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What's new at the  
NGS?

## The NGS is helping to make it happen!

Prof. Peter Coveney, a major user of the NGS, was recently nominated as one of the 25 most influential figures in the world of engineering and technology today.

Some of you may have seen the recent article on The Institute of Engineering and Technology website of who they believed to be 25 of the most influential figures in the world of engineering and technology today ("The People who Make it Happen";

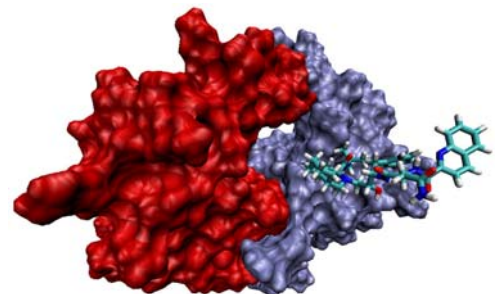
<http://kn.theiet.org/magazine/issues/0901/people-make-it-happen-5-0901.cfm>). We are pleased to see that the NGS had a mention due to the inclusion of Prof. Coveney, a major user of the NGS, who was featured in this list.

Prof. Coveney's research group at the Centre for Computational Science (where he is also Director), University College London has used the NGS for several major projects including the Virtual Physiological Human (VPH) initiative and GENIUS both of which make use of the US TeraGrid resources as well as those from the NGS.

The VPH project has been simulating the efficacy of a HIV drug (saquinavir) in blocking a key protein used by the virus. A large number of simulations were run to predict how strongly saquinavir would bind to three resistant mutants of HIV-1 protease and wild type protease, one of the proteins produced by the virus to propagate itself. Saquinavir is a known inhibitor of HIV-1 Protease as it blocks the maturation step of the HIV life cycle.

Professor Peter Coveney said: "This study represents a first step towards the ultimate goal of 'ondemand' medical computing, where doctors could one day 'borrow' supercomputing time from the NGS to make critical decisions on life-saving treatments".

The Genius project (Grid-Enabled Neurosurgical Imaging Simulation) is using the combined power of the NGS and TeraGrid to produce a 3D model of the blood flow patterns in patients neurovascular structure. Studying the patient's blood flow around the brain with a system like GENIUS before surgery can greatly increase the chances of success.



**The expulsion of saquinavir from a particular HIV-1 protease mutant**



## e-Science – the big chill in Indianapolis

Several members of NGS staff were present at the 4th IEEE International Conference on e-Science which was held in Indianapolis in December 2008. Throughout the five day conference NGS staff gave presentations on many areas including the management of international grid services and projects such as non-CMOS which involves several members of NGS staff.

The conference made the most of new networking technology such as Twitter, blogging, live streaming video etc. The conference website contains a host of information about the event as well as links to all the presentation videos and can be found at <http://escience2008.iu.edu/> so if you were unable to attend you can see what you missed! All members of NGS staff returned without suffering frostbite even in temperatures of minus 12. This year the conference will be taking place in Oxford, UK on the 9<sup>th</sup> – 11<sup>th</sup> of December (<http://www.escience2009.org/>) which we hope will be slightly warmer!



## The NGS goes down under again!

**Steven Young, NGS systems manager at the core node of the University of Oxford, recently visited Monash University in Melbourne, Australia.**

I visited Australia in December last year and had the opportunity to give a presentation about the NGS at the Monash eResearch Centre. The Monash eResearch Centre (MeRC) is a leading centre in Australia for Grid and e-Research activity (notice that in Australia they don't do hyphens). e-Research activity in Melbourne is active and growing.

There is e-research activity at various universities around Melbourne and the Victorian state government has funded VerSI (the Victorian eResearch Strategic Initiative; <http://www.versi.edu.au/>) which provides a coordinated approach to e-research collaborations (and which has Ann Borda, formerly of JISC, as its Executive Director).

My seminar was part of a series and I was in illustrious company. A week before MeRC was visited by Ian Foster (Argonne) and Daniel Katz (Louisiana) (<http://www.monash.edu.au/eresearch/events/index.html>). I gave an overview presentation about the UK NGS. Because I was a long way from home, and I wasn't trying to impress anyone, instead of a sales pitch, I gave a more open presentation. I presented about recent developments in the NGS Software Stack, NGS Inca monitoring and NGS Shibboleth integration with some warts and all information. Slides of my presentation can be obtained by polite request.

I enjoyed meeting the many people who came along to my presentation and would like to thank the Monash eResearch Centre and Anthony Beitz in particular for all the arrangements.

## Fast Upgrades at the University of Glasgow

The NGS partner site, the University of Glasgow, has recently upgraded its Grid cluster. In this article Mike Kenyon, ScotGrid Systems manager, explains how the process went and what the upgrade means for users at the University of Glasgow and beyond.

The University of Glasgow, an NGS partner site, has recently commissioned an extension to its Grid cluster, and in impressive time. The entire process, from completion of tender, to acceptance of the hardware, took just over 4 months.

In parallel with the procurement procedure, and operating to an even tighter schedule, a former workshop in the Department of Physics and Astronomy was converted into a dedicated server environment, utilising underfloor cooling and interfacing with the University's building management system to monitor environmental conditions. Optimal use of the cooling available has been ensured by the use of cold-aisle containment, a method which directs the flow of cool air through the nodes.

