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news from the EGI community

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Please send your comments, feedback and suggestions to: sara.coelho@egi.eu Thanks!

This issue's cover image is a view of the French city of Clermont-Ferrand. (Illustration: Fabien1309 / wikicommons)

Bienvenue Yannick and toodle pip Catherine

Neasan O'Neill welcomes EGI.eu's new director

Yannick Legré has been appointed EGI.eu director and he will take the reins in Amsterdam from the start of February. At the same time the interim director Catherine Gater will be leaving the organisation to take up an opportunity with the Europeana project in London.

Yannick has been involved in the European grid since the very early days with the European DataGrid project in 2001. He now joins EGI.eu as it enters its fifth year and one that could define the European grid, he also knows he has some big shoes to fill.

"I watched EGI.eu grow and flourish when Steven Newhouse was director, what he and the rest of the staff have achieved has been phenomenal, but we now have to look to the future and the Horizon2020 programme," explains Yannick. "I am looking forward to working with the whole collaboration, and the EGI.eu staff, to ensure that we can guarantee the future of the European grid for years to come."

Yannick's appointment is not the only change at EGI.eu. Catherine Gater, who has been the acting EGI.eu director, will be tackling new challenges as project manager for the Europeana Sounds project coordinated by the British Library.

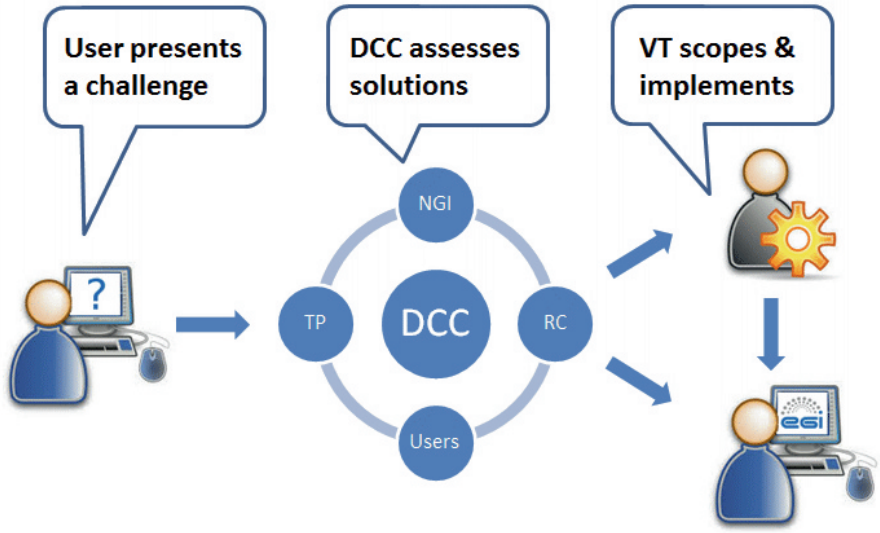
"It wasn't the easiest decision, as I have been working with the grid community for several years now and it has been an exciting and varied time," says Catherine. "But I know that I am leaving EGI.eu in excellent hands and hopefully I can continue to collaborate with the fantastic people I have met over the last five years."

Yannick Legré is the new EGI.eu director

Tiziana Ferrari will continue as the EGI-InSPIRE project director to work with Yannick on the up-coming Horizon 2020 proposals.

The Distributed Competence Centre

Nuno Ferreira and Gergely Sipos introduce a new mechanism to federate technical support to new user communities



DCC, Distributed Competence Centre; NGI, National Grid Infrastructure; RC, Resource Centre; TP, Technology Provider; VT,Virtual Team

One of EGI's most important assets is the experience acquired through years of testing, integrating and using distributed federated services. This knowledge base is diverse and distributed, and is provided by experts from NGIs, Resource Centres, Technology Providers and user communities.

The Distributed Competence Centre (DCC) is a new mechanism, set up to make the most of this expertise and make it more easily available. The DCC strengthens technical support to new user communities and Research Infrastructures, which is one of EGI's strategic objectives for 2014.

The Distributed Competence Centre

The DCC federates EGI's distributed technical support skills to help international research communities facing data handling and processing challenges.

The DCC pools the technical knowhow from the National Grid Infrastructures and Resource Centres which are part of EGI and offers expertise on:

1) core e-Infrastructure services that provide the foundations for community-specific services, such as authentication, authorisation, accounting and information discovery;

2) grid and cloud platform technology,

3) community-specific platforms, such as compute-intensive parallel applications, visualisation, science gateways and workflows.

