IT Services
Supporting your research
A newsletter from the IT Services for Research (ITSfR) group

Welcome to issue #15, June 2014, in a regular series 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.

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

Correction : Confidential Data in Cloud Storage

Data Protection colleagues have confirmed that storing person identifying data outside the EEA may be illegal, regardless of whether or not it's encrypted.

In last month's newsletter it could be inferred that storing personal data in cloud storage was permitted, provided it was encrypted. This is not the case, and the University's guidance on this can be found here: man.ac.uk/nnM9xM.

Where person-identifying data, related to staff, students, research participants or other individuals, is stored by third-party organisations for University purposes, appropriate contractual arrangements between the University and the storage provider must be in place. Further information on procuring such services can be found here: man.ac.uk/PmmQ21.

iPads
We note the growing use of iPads to hold University data; and, if iPads are not synchronised to a local Mac or PC via USB cable, they tend to default to backing up their data to Apple's iCloud. As far as we know, all of Apple's iCloud storage servers are based in the USA (or should be assumed to be outside the EEA).

Individual apps on the iPad may also use cloud storage automatically, such as Apple's Notes and Evernote (to name just two of many).

KPMG Study
The Director of IT recently contracted KPMG to understand and report on:

- What data is held by the University and are transferred to and from third parties?
- Of this information, what is of most value to us and why? What individuals, groups or organisations may want to access this information?
- What controls are established and are they appropriate?

The final output of the project will be an independent report and an information security strategy that will be scalable to accommodate the wide-ranging requirements that we have. Please help KPMG with this study if you are contacted or, indeed, wish to be consulted.

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Isilon Storage:

planned downtime for upgrades

The Isilon network storage requires an upgrade to remain in vendor support. The cluster at Reynolds House will be upgraded on Saturday 12 July 2014 and the cluster at the Kilburn Building will be upgraded on Saturday 19 July 2014. Each upgrade will require an outage of approximately half a day and is scheduled to start at approximately 7am and complete by 2pm. Areas affected include:

Saturday 12 July 2014 – Reynolds House:

- Research data storage (which in turn will affect the Computational Shared Facility and other centrally run High Performance Computing services, excluding Condor)
- Podcasting service

Saturday 19 July 2014 – Kilburn Building:

- P:drives
- Video Streaming
- SharePoint
- Library services e.g. eScholar
- Library Digitisation project
- Electronic Software Delivery System (ESDS)

Research Infrastructure Update

For further information about any of the items below, please contact the IT Services Research Infrastructure team at its-ri-team@manchester.ac.uk.

Computational Shared Facility Update

The Computational Shared Facility (CSF) continues to grow. With end-of-year contributions, the CSF now stands at 5840 CPU cores. For more information, please visit: ri.itservices.manchester.ac.uk/csf.

Maintenance
On 12 July 2014 the system underlying the Research Data Storage service will be upgraded (see above). This requires downtime. All CSF home-directories (and several group shares) are located on Isilon. Some work is required on the CSF nodes that manage the batch/queuing system and on the internal network; we plan to carry out this work on 11 July 2014.

The CSF will be out of service from first thing on July 11th (Friday) until late on July 12th (Saturday). During this time it will not be possible to login to the CSF, and it will not be possible to run any jobs on the CSF. Any jobs still running in the system at the point of downtime will be terminated. We are sorry for the inconvenience; this work will: allow future development of the RDS/Isilon service; improve the CSF's management of an increasing number of computational jobs on the system; and allow us to add many more compute nodes in the future.

Interactive High-Memory Work – on iCSF

Do you have a need to do some interactive computational work – e.g., using Stata, R or MATLAB – that is too big for your desktop? The iCSF now contains two nodes with 256GB RAM and one with 2000GB RAM. If you can make use of these nodes, please email us at the above address.

Hydra – the high-memory/big-data branch of the CSF is now in production. All nodes in this cluster have 512GB RAM; all nodes will be connected via high-bandwidth Infiniband to local high-performance Lustre scratch storage. And, of course, all nodes have access to Research Data Storage (Isilon) over a dedicated, fast and secure network link so that CSF home-directories and shared areas may be used.

A second phase of investment in Hydra has just been made, increasing the size of the cluster – and further investments are certain. If you would like to know more about Hydra, please email us at the above address.

What do we do?

The team develop, maintain and support The University's facilities for computationally-intensive research and related infrastructure – i.e. high performance/throughput clusters, research storage – and of course help researchers make productive use of all this. Please visit our Web site: ri.itservices.manchester.ac.uk/.

We administer and support: the Computational Shared Facility, the University's flagship HPC cluster; Incline, a facility for *interactive* (including GUI-based) computational work (aka the iCSF); and Hydra, the new *big data* (high-memory) cluster. We also support, and are the business owner of, the Research Data Storage (RDS) Service, which provides storage for University researchers.

The University's Computationally Intensive Research Ecosystem

The above facilities are the basis of the UoM CIR Ecosystem, which forms an *integrated* system of infrastructure designed to address all aspects of research groups' computational work and requirements.