The new facility consists of 85 Supermicro servers configured as Grid worker nodes. Each server has two motherboards (i.e. 2 worker nodes) with 2 Quad-core, 64bit CPUs (running at 2.5GHz) per motherboard to give a total of 1360 cores. In terms of Grid storage, 20 Supermicro disk servers, each hosting 20TB of useable storage in a RAID 6 configuration, combine to give a total of 400TB space. These recent additions to the Glasgow site means that it is now the second largest provider of raw computing power (measured in kSI2K) in GridPP, and is one of the largest Tier-2 storage sites, with almost 0.5TB of space available.

Glasgow-based researchers are keen to put the new data, compute and network resources to good use. In particular, the National e-Science Centre (NeSC) at Glasgow is involved in a range of major biomedical related projects including the EU funded EuroDSD project (<http://www.eurodsd.eu/>) which is exploring rare genetic anomalies in children. Key to understanding the genetic mutations that occur are sequence analysis and comparison tools such as BLAST. To facilitate this access to and use of ScotGrid will allow large scale genome BLAST'ing. The expansion of services at Glasgow will also be used to support other projects at NeSC which are looking at small interfering RNAs for therapeutic drug development with specific focus on cancer drugs.



**Andy Elwell (Formerly at Glasgow as Data Management Expert); Mike Kenyon (ScotGrid Systems Manager); Prof. Tony Doyle (Physics & Astronomy at Glasgow University); Dave Power (Viglen Engineer)**

## Case Study

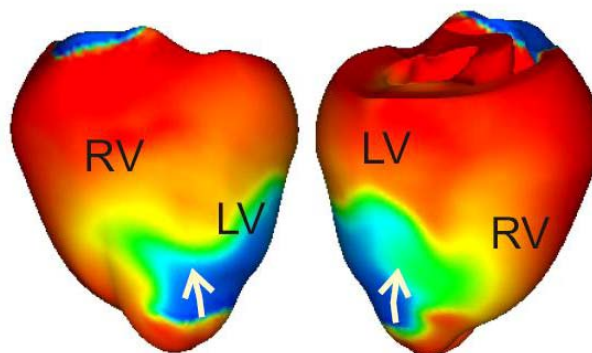
Case studies featuring research carried out by NGS users are regularly featured on the home page of the NGS website. In NGS News we will bring one of the case studies directly to you! If you would like your research to be featured on the NGS website and in NGS News as a case study then please contact Gillian Sinclair ([Gillian.sinclair@manchester.ac.uk](mailto:Gillian.sinclair@manchester.ac.uk)).

### The effects of defibrillation on the heart

Thushka Maharaj is a DPhil Student within the Computational Biology Group (<http://web.comlab.ox.ac.uk/oucl/research/areas/biocomp>) at the University of Oxford. She is part of an international collaboration studying the effects of applying an electrical shock to both healthy and diseased hearts, in an attempt to understand exactly how defibrillation works.

Within a normal, healthy heart the muscle cells (myocardial cells) produce regular, powerful cardiac contractions that allow the heart to pump blood around the body. During fibrillation, these contractions are no longer regular and powerful, but irregular so the heart is unable to pump blood around the body. The standard method today of treating hearts in fibrillation is to shock the heart into stopping completely – defibrillation – so that the myocardial cells have the chance to get back into a regular rhythm again.

Whilst this technique has been used successfully for many years, the mechanisms behind it are still not fully understood. Along with colleagues in the Integrative Biology project (<http://www.integrativebiology.ac.uk>), Thushka hopes to address some of the questions still being asked. In order to do so, she simulates how the application of electric shocks and differing types of tissue properties affects the behaviour of a normal, healthy heart.



**A whole ventricular model showing reentrant activity in the ventricles. The arrows show the direction of wave propagation.**

“We use parallel code with around a million nodes, so it is pretty computationally intensive,” explains Thushka. “But we can get 20ms of animation in 20 minutes using 32 CPUs on the NGS, which is a huge improvement.”

So much so in fact that she feels without the NGS, she would not have been able to even attempt her doctorate research. “I didn’t even know the NGS existed before starting my doctorate, but I don’t think we could have run these simulations without using the NGS. And the benefits of services such as the Storage Resource Broker are immense - it’s fantastic to be able to share data with colleagues all over the world so easily.”

## Are you Engaged?

The NGS and OMII-UK have been working closely together on the JISC-funded Engage project which is working with users to overcome the perceived barriers to using e-research. The project has now funded several short term projects which will provide new services and applications for NGS users. Steve Brewer from OMII-UK provides an update on Engage and introduces some of the newly funded projects. (This article also features in the latest edition of the OMII-UK newsletter).

A detailed picture of the UK's e-Research community has been developed by the JISC-funded Engage Initiative (<http://www.engage.ac.uk>). The Initiative interviewed over 50 researchers to build up a knowledge base of the many ways in which computationally intensive research is being conducted across research domains. Now that the e-Research picture has been created, the Initiative will review best practices and the lessons learned from the interviews, and the most promising technologies will be taken forward by a collection of Engage-funded projects. These projects were chosen because a significant contribution to the community could be achieved in a relatively short time-frame.