How does it work? The DCC in action

The process starts when a research infrastructure or a user community approaches EGI with a specific storage or compute challenge. The problem is passed on to experts in the DCC appointed to help capture, refine and document the technical requirements. Depending on the nature of the problem, the DCC experts can recommend an implementation plan directly, or forward the scoped problem to a Virtual Team (VT). The VT will define a join technical work programme that supports users from the initial requirement analysis phase, to integration, prototyping and testing.

Any user community can benefit from the DCC expertise

Starting from the first quarter of 2014, calls will be opened periodically for participation in user porting projects which will see the involvement of the DCC. The calls will also provide the opportunity to apply for compute and storage resources available through the European grid and the federated cloud platform.

More information

The DCC wikipages: http://go.egi.eu/DCC

Contact: dcc@mailman.egi.eu

How to ask for resources with the new e-GRANT portal?

Sara Coelho writes about the new EGI resource allocation tool

The e-GRANT portal is an allocation tool that sets 5,000 job slots and 170 TB of storage aside for new and existing user communities. To access the resources, researchers just need to fill an online form and ask for what they need and for how long they need it.

The compute and storage resources available through the e-GRANT portal are contributed by five EGI members (Belarus, Croatia, Greece, Poland and Turkey), as well as the International Desktop Grid Federation.

"This is an opportunity for scientists to try out what we have to offer them," explains Peter Solagna, Operations Manager at EGI.eu.

"It gives new and existing user communities simplified access to the resources needed to perform their work, allowing pilot projects or the ability to reserve resources for specific activities."

To streamline the process, applicants are not required to have a grid certificate or to be part of a Virtual Organisation registered in EGI. Applicants just need to give information about the user community or project that they represent, the use case that they want to run, and an assessment of the resources needed. They will then be contacted by the EGI Operations Team to discuss the proposal and allocation of resources to best match needs and available resources.

During this initial phase applications will be processed on a 'first come, first served' basis and will need to be approved by both the EGI Operations Team and the resource providers.

In the event that a request for resources does not match with the pool availability, users will be invited to submit a revised request.

How to submit a request?

> Go to the e-GRANT page: *http://e-grant.egi.eu*

> Log in with SSO (get a free account at: *http://egi.eu/sso/email*)

> Fill the e-GRANT form

> Questions? *operations@egi.eu*

EGI Community Forum: registration is open!

Helsinki, Finland - 19-23 May 2014

The organisers of the Community Forum 2014 invite the European distributed computing community and the researchers with an interest in e-infrastructures to register for the event.

The forum will take place in Helsinki, Finland from 19-23 May 2014. The event will be hosted by EGI.eu in partnership with the University of Helsinki and CSC - IT Centre for Science Ltd.

The leading theme of the event is *Advancing excellent science*. The conference programme will include user-orientated tracks designed to give new and existing user communities an opportunity to present their requirements, report on success stories, get support in porting applications and network with technical providers and other partners.

The Call for Participation is open and abstracts may be submitted via the conference website until 16 February.

The programme committee welcomes proposals for networking sessions to connect the research and technical communities, and hands-on hackathons to tackle software porting and other technical issues.

Submission deadlines

> Presentations, networking sessions, hackathons: 16 February

> Posters and demos: 16 March

> Early-bird registration: 31 March

http://cf2014.egi.eu

More information

> Registration: http://go.egi.eu/CF2014-reg

> Indico pages: http://go.egi.eu/CF2014

A new science gateway for the condensed matter physics community

Antun Balaz on how a SCI-BUS based science gateway is making the difference

Condensed matter physics and materials science address problems highly relevant to fundamental research, as well as to society. The development of high-impact materials or research on quantum information, for example, depends on condensed matter physics and contribute to the IT and smartphone industry, semiconductor technology, and the energy sector, among others.

Typical research problems in this area involve calculating the properties and dynamics of complex quantum physical systems. Parallel large-scale numerical simulations are widely used, and deploy a broad range of algorithms to solve nonlinear partial differential equations, or to apply classical and quantum Monte Carlo techniques, for instance.

The Serbian condensed matter physics community uses scientific computing resources to run three main applications: GP-SCL, SPEEDUP and QSPEEDUP.

GP-SCL is a set of parallel codes for calculating the dynamics and ground states of quantum fluids (e.g. Bose-Einstein condensates and superfluids). These represent macroscopic quantum phenomena where millions of atoms or molecules behave coherently, allowing special properties to emerge.

SPEEDUP and QSPEEDUP codes use, respectively, Monte Carlo- and quasi-Monte Carlo-based path integral algorithms to calculate quantum mechanical transition amplitudes. These calculations are the building blocks in the study of many quantum physics problems.

