

IT Services

Supporting your research

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

Welcome to issue #8, November 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/.

Computationally Intensive Research (CIR)

Around mid November we took a snapshot over the last half-year of CSF and Condor usage, and a summary table is below (just showing the top ten by EPS School or Faculty).

Order	Processor Core Usage (in Years)	Facility	EPS School / Other Faculty
1	803	CSF	EPS MACE
2	303	CSF	EPS CEAS
3	270	Condor	EPS Computer Science
4	152	CSF	MHS
5	121	CSF	EPS Chemistry
6	91	Condor	EPS Physics
7	81	Condor	Humanities
8	41	CSF	FLS
9	23	Condor	EPS Chemistry
10	23	Condor	EPS CEAS

Of over 700 users only 35 use both CSF and Condor, from the EPS Schools of Chemistry and Chemical Engineering. To a rough approximation, the CSF+Condor combination is used by Manchester researchers to compute 2000 years worth of results every 6 months.

The notion of *CIR* incorporates High Performance and High Throughput Computing, amongst other things. Shortly, academic stakeholders will be asked to fill in a survey about their use of CIR facilities (such as the CSF, N8 HPC, EPS Condor, etc), and there will be stakeholder meetings. This is to aid us in producing a clear strategy.

N8 HPC Usage by Manchester Project

This is just over the 3-month period from July through September 2013.

	Project	PI	EPS School / Other Faculty	Processor core usage (In Years)
1	Development and Implementation of Embedded LES into OpenFOAM	Alistair Revell	EPS MACE	173
2	Optimisation algorithms for gait generation	Bill Sellers	FLS	13
3	Large scale parallel computing of complex fluid flows	Xue-Feng Yuan	EPS CEAS	7
4	Protein conformational change using molecular simulation	Richard Bryce	MHS	4
5	Ceramic Composites for Fusion Power	Paul Mummery	EPS MACE	<1 (35 hours)
6	Smoothed Particle Hydrodynamics (SPH) modelling of 3-D Turbulence	Ben Rogers	EPS MACE	<1 (0.3 hours)

N8 HPC Annual Report Released

N8 HPC has recently released its first ever annual report which is now available from the N8 HPC website (www.n8hpc.org.uk). Over the summer Principal Investigators (PIs) of all registered projects on N8 HPC, including those at Manchester, were asked to complete a survey to demonstrate the impact of using N8 HPC on their research. This information has now been collated into a publicly available annual report.

Even though the service had only been open to all for 5 months at the time of the survey, the overall findings show that researchers are happy with the service and facilities. Here at Manchester N8 HPC has made an impact through the inclusion of N8 HPC in Knowledge Transfer Projects and its use in 3 industrial studentships as well as several papers and books.

If you would like to apply for access to N8 HPC then please complete the application form available on the website (n8hpc.org.uk/research/gettingstarted/) or contact Manchester@n8hpc.org.uk.

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.

FLS Academic of the Month

Congratulations to Bill Sellers (Faculty of Life Sciences), who has been awarded access to PRACE Tier 1 systems via the DECI-11 call. The requested computational resource, 15 million core hours, is going to be used to test the scaling of a novel asynchronous genetic algorithm in preparation for a more ambitious bid for PRACE Tier 0 access. The algorithm is used in his software GaitSym, which generates gaits for living vertebrates (including humans), extinct vertebrates (including dinosaurs), robots and more fun applications such as aliens in movies and cartoons. To give an idea of the significance of the award, The University of Manchester EPS Condor Pool has provided 16,572,045 core hours (1891 years) of resource since the service was launched. So Bill has requested almost the entire history of the University's Condor Pool to himself!

Lee Margetts (Research Applications and Collaboration Team) is a co-applicant on the grant and provided "HPC specific advice" on how to ensure the proposal stood out from other submissions. If you are thinking about submitting a proposal to access PRACE facilities, Lee would be pleased to help review the proposal before submission. Lee is Manchester's representative on the PRACE-Manchester Memorandum of Understanding and is a member of the PRACE Industrial Advisory Committee; so he has some unique insights into the difference between success and failure.

Manchester Cancer Research Centre

The University of Manchester was recently awarded – jointly with the University of Cambridge - £8.8 million to become a CRUK & EPSRC Cancer Imaging Centre.

