

MANCHESTER
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The University of Manchester

IT Services

Supporting your research

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

Welcome to issue #5, August 2013, 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 ext.65544 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/.

Visitor WiFi Access

For a long time you have been able to put a request in to the Shared Service Desk for temporary visitor WiFi access (to "UoM_WIFI"). Soon, a visitor here for the day will be able to simply self-serve (if they are a member of staff). Like the DropOff service, this will start off as a *service trial* to make sure there are no problems. If you would like to register your interest in using this service trial, email ian.cottam@manchester.ac.uk.

Note that visitors from institutions that have Eduroam capability should use that, assuming they are based in a building or buildings with Eduroam WiFi access points.

nCrypted Cloud

This is commercial software that provides a layer on top of Dropbox providing *client-side encryption*, without compromising on the ability to share folders, etc. IT staff are starting to test this. It will be offered more widely as soon as we have full confidence in it.

IT Services Research Data Storage Service

The charges for storage over the amount that your Faculty can allocate you free-at-the-point-of-use have been confirmed. They are £150 per TB for unreplicated storage and £300 per TB for replicated. These figures can be quoted on research grant applications, especially where you think you will need more than 20TB over the full lifetime of the project.

Unreplicated storage should only be used if you have a second, secure copy or the data can be easily regenerated. These prices are for research work that is not part of a commercial contract; for information on such, or if you are unsure, full contact details are below.

For more information please visit:

www.rds.itservices.manchester.ac.uk or email its-ri-team@manchester.ac.uk.

Research groups who wish to apply for storage should do so via the form at:

remedy.manchester.ac.uk/cgi-bin/sr.cgi?scid=142.

On completion of the form, your Faculty IT team will contact you.

University Finite Element Club

The next meeting of the University Finite Element Club is being arranged for Thursday 3 October 2013. Visit the following webpage for further details and how to register: wiki.rac.manchester.ac.uk/community/FiniteElements.

The theme of the meeting will be *user subroutines for commercial and open source software*. Dr Hadi Seyed Hosseini, Institute for Surgical Technology and Biomechanics (ISTB), University of Bern, Switzerland has been invited to give a seminar on *Constitutive modeling of bone behaviour, Abaqus umat and uel implementations and their outcomes*. Dr Hosseini is currently contributing interfaces for Abaqus UMATs to the massively parallel ParaFEM software (parafem.org.uk). Attendees will be actively encouraged to contribute to discussion in the meeting and refreshments will be provided. What training/support is available / needed? Are there opportunities for sharing user subroutines?

To subscribe to the University Finite Element Club mailing list, send an email to: listserv@listserv.manchester.ac.uk containing only "subscribe finite-elements" in the main body. Suggestions for future topics or offers to make a presentation can be sent to jonathan.boyle@manchester.ac.uk or lee.margetts@manchester.ac.uk.

Driving UK HPC Enabled Science and Innovation Through UK/US Collaboration

In the next week or so, we are expecting an EPSRC project to be funded that will support attendance at SC13 (Supercomputing 2013) in Denver, Colorado (see sc13.supercomputing.org/). It is planned that this grant will support up to £2,500 per person in travel expenses. The aim is to foster better UK/US research relations and follows on from a BIS/EPSC UK delegation visit made to the US in February 2013. Visit n8hpc.org.uk/news/UScollaborations to read the report.

The application is likely to take the form of a two-page document comprising a short biographical sketch, research area of interest and a description of the collaborations applicants propose to develop at SC13. While applicants at all career levels will be encouraged to apply, a minimum of half the awards will be reserved for post-docs and other early career researchers.

Any UK academic/researcher carrying out research under EPSRC's remit is eligible to apply. If you are interested in this opportunity, please contact: lee.margetts@manchester.ac.uk. Dr Lee Margetts is a co-investigator on the grant and a member of the selection

committee. He will provide further guidance to you directly as soon as EPSRC have provided written confirmation of the funding.

Next IT Services for Research Forum

There is no August forum because of the vacation season and September is a month with a regular IT Services Forum, therefore the next ITS Research Forum we present will be in October. The exact date is to be confirmed, but Mary McDerby will be speaking on Research Data Management.

Computational Shared Facility (CSF)

The agreed policy for the scratch file system on the CSF is that files over three months old may be deleted without notice. Scratch is filling up on the CSF. Some users are using scratch as long-term storage. This is considered an abuse of the file system as scratch is intended as a workspace for current and recent jobs.

Scratch is not backed up and there is minimal resilience. From 30 September 2013 *all scratch files over six months old will be deleted on a regular and frequent basis*.

We will make every effort to warn users of the system about which files will be deleted, but warnings are **not** guaranteed. It is each user's responsibility to ensure older files are safely copied from scratch to CSF home directories (which are suitable for long-term storage), to research data storage (aka Isilon) space – see URL below, or off the CSF entirely. <http://www.rds.itservices.manchester.ac.uk/>.

24th Machine Evaluation Workshop (MEW24)

Registration for MEW24 is open – see: eventbooking.stfc.ac.uk/news-events/mew24.