These applications are developed by scientists from the Scientific Computing Laboratory of the Institute of Physics Belgrade and are used by an increasing number of collaborators from within Serbia, Europe, Brazil, India and China. The applications are deployed on the computing infrastructure provided by the Academic and Educational Grid Initiative of Serbia, part of EGI.

To increase the potential user base of the applications, we created the AEGIS CMPC science gateway to provide seamless access to the software and the data obtained from the calculations. The science gateway hides the complexity of the grid, which was a barrier for many scientists.

The science gateway was developed within the framework of the SCI-BUS project, using the AEGIS infrastructure and relying on the widely-used Liferay-based WS-PGRADE/gUSE portal. We have extended the portal with application-specific workflows, as well as a set of modules, that enables specification of the physical system to be studied numerically, and export of simulation results.

Generic architecture behind this science gateway provides a user-oriented interface that visually unifies SPEEDUP, QSPEEDUP and GP-SCL portlets. The interface portal is developed in the Google Web Toolkit environment. The portal is a workflow developer-oriented interface that allows creation, modification and testing of new and existing workflows. The final element is a document-oriented database that stores configurations and numerical results from all applications supported by the science gateway. We have developed it based on CouchDB technology, as this RESTful web-service is extended with three additional layers responsible for authentication /authorisation, tracking, and merging.

The science gateway is in production and is used by scientists in their everyday research. We have organized several in-house training sessions, and as a result several PhD students are now regularly using the science gateway. So far a number of papers have been published using the results obtained from the AEGIS science gateway, and we plan to extend it with additional applications, currently being developed by scientists from several research groups.

More information

AEGIS CMPC:
http://sci-bus.ipb.ac.rs/

AEGIS: *http://www.aegis.rs/*

Scientific Computing Lab:
http://www.scl.rs/

Institute of Physics Belgrade:
http://www.ipb.ac.rs/

SCI-BUS:
http://www.sci-bus.eu/

WeNMR's solution for identity management

Paul van Dijk on how WeNMR and SURFnet established a Single Sign-On access to distributed services

The management of identities, especially in the context of a distributed service infrastructure, is generally regarded as a major burden.

This burden, however, can easily be reduced because identity is already managed, processed and handled by the user's home institution. By re-using institutional identities, research groups and researchers in virtual communities can focus on those issues they should really focus on. In addition, users in the community will be able to use their trusted institutional account to obtain easy and Single Sign-On (SSO) access to shared resources.

SURFconext and eduGAIN middleware infrastructure

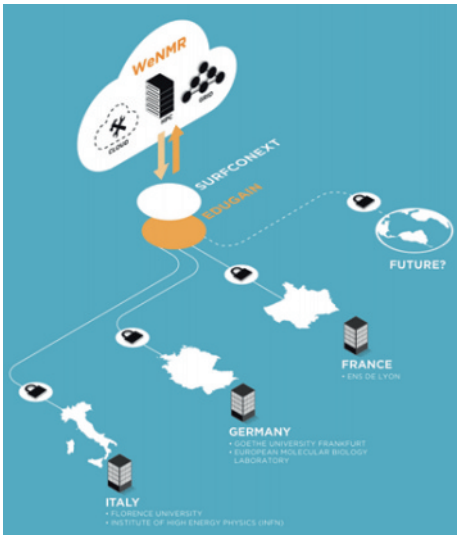
WeNMR was able to apply SAML 2.0 based technology and existing identity federation infrastructure to manage and simplify access to shared resources. In the Netherlands the identity federation for higher education and research is operated by SURFnet and is known as SURFconext. This infrastructure allows users from many institutions to access a wide range of services from many different commercial and non-commercial service providers.

Thanks to the eduGAIN infrastructure, WeNMR was able to extend the coverage area of identity providers and add the home institutions of WeNMR users from Italy, Germany and France.

WeNMR Drupal Portal, a central management and entry point

The SSO support for web(-based) applications was built using the SAML 2.0 Web SSO profile.

High-end distributed computing e-infrastructures such as WeNMR and EGI usually lack the support for web authentication protocols. To circumvent this problem, WeNMR created a Drupal module for SSO for external Services (SSOXS).



This SSOXS module successfully extends Drupal to serve as a SSO authentication, central user management and accounting portal for the external web servers or services of the project. At the same time the Drupal portal acts as a central entry point and virtual collaboration environment for the WeNMR community. In collaboration with SURFnet, the SSOXS module has now been connected to eduGAIN through SURFconext, effectively enabling institutional login into the VRC.

