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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 #14, May 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/.

Cloud Storage: updates

There is news from nCryptedCloud, and also from Janet/Jisc with regard to brokerage negotiations with cloud storage providers.

nCryptedCloud

We still have many licences left for the nCryptedCloud trial – get in touch with ian.cottam@manchester.ac.uk.

nCryptedCloud provides an almost transparent, user-side *encryption* layer on top of cloud storage, and Dropbox in particular. If you are storing University confidential or sensitive data in the cloud, please try it. (With apologies to Linux users as that OS is not yet supported.)

If you are sharing folders with collaborators, you can continue to use the Dropbox mechanism provided your collaborators also use nCryptedCloud (it's free) and you set the folder to "Share Securely" from the nCryptedCloud right-click menu. However, they also provide other sharing mechanisms on top of the Dropbox ones; these allow colleagues access to encrypted files and folders without installing nCryptedCloud or even Dropbox. A video of this in action is here: www.youtube.com/watch?v=_yc9TxZcaD8; and a general case study of nCryptedCloud, based on Brown University, is available: tinyurl.com/mwefda8.

nCryptedCloud works in conjunction with Google Drive, Microsoft OneDrive and Box, as well as Dropbox.

Finally, the latest version of nCryptedCloud turns on a couple of features most people do not want. Click on its icon and select "Preferences...". Under General, untick (if ticked): "Use nCryptedCloud as Cloud Provider Folder View" and "Enforce Privacy on all cloud data".

Janet/Jisc

For a long time Janet have been negotiating with various cloud providers to broker terms that would be suitable for any UK university. They recently announced that the first such provider is Box (www.box.com). Janet also expect Microsoft to join the scheme shortly. Unfortunately, many researchers from The University of Manchester use Dropbox for cloud storage, and Janet's negotiations with them are making little progress.

N8 HPC – High Performance Computing – do you need access to more compute power?

N8 HPC is an EPSRC funded initiative that aims to seed engagement between industry and academia around research using e-infrastructure as well as developing skills in the use of e-infrastructure across the N8 partnership.

The infrastructure consists of a “Tier 2” facility, which is available for use on an equal share basis by researchers from all 8 partner sites including Manchester. The facility is an SGI High Performance Computing cluster with 332 compute nodes. Each node has two of the latest 8 core Intel Sandy Bridge processors, and each node has a compute capability of 320 GigaFLOPS.

Project PIs can apply for access to the facility at any time through a lightweight peer review process. Projects do not need to be funded by EPSRC and do not require an industry component to their research application, although this is preferred. Application decisions are swift and some assistance is available locally to make the most of the facility.

Please visit the N8 HPC website (www.n8hpc.org.uk) for more information, but if you would like to discuss your requirements or if you need assistance with your application, please get in touch (ITS-Research@manchester.ac.uk).

Code Optimisation Service

IT Services (EPS Applications team) run a program optimisation service for researchers who write programs in MATLAB, Python, Mathematica, Maple and R, among other languages. A selection of recent success stories can be found at www.walkingrandomly.com/?page_id=5122. If you would like assistance with your own programs and scripts, contact the team at applicationsupport-eps@manchester.ac.uk.

IT Training for Researchers

IT Services provide a range of training courses, both online and face-to-face, for staff and research students at The University of Manchester. Run by Faculty IT staff, specialised research IT staff and external providers, the training aims to provide researchers with the skills required to carry out their research. Courses range from basic introductory level to more advanced levels and cover a range of skills from programming to specialist research techniques such as Image-based Modelling and visualization.

To browse and book onto any of the courses currently available please visit: man.ac.uk/6d8Gmp

If you have any training requests or queries about IT training then please contact us:

its-research-training@manchester.ac.uk.

Git and GitHub: training in distributed version control

IT Services, in collaboration with the Software Sustainability Institute (www.software.ac.uk), are now offering a course in the use of git and github. Git is one of the most commonly used version control systems in the world, and github has become one of the standard locations in which to store and share your code. Now that github repositories have become citable (<https://guides.github.com/activities/citable-code/>), there has never been a better time to learn how to use these technologies. During the course, you will learn:

- What version control is
- The main benefits of using version control
- How to set up and work with a local repository
- How to work with remote repositories using GitHub
- Topics such as branching, resolving conflicts, merging and rebasing
- Working collaboratively on one repository.

Attendance is free to all postgraduate researchers and members of staff but places are limited and booking is required. For more details, see man.ac.uk/ejK3Q

University Finite Element Club

The next University of Manchester Finite Element Club meeting will be held on Wednesday 11 June 2014 from 1500-1700. A distinguished research scientist from Los Alamos National Laboratory (USA), Professor Curt Bronkhorst, will give a seminar on the computational modelling of advanced composite materials.