The imaging centre at The University of Manchester, led by Professor Alan Jackson, is part of the [Manchester Cancer Research Centre](http://www.mcrc.manchester.ac.uk) (www.mcrc.manchester.ac.uk), a partnership between the University, Cancer Research UK and [The Christie NHS Foundation Trust](http://www.christie.nhs.uk) (www.christie.nhs.uk). Research at this centre will include analysing how second cancer drug treatments may increase the uptake of a first cancer drug and the development of sophisticated, quantitative imaging studies to revolutionise drug development and cancer treatment. One example is their work using radioactively-labelled drugs with positron emission tomography (PET) imaging equipment, which can see whether drugs used to treat brain tumours are delivered where they are needed.

Professor Ian Jacobs, Vice-President of The University of Manchester and Dean of the Faculty of Medical and Human Sciences, said: *"This is an exciting development which will provide added value to our efforts in cancer research by investing in and linking the expertise and research resources in cancer imaging in Manchester and Cambridge. We can anticipate that it will, in due course, result in advances in cancer knowledge and cancer care that will save lives and benefit people in the North West, across the UK and worldwide."*

Humanities Faculty IT Research Development Team

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

The publishing of a new site for the *I Sign, Therefore I Am* project is imminent. The project investigates the history of 9th-12th century Italy via the study of legal documents witnessed by the medical professionals of the day. This site will provide public dissemination of the information input into a database previously developed by the team. The PI was Dr Clare Pilsworth from the School of Arts, Languages and Cultures. Contact is: Phil Bradbury.

Manchester's Turing Fellow Receives Prestigious Award at Supercomputing 13 (SC13)

University of Manchester Turing Fellow, Professor Jack Dongarra, has been awarded the ACM and IEEE Computer Society 2013 Ken Kennedy Award for *Software Technologies that Power Supercomputers to Tackle Big Scientific Problems*. The award was officially presented at the opening of the SC13 Supercomputing Conference in Denver, Colorado on 19 November 2013. See rac.manchester.ac.uk/?p=539 to read the full article.

House of Lords Select Committee Inquiry into Scientific Infrastructure

The report from the *House of Lords Select Committee Inquiry into Scientific Infrastructure* has just been published, with the statement "The potential of the UK's large scale scientific resources is being compromised by the lack of a long term strategic investment plan". See www.parliament.uk/business/committees/committees-a-z/lords-select/science-and-technology-committee/news/scientific-infra-report-published/ and comments on it by the leaders of the Software Sustainability Institute here: www.software.ac.uk/blog/2013-11-18-six-things-funders-can-do-maximise-return-investment-software-development.

There was a collective submission by Professor Luke Georghiou, Vice President for Research, on behalf of N8 and the University. This contained some input from our N8 HPC service on the investment so far in e-infrastructure that is reflected in the findings.

New Fortran Mailing List

A new list for University Fortran users: fortran@listserv.manchester.ac.uk.

To join, those interested can either email lee.margetts@manchester.ac.uk directly or send a message to: listserv@listserv.manchester.ac.uk with: *subscribe fortran* in the body of the message.

Image-based Modelling Club

The next meeting of the Image-based Modelling Club will be held at 2.00pm-4.00pm on Wednesday 11 December 2013. The theme will be *Image Registration and Digital Image Correlation*. With talks from EPS and FLS, the meeting will give the opportunity for EPS researchers to see how the techniques are used in FLS and vice-versa. Please visit the following website for further details and registration: wiki.rac.manchester.ac.uk/community/IBM. If you would like to make a short announcement in the meeting about a recent publication, job opportunity or technical challenge, please contact Lee Margetts beforehand (lee.margetts@manchester.ac.uk). Refreshments will be provided after the talks to encourage networking.

Team Areas

The University will shortly introduce *Team Areas* – an online document management and collaboration work space, built on Microsoft's Sharepoint technology, where you can collaborate on documents, information and ideas with colleagues in a secure environment. These colleagues may be in your own school, in another school or faculty across the University or an external partner, such as another University.

Within a Team Area, you can:

- share documents and files
- contribute to discussion boards
- share calendars
- set up a blog
- create Wikis to log progress or capture ideas

All existing Livelink site owners and users will be able to request a Team Area from December 2013. All members of the University will be able to request a Team Area from early 2014.

University GPU Club

A very informative GPU Club on applicability of GPUs, Xeon Phi and dataflow was held on 13 November 2013, for which the presentations are now available on the GPU Club web site (gpu.manchester.ac.uk). Information on the University's Xeon Phi system is also there.



