Inspired

news from the EGI community

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TOP STORIES

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European Grid Infrastructure

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This Issue

We are on our way to Madrid this Summer, getting ready for the Technical Forum, co-hosted with Ibergrid.

In the meantime, in issue 12 of *Inspired* we have...

> Kitti Varga invites us to get on board with the new science gateways

> Sergio Andreozzi introduces the EGI Solution Portfolio

> Audrey Gerber tells us how the Israeli NGI is helping one company detect genetic mutations

> Carmela Asero highlights where EGI can make a difference for the Digital Agenda for Europe strategy

Plus more about:

The new EGI leaflet on Applications for Biophysics, the GlobusOnline cookbook, the EGI-InSPIRE third year review and Fujitsu, gold sponsor of the Technical Forum

Your comments are always welcome!

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All EGI roads lead to the Technical Forum 2013 in Madrid, Spain.
This issue's picture is a view of Madrid, taken from the M30 motorway.
(Illustration: dr zoidberg / wikicommons)

TF2013 updates: timetable and early-bird registration

The Technical Forum will be held in Madrid, between 16-20 September

Online registration for the event is now open and early bird discount rates are available until 31 July 2013.

All session proposals and abstract submissions have been reviewed by the programme committee, and a timetable is now online in Indico. The main conference tracks are:

> Virtual Research Environments and Enabling Technologies

> EGI's Core Infrastructure Platform

> EGI & Infrastructure as a Service (IaaS) Cloud Platforms

> EGI's Human Networks

> Policies and Business Models for Open Compute and Data Infrastructures

Confirmed keynote speakers

> **Elisa Martín Garijo**, from IBM. Title: *Emerging Technologies and Trends in the IT sector*

> **Ignacio Llorente**, from the OpenNebula Project. Title: *Bringing Private Cloud Computing to HPC and Science: Present and Future*

> **Niklas Blomberg**, from ELIXIR. Title: *The European research infrastructure for life-science data*

> **Afonso Duarte**, from ITQB. Title: *Unveiling the mechanisms behind biomolecules – the role of grid*

> **Xavier Barcons**, from the European Space Observatory. Title: *The most powerful European astronomical observatories and their interplay with e-science*

More information

EGI Technical Forum website - *http://tf2013.egi.eu*

Link to online registration - *http://go.egi.eu/reg-tf13*

Provisional timetable - *http://go.egi.eu/TF2013*

Taking the SCI-BUS around the world

Kitti Varga invites us to get on board with the new science gateways

Photo: F.Guimarães / wikicommons

Science Gateways are frameworks that enable applications to run on grid and cloud infrastructures. They also provide services to upload and share, search, manage or download applications and data. The gateways are integrated via portals or sets of applications. They enable user communities to use resources through a common graphical user interface in an easy and intuitive way. As a result, users can focus on their applications instead of having to manage a complex underlying infrastructure.

The results

As of June 2013, the project has 22 science gateways running using the SCI-BUS gateway technology, and 14 more using application specific portals developed by members of the SCI-BUS community. These gateways support different communities, such as physics, bioinformatics, astrophysics or meteorology.

The workflow applications developed for the SCI-BUS gateways are uploaded and published in the SHIWA Repository. This allows other communities to take advantage not only by using the gateway technology and the portlets, but also the workflow applications.

Update, don't develop

The gUSE/WS-PGRADE portal is the core technology, common between SCI-BUS science gateways. This means that new features and bug fixes are published often and communities can easily update their own gateways. Communities can also develop their own specific portlets based on the core technology, without starting from scratch.

Exploit the Data Bridge

The gUSE/WS-PGRADE framework is being further developed to satisfy the needs of the user communities. The roadmap of these developments is public and any community can contribute. The Italian astrophysics community, for example, is developing a mobile version of the science gateways.

One of the most exciting developments is the Data Bridge service that exposes a simple web service for accessing different types of storage resources. This service will be accessed by an easy-to-use interface integrated into gUSE/WS-PGRADE, allowing users to easily exploit the storage resources supported by the Data Bridge.

STARnet: an advanced SCI-BUS

Some communities have been developing the idea of application specific gateways even further: the astrophysics community has set up the STARnet Federation to create a network of science gateways based on SCI-BUS technology to share a set of services for authentication, computing infrastructure access, and data/workflow repositories.

Ugo Becciani, of STARnet, told us about their federation: "Among the diversified variety of applications related to the astrophysics field we have selected so far some specialised use cases related to scientific visualisation, cosmological simulation, stellar evolution and comets and meteoroid dynamical evolution. Those applications were developed and maintained into the first core sites belonging to the STARnet Federation."

Be a part of it

SCI-BUS is an open project - any organisation is welcome to join as an associated partner.

Associated partners will be supported by SCI-BUS to develop and set up their own science gateway and they can attend the SCI-BUS project meetings.

