

Research IT

Helping you achieve your research outcomes

A newsletter from IT Services: Research IT

Welcome to issue #33, March 2016, in a <u>regular series</u> of updates on IT research support and facilities for postgraduates, researchers and academics of The University of Manchester.

Your main contact email address for research computing support is given on the last page; emailing your queries this way will automatically raise a job for you in the IT Services helpdesk system. Every day, routine work should continue to be submitted through the IT Service Desk on +44 (0) 161 306 5544 or via the Support Centre online at:

www.itservices.manchester.ac.uk/help/

Research IT Twitter

To keep up to date with all the news from Research IT and beyond, please subscribe to our Twitter feed @UoM eResearch.



News

Introduction of Research Virtual Machine Service (RVMS) Platform

In 2015 Research IT ran a pilot for a new Research Virtual Machine Service (RVMS) utilising existing infrastructure. This pilot had only limited capabilities but did allow us to learn more about the best way to use this technology to support researchers and proved the demand for the service.

We now have a dedicated RVMS platform in production. Limited-specification VMs are available free-at-the-point-of-use (e.g. 1 core, 4 GB RAM, 20 GB storage). Research groups who require multiple VMs and/or VMs of higher specification can contribute financially to the platform and they will receive VM capacity equivalent to their contribution.

The platform should be considered complementary to off-campus, commercial services such as Amazon and Azure. The Research IT platform is particularly suited to VMs which: are long-lived and required significant CPU and/or network traffic; require secure, fast access to Research Data Storage (aka Isilon); need tight integration with SCRE@M (the CSF, DPSF, iCSF, etc.).

Two support options are available: VMs on which researchers have root/admin access and there is no guaranteed support from Research IT; VMs on which Research IT will manage the operating system (e.g. patches and security) and basic software stack (e.g. Web server with standard configuration). Support of custom software stacks is NOT included as part of this service and if you have specialised requirements in this area you should discuss with your IT partner.

To find out more about this service and how to access it, please visit our <u>website</u> or email its-research@manchester.ac.uk.

Research IT Core Application Suite

Research IT is inviting feedback on a proposal to implement a 'core suite' for research applications. The intent of this proposal to is to define a set of applications used to advance research in the areas of compute, data analysis and visualisation that are relevant & valuable to a substantial proportion of the UoM research community and potentially warrant central funding and extensive support.

We would welcome your feedback on the following questions:

- Do we have the right mix of applications in the core suite?
- Does the service offering look right is there anything missing that you would consider valuable?
- Do you see value in the broad-based deployment of a highly usable data visualisation tool such as Spotfire or Tableau?

Any feedback or questions should be directed to <u>Kurt</u> <u>Weideling</u> by **11**th **March 2016.** More detailed information is available <u>here</u>.

Food Bug Club Website and Games

The Research Software Engineering (RSE) team within Research IT recently completed a project with Prof. Dan Rigby and Dr. Caroline Millman from the School of Social Sciences to help raise food safety awareness in schools. Food Bug Club brings together inspiring food safety classroom resources for food and science teachers as well as providing a platform for new material as it is developed. Research IT developed the Food Bug Club website and two online games based on MicroTrumps - Top Trumps-style playing cards that depict food-borne microorganisms and important information about them. Why not try playing the games and test your knowledge of food safety on the brand new Food Bug Club website?

Food Bug Club was funded using an Impact Accelerator Award from the <u>ESRC</u> and was developed in association with <u>Chilled Education</u> and the <u>Food Teachers Association</u>.

CSF forges ahead!

This month we are celebrating: the CSF has reached its 5th birthday! We recently replaced the infrastructure servers within the facility (login nodes, fileservers, management nodes).

With the addition of 46 Intel "Haswell"-based nodes (each 24 cores, 128 GB memory) the total core count is now 7300. A further £338k has already been committed by research groups in 2016.

This, together with some investment via the Revolving Green Fund will likely mean an additional 58 Haswell-based nodes. That means we will soon have nearly 8700 cores, from a total investment in the CSF of about 2.5 million pounds!

Simon Hood (Research Infrastructure Manager) will be leaving the team at the end of March to become Head of Research IT at The University of Sheffield. We would like to thank him for his 16 years of service to the research community here at Manchester and wish him all the very best for the future. A new Research Infrastructure Manager will be appointed in due course.

The next procurement of compute nodes will take place in May 2016. Please get in touch with George Leaver and Pen Richardson via its-ri-team@manchester.ac.uk if you would like further information.

