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NGS Adopts Globus Online

The NGS has recently adopted Globus Online as a preferred data movement method for our users.

Many of the computing resources available to the NGS community have been added as transfer endpoints in the Globus Online system,



a hosted service for high performance data movement, and NGS has been enabled as an identity provider for the service. Using their NGS credentials, users can quickly and easily log in to Globus Online and move files among NGS servers, or between an NGS server and the user's local server or laptop.

"We aim through the availability of this service to ensure that our users can quickly and easily access the data they need, regardless of the size or location of the data volume," said David Wallom, NGS Technical Director. "The process to move large volumes of raw information from resources that have generated it, back to the user who needs to manipulate and analyse the results, can be not only time-consuming but also difficult and frustrating for researchers. Enabling Globus Online for NGS data movement will provide a significant value-added service that I know will benefit our users."

Dr. Wallom further explained, "By using a web-based service, we are also ensuring users will have minimum interaction with what they might consider complex ICT tools and technologies -- whilst giving them access to a sophisticated yet easy-to-use capability."

Globus Online is a secure, reliable file transfer service that makes it easy to move datasets of any size, whether between supercomputing facilities or from a facility to a local server or personal computer, without requiring custom end-to-end systems.

"We are very happy to provide this service for the hundreds of researchers who rely on NGS resources," said Ian Foster, Director of the Computation Institute at University of Chicago and Argonne National Laboratory, home to Globus Online. "With the increased capacity for sharing and collaboration that Globus Online provides, NGS users should be able to better focus on their research without the distraction of having to worry about how to move files from here to there."

For more information on Globus Online, please see the NGS website <http://www.ngs.ac.uk/news/uk-national-grid-service-ngs-adopts-globus-online>

SeIUCCR e-infrastructure Summer School Round up

In September 2011 the SeIUCCR project (<http://www.ngs.ac.uk/seiucctr/home>), of which the NGS is a partner along with the Software Sustainability Institute (<http://software.ac.uk/>), held an e-infrastructure summer school for early career researchers.

Over 25 students from all over the UK attended the summer school which was held at Coesner's House in Abingdon. The summer school was massively over-subscribed with 120 applications for the places. In order to make the material available to the large number of applicants who did not manage to get a place, the presentations are now available on the SeIUCCR website at

<http://www.ngs.ac.uk/seiucctr/ss2011presentations>.



We received excellent feedback regarding the summer school such as -

"The summer school was a relaxed and friendly environment. It provided detailed information about the various resources available to researchers both in terms of computer resources and support. The staff were very approachable and keen to show an interest in the attendees work. Overall it was a great experience I would recommend to anyone who has an interest in grid/cloud/HPC or who's work may benefit from such technologies."

All comments and recommendations from this first event will be taken into account for the planning of the next event in 2012. If you would like to see more of the feedback received after the event, please see the NGS blog entry at <http://nationalgridservice.blogspot.com/2011/10/long-long-time-ago-or-so-it-seems.html>.

Interact with the NGS

The NGS has recently updated its presence on Facebook to a new interactive page. Instead of the old-style group page, the NGS now has a new page under the UK NGI banner to reflect our role as the lead in the UK National Grid Initiative.

By "liking" our page you will receive news updates from the NGS in one place as well as articles of interest from the Software Sustainability Institute (SSI) and GridPP. You can share the articles with your friends list and help spread the word about e-infrastructure.

The new page can be found at www.facebook.com/UKNGI

The NGS and the EGI Clouds Federation Task Force

Dr Matteo Turilli from the NGS at the Oxford e-Research Centre (OeRC), University of Oxford has recently been appointed Chair of the EGI Clouds Federation Task Force. In this article he explains what the EGI Clouds Federation is and how it can benefit NGS users.

The EGI Clouds Federation Task Force (<https://wiki.egi.eu/wiki/Fedcloud-tf>) is a European initiative promoted by EGI.eu (<http://www.egi.eu/>) to leverage and coordinate the effort of Resource Providers, such as the NGS, that are experimenting with or deploying already virtualised management environments – i.e. cloud infrastructures. The main goals of the Task Force are to produce a blueprint document for a federation of clouds and a test bed platform accessible to user communities. Our work is contributing to the foundation for the future EGI.eu cloud infrastructure and services.

