Grid TALK GridBriefings
Grid computing in five minutes

The future of innovation: developing Europe's ICT infrastructures

Modern innovation and scientific discovery is increasingly global, fuelled by interdisciplinary teams and dependent on advanced computational resources, massive data collections and shared scientific instruments.

On 5 March 2009 the European Commission (EC) adopted a communication entitled *ICT infrastructures for e-Science*, a document that aims to trigger discussions on the strategic investment and actions needed to ensure the ongoing contributions and success of European e-infrastructures.

This communication has already raised much interest with Member States and discussions under the Czech presidency of the European Union (EU) are underway. These discussions are expected to continue into the second half of this year under the Swedish presidency of the EU, leading to the proposal and adoption of a plan for collaborative action by the close of 2009.

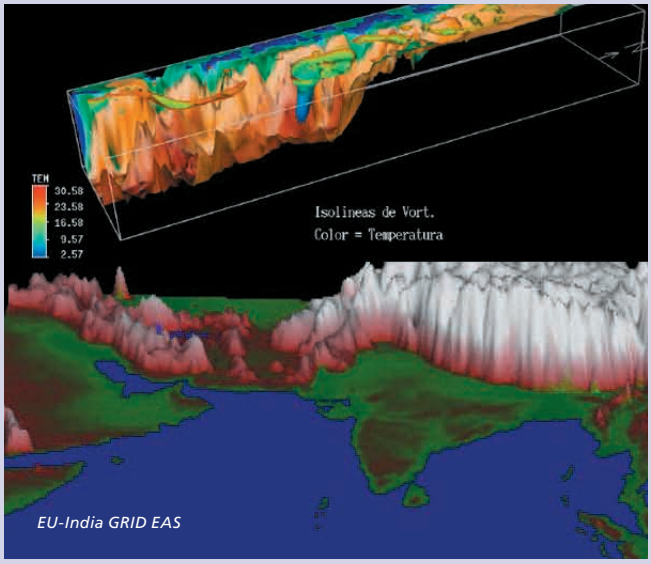
What are ICT infrastructures?

ICT (Information and Communication Technology) infrastructures are also known as e-infrastructures: they are research tools designed to increase the effectiveness of scientific research. Created by combining computer hardware, software, networks, databases and more, ICT infrastructures aim to increase collaboration between countries and scientific disciplines.

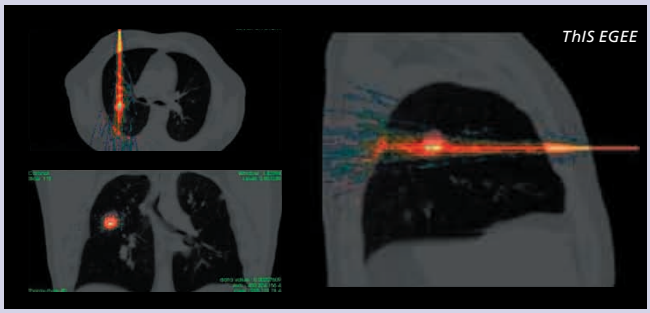
The European Commission and Member States have already made significant investments in e-infrastructures; around 600 million Euros have been earmarked for e-infrastructures investment through the EC's 7th Framework Programme for Research and Technological Development (FP7) (2007-2013). However, the EC sees a renewed strategy as essential if Europe is to continue to achieve leadership in e-science.

New frontiers for scientific discovery

Researchers can now use computer-powered "virtual" simulations to tackle the very small, the very big and the extremely complicated. Research on climate change requires access to data from all over the globe; medical researchers aiming at tailored healthcare use increasingly sophisticated models; disaster management researchers prepare for catastrophes using high-tech simulations in virtual worlds. This 'virtualisation' also leads to unprecedented demand for connectivity, computing resources and information access.



