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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 #7, October 2013, 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 ext.65544 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/).

## Spotfire visualization tool

Several academics are interested in using a powerful data visualization tool called **Spotfire**. If you are interested in visualization of your research data, we would urge you to download and try the trial version of this software ([spotfire.tibco.com/en/download-spotfire.aspx](http://spotfire.tibco.com/en/download-spotfire.aspx)) and let us know your impressions, and if you would support a University bid to purchase licences for this application. Email [ian.cottam@manchester.ac.uk](mailto:ian.cottam@manchester.ac.uk).

## Manchester Blogs

Several academic and support staff write blogs. From time to time, we will feature some here that should be of interest to our readership.

EPS IT's Mike Croucher ([www.walkingrandomly.com](http://www.walkingrandomly.com)).

MHS IT's Mike Taylor and others ([blogs.mhs.manchester.ac.uk/it-matters/](http://blogs.mhs.manchester.ac.uk/it-matters/)).

Professor Nick Higham from the School of Mathematics ([nickhigham.wordpress.com](http://nickhigham.wordpress.com)).

Part of the *Software Sustainability Institute* is based at Manchester (School of Computer Science), and they have an excellent blog site ([www.software.ac.uk/blog](http://www.software.ac.uk/blog)) which your newsletter editor contributes to in his spare time.

IT's RAC Team blog site ([www.rac.manchester.ac.uk](http://www.rac.manchester.ac.uk)).

IT's Lee Margetts *Image-based Modelling Club* LinkedIn Group  
[www.linkedin.com/groups/Imagebased-Modelling-4331572/about](http://www.linkedin.com/groups/Imagebased-Modelling-4331572/about).

Please let [ian.cottam@manchester.ac.uk](mailto:ian.cottam@manchester.ac.uk) know of other sites you would recommend that ought to be of wide interest to Manchester researchers.

## Training Opportunities

IT Services have a variety of courses – including Python – running during November 2013. Bookings and further details: [wiki.rac.manchester.ac.uk/community/Courses](http://wiki.rac.manchester.ac.uk/community/Courses).

## IT Services for Research Forum

The recent ITS Research Forum featured Mary McDerby speaking on the state of *Research Data Management*. We had no academics in attendance and hence we are investigating other channels to disseminate such information, possibly abandoning the research forum.

## Researchers of the Month

Congratulations go to three researchers this month.

Members of the Image-based Modelling Club might remember Llion Evans (Fusion DTN, Materials) practising an interview presentation in front of an audience of 60 attendees at the last meeting. Although the chairman resisted the temptation to give the audience green 'hired' or red 'fired' cards, Llion got some great feedback during questions and coffee. We are happy to announce that Llion's research proposal was successful and he is now working as a Research Fellow at the Culham Centre for Fusion Energy near Oxford. The panel were very impressed with the research Llion carried out during his PhD, particularly his use of the Manchester X-ray Imaging Facility, ParaFEM and the N8 HPC Service. Llion passes his sincere thanks to IT Services for supporting his research and the Image-based Modelling Club for helping him with securing his new appointment where he will be investigating future technologies for reactor designs in continued collaboration with The University of Manchester.

David Arregui, a Conacyt funded PhD student in MACE, has been awarded a prestigious £1,888 travel fellowship by the Science and Technology Facilities Council (STFC) to undertake a research visit to Colorado School of Mines, USA. He will visit the research group of Professor Vaughan Griffiths (a Manchester alumnus) to explore opportunities for international collaboration in the field of stochastic finite element analysis. David is using random fields to define material properties in very large finite element analyses of nuclear reactor cores. He is using ParaFEM, developed at Manchester, and random field generators developed in the USA to run simulations on the N8 HPC Service. David received a little insider help with his application, through the collaborative relationship between the RAC Team and the STFC Hartree Centre, and via Lee Margetts who has just published the textbook *Programming the Finite Element Method* with Professor Griffiths.

Dr Neil Ashton (Turbulence/CFD Group, MACE) has been awarded a £2,500 travel grant to attend this year's Supercomputing Conference in Denver, Colorado, USA. Neil was one of 11 UK applicants who secured the award through EPSRC's UK-USA HPC Collaboration Network. This network was established by Lee Margetts (RAC Team) in collaboration with Imperial College, University of Oxford, NAG Ltd and STFC. Competition was very tough, with two of the awards going to Directors of Regional Supercomputing Facilities in England and Scotland. The

purpose of the network is to help build links so that UK academics can get access to HPC facilities in the US. So, if you are looking enviously at 'leadership class' facilities for HPC and Big Data available to your competitors in the US, contact Lee who may be able to help you get access..