The Engage-funded projects cut across all areas of e-Research, from archaeology to climate modelling, and involve numerous applications of e-Infrastructure. A unifying aim of the projects is to deliver a new set of services and applications for the NGS. The Engage projects will provide greater functionality and an extended user base for proof-of-concept software, by strengthening it and transferring it to the NGS. The first stage of the Engage Initiative identified the projects that could benefit from funding; the future stages of the Initiative will see the community benefitting from software that will be developed to meet their needs.

## Engaging with the Arts and Humanities



**Segolene Tartre from the OERC demonstrating eSAD with David Wallom, NGS Technical Director**

Two notable features of e-Research are the willingness of researchers to embrace large-scale ICT, and the tendency to take up specialist technologies from different fields. The eSAD project is a good example. It is bringing together two multi-disciplinary collaborations to adapt image-processing tools for the study of ancient documents, which will then be provided to a diverse new community.

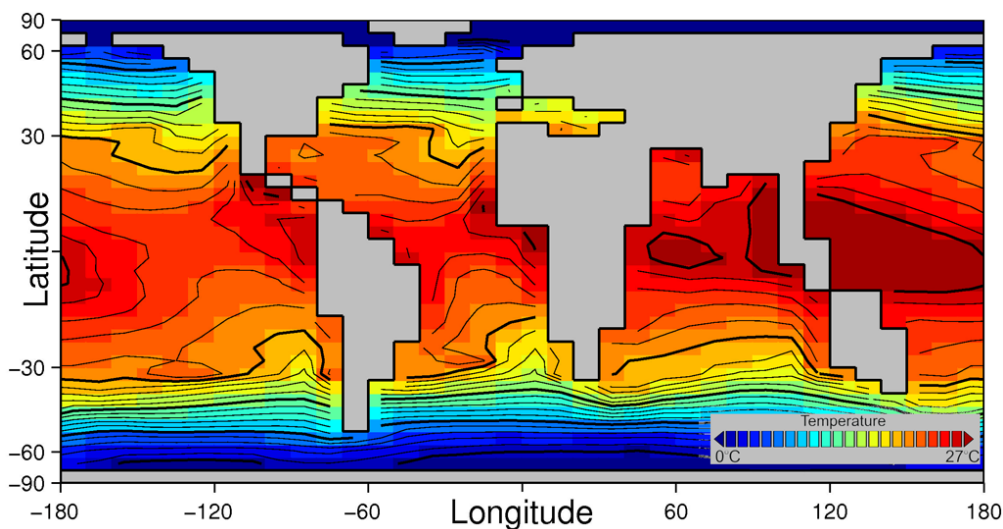
The eSAD project (<http://esad.classics.ox.ac.uk/>) will offer image-processing and interpretation support tools to papyrologists and epigraphers, using the more mature VRE-SDM project (<http://bvreh.humanities.ox.ac.uk/VRE-SDM>), which has developed a pilot portal framework for classicists studying ancient documents.

A user working with the VRE-SDM as a front-end, will have the ability to call upon the new image-processing tools developed by the eSAD project. The aim is to use the same techniques to plug in the functionality of the image-processing algorithms and, ultimately, an interpretation support system into the VRE. Image-processing algorithms will require the use of NGS resources and would ideally be offered as functionalities wrapped in Web Services and presented to the user in the VRE-SDM application within portlets. Migrating resources to the NGS also ensures access to the material by a much larger community, meaning that eSAD will enable a collaborative approach to the analysis and recording of ancient documents.

### Is it getting warmer out there?

A simple, fast-running model of the Earth's climate system was one of the end-products of the GENIE project (<http://www.genie.ac.uk/>). Making this system available to a more diverse research community is the goal of the Engage-funded Aladin2 project.

GENIE allowed users to model the climate over long timeframes – even those stretching over many thousands of years – albeit with a lesser degree of granularity than gained with other climate-modelling systems. The modular construction of GENIE enabled Open University students to acquire a stand-alone simulator that was used to create real-time models of various Earth projections. Funding from the Engage Initiative will help the GENIE project to combine their system with a MatLab toolbox, providing users with far greater control over the climate model.



**Screenshot from the GENIE climate model**

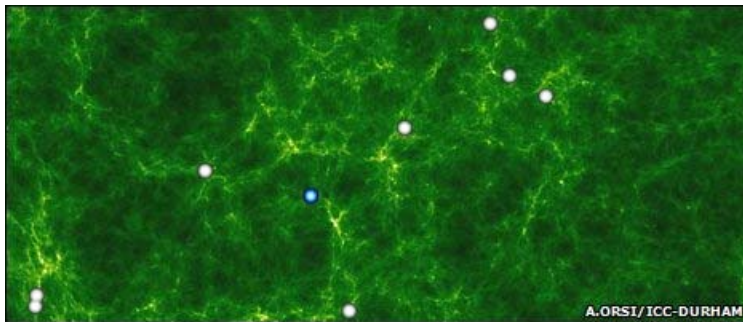
Current climate models, including GENIE, typically require users to possess a significant degree of computing expertise. Aladin2 will be considerably easier to use. The project will provide a prototype of a launch pad application that will help with the set-up and launch of the GENIE climate-modelling system. It will also facilitate the system's use in training workshops for PhD students and other researchers, and in Masters-level teaching units at the Universities of East Anglia and Bristol. The launch pad will be updated following evaluation in these environments, and an improved version will be released. It is anticipated that an NGS-hosted version of the application will appear shortly afterwards. The new application will facilitate the simple set-up and sharing of ensemble experiments, and will remove the need for extensive computing experience, making GENIE accessible, not only to a wider range of scientists, but to the public as well.

