MANCHESTER 1824
The University of Manchester

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

Welcome to issue #3, June 2013, in a regular series of updates on IT research support and facilities for postgraduates, researchers and academics of The University of Manchester.

As we go to press, last month's edition has been downloaded – and hopefully read – 835 times.

Your main Faculty contact email addresses (for research computing support) are given in the section – *News from the Faculties*; 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.

Research Software: Made in Manchester

Many of you will know Mike Croucher from EPS IT's application support group. Mike is also a 2013 Software Sustainability Institute Fellow, and in that role he is curating a *Research Software: Made in Manchester* web site. This lists, both small and large, programs that were developed here at the University and are freely available for anyone to use. Below we present a snapshot of it. (Of course, it is constantly being updated on the actual web site: https://www.applications.itservices.manchester.ac.uk/show_content.php?id=179 and mirrored for external users on Mike's blog www.walkingrandomly.com/?p=4951, where you can find more information and links to all the software mentioned.) It is also linked off the *My Manchester for Staff* site for those of you who are registered for that pilot service.

If you have developed software and would like to be featured on this web site, please email: michael.croucher@manchester.ac.uk. As a courtesy, also tell the software authors if you make use of any of the listed programs.

Finally, please don't forget about software when thinking about your future Research Data Management plans: www.manchester.ac.uk/researchdata.

Faculty of Life Sciences

antiSMASH – Genome annotation tool for secondary metabolite gene clusters.

MultiMetEval – Flux-balance analysis tool for comparative and multi-objective analysis of genome-scale metabolic models.

mzMatch/mzmatch.R/mzMatch.ISO – Comprehensive LC/MS metabolomics data processing toolbox.

Rank Products – Statistical tool for the identification of differentially expressed entities in molecular profiles.

Health Informatics

openCDMS – The openCDMS project is a community effort to develop a robust, commercial-grade, full-featured and

open source clinical data management system for studies and trials.

IT Services

idiffh – A text file differences program. Research software can produce huge text files (e.g. logs). The GNU diff program, for example, needs to read the files into memory and therefore has an upper bound on file size. idiffh might only use a simple heuristic but is only bounded by the maximum file size (and free file store).

ParaFEM – A portable library for parallel finite element analysis. Contributions from MACE, SEAES, School of Materials.

Shadow – This is an Apple Mac OS X shell level application that can monitor Dropbox shared folders for file deletions and restore them.

The Reality Grid Steering Library – A software library for steering and monitoring numerical simulations, APIs available for Fortran/C++/Java and steering clients available for installation on laptops and mobile devices. Developed in collaboration with the School of Computer Science.

Manchester Institute of Biotechnology

Copasi – COPASI is a software application for simulation and analysis of biochemical networks and their dynamics.

Condor Copasi – Condor-COPASI is a web-based interface for integrating COPASI with the Condor High Throughput Computing (HTC) environment.

School of Chemical Engineering & Analytical Science

SurfaceSpectra Identity- is free software that allows you to view and export isotope patterns.

School of Chemistry

DOSY Toolbox – A free, open source program for processing PFG NMR diffusion data (a.k.a. DOSY data).

School of Computer Science

Clinical NERC – Clinical NERC is a simple customizable state-of-the-art named entity recognition, and classification software for clinical concepts or entities.

GPC – The University of Manchester GPC library is a flexible and highly robust polygon set operations library for use with C, C#, Delphi, Java, Perl, Python, Haskell, Lua, VB.Net (and other) applications.

HiPLAR – High Performance Linear Algebra in R. A collaboration between Manchester and Imperial College.

INSEE – Interconnection Networks Simulation and Evaluation Environment

KUPKB (The Kidney & Urinary Pathway Knowledge Base) – The KUPKB is a collection of omics datasets that have been extracted from scientific publications and other related renal databases. The iKUP browser provides a single point of entry for you to query and browse these datasets.

ManTIME – ManTIME is an open-source machine learning pipeline for the extraction of temporal expressions from general domain texts.

MethodBox – MethodBox provides a simple, easy to use environment for browsing and sharing surveys, methods and data.

myExperiment – myExperiment makes it easy to find, use and share scientific workflows and other Research Objects, and to build communities.

Open PHACTS Discovery Platform – Freely available, this platform integrates pharmacological data from a variety of information resources and provides tools and services to question this integrated data to support pharmacological research.