The successful WeNMR experience provides an excellent blueprint of how virtual research communities can share resources in a user-friendly and sustainable way.

In 2014 WeNMR, EGI, SURFnet and other partners will further explore possible models to manage group memberships, attributes and certificates in order to simplify the management of virtual communities and access to shared resources.

WeNMR Virtual Research Community

WeNMR is a FP7 funded project and a Virtual Research Community (VRC) supported by EGI. It has been set up to optimize and extend the use of high-end solutions to determine the structure and properties of proteins and other medically important molecules. The ability to easily manage and share these solutions across institutional and country borders is an important common goal.

The WeNMR federated identity management solution was developed in collaboration with Marc van Dijk, Niels van Dijk and Alexandre Bonvin.

DIRAC for EGI: e-connecting scientists

Ricardo Graciani on the plans to set up a DIRAC pilot

DIRAC is an open source software framework that includes all the necessary components to build complete distributed computing systems. DIRAC allows connection to most grid services, to commonly used cloud managers, to stand-alone clusters and to other distributed data storage and computing solutions.

This integration of different resource paradigms into a single virtual system is seamless to the end user, which means that DIRAC provides interconnection and *de facto* interoperability with a single entry point and a rich user interface.

DIRAC Pilot for EGI

DIRAC, EGI.eu and several NGIs are setting up a pilot service providing a single entry point to EGI's distributed grid and cloud e-Infrastructure.

The aim of the pilot is to develop a prototype of a full-scale DIRAC service for EGI. This experience will be used to develop Horizon 2020 proposals for the deployment, operation, and dissemination of a global DIRAC service connecting researchers to the e-Infrastructure. The service will connect existing science gateway solutions and application/domain specific VREs, as well as from DIRAC interactive portals.

The purpose is to demonstrate how DIRAC can help large well-established communities, as well as small research groups and individual scientists, to exploit the existing e-Infrastructure and boost their scientific output.

The ultimate vision is to lower technical entry barriers and to give scientists transparent access to distributed computing and storage resources. This will bridge the technological gap and promote innovation with a measurable positive impact on scientific output and on society as a whole.

The pilot begins in February 2014, with the contributions from the Polish and French NGIs. A number of communities from different research fields have been contacted to join, including WeNMR, the Pierre Auger collaboration and the EISCAT research infrastructure, amongst others. i-Marine, an e-Infrastructure set up to develop VREs for fisheries management and conservation of marine resources, is also interested and the Greek NGI is evaluating DIRAC to ease the migration of grid users to the Okeanos IaaS. Furthermore, several enginee-ring groups requiring extra computing power for their appli-cations connected to industrial and medical use cases will be served.

"DIRAC can help large well-established communities, as well as small research groups and individual scientists, to exploit the existing e-Infrastructure and boost their scientific output."

The DIRAC pilot will be presented at the upcoming EGI Community Forum in Helsinki, where a DIRAC tutorial will also take place. An interim report on this activity will be presented during ISGC 2014 in Taipei, including a hands-on tutorial session.

The DIRAC project

The DIRAC Project is a collaboration set up to maintain, develop and promote the usage of the DIRAC open source software framework for distributed computing, on a best effort basis.

The main contributors and founders of the DIRAC Consortium are France's CNRS, the University of Barcelona in Spain and CERN. The consortium is open to new institutions interested in ensuring the steady development and continuous support of the DIRAC software.

dirac@diracgrid.org / http://diracgrid.org

EGI - DIRAC collaboration

Initial bootstrap meetings took place in December and January, a work plan has been defined with the support from EGI.eu, and monthly follow up meetings are foreseen. Slides and minutes are available online: go.egi.eu/DIRAC

Call for participation

This is mostly an unfunded effort. NGIs, technology providers and other interested parties are invited to join and contribute to the DIRAC 4 EGI initiative.

dirac@egi.eu

What to expect from the Horizon 2020 ICT Work Programmes?

Sergio Andreozzi reports back from a European Commission Information Day

On 15 January, I attended an Information Day where EC representatives provided insight on Big Data and Open Data related challenges under the ICT Work Programme of Horizon 2020. In the opening presentation, it was made clear that Horizon 2020 is a very different program than FP7. This is no longer "business as usual". Besides some change of terminology (e.g., project is now referred as action), the main shift is from 'Research & Development' to 'Research & Innovation', with the goal of bringing great ideas from the laboratories to the market.

The following topics were addressed:

> ***ICT 15 (Big Data and Open Data Innovation and Take-up)*** with a budget of €50 million and call for proposals by 23 April 2014.