## NGS Applications Corner

In each edition of NGS News we will give an introduction to applications hosted on the NGS website. These may be existing applications or recently added applications that we'd like to bring your attention to. In this issue Jonathan Churchill from STFC-RAL looks at how the NGS is helping out astronomers.

### Astrophysics and Cosmology Research Software on the NGS

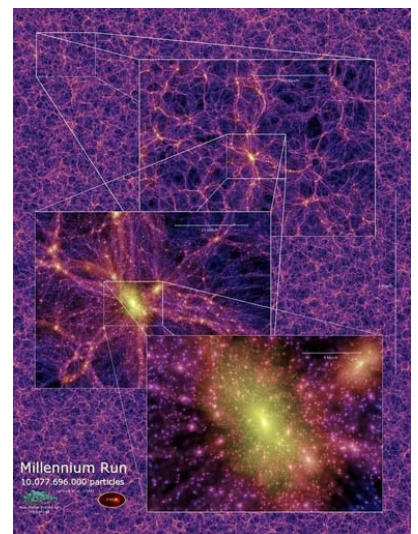
The universe is a big place and simulating how it evolves and how it may have formed in the past are large and challenging tasks. These simulations can help to refine ideas about how "dark matter" affected the early universe and where it might be distributed now. Or for example simulations of the early universe, just as the first galaxies were forming, as in the recent report (Ref. 1) from Durham University's Institute of Computational Cosmology, can be used to predict the kind of structures that improved telescopes may be able to resolve in a few years time.



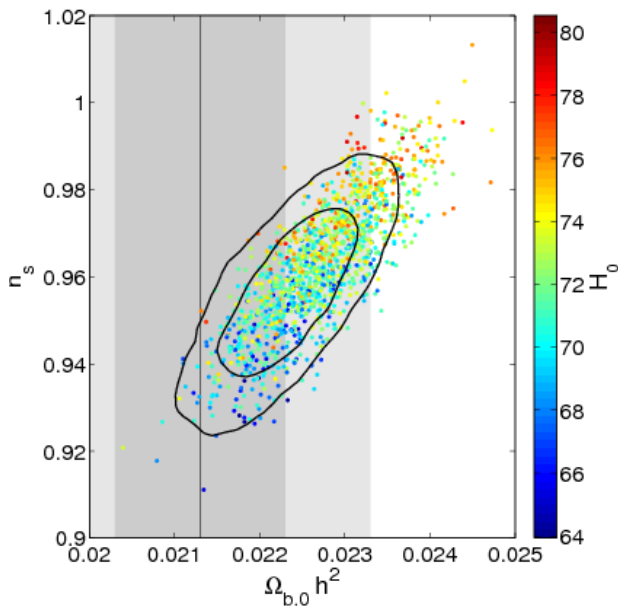
These kinds of simulations require large amounts of multi processor CPU computing. For example the "millennium simulation" run (Ref. 2) by Springel *et al*, which followed the course of around  $1 \times 10^{10}$  particles from the extremely early universe to the present day, took around a month of elapsed time on 512 processors of an IBM p690 computer, using 1 Terabyte of memory.

However this extreme level of detail, and hardware resources(!), are not necessarily required for interesting simulations. A version of the software, 'Gadget2', which was used to produce the "Millennium Run", has been run successfully on the NGS. These simulations may use, for example, a quarter of the numbers of processors of the full run and run for less time (10 hours or so).

However Gadget2 can be used to address a wide array of astrophysically interesting problems, ranging from colliding and merging galaxies, to the formation of large-scale structure in the Universe. With the inclusion of additional physical processes such as radiative cooling and heating, Gadget can also be used to study the dynamics of the gaseous intergalactic medium, or to address star formation and its regulation by feedback processes. It is installed on the RAL and Oxford NGS nodes (See Ref. 3)



Gadget2 is an N-Body / SPH (Smoothed particle hydrodynamics) simulator so it simulates by calculating the static forces between all the particles/bodies or regions, displacing them and then moving to the next time step. However the NGS also has installed a program for analysing the wealth of cosmic microwave background observations, which uses statistical techniques rather than N-body/SPH simulations. This is the 'CosmoMC' program.



CosmoMC (Ref. 4) is a Markov-Chain Monte-Carlo (MCMC) engine for exploring cosmological parameter space. The code does brute force (but accurate) theoretical matter power spectrum and Cl calculations with the fast Boltzman code CAMB. Its aim is to put estimates and error bars on various cosmological parameters which summarize the cosmic microwave background data and to, in principal, start to answer questions such as “Do we observe primordial gravitational waves?” and “Is the universe flat?” CosmoMC is, like Gadget2, a large multiprocessor code which can easily be run on the NGS. For further information on the CosmoMC installation on the NGS, see Ref. 5.

