

IT Services

Supporting your research

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

Welcome to issue #13, April 2014, 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.

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



Web Page: IT Services for Research

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

Mac Usage on Campus Growing

Across campus we are seeing quite a growth in researchers' use of Apple Macs and the OS X operating system – the latest version of which is known as *Mavericks* 10.9.2. In some areas the usage of Macs (cf. Windows or Linux PCs) has passed the 30% level.

UoM IT Services fully support the use of Apple systems.

On 23 January 2014, exactly one day before the 30th anniversary of the Apple Mac, Mike Croucher of the EPS IT Applications Team took delivery of his first ever Apple computer – a late 2013 model MacBook Air. As a long time user of Windows and Linux machines, he had a lot to learn about his new system. As he figured things out, Mike kept detailed notes, which he subsequently turned into a useful guide for other Mac converts. The guide covers:

- General Mac information answers to various questions he raised
- Manchester-centric tips specific to Mac users at UoM
- Linux-centric tips things he was used to on Linux, and how to do them on OS X
- Windows-centric tips things he was used to on Windows, and how to do them on OS X
- Software HowTos general software-related questions
- Software by task the software he likes to use
- Mac OS X environmental changes changes he made to OS X defaults

The guide is continually evolving and the latest version can be downloaded from here:

https://www.dropbox.com/s/nt3l2yktoyceqp5/MacMigrati on_UoM.pdf.

[Ed. note: Like my own, Mike's MacBook is personally owned – a good example of BYOD in action – and therefore the software recommendations in his note reflect that. If you are a member of staff lucky enough to have a UoM-provided Mac, more options are available to you through site-wide licences.]

Emerging Tech Conference Success

On Friday 11 April 2014, 120 people from across Europe attended the inaugural EMiT conference hosted by researchers at The University of Manchester. The keynote speakers were selected from the vendor industry (ranging from MathWorks to NVIDIA and Intel), from academia (Glasgow University and STFC) and from selected businesses (JBA Trust and AllianceBernstein). They outlined their visions for research computing using emerging technologies and techniques, whether GPUs, FPGAs, Xeon Phi or the importance of good coding practices, exascale techniques, energy efficient computing or 'autoaccelerating' compilers.

The <u>EMiT website</u> (<u>emit.manchester.ac.uk</u>) has slides from presentations, a Storify timeline and photographs from the day.

The success of the event confirms the organisers' plans for a larger, 2-day event to be held in 2015. If you would like to get actively involved in organising, please email <u>emit@manchester.ac.uk.</u>

If you would like access to <u>UoM's emerging tech cluster</u> (<u>ri.itservices.manchester.ac.uk/zcsf</u>) to advance your research (support available), please email <u>its-</u> <u>research@manchester.ac.uk</u>.

EMiT thanks NA-HPC and EPSRC for sponsoring the event.

Research Infrastructure Update

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

Funds to contribute to the CSF by end July 2014?

If you wish to make a contribution to the *Computational Shared Facility* with funds that must be spent this University financial year, please contact the IT Services RI team as soon as possible at the above address – it takes longer than you think, so act now.

Big Data CSF – aka Hydra

By the time you read this, a new branch of the CSF will be in production – Big Data CSF, also known as *Hydra*. All nodes in the cluster have 512GB RAM; and all nodes will be connected via high-bandwidth Infiniband to local high-performance Lustre scratch storage. And, of course, all nodes will 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. The initial procurement for Hydra was primarily funded by a NERC grant awarded to Dr Chris Knight from the Faculty of Life Sciences; the Faculty also contributed. Phase II will be procured soon with further funds from the Faculty and a contribution from Prof. Bernard Keavney from the Faculty of MHS. If you would like to know more about Hydra, please email us at the above address.

Confidential and Sensitive Data

Some facilities within the University Computationally-Intensive Research (CIR) Ecosystem are suitable for storing and processing all but the most sensitive data. A combination of encrypted files and exclusive use of compute nodes can satisfy most data security requirements. If you need to process commercially sensitive or pseudo-anonymised data and wish to use the University's CIR facilities, please get in touch at the above address.

INCLINE – the Interactive CSF (iCSF)

The INteractive Computational LINux Environment is growing. Incline is ideal for interactive computationally intensive work including GUI-based, and development and testing job runs.

We now have in production nodes with 256GB of RAM (random access memory), and one node with 2TB of RAM. Priority use of this node will be given to the contributing research group, but others will be able to use spare CPU cycles – and RAM.