## Green Open Access and Help with eScholar

For a limited time (until 22 November 2013), the University Library is able to do most of the work for you in getting an academic paper into the eScholar system. See [www.openaccess.manchester.ac.uk/oaweek/](http://www.openaccess.manchester.ac.uk/oaweek/).

## CAS and University GPU Club

We would appreciate *your* help in promoting the GPU Club to colleagues and researchers.

On **13 November 2013**: The Centre for Atmospheric Science (CAS) are hosting an afternoon discussion on the role of emerging technology. They have key speakers John Michalakes from NOAA over from the States (expert on porting codes to GPUs and FPGAs) and Craig Davies from Maxeler (dataflow solutions on FPGAs). This will be a combined event with the University GPU Club.

Further details: [gpu.manchester.ac.uk](http://gpu.manchester.ac.uk).

## Annual Machine Evaluation Workshop

The annual Machine Evaluation Workshop will take place this year on 27-28 November 2013 at the Adelphi Hotel Liverpool. This year there are more exhibitors than they have ever had before, plus a number of parallel breakout sessions, including one from the Hartree Centre and one from the Applications Division.

If you would like to attend, please make sure you complete the online registration:

[eventbooking.stfc.ac.uk/news-events/mew24](http://eventbooking.stfc.ac.uk/news-events/mew24)

Please also advertise the event to anyone that you think may be interested. Registration is free to delegates from academic institutions.

## Manchester Conference on Application of Emerging Tech

Researchers are looking to hold a national conference in Manchester in Spring 2015 with plenaries and peer-reviewed presentations focussing on emerging technology and the techniques required to obtain near-optimal performance from the likes of GPUs, FPGAs and Xeon Phi. Plans are advancing and researchers who would like to get involved in the planning should contact Ben Rogers on [benedict.rogers@manchester.ac.uk](mailto:benedict.rogers@manchester.ac.uk)

## Support for External Computing Facilities and Services

A broad range of computing facilities that are hosted externally are available to researchers at Manchester. These include the regional centres such as N8 HPC ([www.n8hpc.org.uk](http://www.n8hpc.org.uk)); the Hartree Centre ([www.stfc.ac.uk/hartree](http://www.stfc.ac.uk/hartree)); the UK HPC Service HECTOR/ARCHER ([www.hector.ac.uk](http://www.hector.ac.uk)); European facilities provided by PRACE ([prace-ri.eu](http://prace-ri.eu)) and 'leadership' facilities in the USA. There are also calls for travel fellowships and software development grants that appear from time to time.

IT Services can provide support to help you access these facilities. This support includes: matching research needs with suitable facilities; assistance with writing or critical review of application forms before submission; peer-to-peer networking and introductions; research group development and 'road mapping' to help plan for the transition from one service to another; and support for preparatory work such as skills development, code optimisation and profiling on local University systems.

Your colleagues in IT Services are part of a well connected community of national and international specialist service providers. For example, Manchester leads the N8 HPC service; is a member of HPC-SIG (a network of UK HPC service providers); has signed a Memorandum of Understanding with PRACE and is working with EPSRC to sign a similar multi-laboratory arrangement with the USA. The latter will give access to HPC and Big Data facilities hosted at various places such as Argonne National Laboratory, Lawrence Livermore National Laboratory, NCSA Illinois and FERMI Labs to name a few.

We are very keen to use our knowledge and contacts to help research at Manchester benefit from access to external computing facilities and services. Please contact your faculty support team or Robin Pinning for more information. Contact Lee Margetts regarding PRACE and access to facilities in the USA.

## UK Manycore Developer Conference

The UK Many-Core developer conference (16 December 2013 at Oxford) conference is now in its fifth year, with previous conferences having been held at Bristol, Imperial College, Cambridge and Oxford.

Topics covered by the conference include high-performance computing on accelerators such as GPUs, FPGAs and the Xeon Phi, as well as embedded and mobile parallel systems. Application areas include computational science and engineering, finance, computer vision and beyond. The goal of the event is to strengthen the UK's expertise in many-core computing, in both industry and academia.

