

# IT Services Supporting your research

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

Welcome to issue #4, July 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 contact details is available here: <a href="www.its.manchester.ac.uk/research/">www.its.manchester.ac.uk/research/</a>.

### **GPU Day Success**

Nearly 60 researchers and academics attended the recent (23 July 2013) meeting of the University's GPU Club to hear experts from NVIDIA and MathWorks discuss how GPUs (Graphical Processing Units) can be used to accelerate simulations and how MATLAB's GPU-enabled functionality makes this straightforward.

Michael Bane, IT Services, introduced the day by outlining the variety of GPUs (Kepler and Fermi) available to University of Manchester researchers and the training available to help people get started with GPUs.

Jeremy Purches from NVIDIA, who produce GPUs, underlined the importance of GPUs to performance, citing the number of GPU-enabled machines in the Top500. His colleague, Tim Lanfear, outlined how to use CUDA enabled libraries and applications to obtain good performance from the GPU hardware.

Jos Martin explained his job at <u>MathWorks</u> as "putting the hard, parallel stuff into MATLAB" so that users can benefit from their GPU hardware relatively painlessly.

After a buffet lunch, researchers held one-to-one chats with the vendors to get expert advice on domain specific issues and to build collaborations such as NVIDIA's CUDA Research Centre.

NVIDIA have accepted an invitation to run a one-day, handson training workshop in October 2013 and IT Services will be working with various groups to set up the University as a CUDA Research Centre.

Researchers interested in making use of the GPU-enabled MATLAB can already do so by downloading the latest version from <a href="https://www.itservices.manchester.ac.uk/software">www.itservices.manchester.ac.uk/software</a>.

A training course on best practices will be developed over the coming months.

The event was hosted by IT Services with support from Manchester Informatics. Slides and notes from the day, with information on forthcoming events, are available at <a href="mailto:qpu.manchester.ac.uk">qpu.manchester.ac.uk</a>.

### **Image-based Modelling Club**

The University of Manchester Image-based Modelling Club has recently established a new Steering Group and will be expanding its activities in the 2013/14 academic year.

The members of the Steering Group are Professor Peter Lee, Professor Paul Mummery, Dr Lee Margetts, Louise Lever, David Arregui and Jasmin Stein. Anybody interested in using images as a basis for simulation is encouraged to join the Club and contribute to discussions on the "Imagebased Modelling" LinkedIn group.

There is also a new Twitter feed to follow:
<a href="mailto:alimagebasedmodel">alimagebasedmodel</a>. If you would like to join the Club, please contact <a href="mailto:lee.margetts@manchester.ac.uk">lee.margetts@manchester.ac.uk</a>.

# Nuclear Reactor Simulator Web-application

Dalton Nuclear Institute

(www.manchester.ac.uk/dalton) and the Research Applications and Collaboration team (RAC) have started a project to develop a simple nuclear reactor simulator as a 3D interactive Web-App aimed at children's education and related outreach and engagement activities.

The RAC design and specification is being developed by <u>PlayGen</u>, a third party developer based in London with many years experience developing serious games, simulations and platforms. It is anticipated that this pilot project will act as a catalyst for similarly out-sourced projects in the future. For further information please contact <u>louise.lever@manchester.ac.uk</u>.

### Launch of n8equipment.org.uk

A fully searchable online database has now been launched to promote equipment within the N8 group of universities. This can be used to locate and request access to research equipment and facilities at Manchester and across the N8 university partnership.

#### www.n8equipment.org.uk

A great deal of work has been carried out by Manchester and our N8 Partners to update and improve Equipment Registers across the group and the new database represents a vastly improved resource with information on in excess of 1,300 items of equipment just here at Manchester.

The database classifies equipment according to taxonomy to enable easier searching. It also allows searching by key word, Institution and School.

The shared database will eventually enable us to search for and view details of research equipment held by all our N8 partners as further information is added. The main driver behind this database is the RCUK requirement for universities to become more efficient in the way that they use their equipment. As part of any research application, which includes equipment (items >£10k per RCUK definition), checks should be carried out to ensure that we don't already have access to the equipment being requested, and a Research Equipment Form should be completed. This resource will help greatly in enabling academics and RSS staff to fulfil this obligation.

# 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. 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). Robin is also the contact for the access programme featured in the next item.

