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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 #17, August 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](http://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/](http://www.its.manchester.ac.uk/research/).

## Using Free Software to Replace Simulink

The School of Electrical and Electronic Engineering teaches an *Introduction to Control Theory* course that uses Simulink models to demonstrate various concepts. Since the aim of this course is to teach control theory principles – rather than any particular software solution – it would ideally be software agnostic. Students are not asked to develop models, they are just asked to ‘play’ with pre-packaged models in order to improve their understanding of the material.

A student intern recently demonstrated that all of these models could be implemented in the free Simulink clone, **xcos**. A brief write up of this work is available on Mike Croucher’s blog [www.walkingrandomly.com/?p=5538](http://www.walkingrandomly.com/?p=5538).

## Condor Pool – High Throughput Computing

IT apologise that the Condor Pool is still heavily depleted. This is due to new hardware and software being installed in the undergraduate teaching clusters (which we then have to dual-boot with Linux to support Condor use overnight and at weekends). If this is severely impacting your research, please contact: [ian.cottam@manchester.ac.uk](mailto:ian.cottam@manchester.ac.uk).

## Workshop on High Performance Computing in Health Research

The European Commission is holding a workshop to discuss the role of HPC in health research. It will take place on the 1st and 2nd of October 2014 in Brussels. The objective of the EC is to ensure a broad representation of this area at the workshop. If you are interested in this topic, you can register your interest with the organisers who will then carry out the final selection of participants. The preliminary agenda is here: <https://ec.europa.eu/digital-agenda/news-redirect/17279>.

## CUDA 6.5 Production Release is Now Available

The [CUDA® 6.5 Production Release](#) is now available. Run your application faster with this latest version of the CUDA Toolkit. It features 64-bit ARM support and the simplified programming model enabled by Unified Memory.

Highlights include:

- Support for 64-bit ARM-based systems
- Microsoft Visual Studio 2013 compatibility
- Expanded support for Block Sparse Row (BSR) matrix format in cuSPARSE routines
- cuFFT callbacks for higher performance custom processing on input or output data
- Improved debugging for CUDA FORTRAN applications
- New profiler Application Replay mode reduces the time required to collect multiple metrics when profiling a complex application
- Updated CUDA Occupancy Calculator API provides optimal kernel launch configurations
- New nvprune utility optimizes the size of object files by removing code not needed for target GPU architectures

Download the CUDA 6.5 Production Release at [www.nvidia.com/getcuda](http://www.nvidia.com/getcuda).

Learn more about CUDA 6.5 by attending the webinar:

**CUDA 6.5 Performance Overview** presented by Jonathan Cohen - 17 September 2014 – 10 AM PDT [REGISTER](#).

## Exploiting Multi-core and Many-core Platforms for Atomic and Molecular Simulations

**CECAM workshop** 10-12 September 2014, STFC Daresbury Laboratory.

This European workshop will provide a forum for open discussion to better understand the programming models and strategies that will be needed for the new generation of atomic, molecular, physics, chemistry and materials simulations on current and near-future multi-core and many-core platforms. Confirmed speakers will cover areas including Molecular Dynamics and DFT, Lattice Boltzmann, fast multipole and particle-based methods and will speak about experiences implementing and optimizing codes for Intel Xeon Phi and Nvidia GPU processors.

Further details about the workshop are available at the CECAM website [www.cecam.org/workshop-0-1032.html](http://www.cecam.org/workshop-0-1032.html). The STFC event page also includes details about local arrangements <https://eventbooking.stfc.ac.uk/news-events/many-core-platforms>.

## Efficient Parallel IO on ARCHER 2-3 September 2014 Daresbury

One of the greatest challenges to running parallel applications on large numbers of processors is how to handle file IO: standard IO routines are not designed with parallelism in mind. Parallel file systems such as Lustre are optimised for large data transfers, and performance can be far from optimal if many files are opened at once.

The IO part of the MPI standard gives programmers access to efficient parallel IO in a portable fashion. However, there are a large number of different routines available and some can be difficult to use. Despite its apparent complexity, MPI-IO adopts a straightforward high-level model. If used correctly, almost all the complexities of aggregating data from multiple processes can be dealt with automatically by the library.

