PARALLEL MATERIALS MODELLING PACKAGES

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

Parallel Materials Modelling Packages

Welcome!

- 40 Attendees
  - 24 Institutions, 8 countries

- Course Aims:
  - *"Participants can expect to gain enough experience to decide which code [CASTEP, CP2K, GPAW] is best suited to their particular applications, and the ability to run calculations of moderate complexity using ARCHER, the UK National HPC Service."*

- All lecture slides and practical notes are available at:
  - http://www.epcc.ed.ac.uk/~ibethune/pmmp/

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Course Information

Day 1: CASTEP (Keith Refson, STFC Rutherford Appleton Laboratory)

- 9.30 – 11.00: Lecture - Introduction to DFT and the plane-wave pseudopotential method
- 11.00 – 11.30: Coffee Break
- 11.30 – 13.00: Lecture - Materials modelling with CASTEP
- 13.00 – 14.00: Lunch Break
- 14.00 – 15.00: Practical
- 15.00 – 15.30: Coffee Break
- 15.30 – 17.00: Practical

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Course Information

- Lectures in B17 Lecture Theatre (Basement, Torrington Building)
- Practical Sessions in Computer Suite 113 (1st floor, Torrington Building)
- Tea & Coffee outside Lecture Theatre
  - Please put cups back on the trolley!
- Lunch in Old Refectory, UCL Wilkins Building
  - 5 mins walk from Torrington
- Please don't leave bags, laptops unattended in the rooms.

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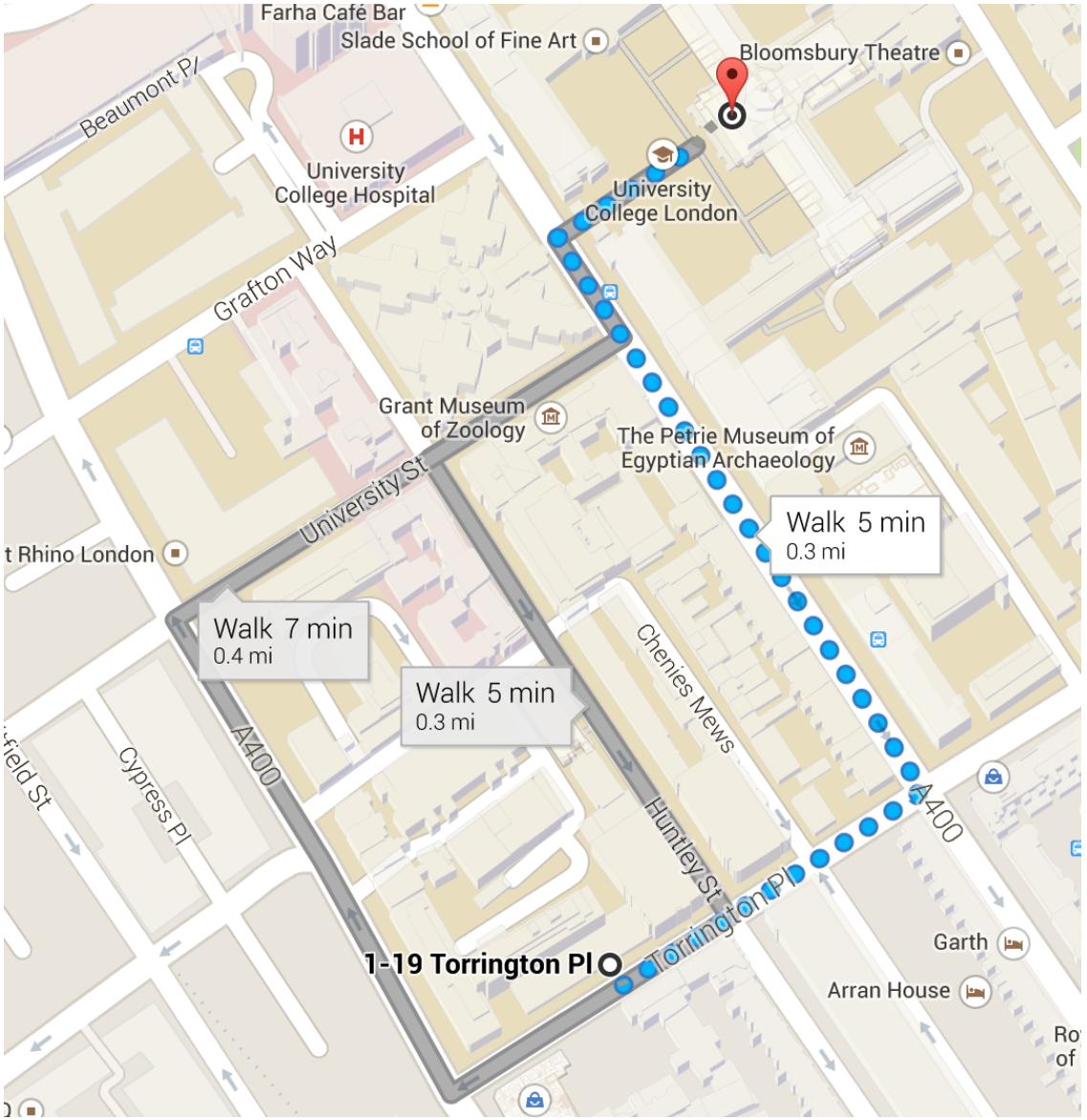
Farha Café Bar
Slade School of Fine Art
Bloomsbury Theatre
Beaumont Pl
University College Hospital
University College London
Grafton Way
Grant Museum of Zoology
The Petrie Museum of Egyptian Archaeology
University St
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Chenies Mews
A400
Cypress Pl
Huntley St
Torrington Pl
A400
1-19 Torrington Pl
Garth
Arran House

Course Information

- Network access:
  - Wifi : UCLGuest (instructions on sheet outside)
  - Wifi : Eduroam (if you already have it set up)
  - Desktop PCs in lab room
- Toilets
- Fire Exits

Course Information

- We welcome your feedback:
  - http://events.prace-ri.eu/confDisplayEvaluation.py/display?confId=280
  - Open until Weds 30th April
- Want more training?
  - General HPC skills
  - Parallel Programming & Software Development
  - Application Specific
  - At a location near you
- Please ask me!

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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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Course Information

Day 2: CP2K (Marcella Iannuzzi, University of Zurich)

- 9.30 – 11.00: Lecture - Introduction to CP2K and Quickstep; Ab initio Molecular Dynamics
- 11.00 – 11.30: Coffee Break
- 11.30 – 13.00: Lecture – Advanced sampling methods with CP2K
- 13.00 – 14.00: Lunch Break
- 14.00 – 15.00: Practical
- 15.00 – 15.30: Coffee Break
- 15.30 – 17.00: Practical

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CP2K Training

- List of upcoming courses:
  - http://www.cp2k.org/events
  - ~3 day course in summer/autumn with NSCCS
  - Email 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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Course Information

Day 3: GPAW (Jussi Enkovaara, CSC)

- 9.30 – 11.00: Lecture - Introduction to GPAW and PAW method
- 11.00 – 11.30: Coffee Break
- 11.30 – 13.00: Practical
- 13.00 – 14.00: Lunch Break
- 14.00 – 15.00: Lecture - Introduction to TD-DFT; parallel calculations with GPAW
- 15.00 – 15.30: Coffee Break
- 15.30 – 16.30: Practical

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