SC15 Conference in Austin, TX

In November last year Simon Hood and Kurt Weideling of Research IT had the opportunity to attend the annual Super Computing conference event, held in Austin, TX.

In addition to plenty of ribs and the great live music that Austin is famous for, the conference offered the opportunity to learn more about developments in the field of super computing and related areas. Kurt and Simon attended a number of workshops on key topics including, HPC architecture, big data analytics, visualisation and super computer procurement, and also held a number of meetings with key suppliers including Dell, DDN and SGI.

During the trip Kurt also had the opportunity to visit the University of Texas at Austin where he toured their state of the art visualisation laboratory and held meetings with academics involved in the digital humanities.

If you are interested in learning more about any of the specific topics covered at the conference or vendor developments, please get in touch with <u>Kurt</u> or <u>Simon</u> or visit conference <u>website</u>.

Upcoming Events

Affordable Virtual Reality Show and Tell

Experts from Samsung will be visiting the University of Manchester on **Monday 14**th **March 2016** to talk about their virtual reality headset – "Samsung GEAR VR". The headset costs less than £100 and is used with a smart phone; the latter providing both the display and the hardware for 3D graphics processing. This affordable price point is really exciting as, until recently, a VR headset would set you back tens of thousands of pounds. The meeting will start at 2pm with a short talk on the potential uses of the Samsung GEAR VR headset within a University setting. The rest of the meeting will have a "show and tell" format. Samsung are bringing a number of headsets along for attendees to try out the technology for themselves.



If you would like to attend, please fill in the online form here. The meeting is organised by Dr Lee Margetts in the School of Mechanical, Aerospace and Civil Engineering.

Data Science Club March Meeting

The third meeting of the UoM Data Science Club will take place **2pm - 3:30pm on Thursday 17th March** in Co-Lab, Kilburn Building.

Following on from excellent feedback from January's event, researchers are once again invited to give a "lightning presentation" highlighting a data problem, solution, tool or database challenge. There will also be updates on the Triangulum "smart city" project as well as discussions on data science training requirements and opportunities.

If you would like to attend the next meeting registration is required (https://dscmar2016.eventbrite.co.uk) or to be kept up to date with Data Science Club activities please join the mailing list here.

Collaborations Workshop 2016 (CW16) + Hackday

CW16 will take place on **21-23 March 2016** at the Royal College of Surgeons of Edinburgh.

The Software Sustainability Institute's annual Collaborations Workshop 2016 (CW16) – focusses on hot topics, sharing of best practice and nascent tools and approaches in research software. If you write, use or have an interest in software that enables better research then CW16 is your must attend event of the year!

The main focus at CW16 will be software and reputational credit. Other themes will also be investigated, including reproducible research, data science, collaborative working, and the sharing of code and data. For more information and registration please visit the event website.

N8 HPC Network Event - Unveiling the impact of HPC in Soft Condensed Matter

Computer simulations and modelling play a crucial role in understanding the complex phase behaviour and dynamics of Soft Condensed Matter. The efficient use of High Performance Computing (HPC) resources, including state-of-the-art software and hardware, can be of paramount importance to address problems that are extremely challenging due to the significant time and length scales associated.



This workshop will take place on 12th April 2016. It will bring together members of the national community with interests in discovering the impact HPC on their research and it is especially designed to promote discussions and future collaborations in the area of computational Soft Matter.

Registration is free of charge, but it is required due to the limited number of places available (40). Registration can be completed <u>online</u>.

EMiT 2016 Conference

EMiT (EMerging Technology) conference series will hold its 3rd annual event on **2-3 June 2016** at Barcelona Supercomputing Centre, which is co-hosted by Mont Blanc and The University of Manchester.



The EMiT conference series brings together experts from all areas of computing to examine how to best take advantage of the changing landscape of computer hardware and novel techniques.

The conference themes include: Device-independent Compilers; High Level Languages; Low Power & Energy Efficient Computing; Advances in Novel Hardware; Numerical Algorithms; Applications.

Registration at just €100 (€75 for students) is now open.

SC16 Conference in Salt Lake City, Utah

SC16, the premier annual international Conference on high-performance computing, networking, storage, and analysis, will be held in Salt Lake City, UT, USA, Nov 13-18, 2016. The SC16 Conference Committee solicits submissions of technical papers that introduce new ideas to the field and stimulate future trends on topics related to high-performance computing, including algorithms; applications; architecture and networks; clouds and distributed computing; data analytics, visualization, and storage; performance measurement, modeling, and tools; programming systems; state of the practice; and system software.

New this year:

Double-blind review: SC16 will use a double-blind review process, which is a change from prior years. Details are available on the SC16 website.

