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

Welcome to issue #10, January 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 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/.

Windows Azure for Research

Microsoft Research will be offering free Azure training to RAs, academics and PhD students who want to use cloud computing.

Microsoft Research and The University of Manchester are delighted to offer a no-cost, two-day, hands-on technical training event for academic researchers interested in cloud computing using Windows Azure. The training will be held 3-4 April 2014 at the School of Computer Science, at The University of Manchester. This is part of Microsoft's Windows Azure for Research programme – please see www.azure4research.com.

Please register now to secure your place bit.ly/1dxZ6Q9.

Attendees will receive a six-month Windows Azure Pass for evaluation purposes and be able to access Windows Azure on their own laptop via a web browser. You will also learn more about receiving significant Windows Azure 12-month grants for your research – for details, please see www.windowsazurepass.com/research.

We would be grateful if you would forward this invitation to your research colleagues and friends, who are welcome to attend (places permitting).

Windows Azure is a general, open and flexible global cloud platform supporting any language, tool, or framework – including Linux, Java, Python, and other non-Microsoft technologies. The programme will cover a variety of hands-on labs with programming examples predominantly in Python and Java. No prior experience of Windows Azure is required. The only prerequisite is basic programming experience in some language. This two-day course is presented by specialised trainers and is geared towards post-doctoral researchers, academics and postgraduate students.

The attendee's laptop does not need to have the Windows operating system installed – Windows Azure is accessed via an Internet browser. After attending the course, researchers will feel confident in applying cloud computing in their current and future research.

For questions about the course please contact azuretraining@microsoft.com.

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

Page 1

Join the Windows Azure for Research community and conversation on LinkedIn & Twitter at linkd.in/18Z5OL4 and twitter.com/azure4research (#azureresearch).

Microsoft course overview: research.microsoft.com/en-us/projects/azure/training.aspx.

Detailed Course Description (pdf) research.microsoft.com/en-us/projects/azure/msr-course-aug2013.pdf.

Logistics and status information about The University of Manchester event: research.microsoft.com/en-us/events/azure4researchtraining-ukman2014/.

Directions to the School of Computer Science at The University of Manchester: www.cs.manchester.ac.uk/about-us/find-us/.

Dr Kenji Takeda, Solutions Architect and Technical Manager, Microsoft Research Limited.

ITSfR Forum 26 February 2014: How IT Services can support Academic Scientific Software

Specialist scientific software is a vital component of academic life for both teaching and research. Not only do academics *use* pre-packaged, specialist software applications (such as MATLAB, R, Mathematica or Abaqus), they also *create* specialist software as an integral part of their research outputs – see for example: www.walkingrandomly.com/?p=4951.

In this talk, Dr Mike Croucher will explore how IT Services can, and do, collaborate with academic colleagues to significantly enhance research (as well as teaching) through the use and creation of scientific software.

The event will be held in Roscoe 1.010 on Wednesday 26 February 2014 at 12:30 for refreshments and a 1pm start. We particularly welcome academics, doctoral students and RAs to the forum, but it is open to all interested parties.

Condor Pool

The High Throughput Computing *Condor* Pool (condor.eps.manchester.ac.uk), provided University-wide by EPS, should be back to full strength by the time you read this, following the on-line examination period. We also predict this facility will have clocked up 2000 years of computational results by end January 2014 matchmaker.eps.manchester.ac.uk/condorstatus/.

Research Data Management – are you compliant?

The University's Research Data Management (RDM) policy is currently being rolled out (www.library.manchester.ac.uk/ourservices/research-services/rdm/implementationtimetable/), beginning with requirements relating to data management planning, storage of data and inclusion of metadata.

The policy has been designed to help you in the management of your research data.

Essentially, what this means to you as a researcher is that you will need to:
- prepare a data management plan using either your funder's template or, if none available, a template provided by the RDM team. To make the process of creating, storing and sharing a data management plan as straightforward as possible we have created an online data management planning tool: www.manchester.ac.uk/researchdata/datamanagementplanning/writing-dmp/odmptool/
- store your data centrally or in a funder compliant repository. To find out more information about central storage please contact your faculty IT or alternatively visit: www.rds.itservices.manchester.ac.uk/
- record basic metadata describing the data, how it was created and how it can be used.