In addition, the iCSF now has a GPU-hosting node for interactive use of graphics-intensive GUI applications such as Abaqus CAE, Paraview and VMD. (This works closely with the Research Virtual Desktop Service, the RVDS.)

The iCSF operates on the same contribution model as the CSF. If you are interested in using the iCSF for a threemonth evaluation period, or contributing funds to the facility, please email us at the address above, or, to learn more, please visit <u>ri.itservices.manchester.ac.uk/icsf</u>.

Big Data event at Rutherford Appleton Laboratory (RAL)

There is a Big Data event at RAL; details are here: www.biginnovationcentre.com/Events/133/Big-Data-OpenFree-data-available-for-use-by-businesses.

The ITSfR group draws its membership from IT and research support staff from the four faculties, the Library, the Directorate of IT Services and the academic community

Maple

The network-licensed version of Maple 18 is now available on campus. Standalone licenses will follow in due course. Downloads and installation instructions can be found at www.applications.itservices.manchester.ac.uk/show_pro_ duct.php?id=12&tab=install.

Notable new features in version 18 include:

Signal Processing -

www.maplesoft.com/products/maple/new_features/maple 18/Signal Processing.aspx

Time Series Analysis -

www.maplesoft.com/products/maple/new_features/maple 18/timeSeriesAnalysis.aspx

Python, MATLAB and Perl code generation www.maplesoft.com/products/maple/new_features/maple 18/Code Generation.aspx

For the full list of what's new, see www.maplesoft.com/products/Maple/new_features/.

MapleSim

MapleSim 6.4 is now available for installation on campus. Currently, this is only for network licences, but standalone will be available soon. Install details are available at https://www.applications.itservices.manchester.ac.uk/s how product.php?id=329&tab=install.

MapleSim looks like Mathwork's Simulink on steroids, but it is based on completely different mathematics. Take a look at its key features at

www.maplesoft.com/products/maplesim/features/.

Our MapleSim license includes MapleSim itself along with the ControlDesign toolbox and connectors to allow it to work with Simulink and Labview.

If anyone would like to discuss this product further, let michael.croucher@manchester.ac.uk know.

Mathematica

The recent seminar and hands-on tutorial given by Wolfram Research at Manchester was a great success, thanks to all who attended. The materials used in the presentation can be downloaded from

https://download.wolfram.com/?key=WZDE86.

Please do not rehost this material anywhere else.

The most common piece of feedback received was that many people were not aware of how much Mathematica could do. It is **much** more than just another computer algebra system. Some highlights from the day include

- Image processing reference.wolfram.com/mathematica/quide/ImagePr ocessing.html
- 3D Volumetric image processing www.wolfram.com/mathematica/new-in-9/3dvolumetric-image-processing/
- Signal processing reference.wolfram.com/mathematica/quide/SignalPr ocessing.html
- **Bioinformatics** http://www.wolfram.com/solutions/industry/bioinfor matics
- **GPU** Computing reference.wolfram.com/mathematica/quide/GPUCo mputing.html
- **Probability and Statistics** reference.wolfram.com/mathematica/quide/Probabili tyAndStatistics.html

Finally, please note that we have an unlimited site license for Mathematica here at Manchester. This means that:

- You can install it on personally owned equipment. These • installs are completely standalone - no network license is required.
- It is installed on all of our High Performance Computing • equipment such as The Computational Shared Facility (ri.itservices.manchester.ac.uk/csf/) and Condor (<u>condor.eps.manchester.ac.uk/</u>).
- It is installed on all managed desktop machines, • including Windows 7 managed desktop and the EPS Linux image for teaching.

For installation details see the following link (only works on campus): https://www.applications.itservices.manchester. ac.uk/show product.php?id=38&tab=install.

Intel Math Kernel Library (Intel MKL) for Linux

You can register and join in the Intel® MKL 11.2 Beta Webinar on 7 May 2014 at 9.00AM to 10.00 AM PDT. If you haven't registered for MKL 11.2 Beta Programme (part of Intel® Software Development Tools 2015 Beta Programme), registration is easy through the softwareproductsurvey.intel.com/survey/150347/2afa/

site. Try out the new features and improvements of MKL 11.2 Beta and help Intel make the product better. More information on new features introduced in MKL 11.2 Beta will be presented in the Webinar

www1.gotomeeting.com/register/496339904.