More information

The SCI-BUS project wants to make the life of e-scientists easier by creating a new way to customise science gateways based on generic gUSE/WS-PGRADE. *http://www.sci-bus.eu/*

The EGI Solutions Portfolio

Sergio Andreozzi introduces five paths to accelerate data-intensive research and engage with user communities

The EGI Solutions Portfolio is based on the EGI.eu Service Catalogue.

The catalogue is available online since May 2013, after an analysis of the EGI ecosystem to document all EGI activities and redefine them as a service, according to their business value.

With the services defined, the next step was to think about how they could be deployed for the benefit of the EGI user community.

The result was a portfolio of five EGI solutions for five common e-science problems and pain points.

We believe that the Solutions will be a powerful outreach tool that will increase the visibility of the EGI added value to e-science and innovation.

There is no clearer way to explain what we do to funders and potential new users: do you have a research data problem? These are our solutions.

> **More information**
>
> **EGI Solutions Portfolio**
> *http://www.egi.eu/solutions*
>
> **EGI.eu Service Catalogue**
> *http://www.egi.eu/services*

Solution #1 - Federated Cloud

Do you need an infrastructure to deploy on-demand IT services for managing and processing your research data?

EGI offers...
A single, standards-based, open system to federate academic clouds from multiple providers, offering scalable computing resources with increased flexibility.

You will get...
Advanced compute capabilities for your research, virtualised resources to run any environment you choose, cloud storage for easier sharing of data, and a number of support services to ensure your applications run as efficiently as possible.

Solution #2 - Federated Operations

Do you need operational services and tools to run a distributed IT infrastructure for research?

EGI offers...
The technologies, processes and people required to manage the operations of a heterogeneous infrastructure and to integrate resources from multiple independent providers with a lightweight central coordination.

You will get...
A cost-efficient framework to manage operations within a federated environment, while retaining responsibility of local infrastructure.

Solution #3 - High-throughput data analysis

Do you need to analyse large datasets, or to execute thousands of computational tasks?

EGI offers...
A global high-throughput data analysis infrastructure, linking hundreds of independent research institutes, universities and organisations delivering top quality computing resources. As of May 2013, EGI offers more than 333,000 CPU cores of installed computing capacity, supporting about 1.4 million computing jobs per day.

You will get...
Large-scale computing, storage and data management facilities to handle big datasets, allow faster results and enable global collaborations.

Solution #4 - Community networks and support

Do you want to discover the best approach to your data-intensive compute needs?

EGI offers...
Established knowledge transfer channels to inform, connect and advise researchers across the globe, and direct engagement with community networks able to solve specific user requirements.

You will get...
Definitive, user-friendly and engaging information and support tailored to your requirements, as well as a network of contacts who are able to show you the best approach to use EGI for your work.

Solution #5 - Community-driven innovation

Do you want to develop new ways to address challenges in the EGI community?

EGI offers...
A mechanism to hear your ideas, find the right experts and bring together a short-term team to address the challenges of an EGI community, or to create a way to help a research group get started with EGI.

You will get...
A focused group of experts from the EGI community that helps you address a technical challenge, resulting in plenty of saved time and an improved user experience.

New sequencing tests to diagnose hereditary diseases

Audrey Gerber tells us how the Israeli NGI is helping one company detect genetic mutations and provide knowledge that can save lives

They say that you cannot escape your genes. But with the help of grid computing, a leading provider of molecular diagnostic products and services from Israel is making it easier to outrun them.

Many diseases are caused by changes, or mutations, in our genes. Some mutations interfere with the proteins responsible for hereditary diseases and or disability, while other mutations increase the likelihood of developing a disease.

The key to understanding, treating and preventing genetic diseases is to identify and map genetic mutations in order to understand the cascade of biological events that occurs when changes are present. To do this, researchers need to decipher DNA sequences and determine the precise order of their basic building blocks. Next-Generation Sequencing (NGS) is a promising new technique that yields reliable results at a competitive cost.

Pronto Diagnostics, a Tel Aviv-based developer of molecular diagnostic products and services, is determined to extend the power of affordable NGS instruments and give doctors feasible diagnostic capabilities.

To do this, Pronto chose two diseases as models: hereditary breast and ovarian cancer, and Congenital Myasthenic Syndromes (CMS), a group of neuromuscular diseases.

The clinical ramifications are clear in both. Knowing which women are at higher risk for breast or ovarian cancer helps to ensure earlier diagnosis and allows informed choices regarding preventive measures. Knowing which mutation causes CMS enables the selection of the most effective therapies.

Pronto's main goal is to develop tests and the accompanying analysis tools for these and additional disease groups. To do this, it needs to create a database of non-pathogenic genetic mutations by aligning sequencing results of selected genes and analysing the data from many perspectives.