> ***ICT 16 (Big Data - Research)*** with a budget of €39 million and call for proposals by 15 April 2015.

ICT 15 aims to develop technologies to increase the efficiency of all EU companies and organisations that manage vast amounts of data, and to boost the competitiveness of EU enterprises. Its two types of action are: an innovation action (ICT-15.a, €39 million) and a coordination and support action (ICT-15.b, €11 million).

For ICT-15a, proposals should contain focused activities to improve existing businesses processes or open new opportunities. Instead of use case they should be structured around clear business requirements from SMEs that can be validated in the market. ICT-15a aims to:

1) Establish a European data incubator for integration and reuse of open data for SMEs, to foster the development of open data supply chains, and to educate and assist new users;

2) Launch collaboration projects focused on innovation and technology transfer in multilingual data harvesting and analytics solutions and services.

ICT-15b will maximise the value of the European data economy by stimulating reuse of data sets, developing skills for big data analytics, and creating big data integrator platforms.

ICT 16 follows a research and innovation action. Proposals should focus on user-defined challenges addressing 'big' dataset, such as: Volume (e.g., PB), Variety, Velocity. Challenges may be related to data structures, algorithms, and visualization tools tackling complex concepts such as energy consciousness in reversible computing. The industry relevance and sustainability strategy are also significant. The target data sets must be European, e.g. from the European Open Data portal, or the Copernicus project. Data sources such as Twitter should only be used as secondary sources.

For a truly digital market in multilingual Europe, it was recommended that language barriers should be removed by achieving automatic language translation, not by adopting one main language. It has been reported that less than half of European citizens speak English.

Dedicated background documents are available online and contain extra information and questions focusing on the key aspects the evaluators will use to assess the quality of the proposals.

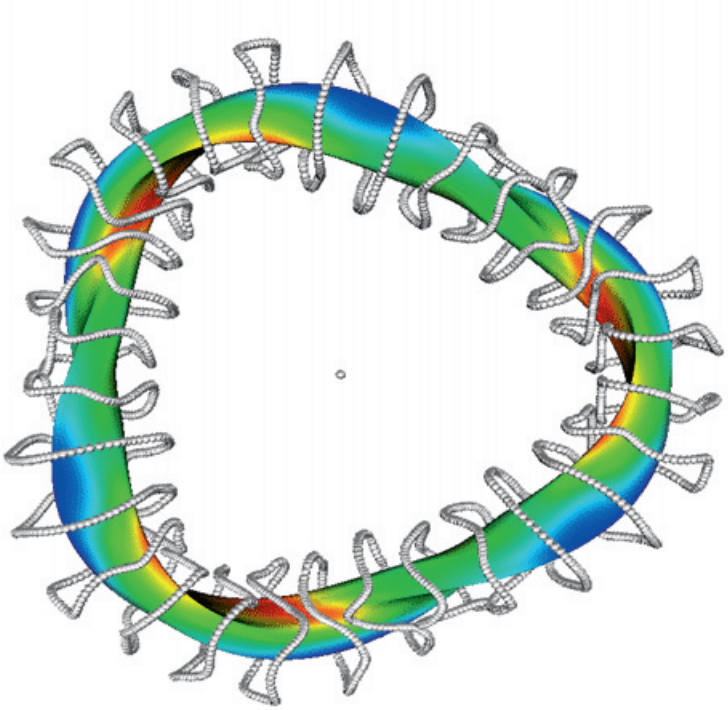
EGI is interested in participating in project proposals with SMEs to offer its infrastructure services and network of experts.

What is Horizon 2020?

Horizon 2020 is the financial instrument implementing the Innovation Union, a Europe 2020 flagship initiative aimed at securing Europe's global competitiveness. A number of work programmes detailing activities for 2014-2015 have been published. The EC is organising several Information and Networking Days to provide insights on specific topics and enable interested participants to network and develop proposals for collaborative action.

Optimization of fusion devices on the grid

Francisco Castejón and Antonio Gómez on the added value of the grid infrastructure for fusion research



The DAB algorithm has run on the grid to produce this optimized three-period stellarator. The plasma shape is shown together with the confining magnetic coils. The colours correspond to the different intensities of the magnetic fields (red is more intense and blue is weaker).

Clean and efficient, magnetic confinement fusion could be the socially and environmentally acceptable energy source of the future. Fusion power does not emit greenhouse gases, and relies on deuterium and lithium, two cheap and abundant fuels.

Yet there are still some problems to solve before achieving commercial fusion. The premise behind fusion power is to create a 'magnetic bottle' to confine the plasma, a fluid fuel superheated to temperatures of hundreds of millions of degrees Celsius.

