}^{\mathrm{SR}} + V_{\mathrm{nl}} \right| \varphi_\nu \right\rangle \\
&+ 2\pi\Omega \sum_{\mathbf{G}} \frac{\tilde{n}^*_{\mathrm{tot}}(\mathbf{G})\tilde{n}_{\mathrm{tot}}(\mathbf{G})}{\mathbf{G}^2} + \sum_{\mathbf{R}} \tilde{n}(\mathbf{R}) V^{\mathrm{XC}}(\mathbf{R}) \\
&= \sum_{\mu\nu} P_{\mu\nu} \left(\left\langle \varphi_\mu \left| -\frac{1}{2}\nabla^2 + V^{\mathrm{ext}} \right| \varphi_\nu \right\rangle + \sum_{\mathbf{R}} V_{\mu\nu}^{\mathrm{HXC}}(\mathbf{R}) \varphi'_{\mu\nu}(\mathbf{R}) \right)
\end{aligned}
$$

From Marcella Iannuzzi,
https://www.cp2k.org/_media/events:2015_cecam_tutorial:iannuzzi_gpw_gapw_b.pdf

epcc

CP2K Features

64 H_2O
32 CPUs IBM SP4

1 SCF iter	DZVP	TZVP	TZV2P	QZV2P	QZV3P
OT	0.50	0.60	0.77	0.87	1.06
Diagonalisation	6.02	8.40	13.80	17.34	24.59

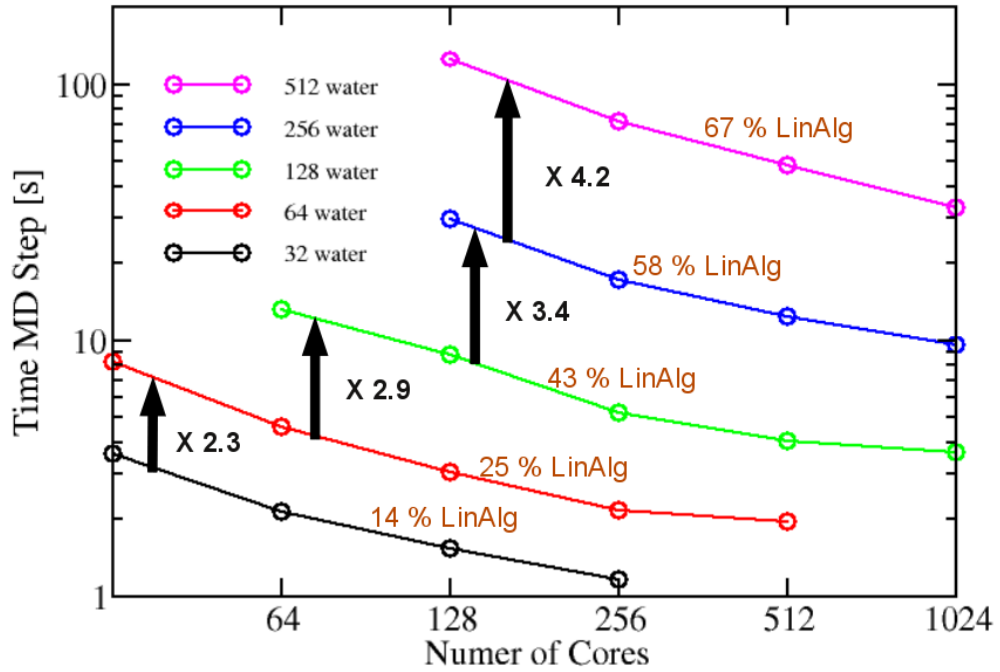


Figure from Jürg Hutter

epcc

THE UNIVERSITY OF EDINBURGH

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 into -> 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
- https://www.epcc.ed.ac.uk/sites/default/files/PDF/CP2K-UK-2015-Hutter.pdf