The STFC Scientific Computing Department is pleased to announce that the 24th annual Daresbury Machine Evaluation Workshop (MEW24) will take place on Wednesday 27 and Thursday 28 November 2013 at the Adelphi Hotel, Liverpool.

As with previous MEWs there will be a full programme of technical presentations, an exhibition of the latest products and technology, and a series of parallel breakout sessions. More information – and an online registration form – can be found on the workshop web pages. Registration is free for delegates from academic institutions.

Videoconferencing for Researchers

The Access Grid servers from Janet are being disconnected at the end of this month. The main users in Manchester – Mathematics and Materials Science – have/are transferred to the approved Janet replacement of **visimeet** by IOCOM (this is the next version of the IG2 software that was in most access grid nodes).

University Provided Training in Research Computing

IT Services offers a range of courses to postgraduates and staff including programming, high end computing and visualization. Please visit the following webpage for information regarding the Autumn 2013 Research Computing Training Programme: wiki.rac.manchester.ac.uk/community/Courses. Bookings and cancellations are now made online for each course through the website.

GPU Club – CUDA Training

NVIDIA are coming to town in October to do intermediate/advanced CUDA training, but if people want an introduction to CUDA, NAG are running a free 3 day course in September (17-19) at their offices in Manchester; please see www.hector.ac.uk/cse/training/cuda3day/ and the article immediately below. In early 2014, we will have NVIDIA back for OpenACC training and Intel will be back for advanced Xeon Phi training. Further details will follow to the GPU Club mailing list and in future editions of this newsletter.

HECToR Training – Autumn / Winter Schedule

Please find below some of the courses in the autumn/winter schedule of HECToR training. Others will be added soon.

- **An Introduction to Unified Parallel C (UPC)**
6 September 2013, Culham Centre for Fusion Energy (CCFE)
- **Parallel Programming with MPI**
10–12 September 2013, Loughborough University
- **Accelerating Applications with CUDA**
17–19 September 2013, NAG Manchester
- **OpenMP** 7–9 October 2013, University of Liverpool
- **Debugging, Profiling and Optimising**
13–15 November 2013, University of Bristol

For further details and registration, please see: www.hector.ac.uk/cse/training/.

ScaleMP Training Course

The Hartree Centre is hosting a ScaleMP User Training Course on 17-18 September 2013 at STFC Daresbury Laboratory. For information and a registration form, please visit: eventbooking.stfc.ac.uk/news-events/scalemp-user-training-course.

BlueWonder provides a large-scale virtual-machine presenting users with hundreds of cores, several TBs of RAM and fast local scratch storage. This capability is based on the vSMP Foundation virtualisation software from ScaleMP. The course provides the student with general knowledge of the architecture, components, and a set of tools and guidelines that will allow the user to execute workloads in an optimal way. The training will include live demonstrations and a hands-on session.

MHS IT Blog: IT Matters

IT staff from MHS Faculty have an interesting blog site. Recent posts are:

- Build it and they will come
- Research Data Storage
- Bring your own device
- Goodbye Windows XP
- iPads in Medical Education

See blogs.mhs.manchester.ac.uk/it-matters/.

Hartree Centre and the University explore Collaboration Opportunities

The Computational Research Stakeholders Group (CRSG) recently hosted a visit by Adrian Wander, STFC Director of Scientific Computing. Adrian gave a brief introduction to the facilities available at the Hartree Centre (www.stfc.ac.uk/hartree) and STFC Daresbury including details of their IBM Blue Gene/Q, the UK's most powerful supercomputer.

Opportunities and methods for collaboration were discussed including the accessibility of these resources to Manchester researchers and the possibility of locally hosting staff from each institution [*this is progressing well since we last reported on it, ed.*]. Discussions will continue and actions from this meeting will be progressed in order to deepen our relationship with the Hartree Centre.

If you are interested in collaborating with Hartree, using their facilities or require more details on the Computational Research Stakeholder Group please contact Dr Robin Pinning (pinning@manchester.ac.uk).

Digital Research 2013

Digital Research 2013 (DR2013) is being held in St Anne's College, Oxford, on 9-11 September 2013. This year's event features a symposium on **The Data Scientist** together with the Digital Research Showcase (9-10 September 2013) and once again they have the UK e-Infrastructure Academic Community Forum collocated with the conference (on 11 September 2013). Please visit the DR2013 website digital-research.oerc.ox.ac.uk for more information.

Digital Research are calling for contributions in two tracks: the Data Scientist Symposium will consider the role, training and career of Data Scientists, and the Digital Research Showcase is an opportunity for researchers and research technologists to present their latest work as in previous years. All submissions that contribute to the scope and purpose of the event will be considered for inclusion in the programme, either as short talks, panels or posters.

An important element of Digital Research 2013 is to continue to develop the collaborations between the Research Technologists who are collaborating to develop novel methods in Digital Research and those whose primary goal is the use of Digital Research to produce novel results and insights. DR2013 will continue the tradition of the e-Science All Hands Meetings in fostering such collaboration.

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 September 2013.

If you have any news to contribute, please contact the IT Services Research Lead, Ian Cottam:

ian.cottam@manchester.ac.uk before 25 Sept 2013.