In addition to the conference on 16 December 2013, on the following day there will be CUDA 'masterclass' sessions to address the interests of CUDA developers. The registration process will include an opportunity to indicate interest in any (or all) of the following: profiling; Nsight IDE; use of new Kepler features such as shuffle; tips for better performance; use of NVIDIA libraries; OpenACC as an alternative to CUDA; and an open session addressing user questions.

Travel details (etc.) are here:

[www.oerc.ox.ac.uk/research/ccoe/ukmac2013/travel](http://www.oerc.ox.ac.uk/research/ccoe/ukmac2013/travel).

## Hartree Centre (Daresbury) Events

*ACitES Chemical Mechanism Computational Workshop*  
[eventbooking.stfc.ac.uk/news-events/acites](http://eventbooking.stfc.ac.uk/news-events/acites)  
12 November 2013.

*DL\_SOFTWARE Training Workshop*  
[eventbooking.stfc.ac.uk/news-events/dlsoftware-training-workshop-179](http://eventbooking.stfc.ac.uk/news-events/dlsoftware-training-workshop-179)  
25-26 November 2013.

*CCPBioSim QM/MM Training Workshop*  
[eventbooking.stfc.ac.uk/news-events/ccpbiosim-qmmm-training-workshop](http://eventbooking.stfc.ac.uk/news-events/ccpbiosim-qmmm-training-workshop)  
28 November 2013.

## CUDA Research Centre

Manchester has been awarded NVIDIA's *CUDA Research Centre* status, which brings our researchers several benefits (please see [gpu.manchester.ac.uk/CRC](http://gpu.manchester.ac.uk/CRC) for details).



## Dropbox Gotchas

Dropbox ([www.dropbox.com](http://www.dropbox.com)) is the gold star service for cloud-enabled file synchronisation. It is so good that there are only a few issues – or 'gotchas' – to watch out for. Here they are.

### 1. Avoiding conflicted copies of documents in Dropbox shares

It is easy to think (wrongly) that one is editing a file on a shared drive when editing a file that is in a shared Dropbox folder. (If it was a shared drive, the single file could be locked for editing by the application concerned, and thus conflicts arising from multiple, simultaneous edits could, in general, be avoided.) In the case of Dropbox, all members of a share have their own local copies, which they could edit whilst offline. When the machine that holds the edits comes back online, Dropbox attempts to synchronise the changes across all member's copies. If more than one user has edited the file since the last sync – or even the same user on two different machines – Dropbox does not know how to resolve the conflict. All it can do is make one of the updates to the original file and leave the rest in separate files of the same name but with "conflicted copy" appended. The users then have to resolve the conflicts manually.

Although not 100% perfect, many users adopt a simple editing protocol for updates to shared folder documents. The two most common are:

- A user intending to edit a file, emails all the people in the share to say he or she has the 'token' for that

file. When the edit is complete a second email can be sent saying the token is free.

- Before editing a file, a user prepends his or her name or initials to the filename. The other users in the share check this before they edit the file. When the user has finished the edit he or she renames the file back to its original name.

Clearly, the reader can imagine scenarios where the above fail, but in practice it has been seen to work moderately well.

### 2. Avoiding sharing issues with Dropbox

There are other sharing issues with Dropbox apart from the "conflicted copies" one described above. The main one arises from the use of shared folders: many users of such do not realize that if they delete or drag out of the folder any file it will be deleted from every other member's local copy of the share (as all users have full and equal access rights, with the possible exception of onward sharing to third parties). You may need to educate your collaborators about this issue.

Sometimes the problem is with the person who shared the files. If the files are not to be updated by others (and possibly infrequently by the owner), the "Share Link" option should be chosen instead. With this, recipients can choose to just view the linked folder through a web browser – and this way they will always see any updates from the owner immediately – or they can choose to download a copy to their own Dropbox (if they have one). With this latter approach it is a good idea to check the web for updates or, better still, the owner can email around when changes are made.

### 3. Windows path length problem

Under Windows (only), Dropbox uses an old interface to the file system that means that files whose path length (e.g. from C:\ onwards) is greater than 260 characters will not sync. If a file was previously in sync across machines and the cloud and its path length is extended over this limit (by moving or changing its name) it will be *silently* deleted from the cloud and all other machines in the share. (It still exists on the machine with the long path length.) Dropbox 'justify' their approach by saying that much of Windows itself has this limitation.

## 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 November 2013.

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

[ian.cottam@manchester.ac.uk](mailto:ian.cottam@manchester.ac.uk) before 25 Nov 2013.