

Research *it*Supporting your research

A newsletter from IT Services: Research IT

Welcome to issue #25, May 2015, in a <u>regular</u> <u>series</u> of updates on IT research support and facilities for postgraduates, researchers and academics of The University of Manchester.

Your main contact email addresses for research computing support are given on the last page; emailing your queries this way will automatically raise a job for you in the *Remedy* tracking system. Every day, routine work should continue to be submitted through the IT Service Desk on +44 (0) 161 306 5544 or via online submission at: www.manchester.ac.uk/servicedesk.

Web Page: Research IT

The web site for our support areas and all contact details is available here:

www.its.manchester.ac.uk/research/.

Clickable Web Links

If you have received a printed copy of this newsletter and wish to follow the links, staff can download an electronic copy with clickable links at:

http://documents.manchester.ac.uk/Doculnfo.aspx?DocID=24111

The link to #24 of the Newsletter was clicked on nearly 1000 times in April. Please help us increase our readership by forwarding the link to colleagues.



Introducing the New Head of Research IT

We'd like to extend a warm welcome to our new Head of Research IT, Kurt Weideling, who joined us on 13th April.

Kurt most recently worked at Monash University in Melbourne, Australia where he managed the IT services group of approximately 200 staff delivering a wide range of IT platforms and services in support of research and teaching activities.

Prior to Monash University, Kurt lived in Raleigh, North Carolina and worked at Quintiles Transnational where he was responsible for the development of clinical informatics solutions in support of clinical trials. He is looking forward to gaining a greater understanding of the many challenges faced by researchers at the University of Manchester and how the Research IT team can work with them to help achieve their research outcomes.

Kurt is a keen rock climber and is looking forward to exploring the various crags of the Peaks and Lakes districts. In early May he will be joined in Manchester by his wife, who is originally from Oxfordshire, and their well-travelled cat.



Research Computing Facilities

IT Services supports University of Manchester researchers and staff on a wide range of facilities including your own desktop, University owned clusters and externally hosted facilities. Links to a range of facilities are provided below. If you would like to find out more about the best option for your particular research needs, please contact us.

- University of Manchester Computational Shared Facility
- University of Manchester Condor Service
- N8 Regional High Performance Computing Service
- ARCHER UK High Performance Computing Service
- <u>UK Hartree Centre Facilities</u>
- PRACE EU High Performance Computing Service
- XSEDE USA High Performance Computing Service

Access to ARCHER

Researchers can request access to test the UK High Performance Computing Service (ARCHER) for suitability for their work all year round via a lightweight application process. <u>Click here</u> for details.

Isight, Tosca and fe-safe

The SIMULIA software *Isight*, *Tosca* and *fe-safe* will be made available for research use to University of Manchester staff and students. In brief *Isight* is used to combine multiple models and applications in a single process flow, *Tosca* is for non-parametric structural optimization and *fe-safe* is for fatigue analysis. Further information can be found here.

If anyone is interested in using these in their research please email <u>EPS Applications Support.</u>

Research Computing Training

PRACE Advanced Training Courses

The Partnership for Advanced Computing in Europe (PRACE) offers <u>free courses</u> at different HPC centres in Europe. Courses offered in May and June 2015 include:

11-12 May	Performance Analysis and Tools	Spain
11-13 May	Introduction to Parallel Computing	Italy
13-14 May	Heterogeneous Programming	Spain
15 May	Programming ARM prototypes	Spain
18-22 May	18th VI-HPS Tuning Workshop	France
20-21 May	PGAS Communications Libraries	Bristol
25-26 May	Introduction to HPC for Women	Ireland
26-28 May	Uncertainty Quantification	France
2-5 Jun	Introduction to CUDA Programming	Spain

Heterogeneous Programming	France
Atomic and Molecular Calculation	France
Hybrid MPI/OpenMP Programming	France
Workshop HPC Methods	Italy
Performance Analysis Workshop	Durham
Programming Paradigms	Italy
	Atomic and Molecular Calculation Hybrid MPI/OpenMP Programming Workshop HPC Methods Performance Analysis Workshop

University of Manchester Courses

IT Services offer a portfolio of short courses in research computing. <u>Click here</u> for the latest schedule. We also tailor courses for doctoral training programmes and arrange on-demand training with external tutors. Please contact us for details.

Upcoming Events

OCF and Manchester Informatics Big Data Symposium 18th June – registration now open!

OCF together with Manchester Informatics, are hosting a Big Data Symposium on the 18th of June at the University of Manchester. This is a one-day event showcasing the important role of big data analytics in a broad range of sectors including biomedical research, astronomy, telecommunications, social media, and security & resilience. The broad and diverse programme aims to highlight to researchers the breadth of multi-disciplinary research currently being undertaken in this rapidly growing field, and to illustrate the value of collaboration across the different sectors.

Speakers include representatives from SKA, Manchester City Council, Oracle, ARM and The Hartree Centre as well as researchers from the University of Manchester. Registration for the event is free but required and can be found on the event website along with the full agenda.

Pint of Science Festival 2015

Have you ever wondered why we haven't found a cure for cancer or Alzheimer's? Whether nuclear power is a better form of energy than solar power? Why our weather forecasts go bad? Or even how schools support children with dyslexia?

Find out the answers to these questions and more at the Manchester Pint of Science Festival, running from 18-20 May 2015. The festival will be held in 5 pubs across Manchester and aims to deliver interesting, fun and relevant talks on the latest science research in an accessible format to the public- all in the pub!

To find out more about the festival please visit the event website.

Registration open for EMiT 2015

EMiT 2015 follows on from last year's successful inaugural conference and focuses on emerging computational technology showcasing how it is revolutionising today's research across all research fields as well as influencing tomorrow's applied computing.

