

Research *it*Supporting your research

A newsletter from IT Services: Research IT

Welcome to issue #22, January 2015, in a <u>regular series</u> of updates on IT research support and facilities for postgraduates, researchers and academics of The University of Manchester.

Your main Faculty contact email addresses (for research computing support) are given on the last page; emailing your research computing queries this way will also automatically raise a job for you in the *Remedy* tracking system.

Every day, routine work should continue to be submitted through the IT Service Desk on +44 (0) 161 306 5544 or via online submission at: www.manchester.ac.uk/servicedesk.



Web Page: Research IT

The web site for our support areas and all contact details is available here: www.its.manchester.ac.uk/research/.

Clickable Web Links

If you have received a printed copy of this newsletter and wish to follow the links, staff can download an electronic copy with clickable links at:

http://documents.manchester.ac.uk/DocuInfo.aspx?DocID=23504

Research Computing Facilities

IT Services provide researchers with support on any facility they are using: from the desktop to the biggest supercomputer on the planet. *This includes help with applications to use externally hosted computers.* Here we provide updates on various systems.

Local Facilities

We are delighted to report that various hardware components on the Computational Shared Facility (CSF) are being updated, securing the service for the next few years. Further details of the refresh are provided here. As well as standard hardware, the University provides access to emerging.com/here. As well as standard hardware, the University provides access to emerging.com/here. Ecceptional According for Securities such as K20 and K40 GPUs, FPGAs and Xeon Phi processors. A large memory facility, Hydra, is also available. This is for solving Big Data problems and an experimental Apache Spark service is being evaluated. Priority use of all these systems is for those who contributed to their purchase. However, all researchers may use the facilities for an evaluation or pump-priming period, and when contributors are not using them. Please contact the research infrastructure team for further information.

Virtual Machines

The University has invested in facilities to support the provision of virtual machines (VMs) for research. The funds will be used to seed a contribution-based VM service running along the same lines as the CSF: any researcher contributing funds will receive VMs equivalent to the hardware procured. VMs can be used for group development areas, web servers, databases and moderate, standalone computational work. Further details are provided in an online article.

Condor Service

Some simulations comprise many hundreds of small, essentially independent jobs. The University provides a Condor Pool for this type of High Throughput Computing. This service, available to all researchers, has run for several years, mainly using time available from teaching clusters overnight and at weekends. Further information about the service is available here.

N8 HPC Regional Service

The N8 HPC regional service provides a stepping stone from local to national resources (i.e. <u>ARCHER</u>), enabling researchers to use large core counts for their simulations. Access is via a lightweight application process that has no deadline. Furthermore applicants receive a quick response regarding the outcome of their application. Further details are <u>online</u>.

Hartree Centre Facilities

The Hartree Centre has announced a further programme of access to its ~98k core IBM Blue Gene/Q supercomputer, Blue Joule. It has also announced its 1st Xeon Phi Access Programme, providing access to a 42 node Xeon Phi cluster. Both programmes provide free usage, but do not provide support or any development effort. Access will be granted for the period 7 April to 26 June 2015. The deadline for applications is 27/28 February 2015. To request an application form, please contact hartree@stfc.ac.uk.

UK National HPC Facility ARCHER

EPSRC has announced a call for <u>ARCHER Leadership Projects</u>, with a closing date of **23 February**. Researchers can also apply for instant access to <u>ARCHER</u> at any time.

Research Computing Training

University Courses

IT Services offer a portfolio of short courses in research computing. <u>Click here</u> for the latest schedule. We also tailor courses for doctoral training programmes and arrange ondemand training with external tutors. Please contact <u>Lee Margetts</u> for details.

PRACE Advanced Training Courses

The Partnership for Advanced Computing in Europe (PRACE) offers a range of <u>free courses</u> at different HPC centres in Europe. Courses offered in February and March 2015 include:

2-4 February	Porting and Tuning	Germany
3-5 February	HPC-Based Simulations	Spain
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6 February	<u>HPC-Based Simulations</u>	Spain
9-13 February	Parallel Computing	Italy
11-12 February	Petaflop System Administration	Spain
19 February	Distributed Computing Platforms	Spain
19-20 February	Intro to Scientific Programming	Italy
23-27 February	VI-HPS Tuning Workshop	Germany
24-26 February	Adv. Threading & Optimization	Finland
25 February	HPC Industrial Services	Germany
2-5 March	Cray XC40 Optimization	Germany
5-6 March	Parallel Filesystems & Libraries	France
9-13 March	Fortran for Scientific Computing	Germany
10-13 March	Computational Chemistry	Finland
11-13 March	HPC Numerical	Italy
12-13 March	Simulation Environments	Spain
25-27 March	HPC enabling of OpenFOAM	Italy

2015 International Summer School on HPC Challenges in Computational Sciences

Graduate students and postdoctoral scholars are invited to apply for the sixth International Summer School on HPC Challenges in Computational Sciences, to be held from **21 to 26 June 2015**, in Toronto, Canada. Expenses for meals, housing, and travel are provided. The deadline for applications is **11 March 2015**. Further information can be found <a href="https://example.com/here-new-march-new-m

Hartree Centre Summer Schools 2015

The 2015 Hartree Centre Summer Schools consist of three separate weeks of study, each focusing on a specific topic.