Running these large simulations is one thing but making sense of the output is just as hard. As can be seen from the ‘Millennium run’

poster above, the details are often hidden by the wealth of data in the results. The developers of Gadget2 have provided useful examples of how to analyse and visualise this output using ‘IDL’ a commercial data analysis package recently added to the NGS node at RAL. This provides simple ways to read in the data, for example from a binary file it uses just two lines to open and read in the data:

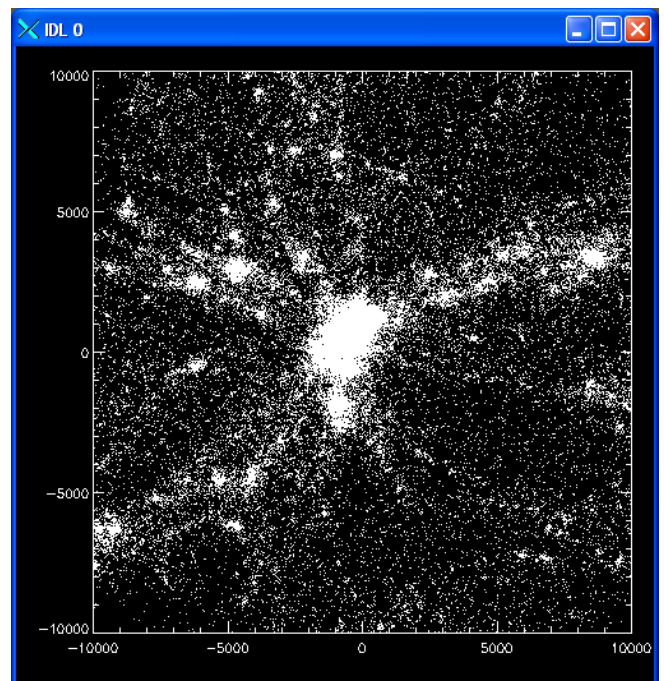
```
openr,1,fname,/f77_unformatted
readu,1,nparr,massarr,time,redshift,flag_sfr,flag_feedback,nparr
Total,la
```

and, after some normalising of the 2D data into two arrays ‘xdisk’ and ‘ydisk’, plot them on the screen using a single line:

```
plot, xdisk, ydisk, psym=3, xrange= [-xlen,xlen], yrange= [-xlen,xlen], xstyle=1,ystyle=1
```

producing a simple plot result as on the right.

As can be seen, there is lots of scope for Cosmology research using the NGS resources. I hope this article provides some food for thought.



Ref 1: <http://news.bbc.co.uk/1/hi/sci/tech/7882364.stm>

Ref 2: Simulations of the formation, evolution and clustering of galaxies and quasars. Nature Vol.435, June 2005, p.629

Ref 3: <http://www.ngs.ac.uk/sites/ral/applications/astrophysics/gadget2.html>

Ref 4: Cosmological parameters from CMB and other data: a Monte-Carlo approach Phys.Rev.D66:103511, 2002 <http://arxiv.org/abs/astro-ph/0205436v3>

Ref 5: <http://www.ngs.ac.uk/sites/ral/applications/astrophysics/cosmomc.html>

## The NGS and Social Networks

The NGS has always kept up to date with the latest in social networking. We already have a NGS blog, Facebook group, Flickr account etc. In this article Mike Jones (<http://twitter.com/nimp0>) explains why the NGS has now joined Twitter.

Over the last few years a number of social networks have sprung into existence and snowballed in popularity. To see what all the fuss is about and to keep our eyes on possible new ways of servicing the community the NGS has joined in.

The latest network we have joined is Twitter; you can find us here [http://twitter.com/uk\\_ngs](http://twitter.com/uk_ngs).



Twitter is a Micro Blogging facility allowing people to post short messages and build up communities. It's thanks to its simplicity, brevity and hooks into all sorts of other technologies -- e.g., other social networks, RSS, blogs, mobile phones -- that has given it its status in this age of social media. Initially a tool used for small social networks Twitter has expanded to help publicize events, manage conferences, promote new activities, help presidents to get elected, build up fan clubs, advertise, and more. Some interesting/relevant examples include:

- <http://twitter.com/stephenfry> - There are a number of celebrities now using twitter, Stephen is probably one of the more famous
- <http://twitter.com/BarackObama> - Folk were able to follow Barack and his campaign all the way to the Whitehouse
- <http://twitter.com/JISC> - Part Funders of the NGS. The JISC Twitter account helps to promote activities and funding opportunities. (A number of JISC's programme staff have also been active)
- <http://twitter.com/escience> - set up for the 4th eScience Conference in Indianapolis last December providing reminders and agenda changes.
- <http://twitter.com/NextGenScience> - almost our namesake!
- <http://twitter.com/LovellTelescope> - Technical data about the position of the Lovell Telescope at Jodrell Bank

For the NGS twitter account ([http://twitter.com/uk\\_ngs](http://twitter.com/uk_ngs)) we have set ourselves up so that we can communicate to followers items of news relevant to NGS business. We've also set a community relay up so that any posts from friends (those we follow) starting "@uk\_ngs" will be relayed to those that follow uk\_ngs.