The Task Force engages resource providers, technology providers and user communities. The resource providers are institutions and private companies that offer staff effort and part of their infrastructure to the Task Force in order to develop the test bed and to write the blueprint.



Analogously, the technology providers bring to the Task Force the required expertise and development effort. User communities are at the core of our activities providing, through the EGI.eu outreach infrastructure, use cases, scenarios and requirements. Currently, the Task Force amounts to more than fifty members coming from twenty four institutions across Europe. Each institution participating to the Task Force activities funds the contributed staff effort and resources. The Task Force will operate for eighteen months, until March 2013.

The Task Force is open to everyone that wants to contribute resources or technologies. User communities and researchers are welcome to join the Task Force and gain free access to the federated resources. To join the Task Force email us at fedcloud-tf@mailman.egi.eu.

The Task Force will fulfil its objectives by delivering a blueprint and a test bed infrastructure. The blueprint document will serve as advice and, where available, full documentation to resource providers and users on how to engage with the federated virtualised environment. The test bed infrastructure will be based on state-of-the-art cloud technologies. This will be useful to test the available standards implementation and to show how much integration can be currently achieved between the available cloud technologies and the centralised services offered by EGI.

The blueprint document is a collaborative effort and can be found constantly updated at <https://wiki.egi.eu/wiki/Fedcloud-tf:Blueprint>. Information on the Task Force test bed – including

instructions on how to obtain an account - can be found at <https://wiki.egi.eu/wiki/Fedcloud-tf:Testbed>.”

I have been involved in the NGS cloud effort for the past two years contributing to the design and the deployment of the NGS cloud test beds. I have participated to several other research projects about Cloud Computing and when the UK NGI decided to collaborate to set up the Task Force I have been asked to lead that effort alongside the NGI.



A federated cloud infrastructure at the European scale is in the interests of the UK research community. The

enthusiastic response to the NGS cloud test beds (<http://www.ngs.ac.uk/accessing-the-ngs-cloud-service>) and the NGS user surveys teaches us that a relevant number of UK research communities are already using cloud services for their research. Meanwhile, the provision of shared computational resources is still undergoing a transition.

From an initial phase in which large amounts of data and computational resources were needed only by few research communities, a new phase is emerging in which many disparate research groups use computation intensely. Life science, humanities, engineering, chemistry, astronomy, space science are just few of the research areas that are routinely using a large amount of computational and data resources.

Such a heterogeneous user base needs a flexible provision of computational resources based on multiple delivery models, recognised standards and federated services for monitoring, accounting, identity and resource management, and information publication.

At the moment, Cloud Computing or, more precisely, virtualisation management platforms, promise to offer a very flexible foundation capable to satisfy all these requirements. Investing now in creating a blueprint and a test bed for clouds federation is an effective way to bring the UK research requirements into the future of computational services for research. But there is more than a strategic edge.

Thanks to the involvement of NGS and the UK NGI into the EGI Clouds Federation Task force, every UK user community has the opportunity to use for free the cloud resources of fifteen cloud providers across Europe. A pretty good deal I think!”

For info and to use resources email fedcloud-tf@mailman.egi.eu.

Case Study

Case studies featuring research carried out by NGS users are regularly featured on the NGS website but in NGS News we will bring one of the case studies directly to you!

Scalable Road Traffic Monitoring using Grid Computing

Recent technological advancements in sensing systems have caused an explosion in the volume of data relating to real world phenomena. For example systems monitoring weather, road traffic and natural disasters such as floods, earthquakes, tsunamis and volcanoes all generate a large amount of data. Typically this data is geographically referenced and is most useful in the short term.



Accessing such data over the internet has been greatly facilitated by the introduction of Sensor Web Enablement (SWE), a specification framework defined by the Open

Geospatial Consortium that provides a standard web service based interface through which to task heterogeneous sensor networks and retrieve their observations. However, processing the large volume of data generated by geographical sensors in a short time period presents an enormous computational challenge. This is where grid computing can help.