epcc

THE UNIVERSITY OF EDINBURGH

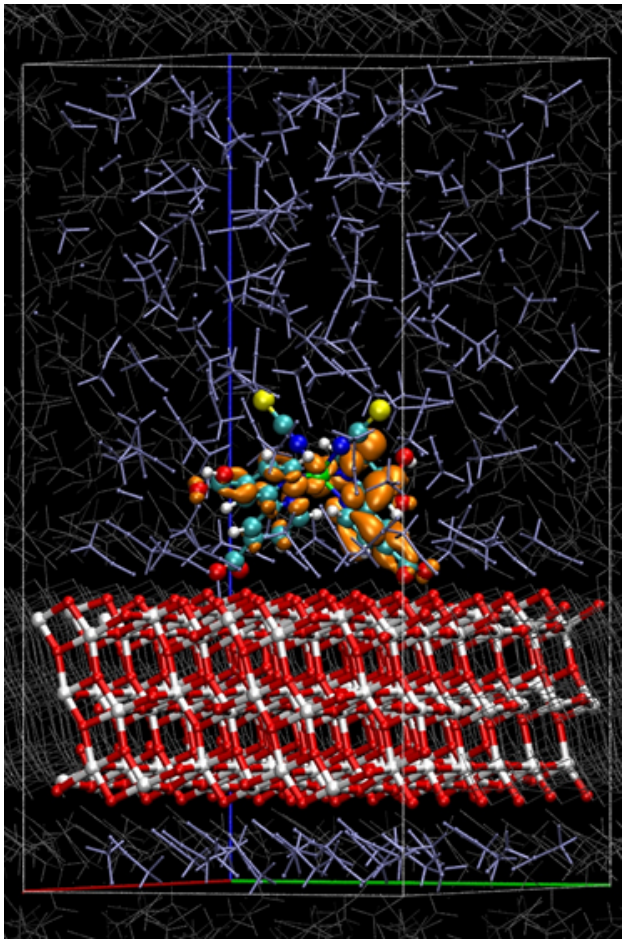
CP2K Features

- And LOTS more…
  - 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!



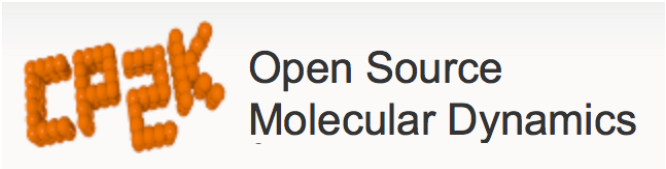
DSSC: see Shiffmann *et al*, PNAS, 2010

epcc

THE UNIVERSITY OF EDINBURGH

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

epcc

THE UNIVERSITY OF EDINBURGH

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…
  - Beta CP2K online input editor
    - http://cp2k-www.epcc.ed.ac.uk/cp2k-input-editor

epcc

THE UNIVERSITY OF EDINBURGH

CP2K Information

- Which version?
  - Current release 3.0 (Dec 2015)
  + stable, major bug-fixes are back-ported
  + source and binaries available from http://www.cp2k.org/download
  + installed on ARCHER
  - missing absolute latest features, minor bugs are not always fixed

  - Previous release 2.6.2 (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

http://www.cp2k.org/version_history

epcc

THE UNIVERSITY OF EDINBURGH

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

epcc

THE UNIVERSITY OF EDINBURGH

Where is CP2K available?

- On ARCHER
  - http://www.archer.ac.uk/documentation/software/cp2k/
- On NSCCS
  - http://www.nsccs.ac.uk/sc_cp2k.php
- Local installations
  - http://www.cp2k.org/download
  - Packages for several Linux distros
  - Source code available
  - Installation help from EPCC

epcc

THE UNIVERSITY OF EDINBURGH

Support for UK CP2K Users

- CP2K-UK: EPSRC Software for the Future
  - £500,000, 2013-2018
  - EPCC, UCL, KCL + 7 supporting groups

EPSRC
Pioneering research and skills

- 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 (next Feb 22nd 2016 @ UCL)
- Updates via mailing list

epcc

THE UNIVERSITY OF EDINBURGH

Access to ARCHER

- ARCHER Driving test
  - Online multiple choice test covering basics of ARCHER and HPC concepts, for new users
  - http://www.archer.ac.uk/training/course-material/online/driving_test.php
  - On completion, get 1200 kAUs (= 3300 node hours)
  - To be used within 12 months

epcc

THE UNIVERSITY OF EDINBURGH

Access to ARCHER

- ARCHER Resource Allocation Panel (RAP)
  - Calls every 2/3 times per year from EPSRC
  - Up to 12 months
  - Large AU allocations (typically ~10s MAU)
  - Technical Assessment + Standard Case for support, Pathways To Impact etc.
  - Also ARCHER Leadership calls for extremely large projects (>100 MAU)

- EPSRC Grants
  - Add ARCHER time as a resource to standard grants
  - Nominal cost does not count towards project total
  - TA form required

- Scientific Consortium Access
  - Materials Chemistry Consortium
  - UK Car-Parrinello Consortium

epcc

THE UNIVERSITY OF EDINBURGH