INTRODUCTION TO MOLECULAR DYNAMICS ON ARCHER

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Intro to Molecular Dynamics on ARCHER

- UK National Supercomputer Service, managed by EPSRC
  - housed, operated and supported by EPCC
  - hardware Supplied by Cray
- Training provided by the ARCHER Computational Science and Engineering (CSE) support team
  - 72 days per year at various locations round the UK
  - free to all academics

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EPCC's Advanced Computing Facility

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What is EPCC?

- UK national supercomputer centre
  - founded in 1990 (originally Edinburgh Parallel Computing Centre)
  - a self-funding Institute at The University of Edinburgh
  - running national parallel systems since Cray T3D in 1994
  - around 65 full-time staff
  - a range of academic research and commercial projects
  - one-year postgraduate masters in HPC www.epcc.ed.ac.uk/msc/
- Get in contact if you want to collaborate
  - many staff are named RAs on research grants
  - joint research proposals
  - European project consortia
  - ...

Key ARCHER Resources

- Upcoming courses
  - http://www.archer.ac.uk/training/
- Material from past courses
  - http://www.archer.ac.uk/training/past_courses.php
- Virtual tutorials (online)
  - http://www.archer.ac.uk/training/virtual/
- Documentation
  - http://www.archer.ac.uk/documentation/

- More courses from ARCHER:
  - http://archer.ac.uk/training/
  - Intro to HPC & Programming with MPI: 13-17 July
  - CECAM Extended Software Development Workshop: 12-25 Oct
- PRACE training:
  - http://www.training.prace-ri.eu
- ARCHIE-WeSt:
  - http://www.archie-west.ac.uk/information/training/

Welcome!

- 20 Attendees from 11 Institutions

- Course Aims:
  - “A comprehensive introduction to MD theory”
  - “practical topics such as setting up a simulation and visualising the results, and using steered MD”
  - “running MD on ARCHER, as well as explore issues such as parallel performance and scaling”

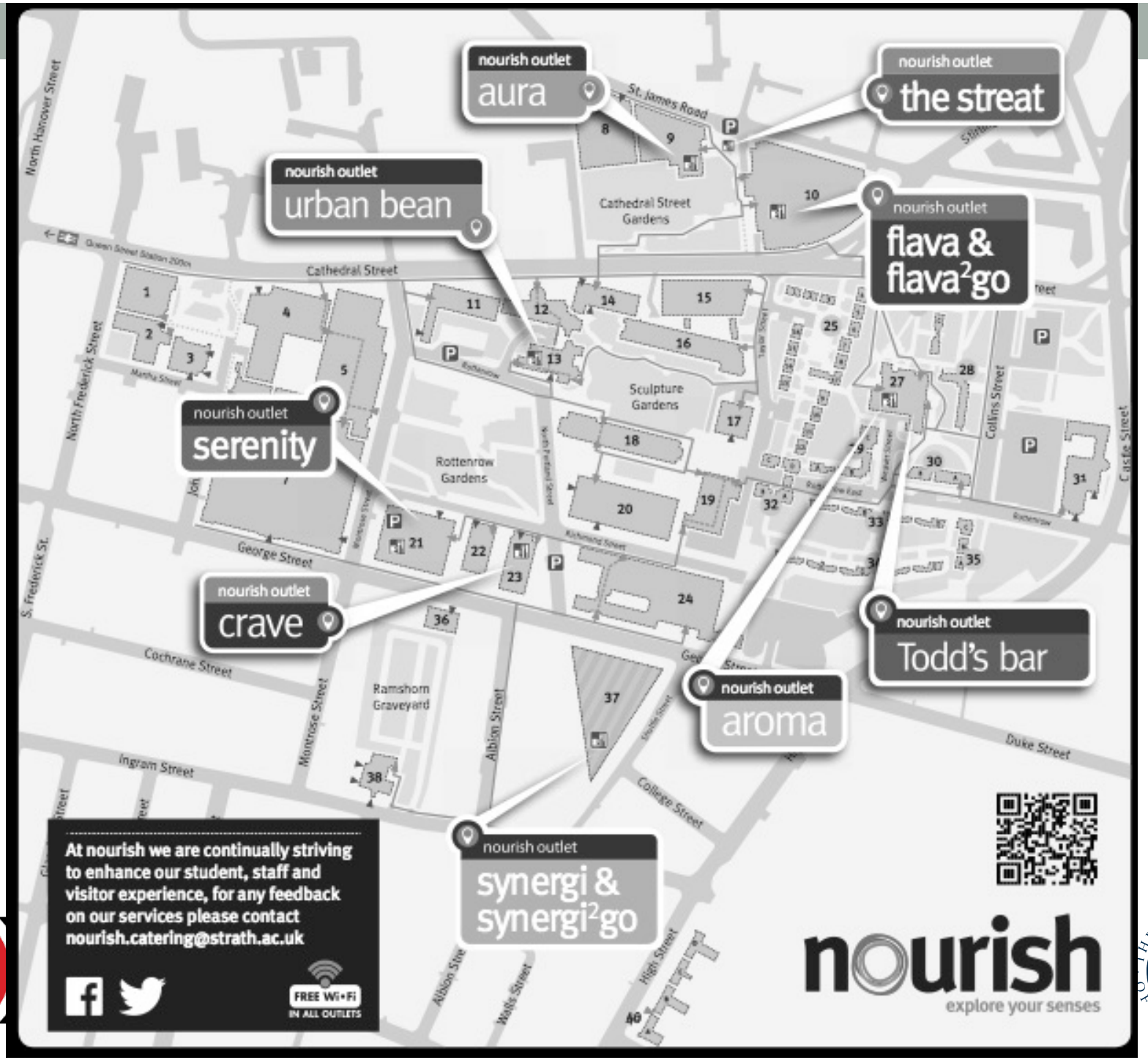
- All lecture slides and practical notes are available at:
  - www.archer.ac.uk/training/course-material/2015/06/MolDy_Strath/
  - **http://tinyurl.com/MDonARCHER**

