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The University of Manchester

IT Services

Supporting your research

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

Welcome to issue #12, March 2014, 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 +44 (0) 161 306 5544 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/.

Monty Python's Flying Programming language and Environment

There has been a surge of interest on Campus recently concerning the use of **Python** as a scientific programming language. The EPS Applications team have developed a basic introductory course in the language: wiki.rac.manchester.ac.uk/community/IntroPython.

We also assist people in migrating from MATLAB, Mathematica and others to Python, and will try to optimise your Python code where necessary. Recent projects include topics such as computer algebra, image processing and differential equations.

For most Python work, we recommend the free Anaconda Python distribution: continuum.io/downloads.

This includes most of the modules required by researchers and is being made available on most managed University systems. A full list of the Modules provided by Anaconda can be found at docs.continuum.io/anaconda/pkg.html.

It also includes the Spyder Integrated Development Environment: <https://code.google.com/p/spyderlib/>.

Finally, we advocate the use of the IPython notebook for teaching and research. This is included in Anaconda and more details can be found at: ipython.org/.

For further support on Python, please email applicationsupport-eps@manchester.ac.uk.

Computationally Intensive Research: Survey

This survey – mentioned in last month's newsletter – has been delayed in order to merge it in with the forthcoming **e-science and big data** one from the group being chaired by Prof. Douglas Kell. We apologise for the number of both local and national surveys being conducted at the moment: it seems just to be "survey season".

IT Services Supports UK Fusion Doctoral Training Network

On Monday 24 to Wednesday 26 March 2014, IT Services delivered an extended version of its *Image-based Modelling with Finite Elements* course. This semester, the course was delivered as part of the UK Fusion Doctoral Training Network with attendees from Manchester, Oxford and Durham. Access to the N8HPC Facility *Polaris* was arranged so that researchers could get first hand experience using the parallel finite element analysis software *ParaFEM* on up to 512 cores.

For further details see www.rac.manchester.ac.uk or contact lee.margetts@manchester.ac.uk.

Understanding the Role of Software in Reproducible Research

Prof. Carole Goble from Computer Science (and a co-investigator of the EPSRC's *Software Sustainability Institute* [SSI] www.software.ac.uk) gave the opening keynote on this topic on 26 March 2014 at the Oxford based *Collaborations Workshop 2014*. She is pictured below flanked on her right by Dr Neil Chue Hong from Edinburgh (and the SSI's Director) and SSI co-investigator Prof. David De Roure from the Oxford e-Research Centre.



Other researchers and research software engineers from UoM attended this annual, popular event.

SSI stickers reading *Better Software Better Research* are available – the T-shirts may be harder to come by.

www.software.ac.uk/news/2014-03-27-softwares-role-reproducible-research-latest-news

New version of PGI C / C++ / Fortran Compiler Suite Available at Manchester

We have released the latest version of the PGI Compiler suite on the Applications Website: man.ac.uk/3dDCJ1

We have licenses for the Linux versions of their C, C++ and Fortran compilers. The principal reason for choosing this compiler over others seems to be its support for OpenACC on NVIDIA and AMD GPUs

www.pgroup.com/resources/accel.htm.

OpenACC is an emerging standard that allows programmers to offload computation to accelerators such as GPUs. More details on the standard can be found at www.openacc-standard.org/.

The PGI Compiler suite is one of a range of compilers offered to researchers at Manchester.

Details of our C / C++ Compilers are here: man.ac.uk/5ICpLg.

Details of our Fortran Compilers are here: man.ac.uk/vG29J4.

Humanities Faculty IT Research Development Team

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

The pilot for the new website for the *National Confidential Inquiry into Suicide and Homicide by People with Mental Illness (NCISH)* will start in April. A new web application has been developed to capture data from mental health professionals based nationwide, both in the NHS and in private practice. This replaces their current paper-based methodology. Six NHS Mental Health Trusts are participating in the pilot.

Contact: Andrew.Jerrison@manchester.ac.uk for further details.

Upcoming ARCHER training

ARCHER is the new UK supercomputing service.

ARCHER Virtual Tutorial on PBS Job Submission: 3pm Wed 9 April 2014

<http://www.archer.ac.uk/training/virtual/>

An online session open to all where you can put questions to ARCHER staff. All you need is a computer and Internet access. This session starts with a talk on how PBS job submission works on ARCHER, which is not as simple as it may first appear, followed by an open Q&A.

Hands-on Introduction to HPC and Introduction to ARCHER: 9-11 April 2014, York

An introduction to HPC for the non-specialist. Learn about the key hardware and software building blocks, and also how to use ARCHER.

Parallel Materials Modelling Packages: 23-25 April 2014, London

Hear from members of the development teams of CASTEP, GPAW and CP2K, and learn how to use these packages on ARCHER.