OWL API – A Java API and reference implementation for creating, manipulating and serialising OWL Ontologies. The latest version of the API is focused towards OWL 2. The OWL API is open source and is available under either the LGPL or Apache Licenses.

OWL Tools – a collection of tools for working with OWL ontologies.

OWL Webapps – a collection of web apps for working with OWL ontologies.

RightField – Semantic annotation by stealth. RightField is a tool for adding ontology term selection to Excel spreadsheets to create templates which are then reused by scientists to collect and annotate their data without any need to understand, or even be aware of, RightField or the ontologies used. Later the annotations can be collected as RDF.

SEEK – SEEK is a web-based platform, with associated tools, for finding, sharing and exchanging Data, Models and Processes in Systems Biology.

ServiceCatalographer – ServiceCatalographer is an open-source Web-based platform for describing, annotating, searching and monitoring REST and SOAP Web services.

Simple Spreadsheet Extractor – A simple ruby gem that provides a facility to read an XLS or XLSX Excel spreadsheet document and produce an XML representation of its content.

Taverna – Taverna is an open source and domain-independent Workflow Management System – a suite of tools used to design and execute scientific workflows and aid in silico experimentation.

TERN – TERN is a temporal expressions identification and normalisation software; designed for clinical data.

Utopia Documents – Utopia Documents brings a fresh new perspective to reading the scientific literature, combining the convenience and reliability of the PDF with the flexibility and power of the web.

School of Electrical and Electronic Engineering
LDLTS – Laplace transform Transient Processor and Deep Level Spectroscopy. A collaboration between Manchester and the Institute of Physics Polish Academy of Sciences in Warsaw.
Raspbian – Raspbian is a free operating system based on Debian optimized for the Raspberry Pi hardware.
Signal Wizard – Digital signal processing software.

School of Mathematics
EIDORS – Electrical Impedance Tomography and Diffuse Optical Tomography Reconstruction Software.
Fractional Matrix Powers – MATLAB functions to compute fractional matrix powers with Frechet derivatives and condition number estimate.
IFISS – IFISS is a graphical package for the interactive numerical study of incompressible flow problems which can be run under Matlab or Octave.
MARKOVFUNMV – An adaptive black-box rational Arnoldi method for the approximation of Markov functions.
Matrix Computation Toolbox – The Matrix Computation Toolbox is a collection of MATLAB M-files containing functions for constructing test matrices, computing matrix factorizations, visualizing matrices, and carrying out direct search optimization.
Matrix Function Toolbox – The Matrix Function Toolbox is a MATLAB toolbox connected with functions of matrices.
Matrix Logarithm – MATLAB Files. Two functions for computing the matrix logarithm by the inverse scaling and squaring method.
Matrix Logarithm with Frechet Derivatives and Condition Number – MATLAB files.
NLEVP A Collection of Nonlinear Eigenvalue Problems – This MATLAB Toolbox provides a collection of nonlinear eigenvalue problems.
oomph-lib – An object-oriented, open-source finite-element library for the simulation of multiphysics problems.
Simfit – Free software for simulation, curve fitting, statistics, and plotting.
SmallOverlap – SmallOverlap is a GAP 4 package which implements new, highly efficient algorithms for computing with finitely presented semigroups and monoids whose defining presentations satisfy small overlap conditions (in the sense of J.H.Remmers).
Symmetric eigenvalue decomposition and the SVD – MATLAB files

School of Mechanical, Aerospace and Civil Engineering
DualSPHysics – DualSPHysics is based on the Smoothed Particle Hydrodynamics model named SPHysics and makes use of GPUs.
FLIGHT – FLIGHT specialises in the prediction and modelling of fixed-wing aircraft performance.
SPHYSICS – SPHysics is a platform of Smoothed Particle. Hydrodynamics (SPH) codes inspired by the formulation of Monaghan (1992) developed jointly by researchers at the Johns Hopkins University (U.S.A.), the University of Vigo (Spain), the University of Manchester (U.K.) and the University of Rome La Sapienza (Italy).
SWAB Online – Innovative and User Friendly Web Application in Running Fortran-based 1-D Shallow Water near Shore Wave Simulation Modelling.

