MANCHESTER 1824
The University of Manchester

IT Services

Supporting your research

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

Welcome to issue #6, September 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/.

Our September issue always contains a repeat of some service information for the benefit of newly joined research students. If you supervise such students, please make sure they receive a copy.

Research Data Service (also known as Isilon)

IT Services' Research Data Service (RDS) is now in full production. This service provides centrally-hosted and administered data storage for research staff and students at the University.

Storage provided by this service is accessible from desktop and laptop machines on campus and may also be accessed from on-campus research computing systems, in particular the Computational Shared Facility.

Files stored on this service can be considered secure. For example, files corrupted or accidentally deleted can be recovered for up to 28 days.

If you have research data storage requirements you can find out more on the RDS site or by contacting your faculty IS research support team, or the Research Infrastructure team, whose email is: its-ri-team@manchester.ac.uk. To apply for storage, you can use the form here: remedy.manchester.ac.uk/cgi-bin/sr.cgi?scid=142

[Editor's note: we are advised by University senior management that, given the above service, and the mandatory need for Research Data Management – www.library.manchester.ac.uk/ourservices/research-services/rdm/ – researchers should *not* be seeking funds to purchase standalone USB external disks.]

IT Services for Research Forum

The next ITS Research Forum we present will be Tuesday 22 October, Mary McDerby will be speaking on Research Data Management. All academic researchers and IT staff are invited.

SciProgramming Email List

This is a listserv email list intended for Manchester researchers who develop software. It is explained further here:
https://www.applications.itservices.manchester.ac.uk/show_content.php?id=180.
The web page also contains a link to the *Research Software: Made in Manchester* site; our thanks to Mike Croucher in EPS IT for setting this up.

Maple and MapleSim

The Faculty of EPS recently purchased a full site license for *Maple* and *MapleSim*, two mathematics and simulation applications. We are making them both available to the entire University.

So far, we have only released network licenses for Maple itself, but MapleSim and home-use licenses for both products will be available soon. Both products are also installed on new versions of the University Windows 7 Managed Desktop.

Maple is available for Windows, Linux and Mac OS X. There is a companion app available for iPad.

The addition of Maple to our portfolio means that academics at Manchester now have access to most of the major, general purpose, commercial mathematical packages: Maple, MATLAB, Mathematica, Mathcad and the NAG library.

The Maple page on the University Applications Website is currently a work in progress, but the basics are there https://www.applications.itservices.manchester.ac.uk/show_product.php?id=12.

If you have any comments or questions, feel free to get in touch with Mike Croucher. Mike is particularly interested in talking to people about the use of these products in teaching and research along with comparisons with their competitors.

Training Opportunities

IT Services have a variety of courses running during October and November aimed at helping researchers with their computational research and data management plans.

Courses are a mix of face-to-face and online, covering Introduction to Research Computing, UNIX, MATLAB, FORTRAN, visualization packages, optimisation & parallelisation techniques, Condor, GPU programming (CUDA and OpenCL) and OpenMP.

Bookings and further details:
wiki.rac.manchester.ac.uk/community/Courses.

University Finite Element Club

The next meeting of the Finite Element Club will be held in the Simon Building 3A (3.62) at 2.00pm on Thursday 3 October 2013. The topic of the meeting will be "user subroutines" for commercial and open source software. Dr Hosseini, Institute for Surgical Technology and Biomechanics (ISTB), University of Bern, Switzerland will give a talk titled "Constitutive Modeling of Trabecular Bone in Large Strain Compression". Dr Hosseini uses X-ray Tomography to capture the geometry of bone and therefore this meeting will also be of interest to members of the Image-based Modelling Club.

The meeting is open to students, researchers and staff. To register, please visit
wiki.rac.manchester.ac.uk/community/FiniteElements.

If you wish to make an announcement during the meeting, please contact Lee Margetts and/or Jonathan Boyle.