This 2-day course will use the national ARCHER supercomputer for exercises, although most aspects of the course are applicable to all large parallel machines. For details, a timetable and to register, please see [www.archer.ac.uk/training/](http://www.archer.ac.uk/training/).

## 3rd eCSE call for proposals now open

Embedded CSE (eCSE) support provides funding to the national supercomputer ARCHER user community to develop software in a sustainable manner. Funding will enable the employment of a researcher or developer to work specifically on the relevant software to enable new features or improve the performance of the code. Examples of this could be:

- Implementation of algorithmic improvements within an existing code
- Improving the scalability of software on higher core counts
- Improvements to code which allow new science to be carried out
- Porting and optimising a code to run efficiently on ARCHER
- Adding new functionalities to existing codes
- Code development to take a code from a Tier-2 to Tier-1 level bringing new communities onto ARCHER

Funding can be requested for existing ARCHER users supported by EPSRC and NERC and can fund staff located at the institution of the PI, third parties, or can include staff from the centralised CSE support team or a mixture of the above.

More details of how to apply are available at [www.archer.ac.uk/community/eCSE/](http://www.archer.ac.uk/community/eCSE/) together with details of the application and review process, assessment criteria eligibility, etc.

Deadline for proposals: 1600 BST Tuesday 16 September 2014

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## Next Image-based Modelling Club Meeting

The University of Manchester Image-based Modelling Club are organising a workshop for “Young Researchers” at the Hartree Centre, Daresbury Laboratory (Warrington) on Tuesday 9 September 2014. We will set off by coach from North Campus at 0900 and return by 1700. The purpose of the workshop is to encourage networking between Manchester PhD students, postdoctoral researchers and recently appointed lecturers who are using or would like to use image-based simulation in their research. Other staff are welcome.

In the morning, we will hear about the >£100M investment in world class supercomputing and visualisation facilities at the Hartree Centre. These are available to Manchester researchers through collaborative projects and European research grants. We will also enjoy a visualisation showcase featuring recent Manchester research in one of the Hartree Centre’s immersive stereo visualisation suites.

Lunch will be provided during a poster session. In the afternoon, we will hold a hands-on workshop to discuss the issues and challenges of image-based modelling. This will inform future Image-based Modelling Club events and help progress the use of this technique at Manchester.

Manchester Informatics and the Harwell Imaging Partnership will cover the costs of attendance. However, there is a caveat. The event is only free to attendees who submit a poster. Posters will describe image-based modelling work that has been completed, is in progress or is being planned. If you would like to participate, please register at the following link: [tinyurl.com/osc74pe](http://tinyurl.com/osc74pe).

Contact [lee.margetts@manchester.ac.uk](mailto:lee.margetts@manchester.ac.uk) or [louise.lever@manchester.ac.uk](mailto:louise.lever@manchester.ac.uk) for further details.

## Subject-specific Email Lists

Please note that these email lists are subject specific discussion forums, rather than a way of contacting IT. For the latter, please see the contact emails in the next section.

[finite-elements@listserv.manchester.ac.uk](mailto:finite-elements@listserv.manchester.ac.uk)

[fortran@listserv.manchester.ac.uk](mailto:fortran@listserv.manchester.ac.uk)

[sciprogramming@listserv.manchester.ac.uk](mailto:sciprogramming@listserv.manchester.ac.uk)

[university-gpu-club@listserv.manchester.ac.uk](mailto:university-gpu-club@listserv.manchester.ac.uk)

## Faculty Contact Emails

### Humanities:

[Hum-ITResearch@manchester.ac.uk](mailto:Hum-ITResearch@manchester.ac.uk).

### Engineering and Physical Sciences:

[EPS-ITResearch@manchester.ac.uk](mailto:EPS-ITResearch@manchester.ac.uk).

### Medical and Human Sciences:

[MHS-ITResearch@manchester.ac.uk](mailto:MHS-ITResearch@manchester.ac.uk).

### Life Sciences:

[FLS-ITResearch@manchester.ac.uk](mailto:FLS-ITResearch@manchester.ac.uk).

## Next edition

The next edition of this newsletter will be circulated at the end of September 2014.

If you have any news to contribute, please contact Dr Mike Croucher: [michael.croucher@manchester.ac.uk](mailto:michael.croucher@manchester.ac.uk) before 25 September 2014.