School of Physics and Astronomy
Herwig++ – Herwig++ is a new event generator, written in C++, built on the experience gained with the well-known event generator HERWIG, which was used by the particle physics community for nearly 30 years. Herwig++ is used by the LHC experiments to predict the results of their collisions and as an essential component of their data analysis. It is developed by a consortium of four main nodes, including Manchester, and its published write-up has been cited over 500 times.
im3shape - Im3shape measures the shapes of galaxies in astronomical survey images, taking into account that they have been distorted by a point-spread function.
MAD8/madinput – Mathematica code and MAD8 installer for performing optics calculations for particle accelerator design.
PolyParticleTracker – MATLAB code for particle tracking against complex optical backgrounds.

Research Software Development – this week's forum discussion

Some research groups have all the skills necessary to develop and maintain research software, but many only have a subset of the experience and skills required. We held an IT Services for Research group forum on 26 June 2013 that discussed this topic and had an external guest speaker from UCL (University College London): Dr James Hetherington.

James explained the role of his research software development team and how its services are accessed, and presented some basic software engineering practices which researchers can adopt to enhance research efficiency, reliability, and impact.

The meeting then went on to discuss: use of tools, such as GitHub; governance and funding approaches; and many other aspects of such a service. If you missed the event, but

are interested in this topic, please email ian.cottam@manchester.ac.uk to find out more. James, at UCL, is also willing to answer questions emailed to him.

Our thanks go to the *Software Sustainability Institute* for funding James' visit to Manchester.

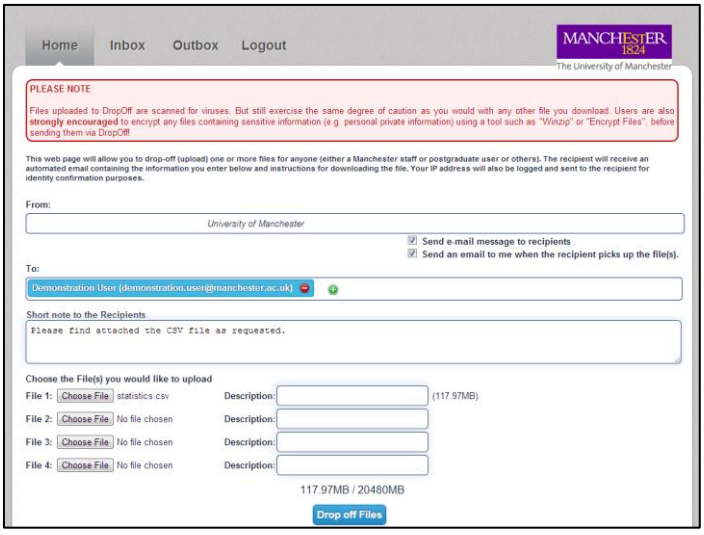
Git – software version control

One key element of any type of (research) software development is automated version control. The research world seem to be largely switching to a system called ***Git*** – developed by Linus Torvalds of Linux fame – and which we could run here on top of the existing SVN (*Subversion*) version control system via a tool called *SubGit*.

Public / open repositories can also be kept on the cloud service *GitHub*, and we will investigate the use of paid for private repositories (as used by University College London, for example).

Please email ian.cottam@manchester.ac.uk if you would like to use such a service.

DropOff and Dropbox



We are now around half way through the service trial of DropOff – a local system that lets you 'drop off' very large files for others to 'pick up'. It can be used to send such large files to external users, as well as within the University. Similarly, your external collaborators can leave files for you. Please contact: dropoff@listserv.manchester.ac.uk for further details and if you would like to use this trial service. (It is also linked off the *My Manchester for Staff* pilot site.)

News on support for the commercial Dropbox for Business service is that Janet's and Dropbox's lawyers are still talking. We are encouraging them to hasten their discussions.

ACM Webinar, Wednesday 17 July 2013, 6pm GMT

Changing How Programmers Think about Parallel Programming, Bill Gropp, NCSA

Does the way that programmers or algorithm developers think about the way a parallel computer works influence the approaches that they take? Can the choice of programming approach lead to inefficient solutions? Do we need new ways to program parallel systems? This session will explore common approaches for developing parallel programs and how they can limit scalability and reliability – whether the programs are for single chip parallelism or the world's largest parallel computers. The importance of an execution model and its relationship to programming models and programming systems will be covered, and why we need to consider new execution models for the parallel systems of the future.

Visit the following website to register: tinyurl.com/nug2njf.