An important topic is the design of the magnetic bottles required to confine the plasma efficiently and prevent power escaping from the fusion device.

Because it's possible to build them in very different shapes, the number of potential fusion devices is huge. The first key point is to define a reliable gauge to measure the quality of the confinement and then to look for designs that could improve this.

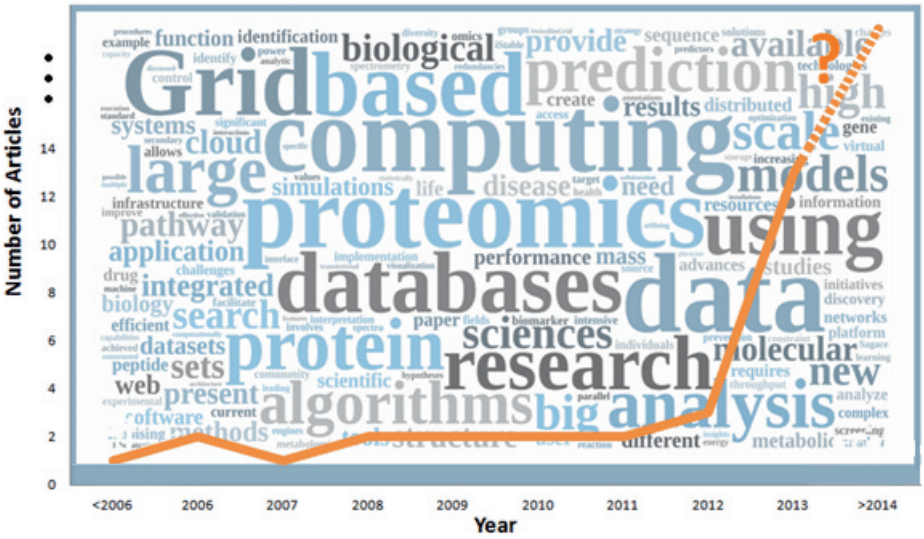
Every fusion device is characterised by a set of parameters called a magnetic configuration. The optimization criteria that are taken into account include reducing the transport of particles and power from the inner to the outer parts of the device, and the stability of the plasma when high pressures are reached. As the evaluations of the different devices are independent, this is a problem suitable to be solved using the grid. The European grid has provided the large CPU time needed to evaluate tens of thousands of magnetic bottles, thoroughly exploring the configuration space.

The strategy we have adopted is based on metaheuristics. We generate new magnetic configurations in a 'master' machine and evaluate the different optimization criteria on the worker nodes of the grid. We store the new configurations on the storage elements. The strategy we have adopted to search for and create new configurations uses two processes: exploration and exploitation of the found optimal configurations (i.e., the search for a set of parameters that obey the optimization criteria) and the variation of these parameters to improve the magnetic configurations. The algorithm follows the behaviour of bees in nature. Because of this, and because of the distributed paradigm of the grid, our algorithm is called Distributed Asynchronous Bees (DAB).

The result of this new algorithm is the generation of new configurations on the grid. These new devices improve the plasma confinement, hence are more suitable concepts for building a fusion reactor. We started with an especially complex type of configuration called stellarators, which are characterised by being more stable, but are difficult to design and build. An example of optimised configuration is shown in the figure. The next step will be to include the coils that confine the plasma in the optimization loop, in order to look for a balance between obtaining a good confinement and developing coils that are not too complex to be built.

Future opportunities and trends for e-infrastructures and life sciences

Afonso Duarte and Fotis Psomopoulos on why e-infrastructures matter



Number of articles in PubMed related to Structural Biology and Big Data (using a high, exclusive threshold). The word-cloud in the background has been produced from the corresponding abstracts.

The goal in science, as the computer scientist Jim Gray said, is not to have the biggest, fastest single computer, but rather "to have a world in which all of the science literature is online, all of the science data is online, and they interoperate with each other". Though we are not quite there yet, life sciences are rapidly transitioning towards a new era of Big Data, where data, algorithms and knowledge are becoming increasingly available to all. Ever since 2007, when genetic sequencing began to release flurries of data, life sciences have been steadily moving towards the analysis of massive data setsthis, i.e., the 'Forth Paradigm'.

EGI has been a key factor in this transition, and will play a critical role in the shape of future research within the life sciences.