University GPU Club

The University GPU Club brings together staff and students to discuss best practice for programming Graphical Processor Units, typically in their use to accelerate the computationally intensive parts of codes ("kernels"). The Club has three speaker events coming up, two of which have been organised by EPS and HUM facilities, and have arranged for NVIDIA to do a day's hands-on CUDA training for those who have tried this GPU programming language and now wish to optimise their codes.

We would appreciate *your* help in promoting the GPU Club and these sessions to colleagues and researchers:

Tues 2 October 2013: Daniel Egloff, QuantAlea, will talk about GPU Applications in the world of HPC Finance. 2-3pm, Crawford 5.1, MBS (hosts).

Tues 29 October 2013: NVIDIA will present the programming language CUDA and their hardware roadmap for GPUs. We also welcome Stephen Longshaw from MACE who will describe the use of Smoothed Particle Hydrodynamics (SPH) on GPUs to model the impact of Minke Whales on turbines.

Weds 30 October 2013: Intermediate CUDA training. (Bookings will be available shortly)

Weds 13 November 2013: The Centre for Atmospheric Science are hosting an afternoon discussion on the role of emerging technology. They have key speakers John Michalakes from NOAA over from the States (expert on porting codes to GPUs and FPGAs) and Craig Davies from Maxeler (dataflow solutions on FPGAs). This will be a combined event with the University GPU Club.

Further details: gpu.manchester.ac.uk.

Royal Society Computing Event

The Royal Society are running a Computing Event in Manchester, which will be of great interest to GPU Club members (and others), on Monday 30 September 2013 and Tuesday 1 October 2013. For more details, please see: www.rac.manchester.ac.uk/?p=427.

Training in PGAS Programming Models

Edinburgh Parallel Computing Centre (EPCC) is organising a set of three events 1-4 October 2013 that all focus on the *Partitional Global Address Space* (PGAS) programming model and its use/future in High Performance Computing applications. Full details of the events can be found at www.rac.manchester.ac.uk/?p=405.

MPI + X = MPI is The Future of Parallel Programming

This month, Lee Margetts (IT Services, Research Applications and Collaborations Team) attended the EuroMPI 2013 conference in Madrid. The main purpose of the conference is to provide a forum to disseminate the latest developments in the Message Passing Interface, the de facto standard in message passing for scientific applications.

High Performance Computing technology evolves very quickly and it is important to keep on top of the latest developments. Lee has posted a blog entry about the conference at: www.rac.manchester.ac.uk/?p=423.

Report on Digital Research 2013

The Digital Research conferences are successors to the UK e-Science All-Hands Meetings, bringing together those interested in data science and research infrastructure. This year's DR2013 was held at St Anne's College Oxford from September 9-11. The first two days featured sessions on Data Science and a Digital Research Showcase, on the last day the Software Sustainability Institute organised a workshop for Research Software Engineers, and held in parallel was the UK e-Infrastructure Academic Community Forum.

This year there was a focus on the issues of being a research technologist, someone who is not an academic researcher, but, on the other hand, works more closely and directly with research projects than the majority of IT support staff. There are a considerable number of staff here at The University of Manchester whose work fits this description, and it was very interesting to meet with colleagues from other institutions and share experiences.

The conference was interesting and lively with excellent keynote speakers who gave presentations concerning key aspects of data science. There was a good balance between presentations of the methods and results of Digital Research and presentations about the software and infrastructure supporting DR. For more information see the web pages at: digital-research.oerc.ox.ac.uk.

N8 High Performance Computing – available for use by Manchester researchers

N8 HPC is an EPSRC funded initiative through the N8 Research Partnership that aims to seed engagement between industry and academia around research using e-infrastructure as well as develop 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. Please visit the N8 HPC website for more information, but if you would like to discuss your requirements or if you need assistance with your application then please get in touch – its-research@manchester.ac.uk.

Computational Shared Facility

The CSF is the University flagship high performance (HPC) / high throughput (HTC) computing facility managed by IT Services for the use of University research groups. It is built on a shared model: all compute nodes are procured using contributions of funds from research groups; the cost of infrastructure such as login nodes, fileservers and network equipment is paid for by the University. University Schools may also contribute so that all members of that School then have access to the facility.