The benefits of this are:
1) Increased efficiency and less duplication of effort when project and data related information are captured at a single point of entry; i.e. project data stored centrally rather than across several storage devices
2) Secure and backed up storage of working data during the life of your project, reducing the risk of data loss and avoiding issues of version control
3) Easier discovery of research data through use of metadata, tagging, linking and search functionalities. This enables data to be reused, maximising its value and increasing the potential for citation and improved reputation
4) Control over allowing access to data within your storage area to your research group and collaborators
5) Compliance with data protection, funder policies, ethical codes and journal requirements

The Research Data Management team at The University of Manchester Library is here to support and advise you on any aspect of your RDM. Researchers can contact the team by email, researchdata@manchester.ac.uk or phone, 275 7853.

Further guidance can be found at: www.manchester.ac.uk/researchdata.

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

Page 2

E-infrastructure Roadmap

EPSRC have published their *E-infrastructure Roadmap*. The document is well worth your time, and EPSRC are seeking comments. (The document and how to respond can be found here: www.software.ac.uk/news/2014-01-22-epsrc-lays-out-plans-e-infrastructure).

What's IT Worth?

The University of Manchester staff IT survey is now live at www.itservices.manchester.ac.uk/survey/, and we are asking you "What's IT worth?". Please take the time to complete the survey. The survey will be available until Friday 7 February 2014, and will take between 5–10 minutes to complete.

Report on first ever MATLAB-based Software Carpentry bootcamp

Software Carpentry bootcamps (software-carpentry.org/bootcamps/) aim to ensure that researchers have a working knowledge of several useful technologies from the world of software development.

On 14 January 2014, The University of Manchester hosted the first ever MATLAB-based bootcamp. For a full report please see www.walkingrandomly.com/?p=5324.

Access to Large Scale Supercomputing Facilities for UoM Researchers

Would you like to access Blue Joule – one of the UK's largest supercomputers? Or, perhaps ARCHER, the new UK HPC national resource? Has your research reached the limits of your currently available computing power? Do you think your research could benefit from access to larger HPC resources? If so, then contact IT's Dr Robin Pinning or Dr Gillian Sinclair (ITS-Research@manchester.ac.uk) from the Research Applications and Collaboration team to discuss your research and how we can help you to access resources such as N8 HPC (www.n8hpc.org.uk) and Blue Joule based at the Hartree Centre at Daresbury www.stfc.ac.uk/Hartree.

N8 HPC is a regional resource managed jointly between the universities of Manchester and Leeds, but shared between the N8 institutions. Access to N8 HPC is through a light-weight review process, and usage is free although priority is given to projects with industrial collaboration.

Through N8 HPC we have been working with the Hartree Centre to give Manchester researchers access to their extensive facilities, as well as helping to develop projects between academia and industry that incorporate the facilities and expertise at Daresbury.

Assistance and advice can also be provided on potential ARCHER projects (www.archer.ac.uk/), European PRACE projects (www.prace-ri.eu/) and even on accessing Tianhe-2, the world's fastest supercomputer.

Please feel free to contact us to discuss any aspect of your computational or data-intensive research at ITS-Research@manchester.ac.uk. The team will work with you to remove any barriers preventing you from accessing the resources your research requires (www.rac.manchester.ac.uk).

ARCHER Training Courses

Upcoming training courses: www.archer.ac.uk/training/.

10-11 February 2014: Introduction to ARCHER and Cray MPI, University of Leeds.

This introductory course will give an overview of the hardware and software environment on ARCHER, focusing on areas where it differs from HECToR. ARCHER-specific features of the MPI library will be explained; for example: ways to make the most of the capabilities of the Aries interconnect. The final session will focus on helping users to port applications to ARCHER.

25-26 February 2014: Data Staging and Data Movement with EUDAT, EPCC, Edinburgh.

This two-day course will describe the mechanisms that can be used to stage data to and from HPC resources such as those available in PRACE, which includes the UK ARCHER system. It will also introduce EUDAT and some of its services that are likely to be of interest to users working with large data files. Subjects that will be covered include: GridFTP, iRODS and Authentication methods.

