

# NSCCS/ARCHER CP2K UK WORKSHOP 2014

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Iain Bethune (ibethune@epcc.ed.ac.uk)

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NSCCS

EPSRC

Pioneering research  
and skills



# Welcome!

- 43 Attendees
  - 22 Institutions, 5 countries
- Course Aims:
  - *“The workshop will provide a survey of the most relevant computational tools implemented within the CP2K program package.*
  - *There will be opportunities to talk to experts and to meet fellow researchers who are interested in CP2K. “*
- All lecture slides and practical notes are available at:
  - <http://www.archer.ac.uk/training/course-material/2014/08/CP2K/>



# Course Information

- Lecturers
  - Iain Bethune, Project Manager, EPCC
  - Dr. Marcella Iannuzzi, Senior Scientist, PCI, University of Zurich
  - Dr. Sanliang Ling, Research Associate, UCL Chemistry
  - Dr. Ben Slater, Reader in Computational Materials Chemistry, UCL
  - Dr. Matt Watkins, Senior Research Associate, UCL Physics
- Hands-on instructors:
  - Dr. Lianheng Tong, Research Associate, KCL
  - Dr. Jörg Saßmannshausen, Computer Officer, UCL Chemistry



# Course Information

## Day 1: Wed 27<sup>th</sup> August

- 9.25 – 9.45: Introduction & Overview
- 9.45 – 11.00: Lecture – Overview of KS-DFT, Introduction to CP2K & GPW/GAPW
- 11.00 – 11.30: Coffee Break
- 11.30 – 12.00: Lecture – Setting up a CP2K Calculation
- 12.00 – 13.00: Lecture – *ab initio* Molecular Dynamics with CP2K
- 13.00 – 14.00: Lunch Break
- 14.00 – 15.30: Practical
- 15.30 – 16.00: Coffee Break
- 16.00 – 17.00: Practical
- 17.00 – 18.30: Drinks Reception and Networking



# Course Information

## Day 2: Wed 28<sup>th</sup> August

- 9.00 – 11.00: CP2K Advanced Topics Lectures:  
QM/MM and NEB calculations,  
Hybrid Functionals, ADMM & Basis Set Optimisation
- 11.00 – 11.30: Coffee Break
- 11.30 – 12.30: CP2K Case Study Lectures:  
MP2 and RPA on ice (XV)  
Surface calculations with Hybrid Functionals
- 12.30 – 13.00: Lecture: Running CP2K in Parallel on ARCHER
- 13.00 – 14.00: Lunch Break
- 14.00 – 15.30: Practical
- 15.30 – 16.00: Coffee Break
- 16.00 – 17.00: Practical



# Course Information

- We welcome your feedback:
  - Please complete the feedback form before you leave!
- Want more training?
  - General HPC skills
  - Parallel Programming & Software Development
  - Application Specific
  - At a location near you
- Please speak to me or NSCCS staff



# Course Information

Any questions?



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# Access to ARCHER

- ARCHER Instant Access
  - <http://www.archer.ac.uk/access/instant-access/>
  - 1.2 MAU (3.3 million node hours)
  - 6 months duration
  - Technical assessment + 2 page case for support
  - For new users i.e. apply once!

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# CP2K Training

- List of upcoming courses:
  - <http://www.cp2k.org/events>
  - Annual CP2K UK User Meeting (Jan/Feb 2015, Location TBC)
  - CECAM CP2K Tutorial (mid-2015, Zurich)
  - Email [ibethune@epcc.ed.ac.uk](mailto:ibethune@epcc.ed.ac.uk) to be added to the notification list
- Also online material (this afternoon):
  - <http://www.cp2k.org/tutorials>
  - <http://www.cp2k.org/exercise>
  - <http://manual.cp2k.org>

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