A good example is the complex network that defines how bio-molecules interact with each other. Understanding the differences between interactions in healthy and unhealthy organisms provides insight into the genesis of disease and how to prevent it. As in many complex problems, multidisciplinary approaches are behind the discovery of such connections and the development of new drugs. Among those approaches, structural biology and bioinformatics are key players in comprehending interactions at the atomic level. However, the rapid expansion of available data on the structure and dynamics of bio-molecules poses new computational challenges. Currently we are trying to sift through all data in a fast and efficient way, bringing computational methods and techniques into the spotlight of cutting edge research. E-infrastructures provide access to these tools and applications, allowing the synergies between life sciences and ICT researchers which are fundamental in moving research forward.

Attempting to quantify this conclusion, we searched the PubMed database for relevant articles and tried to reconstruct the story so far. Starting with the number of published articles, the underlying trend is rather obvious: until 2011 combined structural biology and Big Data processes were few and mainly aiming towards high throughput methods and visualisation tools.

Recently, however, new tools and e-infrastructures such as EGI gave way to a substantial number of publications ranging from large-scale simulations to disease-oriented structural models in proteomics. Although these results are far from new, they do point out a critical change - research has shifted radically from hypothesis-driven studies to data-driven simulations of whole systems.

Besides the development of new applications and the improvement of the existing ones, it is evident that the life sciences and ICT communities need to capitalise on their synergies to strengthen every discipline.

To this end, we will host a discussion of the expected trends, applications and needs of the communities at the upcoming EGI Community forum in Helsinki. This will take place in the form of a dedicated workshop and a networking session to showcase the role of e-infrastructures and promote discussion towards concrete collaborations and sustainable synergies.

CSC – The Finnish HPC Center

Anni Jakobsson profiles the Finnish host of the EGI Community Forum

The new Cray XC30 system located in the new CSC data centre in Kajaani, Finland © CSC

CSC — IT Center for Science Ltd. is a state-owned non-profit company providing services to the Ministry of Education, Science and Culture. CSC provides IT support and resources for academia, research institutes and companies, including modelling, computing and information services. CSC provides Finland's widest selection of scientific software and databases and its most powerful supercomputing environment, which researchers use via the Finnish University and Research Network (FUNET).

CSC is one of the hosts of the EGI Community Forum 2014, together with the University of Helsinki and EGI.eu. For more than 40 years, CSC has provided the Finnish research community with an open access competitive ICT infrastructure for research. With continuous growth since its establishment in 1971, the organisation has today over 250 employees and an annual turnover of around 30 million euros. CSC is a limited company owned by the Finnish Government and is administrated by the Ministry of Education and Culture. All Finnish research relies on CSC through one or several of its services, including: FUNET, supercomputer and computing clusters, storage and data services, software and tools, and training and technical support.

With a vision to "pioneer in the sustainable development of ICT services" CSC has a further role to introduce new technologies and advances within ICT and its applications to benefit Finnish research. Over the years, this has been accomplished by, for example: connecting Finland to the internet in 1988, introducing the Cray T3E parallel computer in 1996, establishing an optical research data network allowing link speeds of up to 100 Gbps in 2009, building a modular free-cooling energy-efficient data centre in 2012, and piloting a high density supercomputer prototype with many-core accelerators in 2013. The capabilities of CSC have enabled a number of advancements for Finnish research. These range from galactic dynamo processes, fundamental aspects of gold clusters and particles, aerosol effects on global warming, analysis of genetic variation in Finland and the Nordic countries, resolving 3D structures of viruses, and more.

CSC represents Finland in EGI and ensures that the grid infrastructure being built is useful for Finnish research and that resources are accessible. All resources provided by EGI are available for Finnish researchers through the EGI-InSPIRE project and the Finnish Grid Infrastructure (FGI).

CSC

More information

url: http://www.csc.fi/english

Anni Jakobsson is a communications officer at CSC

Researchers and networkers draw closer through TERENA and TNC

Laura Durnford on TERENA's success stories of 2013

Research and education has benefited greatly from the development of networked technologies, infrastructure and services that enable international collaboration and access to data and resources in a secure environment.

TERENA, the Trans-European Research and Education Networking Association, helps to further such developments by fostering collaboration among a wide range of researchers and experts in IT, telecommunications, network technologies and more. With almost 1,000 attendees at its workshops, training events and the TERENA Networking Conference (TNC), and around 800 at its open meetings of volunteer Task Forces, 2013 was a good year for 'networking the networkers'.

The gap between the TERENA community and its beneficiaries has been narrowing thanks to a growing collaboration in activities related to accessing online services and resources through 'federations' that verify user identity. A wide range of applications is in use in various research communities, including many that do not have a simple web-browser front-end. This shows the importance of non-browser-based federated access to allow machine-machine interactions in secured workflows. The Federated Identity Management for Research group (FIM4R) also recommended, in a 2012 paper, managing federated access in a user-friendly way that also takes into account open standards, compatibility with licenses, different levels of assurance, and community-controlled authorisation.