Launch of the NAFEMS Professional Simulation Engineer Certification Scheme

NAFEMS, the international association of the engineering analysis, modelling and simulation community, has recently launched the Professional Simulation Engineer (PSE) scheme. PSE Certification allows engineers and analysts within the international simulation community to demonstrate competencies acquired throughout their professional career. The certification enables individuals to gain recognition for their level of competency and experience as well as enabling industry to identify suitable and qualified personnel. To find out more about the scheme, please visit the following website: www.nafems.org/pse. If you teach and would like to consider strategically aligning undergraduate, taught masters or continuous professional development courses with the PSE scheme, please contact lee.margetts@manchester.ac.uk.

IT Service Catalogue

The service catalogue can now be found linked from the main IT Services web page; it includes a section on Research Computing:
www.itservices.manchester.ac.uk/servicecatalogue

Centres For Doctoral Training

A number of responses to EPSRC's latest CDT call have been successful in being invited to submit a full proposal into the next round, with a deadline of 18 July 2013. The call (www.epsrc.ac.uk/SiteCollectionDocuments/Calls/2013/CDTcallfinal.pdf) explicitly included a section of guidance on Computational and Data-Driven Science.

Computational research across the whole of science and engineering is increasingly acknowledged to be the "third leg" of scientific enquiry, alongside experiment and theory. It is therefore a certainty that many of the students being trained through the Centres will be using computational techniques in their projects, and some may have projects aimed specifically at software development. It is essential that they are given appropriate training so that they can confidently use, extend and develop software in a way that supports correct, reproducible and reusable research. The training needs to cover both the tools ("how") and the methods ("why"), as appropriate.

IT Services provide a programme of training courses in computational techniques, both in person and on-line, that can provide the basis of the computational training in your proposed CDT. Due to Manchester's lead involvement in N8 HPC - n8hpc.org.uk, there is also an opportunity to involve partners from across the N8 - n8research.org.uk. If you would like to discuss this, please contact Dr Robin Pinning - pinning@manchester.ac.uk.

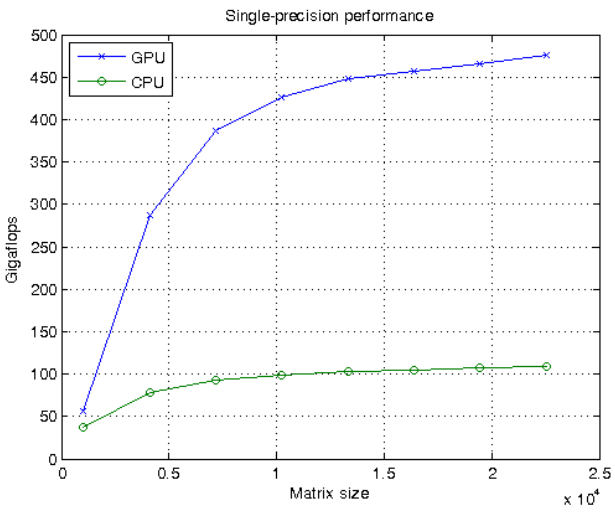
GPU Club Event – Discover how to accelerate your research

Whether you are writing your simulations in MATLAB, Python, FORTRAN, C or one of many other programming languages it is now fairly straight forward to get your results faster by using a General Purpose Graphics Processing Unit: GPGPU or GPU for short.

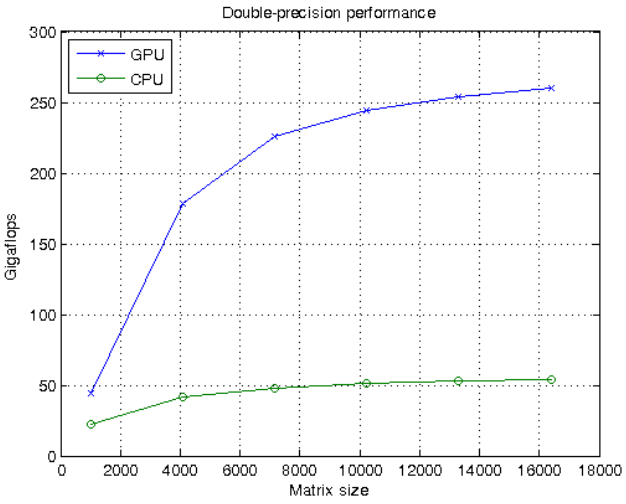
IT Services for Research has speakers from MathWorks (the owners of MATLAB) and NVIDIA (the producers of popular GPUs) coming to talk at the **University GPU Club** on **Tuesday 23 July 2013**.