On Friday 11 July 2014 from 1000-1200, we will be looking at *Faster Simulation for Fracture Mechanics*. The format of the meeting is an open workshop organized and co-chaired by Dr Lee Margetts and Dr Jonathan Boyle. In the meeting, attendees will discuss how to tackle the issue of long run times for engineering simulations involving fracture. Participants are invited to give 'lightning talks' about their research to encourage discussion. The event is open to PhD students, researchers, academic and support staff. Please note that registration is required.

For further details and registration for both events, please visit www.rac.manchester.ac.uk.

Queen's Award for Imaging

The University of Manchester has been presented with the most prestigious award in UK higher education, the Queen's Anniversary Prize for Higher and Further Education (2012-2014), for work in developing world-leading imaging techniques. The award for "New Techniques in X-Ray Imaging of Materials Critical for Power, Transport and Other Key Industries," recognises the special contribution research and expertise at The University of Manchester has made to the UK's strategic development in advanced materials and manufacturing.

We would like to extend our congratulations to Professor Philip Withers and Professor Peter Lee, along with the many academics, researchers and support staff involved in the award. Further details can be found on the Manchester X-ray Imaging Facility website www.mxif.manchester.ac.uk. The website itself is special too. It is a bespoke 'experimental facility management system' designed by Louise Lever from IT Services.

Those working in this area may like to note that Lee Margetts and Louise Lever will be running the next Image-based Modelling course on Wednesday 9 and Thursday 10 July 2014. During the course, attendees will learn how to turn images into computer models for simulation with a hands-on session using the N8 HPC supercomputer: Polaris. Also coming up is a special Image-based Modelling Club meeting in September with a day trip to the Hartree Centre near Warrington. Look out for details in future communications.

To reserve your place on the Image-based Modelling course, please visit man.ac.uk/6d8Gmp. (Note that you may need to login to StaffNet to access this page.)

Nuclear Reactor Simulator

Web-App

The Dalton Nuclear Institute and IT Services' Research Applications and Collaboration team (RAC) have completed the first phase of a project to develop a simple nuclear reactor simulator as a 3D interactive Web-App. It is primarily aimed at children's education, at both GCSE and A-level, but also targets related outreach and engagement activities. The RAC design and specification was implemented by PlayGen, a 3rd party developer based in London, with many years experience developing serious games, simulations and platforms. Participants can take control and make their own decisions to make a modern nuclear reactor run as efficiently as possible to meet energy demands. Players learn about nuclear reactor operation and automatic control systems. The game also incorporates some educational 'Did you know' facts about the various components of a pressurised water reactor (PWR). The simulator can be found and played [here](#). There is also the recent eUpdate/StaffNet article, "[Passing on the spark of](#)

[inspiration to tomorrow's nuclear scientists](#)" which provides a greater overview of the EPSRC grant of which this work was a part. It is anticipated that this pilot project will act as a catalyst for similar web-based application development and/or other out-sourced projects in the future. For further information please contact louise.lever@manchester.ac.uk.

The Janet Network

Janet/Jisc are gathering requirements for the next generation of UK university networking. If you are a researcher who needs to move very large quantities of data around the country and beyond, we would like to hear from you. You can contact the editor (ian.cottam@manchester.ac.uk) and he will pass such requirements on.

Hartree Centre

Summer School 2014

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)

Registration fees are £600 per week. 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.

National supercomputer:

ARCHER

EPSRC are seeking user and stakeholder input to the upgrade of the ARCHER high-performance computer system. A short questionnaire is available via: www.epsrc.ac.uk/newsevents/news/2014/Pages/archer2questionnaire.aspx. This questionnaire asks some questions about your use of the ARCHER machine and the type of technology upgrade you would like to see considered. This consultation questionnaire closes on 30 June 2014.

OpenStack

Do you know someone in the University who is using OpenStack?

<https://en.wikipedia.org/wiki/OpenStack>

DataCentred – one of our Industry Club members datacentred.co.uk – use OpenStack, and are interested to know how it relates (if at all) to Manchester’s teaching and research. Contact the editor ian.cottam@manchester.ac.uk.

PRACE Awards 7 Million Hours to Manchester Researchers

We are delighted to report that another PRACE proposal (for 7,425,000 CPU hours) has been awarded to Manchester researchers for a project titled: “Micro-structurally faithful finite element modelling for fusion energy”. The award is the equivalent of running a simulation for 847 years on a single processor core.