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Future directions

The financial crisis will put pressure on national budgets. Yet the EC say it is now more important than ever to explore "innovative funding for a wide range of infrastructure projects, including transport, energy and high-technology networks." They have identified three goals that will be key to growing Europe's e-infrastructure capacity:

1. **Reinforce Europe's research capacity in e-science**
   Europe must become a hub of excellence for e-science, exploiting multidisciplinary and global collaborations to combine complementary skills and resources.
2. **Ensure sustainability of e-infrastructures as persistent research platforms**
   Researchers must be able to depend on guaranteed access to crucial computing services 24 hours a day, seven days a week, for years into the future.
3. **Explore and exploit the innovation potential of e-infrastructures**
   Existing expertise in e-science should be transferred to areas including e-health, e-government and e-learning, optimising the use of e-infrastructures as cost-efficient platforms for innovation.

Europe's e-infrastructures: towards 2020

European e-infrastructures are currently structured into five intertwined domains.

1) GÉANT is the world's largest multi-gigabit computer network dedicated to research and education.

- **Successes:** GÉANT serves around 3000 universities and research centres, connecting to 32 National Research and Education Networks across Europe as well as linking to similar networks worldwide, thus forming a single global research network to support e-science.
- **Future challenges:** GÉANT needs to meet the challenge of supporting exa-scale computing (10^{18} operations per second), and improve ease of access to encourage increased global collaboration. The network also needs to integrate the latest technologies and contribute to the design of the Future Internet.
- **Actions for the Commission:** The EC will continue to support GÉANT to reinforce its capacity and global perspective.
- **Actions for Member States**: Member States are invited to focus on coordination between relevant national and European policies, and to support and use GÉANT as an experimental platform leading towards the Future Internet.

2) E-science grids combine the power of ordinary computers across multiple scientific communities to provide a massive distributed grid computing resource.

- **Successes:** Europe now hosts the world's largest multi-science grid: EGEE connects over 80,000 computers on 300 sites in 50 countries, and is used by several thousand researchers.
- **Future challenges:** E-science grids must ensure their sustainability to encourage full use of their resources. The European Grid Initiative (EGI) is now building on the success of grids like EGEE to establish a coordinated pan-European grid infrastructure that builds on emerging National Grid Initiatives (NGIs). *[See GridBriefing 3 : European Grid Initiative]*
- **Actions for the Commission:** The EC will support the transition to new, interoperable and sustainable models for European e-science grids, as well as their efficient use in a wide range of research fields.
- **Actions for Member States**: Member States are invited to consolidate and further develop their NGIs as a step towards a sustainable and pan-European grid strategy.

Global real-time astronomy: GÉANT helps astronomers see more than ever

This January, to celebrate the International Year of Astronomy, 17 telescopes from around the world combined to act as a single real-time instrument, providing 33 hours of observation and resulting in images of the universe more detailed than ever before. GÉANT, the pan-European research network managed by networking organisation DANTE, was at the heart of the collaboration, connecting with 27 research data networks across the globe to produce image resolutions up to 100 times better than that possible from the best optical telescopes.

"Working with partners such as DANTE lets us chart evidence of previously unseen astronomical events," said Huib van Langevelde, coordinator of the EC-funded EXPReS project, a collaboration of radio astronomy institutes and national research networks in 14 countries.

Dai Davies, general manager of DANTE, agreed. "Without high speed connectivity, real-time observations such as this would be impossible."

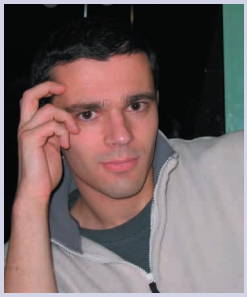


EGEE in the fight against coronary artery disease: the genetics of a killer

Scientists have used the Enabling Grids for E-sciencE grid to move one step closer to understanding the genetic causes of one of the world's biggest killers, coronary artery disease (CAD).

Featured this year in *Nature Genetics*, this research used EGEE to examine genetic marker configurations across nearly 5000 individuals. The researchers discovered a combination of four genetic markers strongly associated with the risk of CAD.

This work aids researchers in their quest to better understand why the disease develops and may offer new approaches for pharmacological prevention and treatment.



"Until recently, we looked at one DNA variation at a time when trying to find new genes associated with coronary artery disease. Here, we looked at the combined effect of several DNA variations located close to each other. We tested more than 8.1 million combinations in less than 45 days. This would have required at least 10 years on a single computer."
David Tregouet, Researcher at INSERM and Pierre & Marie Curie University, France.

3) Data repositories aim to make raw observational and experimental data globally available for virtually all fields of science.

