CP2K-UK 3RD ANNUAL USER MEETING
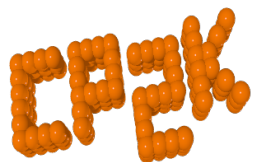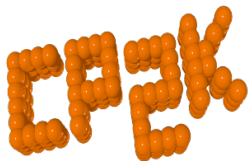
Overview & Project Update
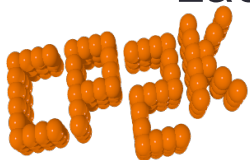
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Introduction

- Welcome!

- 60+ attendees from 30 institutions

- 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)
  - 3rd most heavily used code on ARCHER (8% of machine)
  - Growing users of CP2K on national service:
    - 42 (2Q14) -> 72 (1Q15) -> 116 (1Q16)

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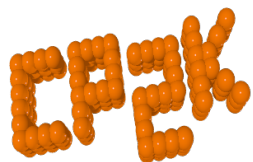 - Lack of documentation

Support for UK 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
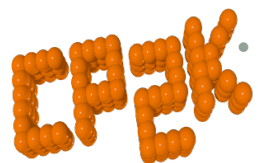 - Extend ability of CP2K to tackle challenging systems

Support for Users

- Training Events
  - Annual User Group Meetings

  - 7 days CP2K training during 2015/16
    - Collaborations with ARCHER, MCC, UKCP & STFC
    - Visits to research groups (Lancaster, UCL, QUB)

  - CP2K CECAM Tutorial
    - 31st Aug – 4th Sept 2015 @ ETH Zurich
    - 50% of lectures from UK people
    - Slides and exercises still available:
      - https://www.cp2k.org/events:2015_cecam_tutorial:index
      - https://www.cp2k.org/exercises:2015_cecam_tutorial:index

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

  - Also notification by email

Support for Users

- Ad-hoc bespoke support
  - Help installing CP2K on your cluster
  - Training days / group visits
  - Debugging
  - Advice on parallel performance - www.cp2k.org/performance
    - We would like more than just Cray machines!

- Documentation
  - Growing set of 'HowTo' guides: https://www.cp2k.org/howto
  - FAQs: https://www.cp2k.org/faq

- Let us know what you want to see in CP2K!
  - Discussion session & feedback forms

Support for Users

http://cp2k-www.epcc.ed.ac.uk/cp2k-input-editor

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

  - Beta CP2K input GUI

  - Validation of input
    - CP2K releases 2.5 – 3.0
  - Keyword Selection
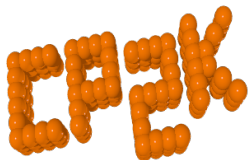 - Show/hide sections
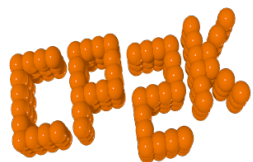 - Templates for common jobs (to come!)

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)
  - REPEAT charge fitting (Campana *et al*, 2008, JCTC)
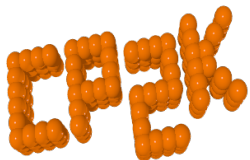 - CP2K Installer

Support for Developers

- External funding
  - Two 12 month funded projects from ARCHER eCSE

  - Linear Response TDDFT with Hybrid Functionals/ADMM
    - Started Dec 2015
    - Sergey Chulkov / Matt Watkins @ Lincoln
    - And more…

  - CP2K performance improvements
    - Started Dec 2015
    - Large, load imbalanced systems, GAPW, K-points
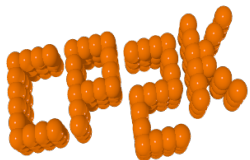   - Mark Tucker @ EPCC

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

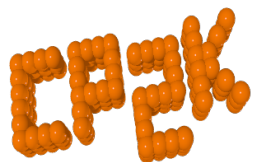   - Present at next year's user meeting

Community Involvement

- Interested in contributing to development?

  - Opportunity to get 6-12 months funding via ARCHER eCSE calls (next May & Sept 2016) 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
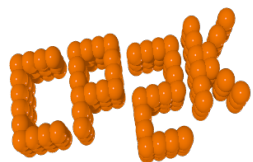
Acknowledgements

- EPSRC (EP/K038583/1)

- Joost VandeVondele & Jürg Hutter

- Lev Kantorovich, Ben Slater & Matt Watkins

- Jochen Blumberger, Patricia Hunt, Jorge Kohanoff, Angelos Michaelides, Philip Moriarty, Carole Morrison, Alex Shluger & Michiel Sprik

Any questions?