# Hartree Centre- new BG/Q Access Programme

The Hartree Centre is pleased to announce a BG/Q Access Programme that will enable use of Blue Joule at the Hartree Centre at no cost.

This call is for work that must be completed by 30 September 2013, and you can commence once approval has been gained.

There will be no charge for use of the system, but in return Hartree will insist on you giving them a report containing full details of the work undertaken, detailing the science/ engineering completed and impact of the project. They will use those materials as a basis of their promotional materials including case studies and future business cases.

# HECToR – a National Computing Facility

Resource Allocation Panel (RAP): Class 1b access to HECToR

Invitation for proposals: This is a call for applications for (class 1b) access to HECToR through the Resource Allocation Panel. Closing Date: 27 August 2013.

www.epsrc.ac.uk/funding/calls/2013/Pages/raphector.aspx

Resource Allocation Panel (RAP): Technical 'top up' applications from existing class 1a grant holders

Invitation for proposals: This is a call for applications to the Resource Allocation Panel for 'top up' HECToR resource.

This call is open only to current class 1a grant holders. Closing Date: 13 August 2013.

www.epsrc.ac.uk/funding/calls/2013/Pages/rapclass1agran tholders.aspx

The Research Applications and Collaboration team can help you with the above application processes: <a href="https://www.wiki.rac.manchester.ac.uk/community/rac">wiki.rac.manchester.ac.uk/community/rac</a>.

#### **Research Councils UK Portal**

RCUK – the Research Councils for the UK – recently launched a new portal: <a href="mailto:gtr.rcuk.ac.uk">gtr.rcuk.ac.uk</a> known as the **Gateway to Research** that allows you to search all 7 research councils at once for 'key data'.

## New High Performance Compilers and Libraries for Windows

New Windows versions of the following compilers and libraries are now available at Manchester. Please note that all the University of Manchester links below will only work on campus.

#### Intel Fortran Compiler

www.applications.itservices.manchester.ac.uk/show\_product.php?id=300

Version 13.1 now available; this includes the Intel Math Kernel Library (MKL), a high performance numerical library with routines in areas such as linear algebra, Fourier transforms, statistics and data fitting. More details concerning the MKL are available at <a href="mailto:software.intel.com/enus/intel-mkl">software.intel.com/enus/intel-mkl</a>.

#### NAG Fortran Library for SMP and Multicore

www.applications.itservices.manchester.ac.uk/show\_product.php?id=323

Mark 24 adds 139 new functions, bringing the total to 1784 routines in areas such as global and local optimisation,

wavelet transforms, statistics, curve fitting, linear algebra, finance, and much more. A full list of routines can be found at <a href="https://www.nag.co.uk/numeric/fl/nagdoc\_fl24/html/GENINT/smpnews.html">www.nag.co.uk/numeric/fl/nagdoc\_fl24/html/GENINT/smpnews.html</a>.

### Dropbox and nCrypted Cloud

As stated in last month's newsletter, JANET's negotiations with Dropbox, with their *Dropbox for Business* cloud storage product, are dragging on.

Given that we know many thousands of our staff are already using Dropbox – either the free version or grant/self-funded – we have decided to go ahead with an extensive trial of **nCrypted Cloud**. This is a layer on top of Dropbox that provides client-side encryption, without compromising on the ability to share folders, etc. More details will be provided soon, once we are passed the end of the financial year, and it is the expectation that anyone who uses Dropbox with University data files will be able to benefit from this technology.

#### **Condor Pool**



Condor is available – free at the point of use – to postgraduates and staff of the University.

The EPS Condor Pool backbone will be further strengthened soon to provide smoother 24/7 operation of this facility and reduce wasted cycles. We were awarded central funds for 10 more computational servers and EPS is adding 3, giving us an extra 104 cores. These servers have now arrived and will be commissioned shortly. You can view further information about Condor at: <a href="mailto:condor.eps.manchester.ac.uk">condor.eps.manchester.ac.uk</a>.

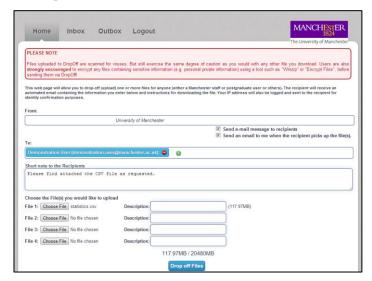
# Computational Shared Facility (CSF)

This summer's procurement for the CSF is the biggest yet: University research groups have contributed £285K. Seventy three new Intel Sandy Bridge compute nodes will soon be in production. Four of these have 256GB of memory; and two nodes each host two NVIDIA Kepler GPUs.

