![Manchester 1824 - The University of Manchester]

Research *it*
Supporting your research
A newsletter from IT Services: Research IT

Welcome to issue #24, April 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 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/DocuInfo.aspx?DocID=23929

The link to #23 of the Newsletter was clicked on nearly 1400 times in March. Please help us increase our readership by forwarding the link to colleagues.

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](#)
- [UK Hartree Centre Facilities](#)
- [PRACE EU High Performance Computing Service](#)
- [XSEDE USA High Performance Computing Service](#)

Access to ARCHER

Researchers can request access to *evaluate* the UK High Performance Computing Service (ARCHER) all year round via a lightweight application process. Applications for larger allocations must be submitted to a Resource Allocation Panel (RAP). The next RAP call closes on **29 April**. [Click here](#) for details.

Energy Efficient Computing

From **1 April**, IT Services will be rolling out new "plug-in and-cycle"desks to researchers across campus. Using this new facility, researchers will be able to turn calories into watts for their laptops and other devices. This initiative will help improve personal fitness as well as support an ambitious drive to reduce the carbon footprint and running costs of IT facilities at the University of Manchester.

Keeping Dropbox Data Secure

Cloud storage folders may optionally be encrypted, for enhanced security, using the service provided by nCryptedCloud.com. It works particularly well with Dropbox. All popular operating systems are supported, except Linux where you have to use the web browser interface. Encrypted folders can be shared with

collaborators around the world. Please keep in mind that "data protection" type data should not be stored outside of the EU even if encrypted; and Dropbox servers are currently all in the USA. Around **May**, a representative from nCryptedCloud will be in Manchester and we are likely run a workshop. For further details please contact Ian Cottam.

Research Computing Training

PRACE Advanced Training Courses

The Partnership for Advanced Computing in Europe (PRACE) offers free courses at different HPC centres in Europe. Some of these could be given in Manchester if there was enough interest. Courses offered in April and May 2015 include:

7-10 April	Advanced Topics in HPC	Germany
7-10 April	Parallel Linear Algebra	France
16-17 April	Programming MareNostrum III	Spain
16-17 April	OpenACC Programming	Germany
16-17 April	ARCHER Software Carpentry	London
20-22 April	Debugging and Optimization	Italy
20-22 April	GPU Programming with CUDA	Germany
23-24 April	Intro to UPC and CAF	Germany
27-29 April	Intel MIC&GPU Programming	Germany
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

Intel Xeon Phi Tools Workshop

Edinburgh Parallel Computing Centre (EPCC) is organising a one day workshop on tools for programming and optimising code on Xeon Phi. The workshop, to be held on **24 April 2015** in Edinburgh, is free to attend but spaces are limited so registration is required. Please click here for details.

Porting and Optimisation Workshop

Edinburgh Parallel Computing Centre (EPCC) is organising a hands-on workshop on **20 April** on porting software to the UK National High Performance Computing Service, ARCHER. The workshop is aimed both at those thinking about using ARCHER and existing users. Further details can be found here.

ARCHER TechForum Webinars

The UK National High Performance Computing Service, ARCHER, provides some useful training through webinars each month. You do not have to be an ARCHER user to register. This month there are 2 webinars on performance tuning, **8 April** and **15 April.** For more information, please visit the ARCHER website.

University of Manchester Courses

IT Services offer a portfolio of short courses in research computing. Click here 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

The Engineering Simulation Show

The Engineering Simulation Show runs from **15-16 April 2015** at the Derby Roundhouse, Derby. Speakers include scientists from the ESA Rosetta Comet mission and engineers from ESI, Jaguar Land Rover, the Virtual Engineering Centre (Daresbury/Liverpool) and Airbus. For more information and to book your free ticket please click here. If you have any questions about this event, please contact David Reeks.

Exascale Applications and Software

Edinburgh Parallel Computing Centre (EPCC) is hosting the 3rd International Exascale Applications and Software Conference from **21- 23 April 2015**. The programme includes invited talks from experts presenting their unique views of the challenges facing HPC. For more information, please click here. Please note that registration closes on 10 April 2015.

1st UK ParaFEM Developer Workshop

ParaFEM is open source finite element software that can solve engineering problems with ~1 billion unknowns on systems with up to 64,000 cores. The workshop will be held from 1300-1700 at the University of Oxford on **Monday 13 April**. Topics include *community led development* for: multiscale modelling of polycrystalline fracture; large strain plasticity; stochastic Monte Carlo simulation; transient thermo-mechanical analysis and interfaces for Abaqus user subroutines. Porting to the Raspberry Pi and Xeon Phi will also be discussed. For further information, please contact Lee Margetts.