As a response to this paper, TERENA's REFEDS (Research and Education Federations) community mobilised to define a roadmap addressing perceived risks and barriers to researchers who use federated access. REFEDS also worked with the GÉANT project's eduGAIN inter-federation service team, which is led by TERENA, to solicit information about specific areas to work on, three of which are now being supported by eduGAIN. This work is set to develop further in 2014.

TERENA's other focus areas in 2013 related to computer and network security and certification, network architecture and operations, media and e-learning and support for collaborative performing arts. TERENA also worked on eduroam® mobile access for students and researchers NRENum.net and number mapping to allow seamless interconnection between multiple technologies. It also published the ASPIRE 5-year foresight study and the 2013 NREN Compendium - a reference document regarding the development of research and education networking in Europe.

Wide-ranging community collaboration

The focal point of the wider research and education networking community was the TERENA Networking Conference – TNC2013 in Maastricht.

TNC2013 drew a record 650 participants and included talks on how the networking community can help meet the demands of 'big data', the use of dynamic Bandwidth-on-Demand to transfer radio-astronomy data, large distance human-robot interaction, improvements to large file transfers between data centres; analysis of medical data and more.

The next TNC will be held in Dublin, 19-22 May 2014, with the theme 'Networking with the world'. Keynote speakers include Tracy Futhey, Barend Mons, Claire Boonstra, Stephen Farrell, David Puttnam and Martyn Dade-Robertson. Early bird registration is available until 24 February. Opportunities are still open to show demonstrations or exhibits, to provide sponsorship, to present lightning talks or posters, and for students to apply for free-of-charge attendance.

More information

TNC 2014: https://tnc2014.terena.org

TERENA: www.terena.org

REFEDS: https://refeds.org/

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When in Rome ... do computational chemistry

Daniele Cesini reports on the first training workshop on grid porting of computational chemistry applications

On the 20th and 21st of January the COMPCHEM Virtual Organisation and the Italian NGI User Support and Training unit ran a hands-on training workshop for computational chemistry researchers. The course attracted 22 researchers from 12 different departments including a remote participant from the Spanish National Research Council in Madrid. Hosted by the Italian NREN, GARR, the workshop was the final phase of a course that had begun with two online meetings to introduce the participants to accessing distributed resources.

Over the two days the workshop focused on porting specific use cases that the students had researched in advance. These use cases were based on three different commonly used computational chemistry applications: VENUS, a classical trajectory direct dynamics computer program, CRYSTAL, a computational tool for solid state physics and chemistry and Quantum Espresso, an open-source software for electronic-structure calculations and materials modeling at the nanoscale. The porting was implemented starting with a command line interface, to finish with the creation of basic graphic interfaces relying on the Italian Grid Portal.

The training was well received with one attendee noting that it had been "very useful to exchange information and share experiences with users belonging to different fields of the chemistry realm."

A follow up to improve the module and a special issue of the VIRT&L-COMM electronic journal containing the event material will be released.

The organisers would like to recognize the support of the National Interuniversity Consortium of Materials Science and Technology who funded three students to attend the course.

More information

COMPCHEM VO - https://www3.compchem.unipg.it/compchem/

Italian Grid Portal - http://portal.italiangrid.it

The applications mentioned in the text are available via the EGI AppDB - http://appdb.egi.eu

Daniele Cesini is the Italian NGI International Liaison

Upcoming event: Cloudscape VI, Brussels

Cloudscape VI is being held in Brussels on the 24th and 25th of February. The meeting focuses on the strategic role of cloud adoption and its socio-economic benefits

Cloudscape VI has a compelling two-day agenda covering topics from security and data regulations to cost efficiency and clouds for a smart economy. The meeting will have talks by Steve McGibbon of Microsoft, Joe Weinman of Telx and other keynote speakers, as well as a series of practical parallel sessions on how to make the transition to the cloud and overcome barriers.

The event is for both public and private sector IT professionals providing a unique opportunity to learn from influential cloud experts. Over the two days there will be talks from companies and institutions at the forefront of the cloud computing industry and research, including Microsoft, EGI, Mobicloud, CERN, VMWare and the European Commission.

More information

http://www.cloudscapeseries.eu/

As part of their 'Circle of Friends' the Cloudscape programme organisers are offering reduced registration to EGI community members. More details on the special rate are available online.