Aengus's research focused on processing near real-time geographic information delivered through SWE interfaces using Grid computing infrastructure. His research is helping to drive technology forward by integrating emerging software standards in Sensor Web and Grid Computing.

Furthermore, his research attempts to classify near real-time processing operations on geographically referenced data with respect to Grid computing architectures, thus outlining the types of application for which this architecture is suitable. Aengus used traffic monitoring and routing as a real-world application case study through which the strengths and weaknesses of current specifications can be evaluated and different types of processing operations can be considered.

One geoprocessing operation Aengus investigated was termed map-matching and involves matching GPS tracks from a fleet of vehicles to the road network. Aengus used the GridSAM job submission service to run open ended compute jobs on the NGS which retrieved GPS tracks in near real-time from a SWE service, combined this with base map data of the road network and publish the matched position to another SWE service.

The map-matching operation is not particularly computationally intensive when data from a single vehicle over a short time period is considered. However, the benefit of executing this computation on the NGS is clear when it is necessary to perform the operation for several hours a day for a large fleet of vehicles. For example when managing a fleet of city council vehicles, map-matching needs to be carried out as a pre-cursor to network analysis functions such as allocating vehicles in response to an incident, or routing vehicles between two location. Aengus successfully tested the system with up to 250 vehicles.

Aengus explained that “The NGS has made endless CPU hours available to me through a standards based interface; it has been an invaluable resource for my research”.

More NGS User Case Studies!

There has been a rush of new user case studies featured on the NGS website over the last few months. The new case studies are –

- Modelling the effect of the peptide sequence on the binding affinity to carbon nanotubes - Susana De Tomasio, University of Warwick <http://www.ngs.ac.uk/modelling-the-effect-of-the-peptide-sequence-on-the-binding-affinity-to-carbon-nanotubes>
- Systematic modelling of ionic liquids - Edward Ballard, University of Wales, Bangor <http://www.ngs.ac.uk/systematic-modeling-of-ionic-liquids>
- Optimisation of imaging during radionuclide therapy using simulations - Maria Holstensson, Institute of Cancer Research <http://www.ngs.ac.uk/optimisation-of-imaging-during-radionuclide-therapy-using-simulations>
- Finding new messages hidden in the genetic code with the NGS - Charlie Laughton, University of Nottingham <http://www.ngs.ac.uk/finding-new-messages-hidden-in-the-genetic-code-with-the-ngs>
- GridQTL – Computational Genetics via the Grid - John Allen, University of Edinburgh <http://www.ngs.ac.uk/gridqtl-computational-genetics-via-the-grid>
- Using the NGS to Help Determine the Suitability of Thoria for a Next Generation Nuclear Fuel - Paul Martin, University of Huddersfield <http://www.ngs.ac.uk/using-the-ngs-to-help-determine-the-suitability-of-thoria-for-a-next-generation-nuclear-fuel>
- Using the NGS to run a computer tournament on social learning strategies - Luke Rendell, University of St. Andrews <http://www.ngs.ac.uk/using-the-ngs-to-run-a-computer-tournament-on-social-learning-strategies>
- Accelerating the Processing of Large Corpora: Using Grid Computing Technologies for Lemmatizing 176 Million Words Arabic Internet Corpus - Majdi Sawalha, University of Leeds <http://www.ngs.ac.uk/accelerating-the-processing-of-large-corpora-using-grid-computing-technologies-for-lemmatizing-176>

Not So Secret Agents

Simon Hettrick from the Software Sustainability Institute (SSI) introduces their agents network consisting of UK researchers from a wide range of disciplines.

If getting good information is difficult, getting good information from across disciplines is damn near impossible. Huge organisations – the Googles and Microsofts of this world – get round the problem by employing lots of experts from different backgrounds. We don't have those kind of resources at the Software Sustainability Institute, so we came up with a different solution.

The institute helps researchers (from all disciplines) build better software. To do this job, we need to know who's using software and who needs our help. The easiest way to learn about these developments is to attend conferences – after all, that's the way the researchers do it.