Reproducibility initiative: As part of an initiative that aims to increase the level of reproducibility and replicability of results, SC16 invites authors of technical papers to volunteer to publish their methodology, code, and data with the paper, if their paper is accepted to SC16.

Important dates:

- Submissions open: March 1, 2016.
- Abstracts due: March 27, 2016 (firm deadline).
- Full papers due: April 3, 2016 (a traditional one week extension will be given until April 10, 2016; no further extensions will be granted).

More information about SC16 Technical Papers is available online.

Email contact: papers@info.supercomputing.org

Other News

Research IT Management Changes

Michael Bane and Robin Pinning are both moving on from the University of Manchester to pursue other opportunities, Michael with his own consulting business and Robin at the Hartree Centre. Research IT is currently implementing a new management structure that will see new roles implemented and appointed, but in the meantime any N8-related queries should be directed to <u>Gillian Sinclair</u>, whilst any research application issues should be directed to <u>Robert Haines</u> or <u>Kurt Weideling</u>. If you have any queries about the new management restructure and what it means for research support in your area please contact Kurt Weideling.

Vacancies

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

Researcher Satisfaction Survey

We value your feedback; please take a moment to tell us how we're doing by completing this <u>short survey</u>.

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 (N8 HPC)
- PRACE EU High Performance Computing Service
- UK Hartree Centre Facilities
- PRACE EU High Performance Computing Service
- XSEDE USA High Performance Computing Service

Access to ARCHER

Researchers can request anything from pump-priming access to full projects on the UK High Performance Computing Service (ARCHER) for suitability for their work all year round via a lightweight application process. Click here for details.

Research Computing Training

University of Manchester Courses

Research IT is running a short series of hands-on training courses which provide skills for researchers to further enhance their research. For information on our courses or other training that we can provide, please take a look at our <u>training catalogue</u> or <u>contact us</u>.

Courses offered in March 2016 include:

3 Mar	Introduction to numerical computing with	
	<u>Python</u>	
17 Mar	Programming in MATLAB	
4 Apr	Introduction to Data Visualization and	
	<u>Analysis</u>	

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 March and April 2016 include:

8-11 Mar	Spring School in	Finland
	Computational Chemistry	
8-11 Mar	Introduction to Modern	Italy
	<u>Fortran</u>	
14-15 Mar	Simulation Environments for	Spain
	<u>Life Sciences</u>	
14-16 Mar	Parallel I/O and Portable	Germany
	<u>Data Formats</u>	
14-16 Mar	C-C++ multicore application	France
	programming	
14-15 Mar	Data Storage and	Edinburgh
	<u>Management</u>	
17-18 Mar	OpenMP and OpenACC GPU	Germany
23-24 Mar	Software Carpentry	London
30 Mar –	Advanced Fortran	Finland
1 Apr	<u>Programming</u>	
4-8 Apr	Fortran for Scientific	Germany
	Computing	
4-7 Apr	Advanced Topics in High	Germany
	Performance Computing	
5-7 Apr	Advanced usage on Curie:	France
	parallelism, optimisation, IO,	
	<u>tools</u>	
6-8 Apr	HPC enabling of	Italy
	OpenFOAM® for CFD	
	<u>applications</u>	
11-12 Apr	Systems Workshop:	Spain
	Programming MareNostrum	
	<u>III</u>	
12-15 Apr	Cray XC40 Optimization, and	Germany
	Parallel I/O Courses	
18-22 Apr	21st VI-HPS Tuning	Germany
	<u>Workshop</u>	
19-22 Apr	Debugging and Optimization	Italy
	of Scientific Applications	
20-22 Apr	Scientific Python	Liverpool
21-22 Apr	Parallel filesystems and	France
	parallel IO libraries	
25-27 Apr	GPU Programming with	Germany
	CUDA	
26-28 Apr	HPC Tools	Durham

Subject-specific Email Lists

Join the email lists below to collaborate and share ideas with a broad network of staff across campus. 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

Useful Links

Faculty of Humanities Blog for Researchers

Faculty of Humanities Training Hub for Postgraduates

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Online Copy

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/display.aspx?Docl <u>D=27031</u>

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Next edition

The next edition of this newsletter will be circulated at the beginning of April 2016.

If you have any news to contribute, please contact Ignas Daugalas <u>ignas.daugalas@mancherster.ac.uk</u> and Gillian Sinclair <u>gillian.sinclair@manchester.ac.uk</u> at any time.

Items received before 25 March 2016 will be included in the next edition. News from academic colleagues and researchers are most welcome.