- The above computational clusters and the RDS are tightly integrated by means of a fast, secure, dedicated network.
- The Research Virtual Desktop Service allows users to: gain secure, off-campus access to all these facilities; do interactive/GUI-based work over relatively slow connections; and re-connect to the same desktop session from office, home and elsewhere.
- Finally, we run a pilot Research Virtual Machine Service providing VMs to academics.

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ARCHER and Training

ARCHER, the new national supercomputing service, offers training in software development and high-performance computing to scientists and researchers across the UK. As part of our training service we are running a 3-day *Software Carpentry boot camp and Introduction to Scientific Programming in Python* at Cranfield University, UK, on 21-23 July 2014.

Software Carpentry boot camps help researchers become more productive by teaching software development skills that enable more to be done, in less time, and with less pain. The presenters will cover skills including version control, task automation, good programming practice and automated testing. These are skills that, in an ideal world, researchers would master before tacking anything with "cloud" or "peta" or "HPC" in their name, skills that enable researchers to optimise their time and provide them with a secure basis to optimise and parallelise their code.

The Introduction to Scientific Programming in Python, will provide an introduction to Python on ARCHER. It will introduce Python's capabilities for scientific computing, in particular the Cython, mpi4py, NumPy, SciPy and matplotlib Python libraries. The course will also introduce how to interface Python with C and Fortran codes.

This course is being run by EPCC, as part of ARCHER, and Cranfield University. The course is in collaboration with EPCC's PRACE Advanced Training Centre (PATC), and Software Carpentry, a Mozilla Science Lab initiative.

For more information and to register please, visit the ARCHER training page www.archer.ac.uk/training/.

Hartree Centre
Summer School 2014

Stop Press: Fee halved to just £300 (per one week course).

This year's event will consist of three weeks of study – each week will focus on a different subject.

• Week 1: Visualization (14-18 July 2014)
Leaders: Hank Childs (Oregon) and Hamish Carr (Leeds)
• Week 2: HPC (21-25 July 2014)
Leaders: Jack Dongarra (Tennessee) and Kirk E. Jordan (IBM)
• Week 3: Big Data (28 July – 1 August 2014)
 Leaders: Chris Williams (IBM) and Alok Choudhary (Northwestern)

The fees include accommodation for 5 nights (Sunday to Thursday inclusive), transport to and from the hotel, meals, refreshments and all course materials. The Summer School will include a mixture of lectures and hands-on tutorials and will take place in the Hartree Centre's state-of-the-art Brunner-Mond Training Suite at STFC Daresbury Laboratory. Go to all three weeks or pick the week that matches your research subject. Further information plus an online registration form is now available at: eventbooking.stfc.ac.uk/news-events/hartree-summer-school-series-2014.

Version Control using git

IT Services, in collaboration with the Software Sustainability Institute, recently ran a course on version control using git. For those of you who missed it, the course materials are available at apawlik.github.io/2014-04-09-GARNET/lessons/garnet/version-control/tutorial.html.

Next Image-based Modelling Club Meeting

The University of Manchester Image-based Modelling Club are organising a workshop for "Young Researchers" at the Hartree Centre, Daresbury Laboratory (Warrington) on Tuesday 9 September 2014. We will set off by coach from North Campus at 0900 and return by 1700. The purpose of the workshop is to encourage networking between Manchester PhD students, postdoctoral researchers and recently appointed lecturers who are using or would like to use image-based simulation in their research. Other staff are welcome.

In the morning, we will hear about the >£100M investment in world class supercomputing and visualisation facilities at the Hartree Centre. These are available to Manchester researchers through collaborative projects and European research grants. We will also enjoy a visualisation show case featuring recent Manchester research in one of the Hartree Centre's immersive stereo visualisation suites.

Lunch will be provided during a poster session. In the afternoon, we will hold a hands-on workshop to discuss the issues and challenges of image-based modelling. This will inform future Image-based Modelling Club events and help progress the use of this technique at Manchester.

Manchester Informatics and the Harwell Imaging Partnership will cover the costs of attendance. However, there is a caveat. The event is only free to attendees who submit a poster. Posters will describe image-based modelling work that has been completed, is in progress or is being planned. If you would like to participate, please register at the following link: tinyurl.com/osc74pe.

Contact lee.margetts@manchester.ac.uk or louise.lever@manchester.ac.uk for further details.

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Academic visitor(s) needing wifi access?

A reminder about the service trial at sponsoravisitor.manchester.ac.uk, where a member of staff can grant a visitor on academic University business one day access to our wifi network. Please note that this is not a public visitor to the campus service.

Subject-specific Email Lists

Please note that these email lists are subject specific discussion forums, rather than a way of contacting IT. For the latter, please see the contact emails in the next section.

finite-elements@listserv.manchester.ac.uk

fortran@listserv.manchester.ac.uk

sciprogramming@listserv.manchester.ac.uk

university-gpu-club@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 end of July 2014.

If you have any news to contribute, please contact the IT Services Research Lead, Ian Cottam: ian.cottam@manchester.ac.uk before 25 July 2014.

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