### Other NGS outreach mechanisms

NGS Blog - <http://nationalgridservice.blogspot.com/> subscribe by RSS

NGS Facebook group - <http://www.facebook.com/group.php?gid=7070195774>

NGS Flickr group - <http://www.flickr.com/photos/ukngs/> please add any photos from NGS events or events where the NGS was present

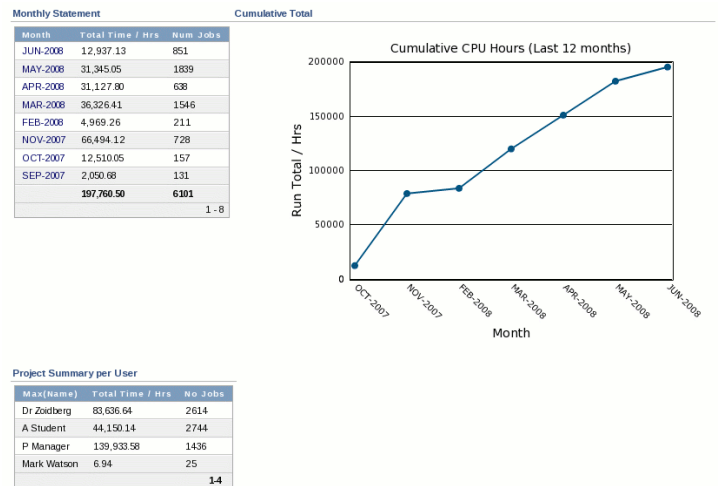
NGS News bulletin – <http://www.jiscmail.ac.uk/NGS-NEWS> a fortnightly email bulletin containing all the latest NGS news direct to your inbox

## Group Accounts at NGS

The NGS has traditionally distributed accounts on an individual basis but all that is about to change as Simon Collins, NGS database administrator at the University of Manchester explains.

Historically, users have been given quota on the NGS (CPU/Disk Space) on a per person basis. Whilst this has been a practical and successful solution, it is evidently more desirable, in certain situations, to allocate and manage quotas at a higher organizational level, e.g. for a group of researchers working on a common project. This simplifies the registration, authorisation and management of quotas in the system. The NGS has recently developed functionality to manage accounting at this level and academics may now apply for project accounts through the standard registration page (<https://www.ngs.ac.uk/apply.php>).

This new alternative utilises the concept of Virtual Organizations (VO). VO's could represent a group of people working on a particular project or at a whole institution. Applications and renewals are managed by a single project/VO administrator cutting down the administration in managing a project with many users. The NGS will create and manage the VO for those who don't have the facilities to manage their own - the application form allows a user to request this. The Manager of the VO account will be able to view a breakdown of the utilisation to the level of an individual working on that project (see diagram).



The single user application is still available (this is appropriate for researchers who are working on their own and are happy to have a dedicated account to be solely managed by them). If you would like more information about project accounts or would like to convert your present account into a project account please contact the NGS helpdesk ([support@grid-support.ac.uk](mailto:support@grid-support.ac.uk)).

## NGS Sysadmins Corner

Every issue we'll be bringing you a handy tip or shortcut from one of the NGS sysadmins. This time it is the turn of Simon Hood from the University of Manchester who shares a tip about Condor.

Many modern computational paradigms use distributed resources to allow for greater performance than can be achieved on a single system. Frequently those resources are located on private networks, rather than the public Internet; the network topology of a traditional HPC cluster is designed to isolate the computational nodes and interconnect for security and performance reasons. Over the past few years, the use of Condor across public/private network boundaries has been of particular and growing interest. Here at the University of Manchester, we (Research Computing Services) have tried the recommended General Connection Broker but found it to have scalability and reliability problems. However, using IP tunnelling to create a Condor pool across private and public networks has proved to be much more successful. Details (including links) can be found at <http://wiki.rcs.manchester.ac.uk/community/IPTunnelingInPlaceOfGCB>

## Collaboration Focus

Each issue we will introduce you to one of the institutions that make up the UK National Grid Service. In this issue the NGS partner site of the University of Westminster tell Gillian Sinclair why they got involved with the NGS.

**Gillian: Where is the Westminster team based?**

**Westminster:** The team is part of the Centre for Parallel Computing (CPC), one of the research laboratories in the School of Electronics & Computer Science.

**GS: Who is in the team?**

**W:** CPC is led by Prof. Stephen Winter (Director) and Prof. Peter Kacsuk (Technical Director). Dr. Gabor Terstyanszky and Tamas Kiss (new Grid services and application porting); Dr. Thierry Delaitre, Systems Manager (CPC infrastructure); Florent Daigniere and Zsolt Lichtenberger (NGS infrastructure); Noam Weingarten (application porting and testing).



**Back row from left: Zsolt Lichtenberger, Thierry Delaitre, Gabor Terstyanszky, Steve Winter and Florent Daigniere. Front row from left: Tamas Kiss and Noam Weingarten**

**GS: How long have you been a member of the NGS?**

**W:** CPC joined the NGS in February 2006 as a Partner site, providing the 32-node Tristan cluster. In 2008 it was replaced by a new Carmen cluster of 64 nodes with multi-core processors.

