

INTRODUCTION TO MOLECULAR DYNAMICS ON ARCHER

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Access to ARCHER

- ARCHER Instant Access
 - <http://www.archer.ac.uk/access/instant-access/>
 - 1,200 kAU (3,300 node hours)
 - 6 months duration
- Technical assessment + 2 page case for support
- Pump-priming, exploratory projects
 - Generate data for a larger peer-reviewed allocation



Access to ARCHER

- ARCHER Driving Test
 - http://www.archer.ac.uk/training/course-material/online/driving_test.php
- Work through online training and pass the test to get:
 - 1,200 kAU (3,300 node hours)
 - 12 months duration
- For new users – you can only do this once!
 - Open to students, postdocs... not just for PIs



Course Information

- We welcome your feedback:
 - <http://archer.ac.uk/training/feedback/>



Course Information

Day 2:

- 9.30 – 10.30: Advanced NAMD – PME, Steered MD
- 10.30 – 11.00: Parallelisation & Scaling of NAMD
- 11.00 – 11.30: Coffee Break
- 11.30 – 13.00: Practical – NAMD on ARCHER
- 13.00 – 14.00: Lunch Break
- 14.00 – 15.30: DL_POLY - Introduction & Overview
- 15.00 – 15.30: Coffee Break
- 16.00 – 17.00: DL_POLY – Features & Performance



