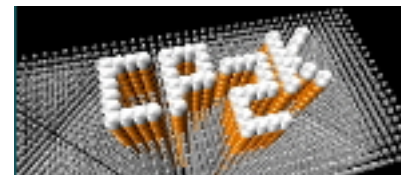


CP2K-UK 1ST ANNUAL USER MEETING

Introduction & Overview

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Introduction

- Welcome!
- 55 attendees from 16 institutions
- Chemistry, Physics, Materials, Engineering, Bioscience
- Experienced and novice users
- All interested in learning more about CP2K

Background: CP2K-UK

- CP2K is a powerful tool
 - DFT, Classical, Hybrid-DFT, Many-body correlation, QM/MM
 - MD, MC, Relaxation, NEB, Free Energy Tools
 - Suitable for simulations in range of EPSRC target areas
- CP2K is popular (and growing)
 - 2nd most heavily used code on HECToR (>£3m compute time)
 - 10+ research groups already using CP2K on national service
- CP2K is hard to use
 - Large feature set leads to complexity
 - Lack of documentation



Background: CP2K-UK

- EPSRC ‘Software for the Future’ funded project:
 - 2013-2018
 - EPCC : Iain Bethune, Fiona Reid
 - KCL : Lev Kantorovich, Lianheng Tong
 - UCL : Ben Slater, Matt Watkins
 - + 7 supporting group leads
- 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



Support for Users

- Knowledge Transfer
 - Lots of collective experience exists within research groups
 - Provide forums to share, capture and disseminate best practice
 - Foster interaction between users and developers
 - Users should influence development
 - Enable users to *become* developers!
 - Let us know what features you *need* for your research
- Improve the contents of the CP2K website
 - <http://www.cp2k.org>
 - Now a wiki – so please contribute!
 - Enable self-support

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Support for Users

- Documentation
 - Address the 'documentation gap'
 - Input file format: <http://manual.cp2k.org> – editable!
 - User guide / tutorials for core functionality: <http://www.cp2k.org/tutorials>
 - Case studies of advanced features
 - Exemplar science articles: <http://www.cp2k.org/science>
- Performance
 - CP2K is designed to take advantage of HPC resources
 - Architecture-specific tuning, communication schemes...
 - Generate and publish benchmark data
 - Advice on building/tuning/optimising CP2K

Support for Users

- Training
 - Series of annual user meetings
 - Will evolve in line with community needs & expectations
 - CP2K training course
 - Similar format to existing CECAM training
 - To be held in London, 2015
- Publicise other training opportunities
 - e.g. Parallel Materials Modeling Packages course
 - 22-24 April 2014 @ EPCC
 - Covering CP2K, CASTEP & GPAW
 - Theory and practicals



Support for Users

- Tools & Usability
 - Integration with community tools
 - e.g. VMD, Avogadro...
 - Pre- and post- processing (*lev00*, *tetr*)
 - Your suggestions welcomed!
- Input file editing
 - Bindings for emacs, vim ...
 - GUI for creating and editing

Support for Developers

- Underpinning support from EPCC
 - Get new developers quickly up to speed
 - Bespoke training & visitor opportunity
 - Improved developer documentation on CP2K website
 - Provide route for patches to be fed back into trunk
- Improved regression test environment
 - Find bugs quickly in a multi-platform & parallel environment
 - Once things are fixed, they should stay fixed
 - Status online: <http://cp2k-www.epcc.ed.ac.uk>



Support for Developers

- Development projects
 - 3 year PDRA developer post at KCL (LT)
 - Trailblazer for future (externally funded) projects
- Implement new algorithms and methods beneficial to wide community:
 - Filter Matrix Diagonalization (Rayson & Briddon, 2009, Phys Rev B)
 - Adaptive KMC
 - System Partitioning (He, Di Paola & Kantorovich, 2009, J. Chem Phys)
 - Embedding TDDFT within ground-state DFT
- Ideas for future projects welcome!

Community Involvement

- CP2K-UK Project exists to support and grow the CP2K user community - how can you get involved?
 - Let us know what support you need
 - Via discussion session & feedback forms, or ad hoc
 - Provide support visits to individuals & groups
 - Contribute to the CP2K website / wiki
 - Join the CP2K discussion forum
 - <http://groups.google.com/group/cp2k>
 - Present at next year's user meeting

Community Involvement

- Interested in contributing to development?
 - Opportunity to get 6-12 months funding via ARCHER eCSE calls (next May 2014) for *“Improvements to code which allows new science to be carried out”*
 - Have a ‘killer feature’ that you *need* in CP2K?
 - Interested in working on a development project? Let me know...
 - Acknowledge support from CP2K-UK grant (EP/K038583/1) in publications (and tell me!)
 - More impact = better chance of future funding
 - Cite CP2K reference papers (check your output!)
 - Letters of support available to projects who will use/develop CP2K

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Summary

- CP2K-UK exists to support your research using CP2K!
- Aim to improve confidence and competence in the user community
- User engagement and feedback is key
- Opportunity to get bespoke support for new development projects within your group

Acknowledgements

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