Jeremy Purches and Tim Lanfear of NVIDIA will outline the use and potential of GPUs for research, including tips on programming for best GPU performance.

Jos Martin of Mathworks will outline the use of MATLAB in simulation and how using the GPU-enabled functions already in MATLAB will result in substantial performance improvements for researchers' codes.



The morning presentations will be followed by a buffet lunch. In the afternoon you can arrange to speak with Jeremy, Tim and Jos about their products with a view to strengthening the University's research collaboration with MathWorks and NVIDIA.



To register your attendance and to request an afternoon appointment with the speakers, please visit the GPU club website: wiki.rac.manchester.ac.uk/community/GPU/Club/Meetings/23July2013.

N8 High Performance Computing

Project Principal Investigators can apply for access to this facility through a lightweight peer review process, the details of which can be found on the N8 HPC website: n8hpc.org.uk.

INteractive Computational LINux Environment–*INCLINE*

The Computational Shared Facility (CSF) has been a great success, but is configured primarily for batch work. Interactive (e.g., GUI-based) work can be done, but an environment *designed* for development, testing and post-processing would be more productive.

The Research Infrastructure team has secured £25k of seed funding to kick-start an interactive shared facility based on the same financial model as the CSF. If you are interested in such a service, please contact its-ri-team@manchester.ac.uk.

Computational Shared Facility (CSF)

For CSF information, please contact the IT Services Research Infrastructure team at: its-ri-team@manchester.ac.uk.

The CSF website is also available at: ri.itservices.manchester.ac.uk/csf.

Condor Pool Backbone Servers

The EPS Condor Pool backbone will be further strengthened in July to provide smoother 24/7 operation of this facility and reduce wasted cycles. We have been awarded central funds for 10 more computational servers and EPS is adding 3, giving us an extra 104 cores (assuming provisioned at 8 cores per server).

You can view further information on Condor at: condor.eps.manchester.ac.uk.

PRACE Industrial Advisory Committee

Dr Lee Margetts will be attending the next meeting of the PRACE Industrial Advisory Committee on 3September 2013. PRACE is the Partnership for Advanced Computing in Europe - www.prace-ri.eu. The purpose of the meeting is to help PRACE review how it promotes the use of High Performance Computing in Industry. If you work with industrial partners and have ideas or suggestions as to how joint industrial-academic use of European HPC facilities could be improved, or if you have experienced 'issues' that need help resolving, please contact lee.margetts@manchester.ac.uk.

News from the Faculties

Humanities

Your contact email is Hum-ITResearch@manchester.ac.uk.

Humanities Faculty IT Research Development Team
The team specialize in providing bespoke web applications and databases compliant with funding bodies' requirements for security, resilience and archiving of project data.

Members of research staff in the Faculty have been asked to update their publically available research profile for REF 2014. Theresa Teng from the team will be at a drop-in session for School of Law staff to demonstrate how to update profile details (*1 July 2013, 2-4pm Williamson 4.08*). No need to book, just drop by. If anyone from other Schools would also like such a session, please ask your External Relations Manager or Research Support Manager to contact Theresa Teng to arrange a date.

Humanities IT are currently cataloguing the large number of datasets on Faculty servers to ensure compliance with data protection legislation. If any researchers use either Access or spreadsheets (or equivalent desktop software) for small research databases, and keep them on a shared drive or your own P: Drive, please inform us what the database is used for, whether there is personal or sensitive data on it, and whether it is still necessary to keep this database. Contact: Theresa Teng or Phil Bradbury.

Current Projects News

Work has started on a major new project for the National Confidential Inquiry into Suicide and Homicide by People with Mental Illness (NCISH), which will last several months. A new web application will be developed to capture data from mental health professionals based nationwide, both in the NHS and in private practice. This replaces their current paper-based approach. Contact: Andrew Jerrison.

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Next edition

The next edition of this newsletter will be circulated at the end of July 2013.

If you have any news to contribute, please contact the IT Services Research Lead, Ian Cottam: ian.cottam@manchester.ac.uk before 25 July 2013.