For details and to register: www.archer.ac.uk/training/.

Social Media Research Workshop on Technical Challenges

The new University of Manchester Social Media community recently held a workshop about the technical challenges facing the procurement of an International Centre for Social Media Research. More details and links to the workshop presentations and notes from the event, including the challenges facing IT Services, can be found at the RAC Blog (www.rac.manchester.ac.uk/social-media-research-workshop-on-technical-challenges/).

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

Page 3

zCSF (aka *Zrek*) – the Emerging Technology Branch of the CSF

Several research groups at the University have procured examples of emerging technology over the last year. These include Xeon Phi systems, the latest Nvidia computational GPUs and also some FPGA cards. With Zrek – the latest branch of the Computational Shared Facility – we hope to pull these disparate systems together into one loose-knit cluster. As a cluster: it is much easier to share and promote use of each system between University research groups; and the individual systems can be integrated into the University Computationally-Intensive Research Ecosystem ri.itservices.manchester.ac.uk/the-cir-ecosystem/ For example, RDS (aka Isilon) storage can be made accessible so that users have the same home-directory (i.e. see the same files) as on the CSF, Redqueen, iCSF, etc.

Zrek will be in production by the time you read this!

If you would like to know more about Zrek, please contact the IT Services Research Infrastructure Team its-ri-team@manchester.ac.uk.

More Old Beowulf Clusters Replaced Using the *Revolving Green Fund* – Ivy Bridge Nodes for the CSF

Four old computational clusters have been replaced by making use of the University's Revolving Green Fund to procure newer, more powerful and more efficient compute nodes. The old clusters are from Chemistry (three) and Chemical Engineering and Analytical Science.

As a result of the replacement, over the next five years, there will be an energy saving of approximately 1.3 million kW-hours equivalent to almost 700 tonnes of carbon-dioxide.

Twenty-four Ivy-Bridge-based compute nodes have been procured and these have been added to the Computational Shared Facility. (We are also expecting a further 12 Ivy-Bridge-based nodes from other contributions in the next few weeks.) The 24 new nodes offer far greater computational power than the old hardware they replace.

If you are the owner of an old computational cluster on campus and would like to investigate its replacement with new, centrally-hosted hardware by means of the RGF, please contact the Research Infrastructure Team at its-ri-team@manchester.ac.uk.

Image-based Modelling Club

The next meeting of the University of Manchester Image-based Modelling club will be held from 12.30–13.30 on Tuesday 4 March 2014 in the Michael Smith Building. The theme of this meeting will be composites. In the natural world, composite structures have evolved over millions of years in both plant and animal tissues. Engineers are trying to follow this lead, combining two or more constituents to design materials with special engineering features such as low weight and high strength. Professor Constantinos Soutis (Director of UMARI and the Northwest Composites Centre) will give an invited talk on polymer composites. Many of the images presented may leave attendees scratching their heads as to whether they represent biological or manufactured structures. The aim of the talk is to foster cross-faculty collaboration between researchers in EPS, FLS and MHS. What can life scientists learn from engineering techniques and vice-versa? If you would like to make an announcement during the club meeting about a recent paper, job opportunity or event, contact lee.margetts@manchester.ac.uk. Please visit the following website for further details and registration: wiki.rac.manchester.ac.uk/community/IBM.

Future UK / US Collaboration in High Performance Computing

Manchester is one of the lead organizations in an 'exploratory' EPSRC project (tinyurl.com/pd8qorh) that is looking at how collaborating with US HPC Centres could benefit UK Science. This is an initiative started by the British Embassy in Washington DC and the UK Ministry for Business Innovation and Skills.

Dr Lee Margetts, one of the investigators, is currently documenting recommendations to EPSRC regarding possible targets for future joint NSF/EPSRC funding calls. If you would like to see UK/US HPC Collaboration supported in a particular line of research or activity, please email lee.margetts@manchester.ac.uk.

Source Code and Data Version Control

The UoM central repository now supports the popular *Git* distributed version control system, as well as Subversion. Details are here: https://scm.manchester.ac.uk.