15-19 June Visualization 29 June - 3 July Big Data

6-10 July High Performance Computing

The Summer Schools are aimed at researchers in academia and industry encountering complex application problems that require significant HPC/Visualization/Big Data resources. For more information – and to register – please <u>click here.</u>

Upcoming Events

ACM WomENcourage Conference

WomENcourage is a scientific event sponsored by the Association for Computing Machinery aimed at networking and exploring career opportunities for women in computer science and related disciplines. The deadline for papers, panel and workshop proposals is **8 February**. Further details are online.

Standing Up for Science Media Workshop

Sense About Science will be holding a Standing up for Science media workshop at the University of Manchester on **Friday 27 March 2015**. This full day event is free and for early career researchers in all sciences, engineering and medicine (PhD students, post-docs or equivalent in first job). The workshop combines discussion about science-related controversies in media reporting with practical guidance and tips on how to deal with the media. Click here for details on how to apply.

UK Data Service Webinars

The UK Data Service offers a programme of webinars throughout the year. <u>Click here</u> to book or to find out more. Webinars offered in February and March 2015 include:

4 February Census

3 March Introduction to the UK Data Service

10 March Finding & Accessing Data in the UK Data Service

11 March Longitudinal Surveys

17 March Getting Started with Secondary Data

24 March Data Management Basics

ARCHER Tech Forum

The ARCHER service runs an online technical forum. This starts with a short presentation on a technical topic followed by open discussion. The meetings are organised by EPCC and published on the ARCHER website. <u>Click here</u> for more information on the meeting schedule and how to connect. The next meeting is on **8 March**, titled Not so old Fortran.

PRACEDays15

The European Supercomputing Service PRACE holds its biennial conference, <u>PRACEDays15</u>, in Dublin on **26-28 May**. Two of the keynote speakers are from Manchester: Dr Bill Sellers (FLS) and Dr Lee Margetts (IT Services).

European Exascale Software Initiative

The EESI2 project will present all its works, vision and recommendations in a final two day conference on **28-29 May**. The conference will be held back-to-back with PRACEdays15 in Dublin. More information on the conference will be available soon on the EESI2 website.

ACM Web Science

The ACM Web Science event, to be held in Oxford from 28 June to 1 July aims to draw together theories, methods and findings from across academic disciplines, and to collaborate with industry, business, government and civil society, to develop our knowledge and understanding of the Web. The deadline for paper and poster submissions is 20 March. For more details visit Web Science.

Other News

Open Call for UK/USA Travel Awards

Travel awards of up to £2.5k are available to researchers to encourage UK/USA networking in HPC. Please contact <u>Lee Margetts</u> for details or <u>read the open call</u>.

Quantum Materials Network Event

N8 HPC recently held the first N8 HPC network event, "HPC for Quantum Materials Simulation" which took place at the University of York on **9 January**. The event brought together researchers from across the N8 universities to network, present their research and to discuss current issues and limits within their research area and how these could be overcome. Over 40 researchers from across N8 took part, ranging from PhD students to Professors, with the day consisting of invited keynotes, research presentations, discussion sessions and poster displays. Feedback received from attendees was very positive with particular emphasis being placed on the new research contacts made and the relevance of the research presentations. Presentations are now available on the N8 HPC website.

If you are already part of a research network, N8 HPC would be happy to discuss participating in a similar event within your research area, just contact enquiries@n8hpc.org.uk.

Research IT Seminar- Rspace

A presentation by ResearchSpace on their electronic lab notebook (ELN) solution Rspace, held on **15 January**, proved to be very popular. RSpace enables the streamlining of record-keeping by replacing paper lab notebooks with a flexible, searchable, secure and easy to use ELN. Concerns about IP protection, secure collaboration and other technicalities were addressed in the thorough and interesting talks and through Q&A discussions. If you were unable to attend, the slides are available here.

If you have any feedback, questions or would like to be included on a mailing list for relevant news and events, please contact Mary McDerby or Cerian Lindsay.

Condor Service Usage

Over the Condor Pool's lifetime, there have been 256 users. Around just under half that number (110) have run jobs relatively recently, although it is rare for more than a dozen people to have jobs queued at one time. Of those 110 users the processor core time usage varies from just 0.01 hours through to an impressive 216 years. In fact half of this set of users have benefitted from more than a computational year each. Computer Science and Physics are the biggest users (in terms of core hours/years) with Chemistry and Chemical Engineering closing the gap. However, Humanities researchers use the Pool too, with one user clocking in over 100 computational years. Similar stats apply to users from FLS and to a lesser degree MHS. There is still capacity for new users. Click here to find out more.

Subject-specific Email Lists

Please note that these email lists are subject specific discussion forums, rather than a way of contacting IT Services.

finite-elements@listserv.manchester.ac.uk
fortran@listserv.manchester.ac.uk
sciprogramming@listserv.manchester.ac.uk
university-gpuclub@listserv.manchester.ac.uk

Faculty Contact Emails

Humanities:

Hum-ITResearch@manchester.ac.uk

Engineering and Physical Sciences: EPS-ITResearch@manchester.ac.uk

Medical and Human Sciences: MHS-ITResearch@manchester.ac.uk

Life Sciences:

FLS-ITResearch@manchester.ac.uk

Next edition

The next edition of this newsletter will be circulated at the beginning of March 2015.

If you have any news to contribute, please contact Lee Margetts: lee.margetts@manchester.ac.uk at any time.

Items received before Friday 20th February 2015 will be included in the next edition. News from academic colleagues and researchers are most welcome.