Once the new nodes are in production, the CSF will comprise 2792 Intel cores and 2144 AMD cores.

For more information about the CSF, please visit <u>ri.itservices.manchester.ac.uk/csf</u>, or email <u>its-ri-team@manchester.ac.uk</u>.

### **DropOff**



#### https://dropoff.manchester.ac.uk

We are now around 75% through the service trial of **DropOff** – a local system that lets you 'drop off' very large files (up to 20GB) for others to 'pick up'. It can be used to send such files to external users, as well as within the University. Similarly, your external collaborators can leave files for you.

Please contact: <a href="mailto:dropoff@listserv.manchester.ac.uk">dropoff@listserv.manchester.ac.uk</a> for further details and if you would like to use this trial service. (It is also linked off the My Manchester for Staff pilot site.)

As we go to press, DropOff has 174 users with 51 files for pick-up occupying 87GB.

#### Top Tip!

Some users want to email a set of large files to various people, but include a different email message for each recipient, and also do most of this from their favourite email client.

- 1. Use the secure web site to drop-off the file(s) with the single recipient being yourself.
- 2. You will see *ClaimID* and *Passcode* for the drop-off as per the example below:

# Claim ID: HJczMah9TzJBZy9y Claim Passcode: c58KB7PtyDhprrwq

- 3. Cut and paste these.
- 4. Write your separate emails, using your normal email client, to whomever and include the *ClaimID* and *Passcode*. Tell them to go to <a href="https://dropoff.manchester.ac.uk">https://dropoff.manchester.ac.uk</a> and

click Pick-up.

They enter the *ClaimID* and *Passcode* and get the files. You should include in the emails a request for the recipients to **not** delete the drop-off.

5. When you have received emails that all parties have picked up, you can log in to DropOff and delete the files, or the files will automatically deleted after 14 days.

#### **Another Top Tip!**

Warn recipients of your drop-offs that the notification email from the DropOff service may end up in their spam / junk email folder.

### **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 <a href="digital-research.oerc.ox.ac.uk">digital-research.oerc.ox.ac.uk</a> 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.

# N8 High Performance Computing (HPC)

N8 HPC currently offers a shared 'Tier 2' HPC facility underpinning world-class research, enabling collaborations between institutions and creating the opportunity to engage more effectively with business and the community. The facility – **Polaris** – is an SGI High Performance Computing cluster with 332 compute nodes. Each node has two of the latest Intel Sandy Bridge processors, and these nodes have a capacity of 320 GigaFLOPS/second. Project Principal Investigators can apply for access to this facility through a lightweight peer review process.

If you wish to know more about N8 HPC, please see the website (<a href="www.n8hpc.org.uk">www.n8hpc.org.uk</a>) or contact <a href="mailto:enquiries@n8hpc.org.uk">enquiries@n8hpc.org.uk</a>. Robin Pinning (<a href="mailto:pinning@manchester.ac.uk">pinning@manchester.ac.uk</a>) and Gillian Sinclair (<a href="mailto:gillian.sinclair@manchester.ac.uk">gillian.sinclair@manchester.ac.uk</a>) are the local contacts for Manchester researchers.

### IT Services Research Data Storage Service

The first annual procurement for the new IT Services Research Data Storage Service has been made. One petabyte of new storage is now ready for use (equivalent to 0.5PB of resilient storage). Faculties each have around 100TB they can allocate. This storage can be mapped as a network drive to desktop and laptop computers in the usual way (i.e. is available via the standard Windows share technology). It is also available for use in the Computational Shared Facility via a fast network link.

For more information please visit: <a href="https://www.rds.itservices.manchester.ac.uk">www.rds.itservices.manchester.ac.uk</a> or email <a href="https://www.rds.itservices.manchester.ac.uk">its-ri-team@manchester.ac.uk</a>.

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

<u>remedy.manchester.ac.uk/cgi-bin/sr.cgi?scid=142</u>. On completion of the form, your Faculty IT team will contact vou.

# Is Your Computational Data Photogenic?

A chance to win a prize here:

www.staffnet.manchester.ac.uk/news/display/?id=10439

### **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 August 2013.

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

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