Using NGS, each nucleotide must be sequenced at least 100 times on average to get high-certainty data. So to find the sequence of a target region that has half of million nucleotides, at least five million nucleotides need to be sequenced. That requires quite a lot of computing power.

How Isragrid is helping

Pronto Diagnostics does not have in-house bioinformatics capabilities of the scale required for NGS-based research. In fact, few commercial companies do outside of global pharmaceutical conglomerates or academic-based laboratories and institutions.

The company turned to Isragrid, Israel's National Grid Initiative (NGI), for assistance. Isragrid is a cooperative initiative of three government ministries: Industry & Trade, Finance and Defense, and Israel's Council for Higher Education. And to extend capacity, Isragrid is fully integrated with the European Grid Infrastructure (EGI), providing full access to this enormous resource.

A typical sequencing output is a text file between 3 to 7 Gb that must be compared and aligned to the human genome sequence, in itself a 3.17 Gb file. This process could take several days on a standard personal computer. But on the grid, it can be allocated and divided into many parallel threads and completed in up to 12 hours – or overnight.

In contrast to less costly and commonly used tests that scan only for known mutations, next generation sequencing is able to identify new mutations. Pronto Diagnostic's work is leading toward diagnostic-grade NGS tests to discover and diagnose all the genetic mutations associated with diseases, rather than just the more common ones, and making this both and accurate and affordable option for more and more patients.

More information

Audrey Gerber is the Communications Officer for Israel's IUCC and Isragrid.

Isragrid: http://www.isragrid.org.il/

This story has been previously published on iSGTW (http://www.isgtw.org) and as an EGI case study (http://go.egi.eu/cst)

Digital Agenda for Europe: why it is important for research communities

Carmela Asero highlights where EGI can make a difference

On 19-20 June 2013, the Digital Agenda Assembly met in Dublin to reflect on recent milestones. What does this mean to the EGI community?

Virtual Research Environments

The focus of the Digital Agenda Assembly was on how key technologies can help economic growth and create jobs. One of these is high-speed broadband and another example is the growing use of cloud computing services, collaborative platforms as well as the increase of data shared through internet networks.

This is not news to the research communities that pioneered the use of grid computing ten years ago, and are now at the forefront of cloud technologies. The trend now is a call for easy-to-use platforms and interfaces that can facilitate access and exploitation of distributed computing resources and cloud resources.

EGI has been doing just that by promoting the development and uptake of Virtual Research Environments to lower entry barriers and help scientists to make the most of the computing resources available to them.

More collaborations

The EU Commissioner for the Digital Agenda, Neelie Kroes, also made clear in her speech that the new paradigm for economy and society is "*sharing and joining*" instead of the old-fashioned "*ring-fencing and protecting*".

EGI's Research Communities are pioneers of this approach, sharing resources and good practices to achieve excellent results in many scientific domains.

NGIs can play a key role here by joining forces and working together to develop advanced tools and services for improved collaborative research.

This will help countries to fully exploit the potential for distributed and multi-domain data-driven research, and contribute actively to the strategy.

A seamless cloud

Action 53 of Digital Agenda for Europe, explicitly calls on governments to "*financially support joint ICT research infrastructures and innovation clusters*" to foster innovation.

It also stresses the importance of "*virtual research communities transcending national, administrative and scientific discipline borders*", while recognising that "*limited interoperability and data protection concerns hamper the development of cloud infrastructures and services that could energize economic activity*".

This is a problem at the top of the EGI.eu and the NGI's priorities. The work done by Federated Cloud Task Force to integrate existing communities' resources and making them interoperable with use of open standards, will pave the way to an highly valuable and flexible European model to deliver innovative cloud services.

This is also the key goal of the Helix Nebula project, setting up a European cloud for science.

EGI.eu is contributing to this effort, by leading the interoperability activities.

The Digital Agenda for Europe (DAE) and EGI

The DAE is a strategy set by the European Commission in 2010. Together with the Innovation Union policy, the DAE is at the core of Europe 2020, the EU strategy for jobs and economic growth.
The DAE wants to establish world class e-infrastructures as a way to promote innovation and growth.
EGI is contributing to this vision with a portfolio of services aimed at the research community and computing resource providers.

Want to know more about EGI Applications for Biophysics?

Biophysics is an interdisciplinary science that looks at the physics behind biological processes. It's a fast-evolving field of research and a fast-growing community within EGI.

The EGI Applications Database (AppDB) stores many grid-based computing tools for biophysics, especially for researchers interested in structural biology problems. The applications filed in AppDB are ready-to-use products.