The project is a collaborative effort involving Professor Paul Mummery (MACE, EPS), Dr Llion Evans (Culham Centre for Fusion Energy) and David Arregui-Mena (CONACyT PhD Student), as well as a number of European collaborators. Dr Lee Margetts from IT Services provided support and guidance with the application process.

The objective of the project is to undertake thermo-mechanical analysis of (i) the first wall of the Joint European Torus (JET) and (ii) components of candidate materials for the ITER first wall. The proposed work will also couple neutronic simulations with finite element analysis to investigate neutron irradiation effects on thermo-mechanical performance. The geometries for the simulations will be derived from 3D tomography images captured using Manchester facilities and the resulting finite element problems will be solved using ParaFEM (parafem.org.uk).

If you would like assistance with a future application to use PRACE facilities, please contact Dr Lee Margetts (lee.margetts@manchester.ac.uk) who represents The University of Manchester in a number of PRACE activities.

US Department of Energy INCITE Programme

The U.S. Department of Energy (DOE) Office of Science provides a portfolio of national high-performance computing facilities housing some of the world’s most advanced supercomputers. These lead computing facilities enable world-class research for significant advances in science.

Open to researchers from academia, government labs, and

industry, the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) programme is the major means by which the scientific community gains access to some of the fastest supercomputers. The programme aims to accelerate scientific discoveries and technological innovations by awarding, on a competitive basis, time on supercomputers to researchers with large-scale, computationally intensive projects that address “grand challenges” in science and engineering.

The INCITE Programme is open to applicants from outside the U.S. and projects do not need a U.S. collaborator.

For further details see

www.doeleadershipcomputing.org/incite-program/. If you would like to talk through ideas for a proposal before submission, please contact Dr Lee Margetts (lee.margetts@manchester.ac.uk). Lee knows the INCITE Programme Manager through PRACE and the UK-US-HPC Network and can provide some direction regarding ensuring success in your application.

Manchester’s myGrid team announce the release of Taverna Player

Taverna Player is a Web-based interface (implemented as a Ruby on Rails plugin) for executing existing workflows through a Taverna Server. It can be considered analogous to playing videos on YouTube. Workflows can be run with data supplied by the creator, or with new data uploaded by the user, but the workflows themselves cannot be altered. The Taverna Player functionality can also be embedded into other HTML pages to run specific workflows with pre-defined data.

As a plugin Taverna Player will reside within your host application but requires a minimum of prerequisites for use.

Package: <https://rubygems.org/gems/taverna-player>.

Developer docs: mygrid.github.io/taverna-player/.

Embedding: <https://github.com/myGrid/taverna-player/wiki>.

Source code: <https://github.com/myGrid/taverna-player>.

An example of Taverna Player in an analysis portal is here: <https://portal.biovel.eu/>.

For more information, comments or questions, please see www.taverna.org.uk/documentation/taverna-2-x/taverna-player/ or contact support@mygrid.org.uk.

Isilon network storage: maintenance

There is likely downtime for this system on Saturday 12th and Saturday 19 July 2014 for necessary updates. Research storage and P-drives, amongst many other services, are on this system. There will be detailed communications closer to the time.

Big Data Day at Daresbury

For details of this event on 24 June 2014, see: <https://www.events.ukti.gov.uk/international-festival-for-business---ict-day>.

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.

Last call for CSF contributions before 31 July 2014

If you wish to make a contribution to the Computational Shared Facility ri.itservices.manchester.ac.uk/csf/ (or iCSF, etc.) with funds which must be spent this University financial year, please contact the IT Services RI team as soon as possible at the above address – it can take longer than you think!

Hydra – the high-memory/big-data branch of the CSF is now in production

All nodes in this cluster have 512 GB 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 – further investments are certain. If you would like to know more about Hydra, please email us at the above address.

The Research Infrastructure Team: What do we do

The RI Team develop, maintain and support the University's on-campus facilities for computationally-intensive research and related infrastructure – i.e., HPC clusters, research storage – and of course help researchers make productive use of all this.

To find out more about what we do, please visit our Web site: ri.itservices.manchester.ac.uk/

In more detail – computational resource and storage: we administer and support: the Computational Shared Facility (CSF), 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 UoM CIR 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.
- We run a pilot Research Virtual Machine Service providing VMs to academics.

And Finally...

If this is your first exposure to our newsletter – and it may be as we have increased the email circulation this month – there are many useful articles in back issues.

They are all here:

www.itservices.manchester.ac.uk/research/newsletter/.

Note that our September issue always contains an update on computational facilities: such as: Condor, CSF, N8 HPC, iCSF, Archer, etc.

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 June 2014.

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

ian.cottam@manchester.ac.uk before 25 June 2014.