The aim of the event is to bring together leading key figures in the computing communities as well as the end users of new software & hardware in industry and universities to address aims including identifying the latest trends in hardware development for novel computing; sharing how best to exploit Emerging Tech for application; and a focus on new techniques, their development and transfer to new areas.

The full programme, including details of the international keynote speakers, is now available on the <u>EMIT website</u>. To register for the event please visit the website.

nCryptedCloud Workshops

During the period 18 to 20 May 2015 IT Services will be hosting Tom Murphy from nCryptedCloud of Boston, MA, USA.

We have a site-wide licence for their <u>software</u> <u>encryption layer</u>, which works on top of Dropbox, Google Drive, etc. Tom will be running a series of short workshops on the use of their software. The short (repeated) sessions will be held in room 205 of the Williamson Building. Please let <u>lan Cottam</u> know your preferred day (of the current three on offer) and time(s); and we will get back to you when we have further details.

Other News

New social network for PhD students using HPC

If you are a PhD student using High Performance Computing (HPC) facilities for your research, would you find it useful to be part of a broader network of likeminded folk across campus to collaborate and share ideas with? If so, please subscribe to the accelerate-phd@listserv.manchester.ac.uk list or contact Lee Margetts to be added. In this context, HPC includes the use of any computing facility beyond a standard desktop PC that is used to carry out research, including emerging technologies such as the Intel Xeon Phi, GPUs, FPGAs and ARM processors.

Do you host data for University academics and external bodies?

Do you need to share or look after research data generated by external collaborators? If so, please respond to this <u>survey</u> from IT Services on SharePoint to share your experiences (good or bad) or future requirements so that IT Services can help support you in the future.

When logging into SharePoint please use the following approach-

Username: ds\your university username Password: your university password

If you have any questions please contact <u>Mary McDerby</u> in the Research IT team.

The Condor Clock

By the time you read this the clock on our Condor High Throughput Computing pool will have ticked over the 2,500 mark. That's 2,500 years of accumulated computational results for UoM researchers, from contributing to the search for exoplanets to helping to combat cancer - just two of many exciting research topics that this service contributes to.

If you want to find out more about the Condor pool please contact <u>lan Cottam</u>.

Out now - Industrial Applications of High-Performance Computing: Best Global Practices

Of potential interest to many researchers who collaborate with industry as well as HPC support staff, this recently released book offers a global overview of high performance computing (HPC) for industrial applications, along with a discussion of software challenges, business models, access models (e.g., cloud computing), public-private partnerships, simulation and modelling, visualization, big data analysis, and governmental and industrial influence. Also included are testimonials of industrial users whose R&D has benefitted from HPC resources via PRACE, or from national HPC resources hosted by PRACE partners.

For more information and to order please click here.

High Throughput Computing on Windows

This month we have a guest article from IT Relationship Manager Ian Cottam, who writes:

Users of the Condor Pool, as well as regular readers of this newsletter, will know that the University Condor Pool runs on the Linux operating system. This decision was taken years ago to differentiate cleanly the use of clusters of PCs for teaching (under Windows) and high throughput computing for researchers (out of hours: evenings and weekends). That is, it has been impossible to argue that Condor negatively impacts the "student experience": the worst case being that a student has to restart a PC she wants to use should she be in late and finds it running Linux.

This design also means that Windows-only applications could not benefit from Condor and high throughput computing.

Recently, IT Services have added 5 high performance PCs, running Windows 8 and some Windows-only applications, to the Pool for a research group in the School of EEE. These PCs can only be accessed by that group, but being part of the Pool gives the research group access to the entire Condor infrastructure (submit node, storage, etc.).

This addition of Windows-based compute nodes proved to be straightforward, and we observed that no special rights to join the Condor Pool were needed, other than being a registered on-campus computer. (Note: such special admin rights are needed, for security and management reasons, to add new submit nodes, but that is not the case under discussion).

We are therefore thinking of documenting how this is done, so that similar research groups to the above can choose to add their Windows-based PCs, and likely Windows-only applications, into the Pool. This would be documented for self-service by the research groups concerned, although IT could advise on any issues. It is possible to add Windows compute nodes either for general community access or dedicated to the owning research group.

The expectation is many will start off fully dedicated, but over time some subset could become generally available. Clearly, software licence conditions need to be reviewed and respected as part of making such a choice.

If this is of interest to you, please let <u>lan Cottam</u> know.

Finally, note that we are talking about unmanaged PCs in research groups running Windows 7 or 8 (and soon 10, we expect), not the Managed Desktop.

Vacancies

Are you trying to recruit someone? Let us know and we will help you advertise here.

For jobs in Research IT, please contact <u>Dr Michael Bane</u> (research applications) for details.

Useful Links

Faculty of Humanities Blog for Researchers

Faculty of Humanities Training Hub for Postgraduates

Subject-specific Email Lists

Please note that these email lists are subject specific discussion forums, rather than a way of contacting IT Services.

University HPC PhD Network

finite-elements@listserv.manchester.ac.uk

fortran@listserv.manchester.ac.uk

sciprogramming@listserv.manchester.ac.uk

university-gpuclub@listserv.manchester.ac.uk

Contact Emails

Research IT:

its-research@manchester.ac.uk

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 beginning of June 2015.

If you have any news to contribute, please contact Gillian Sinclair gillian.sinclair@manchester.ac.uk and Dalinder Sall dalinder.sall@manchester.ac.uk at any time.

Items received before 22nd May 2015 will be included in the next edition. News from academic colleagues and researchers are most welcome.