Hands-on Introduction to High Performance Computing: 23-24 April 2014, Edinburgh

An introduction to HPC for the non-specialist. Learn about the key hardware and software building blocks and run real examples on ARCHER.

Tools for Large-Scale Debugging and Profiling: 29 April - 1 May 2014, Edinburgh

Learn from the developers how to debug codes on ARCHER using DDT, and how to do parallel performance analysis with Scalasca and Vampir.

Advanced OpenMP: 6-8 May 2014, Oxford

For those seeking to deepen their OpenMP understanding. Topics include the OpenMP memory model, performance tuning, OpenMP+MPI and OpenMP 4.0.

Introduction to Fortran 90/95: 12-13 May 2014, STFC Daresbury Laboratory

An introduction to features of Fortran 90/95 relevant for numerical applications e.g. program control, subprograms, variables, I/O, arrays.

Parallel Computing with R: 29-30 May 2014, Swansea

SPRINT provides easy access to HPC from the R language. This course introduces HPC followed by a detailed practical introduction to SPRINT.

To register, see www.archer.ac.uk/training/. Attendance is free for all academics.

Women in HPC (WiHPC)

WiHPC is a new network initiative that aims to support collaboration and networking by bringing together female High Performance Computing (HPC) scientists, researchers, developers, users and technicians from across the UK.

We encourage women in HPC to engage in outreach activities and improve the visibility of inspirational role models. Our activities are complemented by research into the influence of UK equality initiatives on the HPC community.

Women in HPC Launch 24 April 2014 – 13:00 to 18:00 Venue: EPCC, The University of Edinburgh

This is an opportunity to find out more about the network that aims to inspire, connect and train women in HPC. The event will discuss the obstacles facing women in HPC today, how to broaden participation and talks from HPC professionals. Refreshments and a buffet lunch will be provided.

You might also like to attend the 1.5 day *Hands-on Introduction to HPC* course, which precedes the launch. No programming, Linux or HPC experience is required although familiarity with desktop computers is presumed. Open to anyone in the UK, this course will prioritise participation by female academics, post-doc researchers and postgraduate students, and will finish with lunch prior to the WiHPC Launch.

For more information, email info@womeninhpc.org.uk, or visit www.womeninhpc.org.uk.

Software for the Future

EPSRC have just released their Software for the Future call www.epsrc.ac.uk/funding/calls/2014/Pages/softwarefuture.aspx. The deadline for registering an intent to submit is 28 April 2014 and the deadline for proposals is 28 May 2014.

Snow Leopard

Are you still running Apple's OS X 10.6 Snow Leopard? IT Services are concerned about two issues. The first is that Apple may no longer be issuing security updates to this (three generations back) version of OS X. Unfortunately, it is Apple policy not to answer such direct security-related questions. Secondly, and relatedly, it may be that you keep Snow Leopard for the Rosetta translation layer (from PPC to X86 code). If so, we would like to know which old applications are stopping you from upgrading; and in return, hopefully, offer you advice on alternatives. You can contact ian.cottam@manchester.ac.uk.

Emerging Technology

Conference: EMiT

Computational hardware is changing rapidly, with new and novel highly parallel computing architectures that are in a state of constant flux being unveiled all the time.

This forces significant questions about re-coding and future proofing existing scientific software. The term **Emerging Technology** is beginning to be used to describe this continual state of hardware change.

The Inaugural EMiT Event will take place on Friday 11 April 2014 at The University of Manchester and will focus on application in research of new methods and techniques to exploit this technology.

For more details please see: emit.manchester.ac.uk/.

And finally

Congratulations to Joe Gavin and Richard Mervin, the current IT Services Research and Application Collaboration (RAC) team interns in securing further studies, after their internships end in September.

Joe will be heading to the University of Birmingham to start a graduate entry medicine course with the intention of becoming a doctor. It was a tough interview process with only 40 places available to over 700 applicants. Joe puts part of his success down to the communication and people skills he developed during his internship.

Richard is off to the University of Cambridge to study for an MPhil in Advanced Computer Science, with the intention of eventually pursuing a PhD in the field. He was attracted to the course due to the focus on machine learning applied to natural language processing, an area he would like to focus on during a PhD. His internship in the RAC team proved to be

good preparation as it featured heavily in the interviews and the interviewer noted the excellent preparation it provides, particularly for the programming elements of the course.

The RAC team (and the research community at Manchester) has benefited enormously from our interns through the addition of extra resources to tackle new projects, as well as a fresh perspective on our operations and valuable, not to mention younger, alternative viewpoints. We are very proud of both our interns and the progress they have made over the last 5 months. We look forward to working with them over the summer before they leave to take up their new challenges.

More information about internships can be found on the Manchester Graduate Internship Programme website. Alternatively, contact Robin Pinning or Gillian Sinclair for information specifically related to internships within RAC.

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 April 2014.

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

ian.cottam@manchester.ac.uk before 20 Apr 2014.