MANCHESTER 1824
The University of Manchester

IT Services

Supporting your research

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

Welcome to issue #9, December 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/.

CIR – Computationally Intensive Research

An ITSfR Forum was held on 18 December 2013 where the state of support for computationally intensive research (CIR) was presented, along with information about the on-going review of how we might improve planning. The former was led by Ian Cottam from IT Services, and the latter by Professor Chris Taylor.

The forum was well attended – around 40 people – by both academic researchers and the IT support community. Powerpoint slides can be found here: https://www.dropbox.com/s/d3ee7eznn6csm3s/ITSfR-talk-CT-IC.pptx.

Some highlights:

- There is a national eco-system of CIR: we need to understand UoM's place in this context
- The previous review of CIR in 2010 resulted in the *Computational Shared Facility*; we need to build on that work and produce a coherent plan
- We need to know current and future needs, via surveys and otherwise consulting stakeholders (for size of jobs, number of cores needed, *etc*)
- We need to invest where/when/what, using and maximizing external funding opportunities
- Barriers to use should be reduced
- Change culture and "commoditise" CIR – support researchers and not hardware
- Software is more important than hardware
- We need to be more provider agnostic
- We should have local control and regional collaborations
- Local user communities of software and technologies are important
- Local is good for, *inter alia,* "nursery slopes" work; sensitive data; network bandwidth; and agility

Further discussions and consultations with academics will continue in January 2014.

Weather Forecasting – made locally

ManUniCast is a real-time weather and air-quality forecasting website, teaching portal for students, and outreach tool. Every day, two model forecasts are performed – one meteorological and one chemical – using the most popular open-source models in the world: WRF and WRF-Chem. The forecast model runs are carried out on the Redqueen HPC cluster. These 54-hour forecasts are computationally expensive; each WRF and WRF-Chem model run takes ~6 and ~10 hours respectively (each on 80 computational cores). Once these forecasts complete, plots of key forecast variables are generated and pushed to the webserver for users to access through the ManUniCast website. The beta version was launched on 4 November 2013.

This project was carried out by researchers at the Centre for Atmospheric Science, in collaboration with the eLearning team in the Faculty of Engineering and Physical Sciences, and supported by IT Services. Particular thanks go to Simon Hood and his team for their expertise and help setting up the models on Redqueen – installing the computational nodes, configuring the required software modules and optimising the model code. Thanks also go to Chris Paul for setting up, configuring and maintaining the Virtual Machine and webserver which hosts the ManUniCast site. Visit manunicast.seaes.manchester.ac.uk for your latest weather and air-quality forecast and for more information about the project. [Stuart Anderson]

Source Code and Data Version Control

We are pleased to announce that 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.

Hartree Centre – access to Blue Joule

The Hartree Centre is pleased to make available time on Blue Joule, the IBM BG/Q supercomputer, to industry and academia for projects that need large scale.

Projects are able to use the facilities between Monday 13 January 2014 and Friday 11 April 2014.

It is a pre-requisite that, if you have been a member of a project on the previous BG Access Program, the Project has provided the feedback requested by the Partner Support Team, i.e. a report with full details of the work undertaken, detailing the science/engineering and impact of the project.

This programme will provide free usage of the super-computer but will not provide support or development effort.

More information about Blue Joule can be found at: community.hartree.stfc.ac.uk/wiki/site/admin/home.html.

We have helped a number of people from Manchester onto previous programmes (we can usually get UoM projects fast tracked), so please get in touch with robin.pinning@manchester.ac.uk or ITS-Research@manchester.ac.uk.

The same also applies for the new national ARCHER service that replaces HECToR.

ARCHER: 1st eCSE Call for Proposal

ARCHER, the new UK National HPC Service, has launched its first embedded CSE (eCSE) call. The closing date is 4pm, Tuesday 14 January 2014. 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. For further details of the application and review process, see www.archer.ac.uk/community/eCSE/. Local assistance in preparing applications is offered by the Research Applications and Collaboration Team. Contact lee.margetts@manchester.ac.uk if this is required.

The World's Number 1 Supercomputer

Congratulations to Dr Xue-Feng Yuan, from the MIB and the School of CEAS, in his new job as *Director of the National Supercomputing Centre at Guangzhou*. Xue-Feng will be leaving us at the end of January and we all wish him well.

Future collaborations with the Guangzhou Centre are, of course, a possibility!

Humanities Faculty IT Research Development Team

The team specialise in providing bespoke web applications and databases compliant with funding bodies' requirements for security, resilience and archiving of project data.

The website and database for the *Lexis of Cloth and Clothing Project* has gone live this month. The database allows visitors to the site to discover what items of clothing were authentic for a specified period between the 8th and 15th centuries in Britain. They can also search for the terms used to describe cloth and clothing in that period. The PI was Professor Gale Owen-Crocker from the School of Arts, Languages and Cultures. Contact: Dave Risley.

CUDA course

Some readers may be interested in an online hands-on introductory CUDA tutorial posted on the EPCC web site: *Learn CUDA in an Afternoon*, www.epcc.ed.ac.uk/online-training/learnCUDA.

SciProgramming

Mike Croucher writes "*I often get asked how to perform nonlinear least squares curve fitting in various systems, and so documented how to do it in several languages.*"

Below are all the links.

For commercial software that's site licensed at Manchester:

Maple - www.walkingrandomly.com/?p=5218

Mathematica - www.walkingrandomly.com/?p=5180

MATLAB - www.walkingrandomly.com/?p=5196
(Note, we don't have the curve fitting toolbox at Manchester but we have all of the others mentioned in this article.)

Additionally, this type of analysis can be performed in Origin – a Windows-only, site licensed data analysis package that is available from (on campus only): www.applications.itservices.manchester.ac.uk/show_product.php?id=301.

For open source languages:

Python – www.walkingrandomly.com/?p=5215

R – www.walkingrandomly.com/?p=5254

Julia – www.walkingrandomly.com/?p=5181

Comments welcomed and to: Dr Michael Croucher, Head of EPS IT Applications Support, Michael.Croucher@manchester.ac.uk.

Faculty Contact Emails

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Next edition

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

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