There is no barrier to entry: all contributing research groups from The University may use the CSF – there is no review process.

The CSF currently has almost 5000 processor cores and it is tightly integrated with the Research Data Service (see below) forming a complete compute/storage research computing package ideal for those whose work involves large quantities of data.

Support for users of the CSF is provided by both central IT Services and the faculties with particular focus on helping those new to using HPC/HTC systems becoming

productive; we are happy to provide face-to-face help for small groups and individuals.

The CSF originated to provide a professionally managed alternative to individual research groups building and running their own small clusters. For this reason (that is to accommodate the differing needs of research groups), the service provided is very flexible and responsive – the CSF is run as an agile service.

If you would like more details about the service or how to contribute to the CSF, please visit the web site ri.itservices.manchester.ac.uk/csf/ or contact the Research Infrastructure team via its-ri-team@manchester.ac.uk.

Incline (also known as iCSF)

Incline (aka iCSF) is a new, experimental service which will soon be in production. The service is designed specifically for interactive computationally-intensive work, such as code development and testing, or interactive (GUI-based) use of applications such as Stata and R.

Users of Incline will have access to the same home directory (and other RDS/Isilon-based filesystems) as they have on the CSF.

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

Condor High Throughput Computing

Condor is free-at-the-point-of-use to any researcher in any faculty. It provides High Throughput style computing (only – there are no fast interconnects or shared storage facilities). As well as bespoke code, Condor can run any application that has a batch mode.

Although we have some active professorial users, by far the main user community is PhD students (and also some research assistants). Graduate (PGR) students like the service as they can get more or less instant access without having to go through supervisor or application approval.

At any given time there are usually over 100,000 jobs queued up (over 200,000 at the time of writing). The number of simultaneous users of the system typically varies from around 8 to 20. The total number of processor cores varies during the day: circa 250 during normal office hours, 2500-3500 out of office hours.

Apart from a backbone of some 250 cores, we make use of existing PCs in (some of) the EPS Faculty teaching clusters (over night and at weekends, to avoid impacting undergraduate use – we also use Linux rather than Windows as the underlying system to get the full Condor features and further disambiguate it from the undergraduate teaching environment).

IT staff provide training courses and one-to-one support, as well as a code optimization service. We have added a GUI – called *DropAndCompute*, as well as an active web-based monitoring tool that is clickable down to a fine level of detail per job. We have also developed a tool that automatically checks all users' jobs have been adequately described in their submission files. Full details of the Condor system can be found here: condor.eps.manchester.ac.uk.

Report on Numerical Python Seminar

The EPS IT Applications team recently delivered a seminar on numerical Python to the School of Mathematics. We covered the basics of the language along with demonstrations and discussions of technologies that are of particular interest to scientists. Python is a mature, free scripting language which can be used as an effective replacement for commercial mathematical and statistical products such as MATLAB and Mathematica. If you are interested in learning more, contact the EPS Applications team at applicationsupport-eps@manchester.ac.uk.

Manchester Conference on Application of Emerging Tech

After the success of the GPU Club and Manchester's past involvement in the MRSN, researchers from across the University are looking to hold a national conference in Manchester in Spring 2015, with plenaries and peer-reviewed presentations focusing on emerging technology and the techniques required to obtain near-optimal performance from the likes of GPUs, FPGAs and Intel Xeon Phi. Plans are at an early stage and researchers who would like to get involved in the planning should contact Dr. Ben Rogers.

Faculty Contact Emails

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MHS-ITResearch@manchester.ac.uk.

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FLS-ITResearch@manchester.ac.uk.

Next edition

The next edition of this newsletter will be circulated at the end of October 2013.

If you have any news to contribute, please contact the IT Services Research Lead, Ian Cottam: ian.cottam@manchester.ac.uk before 25 Oct 2013.