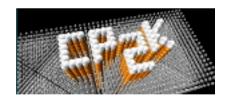# CP2K-UK 2ND ANNUAL USER MEETING

Overview & Project Update

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Introduction

- Welcome!

- 70 attendees from 28 institutions
  - Up from last year (55 / 16)
  - Including overseas and industry

- Experienced and novice users
  - Network, learn from others' experience

- Highlight opportunities for training & support

- Update on latest developments

Background: CP2K-UK

- CP2K is a powerful tool
  - DFT, Classical, Hybrid-DFT, LS-DFT, MP2/RPA, 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 ARCHER (5-10% of machine)
  - Growing users of CP2K on national service 42 (2Q14) -> 72 (1Q15)

- CP2K is hard to use
  - Large feature set leads to complexity
  - Lack of documentation

Support for Users

- Training Events
  - Annual User Meetings

  - 3 days CP2K training during 2014
    - Collaboration with ARCHER and NSCCS & TYC
    - Slides and exercises still available:
      - http://archer.ac.uk/training/course-material/2014/08/CP2K/
      - http://archer-www.epcc.ed.ac.uk/training/course-material/2014/04/PMMP_UCL/

  - CP2K CECAM Tutorial
    - 31st Aug – 4th Sept 2015
    - ETH Zurich
    - http://www.cecam.org/workshop-1122.html

  - All CP2K events at www.cp2k.org/events

  - Also notification by email

Support for Users

- Ad-hoc bespoke support
  - Example: Macgregor Group at Heriot-Watt
    - Solid-state catalytic chemistry
    - Experience running CASTEP on NSCCS

  - Attended CP2K training day in April 2014
  - Visit to HW in May
    - Installed CP2K on department cluster
    - Worked through basic capabilities, running jobs …

  - Instant Access to ARCHER, 1.2 MAU, Jun-Nov 2014
  - ARCHER RAP, 65 MAU, Nov 2014
  - PDRA currently visit J. Hutter in Zurich.

Support for Users

- Performance
  - Systematic benchmarking method covering a range of methods
    - Classical, DFT, LS-DFT, HFX, MP2

  - Performance paper published at CUG
    - http://www2.epcc.ed.ac.uk/~ibethune/files/cp2k_cug2014.pdf

  - Benchmark data available on CP2K website
    - www.cp2k.org/performance

  - Instructions to run on your own machine
    - We can help with tuning & running benchmarks
    - Please add your data to the web page.

Support for Users

- Tools & Usability
  - Feedback from tutorials - building an input is hard!

  - Developing a GUI
    - based on LibHPC project

  - Validation
  - Keyword Selection
  - Show/hide sections

  - Templates for common jobs

Support for Developers

- Automated regression testing
  - Now covers Intel compilers
  - Working arch files for Intel builds now available
    - http://cp2k-www.epcc.ed.ac.uk
  - Good relationship with Intel – code quality improving
    - http://www.cp2k.org/static/dashboard/

- Automatic doxygen generation
  - All routines in CP2K now document their parameters (in and out)
    - doxygen.cp2k.org
  - Avoids 'comment rot' during refactoring

Support for Developers

- Development projects
    - 3 year PDRA developer post at KCL (LT)
        - Trailblazer for future (externally funded) projects

    - Langevin Dynamics regions (Kantorovich, 2008, Phys Rev B)
    - BSSE calculations with arbitrary fragments
    - Filter Matrix Diagonalization (Rayson & Briddon, 2009, Phys Rev B)
        - More later…

Support for Developers

- External funding
  - Awarded 12 months funding from ARCHER eCSE
    - Matt Watkins, starting Apr 2014
    - Linear Response TDDFT with Hybrid Functionals/ADMM
    - And more…

  - Submitted 6 month project to current eCSE call
    - Martin Paterson (Heriot-Watt Chemistry)
    - Load balancing + extended Implicit Solvent models
    - Emphasis on early-career researcher training

  - Letters of support for 2 EPSRC proposals

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 & Sept 2015) 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

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