**GS: Why did you decide to become involved?**

**W:** Membership has brought us closer to the NGS community, users and providers. We are interested in the research and development issues, as well as the pragmatic practicalities, of effective user/provider interaction and engagement.

**GS: What advantages has being a partner brought Westminster?**

**W:** We have developed robust technology and sound processes for delivering services to research communities and to our industry contacts. We have established strong collaborative relationships with researchers in bioscience, engineering, healthcare, media, transport, and social science through W-GRASS (Westminster Grid Application Service) (<http://wgrass.wmin.ac.uk>). The feedback we acquired from NGS users and fellow providers has been extremely valuable and has helped us to create an increasingly appreciated service within the university and beyond. Our grid technology research has benefited tremendously!

**GS: What projects are the Westminster team participating in that involve the NGS?**

**W:** CPC is involved in the EDGeS (Enabling Desktop Grids for e-Science; <http://wgrass.wmin.ac.uk>) FP7 project which connects BOINC-, XtremWeb-based Desktop Grids and gLite-based Service Grids via bridges. Users are able to run their applications on the EDGeS infrastructure without being aware of where the applications are executed. The ProSim (Protein Molecule Simulation on the Grid) JISC Engage project to run protein molecule simulation on the NGS (<https://engage.cpc.wmin.ac.uk>). The project is based on effective collaboration between computer scientists bio-scientists. The project is porting the simulation to the NGS and developing application portlets to run the simulation seamlessly on NGS.

## NGS presents...

**Each issue we introduce a member of NGS staff who will explain their role within the organisation. In this edition we are delighted to introduce Hamza Mehammed who works for the Training, Outreach and Education (TOE) team at the National e-Science Centre based at the University of Edinburgh.**

Starting from last October, I have been working as a senior trainer of Grid computing primarily for the EGEE (Enabling Grids in e-Science; <http://www.eu-egee.org/>) and NGS projects at the National e-Science Centre (NeSC; <http://www.nesc.ac.uk/>) in Edinburgh. As a trainer in the NGS, I provide NGS and Grid Induction courses which can be general or tailored to a required discipline e.g. geosciences, biochemistry, biomolecular simulation, using application examples like AMBER, NAMD, GROMACS etc. Currently, we are preparing NGS induction courses and presentations to be held in Aston, Bath and London in the coming months. In addition to this, we also provide on-line courses which can be found on our website (<http://tc03.nesc.ed.ac.uk:8080>).



I am also a tutor in the International Winter School of Grid computing (IWSGC09; <http://www.iceage-eu.org/iwsgc09>) and will also take part in the international summer school of Grid computing (ISSGC09; <http://www.iceage-eu.org/issgc09>), both of which are organized by NeSC. Through the EGEE project, I am going to be one of the three main speakers in "Computing School 2009 CEA-EDF-INRIA '09" (<http://www.inria.fr/actualites/colloques/cea-edf-inria/index.en.html>) in France where I will give a series of talks and organise hands on sessions about grid services (computing, storage and information) and standardisation and interoperability issues of the globus, glite, and unicore middleware. I am also a member of the eUptake project (<http://www.e-researchcommunity.org/projects/e-uptake/>), with the National Centre for e-Social Science (NCeSS) and Arts & Humanities e-Science Support Centre (AHeSSC), in the JISC project, "Enabling Uptake of e-Infrastructure Services". In addition to this, I am providing a lecture support in the MSc course: distributed computing for e-Science.

I worked as a computer scientist researcher at the technical university of Munich (TUM), Germany, for three years. There, I was involved in the CrossGrid project (<http://www.eu-crossgrid.org/>) especially by the development of a performance analysis tool for Grid applications. I was also working at the Leibniz Computing Centre (LRZ) in the national grid project of Germany (D-Grid; <http://www.d-grid.de/>) for two years where I was responsible for the installation and training of Globus Toolkit 4 and also in the DEISA project by the integration of Globus services specially GridFTP. I have given some training courses specially GT4 in, e.g., Gridka and CoreGrid summer schools. My interest lies on specially the service oriented architecture of grid computing. I like to visit different cities and have visited many of the cities in Europe and USA. In my free time, I like swimming, reading and hiking.

## What's new at the NGS?

Jonathan Churchill, STFC, RAL updates us on new applications recently installed or updated at the NGS.

**GROMACS 4.0** – the latest version of this popular molecular dynamics package was recently released by the developers boasting improved scalability, full checkpointing support, REMD, and various optimizations. GROMACS is a versatile millions of particles. It is primarily designed for biochemical molecules like proteins and lipids that have a lot of complicated bonded interactions, but since GROMACS is extremely fast at calculating the non-bonded interactions (that usually dominate simulations) many groups are also using it for research on non-biological systems, e.g. polymers. This package is currently installed on the RAL node.

<http://www.ngs.ac.uk/sites/ral/applications/bioinformatics/Gromacs.html>

**IDL v7.0** - installation of IDL has recently been completed. This is a tool for rapid data analysis, data visualization, and software application development. IDL requires less code and programming expertise to produce visualizations and analyses than traditional programming languages. RAL have made available 2 licenses for batch mode analyses but not the GUI IDE. This tool is currently installed on the RAL node.

