

Research IT

Helping you achieve your research outcomes

A newsletter from IT Services: Research IT

Welcome to issue #30, October 2015, in a regular series 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/

New Website for Research IT

We are currently redeveloping the Research IT website to bring it in line with our new platforms and services. The link will be posted in the newsletter when it's ready.

Research IT Twitter

The Research IT team now have a voice on Twitter. We will be tweeting about a wide variety of exciting topics from the world of e-Research to help keep you informed of the cutting edge of the field. From the very latest news on our fast developing platforms and services, to hand-picked tweets from the rest of the world. Please follow us at @UoM_eResearch.



Research Data Storage Update

The Research Data Storage Service provides centrally hosted resilient storage for academic-led research projects. As part of a recent review it has been decided to reduce the maximum amount of storage available free at the point of use from 20TB to 8TB. This will help share the amount of University funded storage more equitably across researchers whilst still ensuring that the substantial majority of projects do not incur any additional costs.

This amended limit will only affect new requests for storage made from 22 September 2015 and will not impact any previous allocations. For those research projects requiring additional research data storage beyond 8TB, this may be purchased. Please see the RDS website for costs of storage over and above the University funded allocation.

Please contact your faculty IT Partner if you have any questions about this change. Contact details are given on the last page of the newsletter.

News

Researcher Satisfaction Survey

We've recently launched a survey to assess the use of our facilities by you, our users. Please help us to evaluate and improve our services by taking a couple of minutes to complete this <u>short survey</u>.

PRACE Call for Proposals for Project Access

The 12th call for proposals for PRACE Project Access is now open and will close on **11 November 2015**. Proposals can be based on a 12-months schedule, or, for Multi-year Projects, on a 24- or 36-months schedule.

The allocation of awarded resources is made for 1 year at a time with provisional allocations awarded for the 2nd and 3rd year.

The 12th Call will offer resources on:

- **FermiFERMI**, an IBM Blue Gene/Q supercomputer operated by CINECA, Italy
- **MareNostrum**, an IBM System x iDataPlex supercomputer operated by BSC, Spain

The 12th Call Technical Guidelines for Applicants can be found <u>here</u>. To apply, <u>click here.</u>

The Condor Pool Citied in Publication

J. M. Garland, R. B. Appleby, H. Owen, and S. Tygier from The University of Manchester cited the use of the UoM Condor Pool in a recently published paper which investigates a new lattice design for proton therapy and tomography. You can read the paper here.

Upcoming Events

N8 HPC Network Event- Multiscale Computational Mechanics

This one day networking event on the 30 October at the University of Sheffield will bring together members of the research community who share a common interest in the topic of 'Multiscale Computational Mechanics' with a focus on structural continuum computational methods.

This free event is open to all researchers at the University of Manchester and is an ideal way to find out more about the use of N8 HPC in this field. Registration can be completed <u>online</u> and closes on **19 October**. Please note that you **do not** have to submit an abstract to attend the event.

Vacancies

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

Computational Physicist- STFC

<u>Computational Scientist in Computational Mechanics</u> <u>and Industrial Applications- STFC</u>

Data Repository Developer- STFC

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
- <u>UK Hartree Centre Facilities</u>
- 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. <u>Click here</u> for details.

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 October and November 2015 include:

20-22 Oct	Introduction to Parallel	Finland
	<u>Programming</u>	
26-28 Oct	Debugging and Optimisation	Italy
28-29 Oct	Advanced MPI	Edinburgh
29-30 Oct	<u>Data Carpentry</u>	Leeds
18-20 Nov	High Performance Molecular	Italy
	<u>Dynamics</u>	
23-24 Nov	Share Memory Programming	York
23-27 Nov	Parallel Programming	Spain
	Workshop	
24-25 Nov	<u>Practical Software</u>	Edinburgh
	<u>Development</u>	

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:

Introduction to the CSF (7 Oct) - an introduction to using the University's eResearch infrastructure (including the Computational Shared Facility) including how to access and transfer files, submitting jobs, and principles of parallel computing in order to know what's possible from the 6,000+ processor cores available

<u>Introduction to Unix Shells & Processes</u> (14 Oct) – an intensive half day exploring use of ssh (to login to remote computers), file permissions (how to share, or prevent sharing), shells (scripting) and processes (controlling what is running and how).

Introduction to Writing and Running Programs (20 Oct)

- a half-day introduction to programming terminology, the principles of compiling and how to use compiler flags to optimise your code for faster results. The course discusses methods for parallelism, outlines how OpenMP and MPI can be used and sketches additional programming tools.

Introduction to Python (21 Oct) – covers the free and popular general purpose programming language Python which is widely used for scientific programming. The course covers using iPython Notebook, the command line interface, scientific libraries, programming constructs and some basic plotting

Introduction to Optimisation (28 Oct) – a half day course outlining the role of compilers and how they can be used to get simulations to run faster. Materials include looking at the causes of slow programs and how to address the key problems either by approaches to programming or by appropriate use of the compiler, debug and performance tools

Introduction to Parallel Programming (4 Nov) - covers the whys and hows of parallelising code, with hands-on examples. Useful for learning the aims & principles of getting your code to run much faster, or to expand the capabilities of your model simulation by accessing more memory, by porting it to parallel computers such as multicore desktops, high performance computing

clusters (CSF, Polaris and Archer) as well as on Intel Xeon Phi and GPU cards.

Extended Introduction to CUDA (10-12 Nov) - covering the basics of programming GPUs with NVIDIA's "CUDA" language. CUDA allows one to exploit the full power available (over TFLOPS/sec) from GPU programming. The course will also discuss how to profile code and use the results to drastically improve the performance.

Introduction to Data Visualization & Analysis (18 Nov) – following a discussion on the purpose and general principles of visualization, attendees will gain hands on experience in key functionalities of the popular software ParaView.

For more information on these courses or other training that we can provide, please <u>contact us.</u>

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/DocuInfo.aspx?DocID=25417

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Next edition

The next edition of this newsletter will be circulated at the beginning of November 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 30 October 2015 will be included in the next edition. News from academic colleagues and researchers are most welcome.