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

Page 4

Improve your computational science – do more, faster!

IT Services has a variety of introductory and intermediate courses on programming, visualization and code optimisation run by support staff from across IT Services.

Skills learned during these workshops and online courses can be applied to computational research codes, to both obtain results faster and to increase the size (or increased resolution) of the problem being solved.

Such techniques are invaluable on resources such as the CSF (ri.itservices.manchester.ac.uk/csf/), Condor (www.condor.eps.manchester.ac.uk) and N8 HPC (n8hpc.org.uk) as well as ARCHER (www.archer.ac.uk) and beyond.

But it's not just about high end computing, you can apply the skills you learn to codes running on modern multicore or GPU-enabled desktops to gain better utilisation of the resources available at your fingertips.

For bookings and background info please see: wiki.rac.manchester.ac.uk/community/Courses.

List of Forthcoming Training Opportunities (2014)

An introduction to using UNIX Shells (Bash scripts, environment variables)	Tue 04 Feb
An introduction to research computing	Wed 05 Feb
How to optimise your codes	Fri 07 Feb
Introduction to FORTRAN programming language	Tue 11 Feb
Programming in MATLAB	Thu 13 Feb
An introduction to Python	Fri 14 Feb
The theory of parallel programming	Mon 17 Feb
FORTRAN programming language	Tue 18 Feb
Introduction to FORTRAN programming language	Tue 25 Feb

Using Paraview for visualization	Thu 27 Feb
FORTRAN programming language	Tue 04 Mar
High throughput computing using Condor	Wed 05 Mar
An introduction to OpenCL	Thu 06 Mar
Image-based modelling	Mon 24 Mar

Programming the Finite Element Method

Dr Lee Margetts (IT Services, Research Applications and Collaboration) has published a new textbook titled *Programming the Finite Element Method*. The aim of the book is to help researchers learn how to use or develop software to solve 'large' engineering problems on 'massively parallel' computers. This is particularly important given that a 100,000 core HPC system is predicted to cost £150,000 in 2018: a budget affordable by many companies and research groups. The book documents the open source software ParaFEM, which has been developed by UoM researchers in the Schools of MACE, SEAES, Mathematics and Computer Science. Lee will be using the book to teach 'parallel' finite element analysis to the *UK Doctoral Training Network for Fusion* in March 2014. He will also project manage software development effort funded by the Software Sustainability Institute (SSI). This has been awarded to help improve usability and uptake. The full reference of the book is Smith IM, Griffiths DV and Margetts L, *Programming the Finite Element Method*, 5th Edition, Wiley, 2014. Two copies are available in the University Library. Please contact lee.margetts@manchester.ac.uk for further details.

Researcher of the Month

PhD student David Arregui Mena (Nuclear Graphite Group, School of MACE) is currently braving the cold and snow during his STFC Battery Network funded research visit to the Colorado School of Mines, USA. David is a CONACyT funded student applying stochastic finite element modelling techniques to his studies of nuclear graphite bricks (work that initially used Windows Azure). Professor Vaughan Griffiths, who is hosting the visit, is one of the leading international experts in this area, recently publishing work on random fields for porous materials (as well as being one of the authors of *Programming the Finite Element Method*). David will be giving a talk about his visit at a **Finite Element Club** meeting in March 2014, hopefully alongside our own local experts from the School of Mathematics.

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

Page 5

The University of Manchester presents the Emerging Technology Conference: EMiT

Computational hardware is changing rapidly, with new and novel highly parallel computing architectures that are in a state of constant flux being unveiled all the time.

This forces significant questions about re-coding and future proofing existing scientific software. The term *Emerging Technology* is beginning to be used to describe this continual state of hardware change.

The Inaugural EMiT Event will take place on Friday 11 April 2014 at The University of Manchester and will focus on application in research of new methods and techniques to exploit this technology.

For more details please see: emit.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 February 2014.

If you have any news to contribute, please contact the IT Services Research Lead, Ian Cottam: ian.cottam@manchester.ac.uk before 20 Feb 2014.

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

Page 6

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

Page 7