Discounted NVIDIA cards, as per our CUDA Research Centre award, are now available. For now, please email its-research@manchester.ac.uk (details will soon be available via the ITS Knowledge Base).

Please let us know what topics you would like the club to discuss in 2014.

Interactive Computational LINUX Environment (INCLINE)

INCLINE, also known as the iCSF, is a new service for researchers who have a need to run **interactive**, computationally intensive jobs. Examples include: development and testing of parallel or data-intensive code; GUI-based use of applications such as Abaqus, MATLAB, R, and Stata, particularly where a lot of memory is required.

INCLINE is currently in user-testing.

The system will be run on the same sustainable, financial model as the CSF: access is limited to members of groups that have contributed funds to the facility.

Academics are encouraged to contribute to INCLINE instead of purchasing computational workstations. For more information about this new service, please visit the Web site at ri.itservices.manchester.ac.uk/icsf/ or email the Research Infrastructure team at its-ri-team@manchester.ac.uk.

CSF Downtime

The CSF will not be available on 3–4 December 2013. This is primarily because of a major network upgrade taking place in one of the University data centres on the 3rd. We are taking the opportunity to apply some operating system patches on the 4th.

It will be possible to login to the system and submit jobs until immediately before it is taken down. However, jobs which are still running when the system is taken down will be killed. (Jobs that are queued-waiting at this time should be considered at-risk.)

For updates on 3 December 2013, and thereafter, please monitor ri.itservices.manchester.ac.uk/csf/overview/service-news/. If you have any questions about this downtime, please email its-ri-team@manchester.ac.uk.

National Instruments' Labview

The University of Manchester has a full site license for National Instruments' Labview software, which makes it available for all staff and students here. A recent addition to the benefits of our site license is a set of free, online training courses for Labview and its many add-ons. More details can be found on the IT Services applications website: https://www.applications.itservices.manchester.ac.uk/show_product.php?id=245&tab=training.

SciProgramming

You may have seen in the news that Wolfram Research have made their flagship product, Mathematica, available for free for personal use on the low-cost Raspberry Pi computer. news.cnet.com/8301-1001_3-57613462-92/premium-mathematica-software-free-on-budget-raspberry-pi/.

The University of Manchester has a full site license for Mathematica, which allows all staff and students to install it. Full Installation details are available at (link only works on campus): https://www.applications.itservices.manchester.ac.uk/show_product.php?id=38&tab=install.

If your machine is permanently connected to the University network, you should use the network licenses. Otherwise you can use the standalone licenses. Mathematica is also available on all cluster PCs running the University managed desktop as well as on high performance hardware such as the Computational Shared Facility and Condor.

Finally, Mike Croucher (from EPS IT) spent a couple of hours playing with the Raspberry Pi version over the weekend and wrote up his thoughts on his blog: www.walkingrandomly.com/?p=5220.

Also In Progress...

Core Wired Network

Progress details are being posted here www.staffnet.manchester.ac.uk/news/display/?id=11177.

DropOff – large file transfer

The service trial was used successfully by some 600 people (400 at Manchester and 200 off site), and is now being developed as a production service. We will likely change its name to *ZendTo* to distinguish it from cloud storage systems like Dropbox.

Cloud (Encrypted) Storage

Dropbox users will soon be able to use the secure encryption layer *ncrypted Cloud* as part of a trial period. We are just awaiting an update to the iPad version and improvements to the "invite to join in" system. Contact ian.cottam@manchester.ac.uk for details. Note that such an encryption layer does not stop you sharing folders with external collaborators (although they do need to use a free download).

Sponsor a Visitor's WiFi Account

A service trial will be starting shortly: you can contact ian.cottam@manchester.ac.uk if you would like to be an early adopter.



An open invitation to all
University of Manchester
Academics and Researchers:

IT Services for Research Forum

Wed 18 December, 1pm - 2pm, 6.207 University Place.
No booking required - just drop in.

Prof Chris Taylor and Ian Cottam (IT Services Research Lead)
will speak on:

COMPUTATIONALLY INTENSIVE RESEARCH (CIR)

How CIR can help your research

The current state of CIR

Moving towards a CIR strategy

Followed by an open Q&A session

www.itservices.manchester.ac.uk/research

Lunch provided - served from 12.30pm

**ENGINEERING AND PHYSICAL SCIENCES · HUMANITIES
LIFE SCIENCES · MEDICAL AND HUMAN SCIENCES**

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 December 2013.

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

ian.cottam@manchester.ac.uk before 18 Dec 2013.