CP2K-UK 2\textsuperscript{ND} 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)
  • 2\textsuperscript{nd} most heavily used code on ARCHER (5-10\% of machine)
  • Growing users of CP2K on national service 42 (2Q14) \rightarrow 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](http://www2.epcc.ed.ac.uk/~ibethune/files/cp2k_cug2014.pdf)

• Benchmark data available on CP2K website
  • [www.cp2k.org/performance](http://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
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