CP2K-UK 5th Annual User Meeting

Welcome & Project Update

Iain Bethune
iain.bethune@stfc.ac.uk
@ibethune @CP2Kproject
Introduction

• Welcome!

• 30+ attendees from 20+ 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, TDDFT, LS-DFT, MP2/RPA/G0W0, QM/MM
  – MD, MC, Geometry Optimisation, 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 (£0.5m per year)
  – Growing users of CP2K on national service:
    • 42 (2Q14) -> 72 (1Q15) -> 116 (1Q16) -> 132 (1Q17) -> 173 (1Q18)
    • EPSRC: Materials Chemistry Consortium, UKCP
    • NERC: Mineral Physics

• CP2K can be hard to use
  – Large feature set leads to complexity
  – Few default settings -> hard to set up systems from scratch
  – Lack of documentation
Support for UK CP2K Users

• CP2K-UK: EPSRC Software for the Future
  – £500,000, 2013-2018
  – EPCC (+ STFC), UCL (+ Lincoln), 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
  - CP2K User Tutorial 2017
    - 3 day workshop at Zurich
    - CP2K-UK travel funding
  - All CP2K events at [www.cp2k.org/news](http://www.cp2k.org/news)
    - Growing archive of lecture, example material: [www.cp2k.org/docs#workshops](http://www.cp2k.org/docs#workshops)
  - Also notification by email
  - Planning CP2K Summer School 2017
Support for Users

• Ad-hoc bespoke support
  – Help installing CP2K on your cluster
    • Iceberg @ Sheffield, Lancaster HEC, KCL Physics Cluster, QUB, Cambridge ...
  – Training days / group visits
  – Debugging
  – Adding functionality
    • Merging in user contributions (OPLS torsions, CDFT...)
  – 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 me know your pain points!
Support for Users

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

• Tools & Usability
  – Feedback from tutorials:
    • building an input is hard!
  – CP2K input GUI
  – USCF Chimera plugins for TETR and LEV00

https://www.cp2k.org/tools:tetr
Support for Developers

- Development projects
  - 3 year PDRA developer post at KCL (2013-2016)
    - 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 / toolchain
  - Vibrational Initialisation for MD (West & Estreicher, 2006, PRL)
Support for Developers

• External funding
  – Three 12 month funded projects from ARCHER eCSE
  – LR-TDDFT with Hybrid Functionals/ADMM (2015-2016)
    • See https://www.archer.ac.uk/training/virtual/2016-11-23-CP2K-Improvements/TDDFT.slides.html
    • 3.6x speedup for GAPW calculations
    • 10% speedup and GBs memory saving for load-imbalanced systems
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 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](http://groups.google.com/group/cp2k)
  
  – Present at future user meetings
Community Involvement

- Interested in contributing to development?
  - ARCHER eCSE is now closed... but opportunities from PRACE, EPSRC...
    - 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/K038583/2) 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
  – Support requests to iain.bethune@stfc.ac.uk
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Any questions?
Lightning talks

• 3 minute summaries of research using CP2K:
  – Stephen Cox, University of Cambridge
  – Matthew Krzystyniak, STFC
  – David Benoit, University of Hull
  – Natalia Martsinovich, University of Sheffield
Interfacial ion solvation: Obtaining the thermodynamic limit from molecular simulations

- Potential future user of CP2K.
- Using the constant $D$ ensemble to probe the statistical mechanics of electrolyte solutions.
- Hoping to investigate acidity of liquid/solid interfaces in future [see e.g. Zhang & Sprik, PRB 94, 245309 (2016) and Sayer, Zhang Sprik JCP 147, 104702 (2017)].
- Recent work on finite size effects in slab geometry…

simple finite size correction.
related to polarization fluct’s/response at interface.
disambiguates contributions of surface potential in solvation.

sjc236@cam.ac.uk
Mass-selective neutron Compton spectroscopy

No coupling constant weighting as PVDOS and cross section are separate parameters!

In many respects, an ultimate ab initio benchmarking tool!

width : \[ M^2 \approx \int_0^\infty E \cdot G_M(E) \cdot \coth \left( \frac{E}{2kT} \right) \cdot dE \]

First moment of the pVDOS!

partial VDOS

\[ p \text{VDOS} = G_M(E) \cdot E \cdot \coth \left( \frac{E}{2kT} \right) \]

\[ E \gg \text{binding energy} \]

\[ Q \gg \text{inverse interatomic distance} \]
Dusty Interstellar Ices

• Do large carbon-rich molecules stick to ice?
• What is their vibrational signal?
Photocatalytic TiO$_2$/graphene-based charge-transfer interfaces

Peter Gillespie, Natalia Martsinovich
Department of Chemistry, University of Sheffield

Research question: Explain the high efficiency of TiO$_2$/reduced graphene oxide photocatalysts

Computational challenges:
- Commensurability => large systems: 180 atoms TiO$_2$ + 72 atoms C
- Need hybrid functionals to describe TiO$_2$
- Need dense k-point grid to describe graphene

Our approach:
- Geometry optimisation using CP2K (first PBE, then HSE06 using ADMM)
- Electronic structure analysis using CRYSTAL

1. TiO$_2$ (rutile)/graphene

2. TiO$_2$ (rutile)/reduced graphene oxide (RGO)
RGO model: C:O ratio =12:1; 4 OH, 2 epoxy groups

DOS

Energy (eV)
Summary

• Thank you very much for coming

• Thanks to all our our speakers

• Please complete feedback forms and return them before you leave

• See you again next year (maybe)!