But what are the right conferences to attend and, when you get there, who are the right people to talk to? Unless you're

already an expert in the field, these questions are difficult to answer. To solve our information problem, the institute needed experts. We don't have the resources to employ them, so we sent them packing instead.

We came up with the idea of a swap: the institute needs information and researchers want to travel. We agreed to pay researchers up to £3000 a year in travelling expenses in exchange for the benefit of their expertise. It's a fair deal: we get information that has been sifted and verified by experts in the field, and the researchers can go to conferences that they would not otherwise have been able to attend.

In July this year, the hunt for our Agents began. We based the application process around the two skills that an Agent must possess: they have to learn new information quickly, and they have to effectively communicate that information to non-specialists (i.e. us). In the first round of judging, we asked the applicants to describe their research, and the way they use software, in a way that a non-expert audience could understand.

The second round was more difficult: we asked the applicants to write a blog about someone else's research. There were other factors to consider. We needed a good coverage of the research community, so we wanted researchers from a wide range of organisations and as wide a range of backgrounds as possible. We also gave preference to early career researchers, because we have found that they tend to be active in emerging technologies and are more likely to write the reports we need.



The application process was a great success. We were inundated with applications in the first round – over 130 of them for the 10 places we had on offer. This was whittled down to 30 applications in the first round of judging and then, with the help of the NGS's Claire Devereux as our independent adjudicator, we chose our 10 Agents.

Now that we've recruited our Agents, getting good information just got a lot easier. We have access to experts in fields as diverse as climate change and sports science. This is an incredible resource for the institute. We have massively increased the breadth of research that we can deal with (and that we have exposure to), and we have a team to call on when we face problems that are outside of our field of expertise.

Details about our Agents are available on the Software Sustainability Institute's website. If you would like to meet the Agents, the best opportunity will take place next March at the Collaborations Workshop 2012.

For more information about the SSI agents, visit <http://www.software.ac.uk/agents>

Dinosaurs Marching Over Europe

The research of NGS users was recently featured as a "success story" by EGI (http://www.egi.eu/results/success_stories/how_fast_could_a_T-rex_run.html).

The research of several NGS users was recently featured as a "success story" on the EGI website. William Sellers, Phil Manning (both University of Manchester, UK) and Karl Bates (formerly University of Manchester, now University of Liverpool, UK) used Grid computing to better understand dinosaur locomotion.

As there are no similar animals around today to compare to dinosaurs such as a T. Rex, the solution is to create a detailed computer simulation of the animal's skeleton and muscles.

Their research has featured heavily in Grid publications around the world as a fantastic example of the work that can be done on Grid resources. For more articles on their research see the links below:

- Exploring the locomotor dynamics of extinct animals using evolutionary robotics – NGS Innovation Forum 2009 http://www.ngs.ac.uk/sites/default/files/file/ngsif09_presentations/NGS_IF09-loco.pdf
- Answering a truly big question: How did dinosaurs move? <http://www.isgtw.org/feature/feature-answering-truly-big-question-how-did-dinosaurs-move>
- How fast could a T. rex run? <http://www.isgtw.org/feature/how-fast-could-t-rex-run>



Event	Date	Location	Website	NGS Presence
Workshops on e-Science Workflows	9 th – 10 th Feb 2012	Budapest, Hungary	https://www.egi.eu/indico/conferenceDisplay.py?confid=656	
OGF 34	12 th – 15 th March 2012	Oxford, UK	http://www.gridforum.org/OGF34/	
EGI Community Forum	26 th – 30 th March 2012	Munich, Germany	http://cf2012.egi.eu/	
Digital Research 2012	10 th – 12 th Sept 2012	Oxford, UK		
8th IEEE International Conference on eScience (eScience 2012)	8 th – 12 th October 2012	Chicago, USA	http://www.ci.uchicago.edu/escience2012/	

How to get involved

We hope you have enjoyed this latest edition of NGS News. If you have any NGS-related or grid computing news that you would like to see published in the next edition (March 2012) then please contact Gillian Sinclair (gillian.sinclair@manchester.ac.uk).

We are always looking for research papers, conference presentations and posters to feature on our website. If you are interested in distributing your research findings to a wide UK and international audience then please contact Gillian at the address above.