The new EGI leaflet introduces the most useful six AppDB applications for biophysics. They are:

For protein-protein/ligand interactions...
HADDOCK - High ambiguity driven biomolecular docking
AutoDock - Science gateway for molecular docking simulations
For protein structure and dynamics...
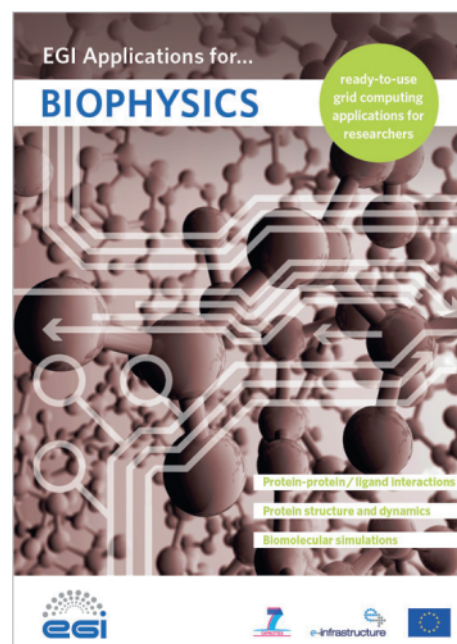**CYANA** - Automated NMR protein structure calculations
CS-ROSETTA - NMR chemical shift-based structure prediction
For biomolecular simulations...
GROMACS - A versatile package to study molecular dynamics
For quantum chemistry...
Gaussian - Expanding the limits of computational chemistry

More information

Download the leaflet at
http://go.egi.eu/bioph

Or go straight to the applications on AppDB
http://appdb.egi.eu

Cookbook: how to use file transfer services

The UCST prepared a step-by-step Globus Online guide to help VOs get started

Globus Online provides a robust way for scientists to transfer and share files across multiple locations.

The EGI.eu User Community Support Team (UCST) published the 'Globus Online cookbook' to help Virtual Organisations (VOs) to make the most of the service.

EGI provides access to Globus Online file transfer services via a portal front-end. This is straightforward for the end-users, but adding EGI resource centres as endpoints is not a trivial task for VO managers and system administrators.

The cookbook provides step-by-step instructions on how to register EGI 'SRM-type' storage services as endpoints of file transfers managed by Globus Online. This will help VO managers to set up the system and make the Globus Online file transfer service available to their VO members.

The second part of the cookbook was designed to help individual researchers to move data and files securely across resource centres and institutions.

The service and the cookbook will be demonstrated at the EGI Technical Forum in September.

More information

Globus Online cookbook
http://go.egi.eu/gocookbook

Globus Online
https://www.globusonline.eu/

Questions?
ucst@egi.eu

EGI-InSPIRE: third year review

Neasan O'Neill

At the end of another project year, EGI.eu hosted the third review of the EGI-InSPIRE project.

One year is a long time in the world of grid and the work accomplished by the whole community during this time is not easily summarised into a handful of slides. With 15 presentations over two days (25-26 June), the team in Amsterdam presented the previous year's achievements and the plans for the future. Every aspect of the collaboration was covered, from the heavy user communities and new ways to engage with the 'long tail of science', via sustainability and communications.

The scene was set with a talk from project director Steven Newhouse, "Building a sustainable EGI", highlighting what EGI has done to move towards sustainability and how the collaboration sees its place in the European Research Area. The talks that followed, given by EGI.eu staff and various members of the project, expanded on the areas.

By the end of the first day there had been talks on EGI's solution portfolio, including a short presentation on each of the five solutions, the communications team, EGI's policy and strategy work, technical outreach and the project's finances and administration. The second day was dedicated to the technical and operations side of the collaboration and a final presentation on the plans for the 4th year of EGI.eu and beyond.

The reviewers were interested in many of the changes made with a particular interest in the EGI Champions scheme, the new approaches to support and attract new user communities, and the EGI Service and Solutions portfolios.

The EC reviewers are now working on their comments and suggestions to report back their findings in late July.

> **More information**
>
> Slides from the review presentations are available at:
> *http://go.egi.eu/Review2013*

Fujitsu: Leadership in the Exaflop Race

The impact of HPC solutions will continue to grow significantly as more and more scientific and engineering problems must be tackled by computer simulation. High Performance Computing gives analysts, engineers and computer scientists the resources they need to make better decisions, promote product innovation, accelerate research and development, and reduce time to market. The solutions of High Performance Computing (HPC) from Fujitsu offer intelligent performance which aims to meet the most complex challenges of high-performance computing today, with expansion capabilities for the growing future expansion needs.

We are in a leading position in the field of supercomputing. With 30 years experience in the successful development of high performance systems. Cooperating with leading research institutions, we believe that supercomputing has the potential to solve the world's most pressing problems. In November 2011, the K supercomputer broke the petaflop barrier speed 10. And even today, two years later, continues to lead several categories of performance and efficiency in the Top 5 of the most powerful supercomputers.

Fujitsu is a Gold Sponsor of the EGI Technical Forum in Madrid