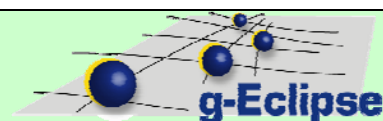
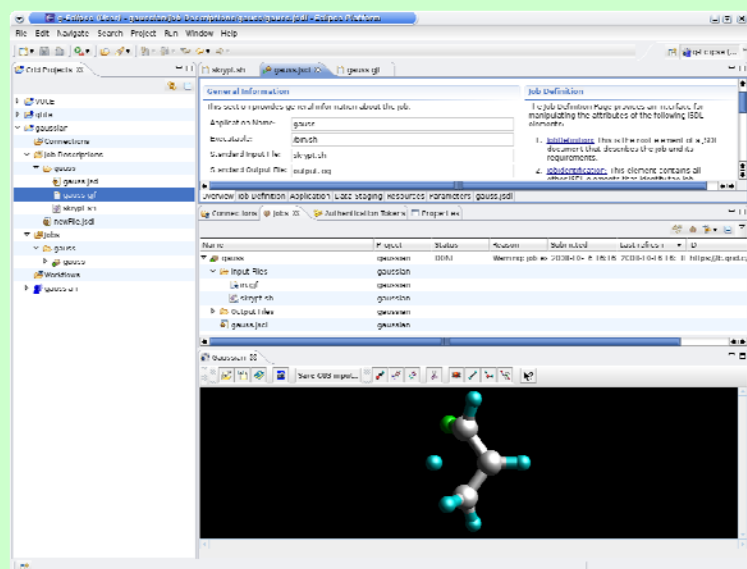
<http://www.ngs.ac.uk/sites/ral/applications/analysis/idl.html>



**PC-GAMESS/Firefly** – this is a freely available ab initio and DFT computational chemistry program. The recently released version 7.1.E is now installed on ngs.rl.ac.uk and ngs.leeds.ac.uk.

<http://www.ngs.ac.uk/sites/ral/applications/Chemistry/pc-gamess.html>

## First major release of g-Eclipse



The g-Eclipse project

has released version 1.0 of their framework – an easy-to-use workbench environment enabling end-users, application developers and operators to access and work with Grid and Cloud infrastructures. Built around a middleware-independent core, g-Eclipse currently supports the gLite and GRIA Grid middlewares and Amazon's Cloud platforms, EC2 and S3. Starting as a project funded by the European Commission, g-Eclipse is also an open-source Technology project at the Eclipse Foundation.

More information is available at <http://www.geclipse.eu/> and <http://www.eclipse.org/geclipse/>



## Event Diary

Event	Date	Location	Website	NGS presence
EGEE User Forum/OGF25 & OGF Europe's 2nd International Event.	2 <sup>nd</sup> – 6 <sup>th</sup> March 2009	Catania, Italy	<a href="http://www.ogf.org/OGF25/">http://www.ogf.org/OGF25/</a>	Part of the UK & Ireland Federation exhibition stand
JISC Conference 2009	24 <sup>th</sup> March 2009	Edinburgh, UK	<a href="http://www.jisc.ac.uk/events/2009/03/jiscconference09.aspx">http://www.jisc.ac.uk/events/2009/03/jiscconference09.aspx</a>	Exhibition stand
NGS Roadshow Aston University	7 <sup>th</sup> April 2009	Birmingham, UK	<a href="http://www.ngs.ac.uk/events/roadshows.html">http://www.ngs.ac.uk/events/roadshows.html</a>	Organiser
NGS Roadshow University of Bath	15 <sup>th</sup> April 2009	Bath, UK	<a href="http://www.ngs.ac.uk/events/roadshows.html">http://www.ngs.ac.uk/events/roadshows.html</a> (only open to University of Bath staff)	Organiser
Higher Education Academy Annual Conference	30 <sup>th</sup> June – 2 <sup>nd</sup> July 2009	Manchester, UK	<a href="http://www.heacademy.ac.uk/events/conference">http://www.heacademy.ac.uk/events/conference</a>	Exhibition stand
International Summer School on Grid Computing (ISSGC) 2009	July 2009	Nice, France	<a href="http://www.iceage-eu.org/issgc09/index.cfm">http://www.iceage-eu.org/issgc09/index.cfm</a>	Supporter
Advanced Distributed Services Summer School 2009 (ADSSS)	24 <sup>th</sup> August – 4 <sup>th</sup> September 2009	Oxford, UK	<a href="http://www.ngs.ac.uk">http://www.ngs.ac.uk</a>	Organiser

## How to get involved

We hope you have enjoyed this edition of NGS News. If you have any NGS-related news that you would like to see published in the next edition (June 2009) then please contact Gillian Sinclair ([gillian.sinclair@manchester.ac.uk](mailto:gillian.sinclair@manchester.ac.uk)). The deadline for content for the next issue is the 11<sup>th</sup> of May 2008.

If you are a researcher currently using the NGS or if you have recently used the NGS, we would like to feature your research as a case study for our website and to possibly use it as promotional literature for the NGS. If you are interested in distributing your research findings to a wide UK and international audience then please contact Gillian at the address above.