Course Information

- Instructors:
  - Iain Bethune, EPCC
    - HPC, Parallel Performance, Classical (GROMACS, LAMMPS, NAMD) and Ab-initio MD
  - Karina Kubiak-Ossowska, Strathclyde
    - ARCHIE-WeSt User Support & Training, Classical MD (NAMD), VMD, Protein modelling
  - Ilian Todorov, STFC Daresbury
    - STFC Computational Chemistry Group Leader, DL_POLY Developer, Radiation damage in crystalline solids

Course Information

- Lectures & Practicals in Royal College Building Room 473
- Tea & Coffee provided
  - 30 min breaks morning (11.00-11.30) and afternoon (15.30-16.00)
- Lunch not provided (sorry!)
  - 1 hour break (13.00-14.00)
  - http://www.strath.ac.uk/nourish-catering/wheretoeat/
  - Map on next slide
- Please don’t leave bags, laptops unattended in the room.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North Frederick Street
S. Frederick St.
Montrose Street
Albion Street
Collins Street
Castle Street
High Street
Wells Street
At nourish we are continually striving to enhance our student, staff and visitor experience, for any feedback on our services please contact nourish.catering@strath.ac.uk
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Course Information

- Accounts:
  - Local workstations
  - ARCHER – for running NAMD & DL_POLY
  - ARCHIE-West – for visualisation with VMD
- Network access:
  - Wifi : conference accounts (instructions available)
  - Wifi : Eduroam (if you already have it set up)
- Toilets & Fire Exits

Course Information

Day 1:

- 9.30 – 9.45: Introduction
- 9.45 – 11.00: MD Overview - Motivation, Force-field model
- 11.00 – 11.30: Coffee Break
- 11.30 – 13.00: MD Continued - Minimisation, Integration & Ensembles
- 13.00 – 14.00: Lunch Break
- 14.00 – 15.30: Introduction to NAMD
- 15.30 – 16.00: Coffee Break
- 16.00 – 17.00: Practical – NAMD on ARCHER

Any questions?

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