EU-China Research and Innovation Partnership (ECRIP): 4 Million Euros to fund mobility of EU researchers to China

A new major programme of the European Commission to fund specifically mobility of European researchers to China has been launched on 4 April 2014.

The objective of this programme called *EU-CHINA RESEARCH AND INNOVATION PARTNERSHIP (ECRIP)* is to create, strengthen and intensify the EU-China Research and Innovation (RI) partnerships by supporting the mobility of EU researchers to China and strengthening people-to-people contacts, from both the public and private sectors, in strategic RI sectors.

The overall indicative amount made available under this Call for Proposals is EUR 4 000 000.

The Call for Proposals is divided into five lots of EUR 800 000 each, corresponding to five identified strategic areas:

- Lot 1: Renewable energy, energy efficiency, sustainable energy solutions for cities
- Lot 2: Sustainable urban development and urban planning, green urban mobility and transport
- Lot 3: Health, public health and welfare policies life sciences
- Lot 4: Information and communication technologies, smart cities
- Lot 5: Food, agriculture, biotechnologies and water

Any grant requested must be comprised between EUR 600 000 and EUR 800 000. The proposed project must aim to set up or strengthen partnerships in the targeted areas between European and Chinese research organizations (higher education and research entities from public and private sectors), by supporting the mobility of EU researchers to China.

Each project funded under this call will be a combination of an identified number of individual mobility schemes complemented by supporting activities. The funding of the mobility of EU-based researchers to China is the main aim of this programme.

Hence, individuals financially supported in the framework of the mobility scheme must be nationals from one of the EU Member States and shall not be already based in China or have previously spent an extended period undertaking research in China. Doctoral and post-doctoral students, research and academic staff, as well as engineers, innovation managers and RI personnel are all eligible to be funded.

While in light of the nature of this programme, the participation of EU and Chinese public or private research entities is compulsory, the mobility of Chinese researchers or Chinese visiting professors or travel / per diem for Chinese nationals is not eligible for funding.

In order to implement the project, the applying organizations will organize themselves in a partnership composed of at least two European organizations, from two different EU Member States, and a minimum of one Chinese organization.

Participation of research organizations from the European private sector is strongly desired.

In order to be eligible, the applicant must be legal persons and be organisations carrying out research activities from one of the EU Member States or Partner Countries.

Deadline to submit the proposal's concept note is 23 May 2014.

Access the call and all the application details on the European Commission Development & Cooperation website. (https://webgate.ec.europa.eu/europeaid/onlineservices/index.cfm?ADSSChck=1397180276530&do=publi. welcome&NBPUBLILIST=15&SEARCHTYPE=RS&ORDERBY =upd&AOFR=135587&ORDERBYAD=Desc&userlanguage=e n)

National supercomputer: ARCHER

Proposals to the 2nd ARCHER embedded CSE (eCSE) call are invited. Embedded CSE (eCSE) support provides funding to the ARCHER user community to develop software in a sustainable manner for running on ARCHER. Funding will enable the employment of a researcher or code developer to work specifically on the relevant software to enable new features or improve the performance of the code. Examples of this could be:

- Implementation of algorithmic improvements within an existing code
- Improving the scalability of software on higher core counts
- Improvements to code which allow new science to be carried out
- Porting and optimising a code to run efficiently on ARCHER
- Adding new functionalities to existing codes
- Code development to take a code from a Tier-2 to Tier-1 level bringing new communities onto Archer

Funding can be requested for existing ARCHER users supported by EPSRC and NERC and can fund staff located at the institution of the PI, third parties, or can include staff from the centralised CSE support team or a mixture of the above. More details of how to apply are available at www.archer.ac.uk/community/eCSE/ together with details of the application and review process, assessment criteria eligibility, etc.

The 2nd eCSE call opened: Tuesday 1 April, 2014. Deadline for proposals: 1600 BST Tuesday 13 May 2014

Proposals received after the deadline cannot be accepted. More information is available from the ARCHER helpdesk (support@archer.ac.uk).

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: <u>Hum-ITResearch@manchester.ac.uk</u>.

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

Medical and Human Sciences: <u>MHS-ITResearch@manchester.ac.uk</u>.

Life Sciences: FLS-ITResearch@manchester.ac.uk.

Next edition

The next edition of this newsletter will be circulated at the end of May 2014.

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