COMSOL Multiphysics Workshop

COMSOL is running a free workshop on **Wednesday 15 April** in the Mercure Manchester Piccadilly Hotel, focusing on the simulation capabilities of their multiphysics software. Register online.

Seminar: "Apps for Mental Health"

Registration is now open for the next Connected Health Innovation Centre Seminar on "Apps for Mental Health" on **16 April 2015**. The seminar will be held from 3-5pm in Room 306A, Jean McFarlane Building and includes a presentation from John Ainsworth, Deputy Director of the Centre for Health Informatics and the Health e-Research Centre.

Other News

UK e-Science CA User Survey

The UK e-Science CA have released a short survey to assess who their current users are and hope to use the information to improve the sustainability of the CA, or alternatively, assess the impact of closing the service. If you are a user of the CA, please fill in the survey about what projects you are using your certificates for.

EPSRC Call for Healthcare Technologies

The EPSRC Healthcare Technologies theme invites applications from early career researchers under 4 grand challenges: Developing Future Therapies; Frontiers of Physical Intervention; Optimising Treatment and Transforming Community Health and Care. £10 million is available to support around ten personal awards. The closing date for applications is 14 May 2015. For further information please click here.

Opinions

Just fancy that: who needs a supercomputer?

Ian Cottam writes: " … IT Services recently tested a top of the range Windows 8.1 PC. We should point out that it cost quite a bit more than many researchers are prepared to pay. Nevertheless, it benchmarks at 370 Gflop/s: that's 370 billion double precision floating point operations per second (just using the CPU, rather than GPU). Makes you think! The benchmark was matrix matrix multiply written in MATLAB. As recently as 1996, this under the desk PC would have been the

fastest computer in the world. And it would have stayed in the Top 500 until 2003."

To give balance to our editorial, we have shared the following article, published by the online magazine insideHPC, in order to present both points of view - Editor

How Supercomputers Give Universities a Competitive Edge

A recent US study, based on a survey of 212 research intensive institutions, shows that the fields that benefited the most from access to supercomputers were chemistry, civil engineering, physics and evolutionary biology. Click here for the full article.

Case Studies

We'd like to thank Egor Zindy for contributing the following short article about his experiences using the iCSF cluster. The iCSF is also known as INCLINE: the INteractive Computational LINux Environment. The systems is specifically configured for **interactive** computationally-intensive work - Editor

Tracking Maggots

Egor writes: " … My main job, as a Senior Experimental Officer for Bioimaging, is to help people analyse large sets of images or movies acquired on our microscopes. Typically, there are multiple conditions and multiple repeats to explore, and quite often these are processed independently. Looking at how these images are processed, you will often find a loop scanning through all the pixels, processing one at a time, independently of all the others.

With my next task looming (tracking maggots in hundreds of movies, each consisting of thousands of frames), I am evaluating the possibility of using the university computer clusters rather than my own tired workstation. Fast forward to this week, I have *just* been given access to the iCSF cluster, which is designed specifically for _interactive_ computationally-intensive work.

The iCSF has three types of node. The biggest, _incline2000_, has 40 CPU cores and 2 TB of RAM. I used incline2000 for my tests. I designed a quick test to get a feel for "how fast" these machines are. I used a contrast enhancement method called weighted region ranking (WRR), which I have optimised to run on multiple cores using OpenMP. See here for my blog.

The first result of this experiment was that running the algorithm on a single core was 25% slower than running it on a single core of my desktop machine.

The incline2000 contains Intel Westmere CPUs which are slower than newer IvyBridge and Haswell CPUs - Editor

I think this is a very important result, as people may be disappointed if the software they try to run on these "big iron" machines is not in some way tailored to take advantage of a large number of cores. The incline2000 has 40 cores and this is where it really shines. Using all the cores (40 on incline2000 versus 12 on my workstation), my WRR implementation ran about 4 times faster compared to running it on all the cores of my desktop machine.

With these very preliminary results, this is where I'm at. I still need to optimise my code for the iCSF, and better understand how to balance the number of cores used in my process, versus running multiple instances of the code on separate images, versus profiling and optimising parts of my code to fully take advantage of these amazing machines. In any case, a very encouraging result ! "

The iCSF is ideal for development work of this kind, but once the software is fully optimised, processing hundreds or thousands of images using the original CSF system will be more productive for Egor - Editor

Vacancies

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

PDRA at Barcelona Supercomputing Center

Support Engineer at Barcelona Supercomputing Center

PhD position at Barcelona Supercomputing Center

For jobs in Research IT, please contact Dr Simon Hood (system administration) or Dr Michael Bane (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.

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 May 2015.

Lee Margetts has left IT Services to take up a lectureship in the School of MACE and Gillian Sinclair joins Dalinder Sall on the editorial team.

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 24th April 2015 will be included in the next edition. News from academic colleagues and researchers are most welcome.