- **Successes:** Most data repositories across Europe still do not interoperate, but the scientific community are working to develop new tools and methods to ensure the availability and preservation of unprecedented quantities of scientific data.
- **Future challenges:** Europe needs to define consistent policies to enhance access to growing volumes of scientific information. By 2012, the average bioinformatics data repository will grow by 4 petabytes per year, equivalent to a 10 kilometre stack of CDs. Unmanaged, such growth could undermine the efficiency of scientific discovery. Europe must address this challenge, and manage the accessibility, quality assurance and preservation of its key data collections.
- **Actions for the Commission:** The EC will reinforce investment in scientific data infrastructure, to support accessibility and preservation policies.
- **Actions for Member States**: Member States and scientific communities are invited to step up investment in scientific data infrastructures and promote the sharing of best practices.

4) Supercomputing e-infrastructures apply the latest and most powerful computing and simulation technologies via centralised supercomputers.

- **Successes:** DEISA has developed and operates an e-infrastructure that links the twelve most powerful supercomputers in Europe and is already used by more than 160 universities and research institutes. The PRACE project is preparing a persistent pan-European high performance computing infrastructure, commencing operation with peta-scale machines (10^{15} operations per second) in 2010. PRACE builds on DEISA's middleware developments and operational experience.
- **Future challenges:** Supercomputing is now a key priority for Europe's scientific performance. Europe needs to focus on developing new software, simulation models, and organisational structures. Investment in supercomputing should have clear industrial impact, allowing public-private partnerships and pre-commercial procurement opportunities.
- **Actions for the Commission:** The EC will define and support an ambitious European strategic agenda for supercomputing.
- **Actions for Member States**: Member States are invited to scale up and pool investment in support of PRACE and related research areas, in full cooperation with the Commission.

5) Global Virtual Research Communities are cross-border multi-disciplinary research collaborations.

- **Successes:** Virtual research communities are increasingly allowing researchers from around the globe to work together.
- **Future challenges:** There is a need to manage potential clashes between the different disciplines, cultures and philosophies, and to set up appropriate organisational styles, quality assurance mechanisms and business models. Improved training is needed to ensure that researchers can make optimal use of e-infrastructures.
- **Actions for the Commission:** The EC will promote the emergence of stronger European virtual research communities and encourage sharing of best practices, software and data.
- **Actions for Member States** Member States are invited to encourage their research communities to fully utilise the benefits of e-infrastructures.

PRACE supercomputer calculates the origin of the visible mass of the universe

Thanks to JUGENE, a supercomputer that also serves as a prototype for the Partnership for Advanced Computing in Europe (PRACE), an international team of scientists has for the first time computed the masses of protons and neutrons. Reported in *Science* magazine, the calculation allowed researchers to confirm a fundamental theory of physics.

JUGENE can perform 180 billion operations in a second, allowing it to power the elaborate simulations required. The calculation used a four-dimensional lattice, solving multiple equations on different sites within the lattice to bring the result closer to the reality of continuous space-time.

"This is one of the most CPU-demanding calculations known to mankind," said Zoltan Fodor, the Hungarian physicist who led the project. "The origin of the vast majority of the visible mass is now settled." There are, however, further riddles to be solved. "We do not know yet what dark matter is and how it gets its mass," Fodor said.

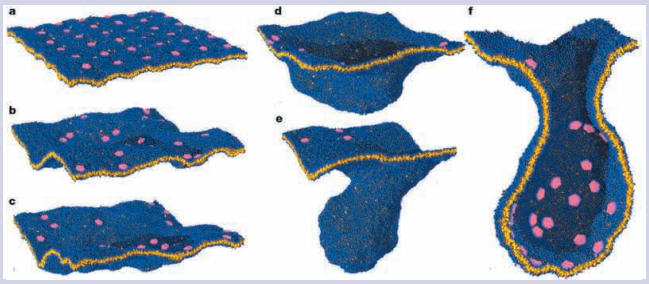


Image : JUGENE

Space-time curvature and the human body: the POLYRES project on DEISA

The German-British POLYRES collaboration used DEISA to uncover a mechanism that had eluded scientists for two decades. One of more than 90 research projects to have collectively used more than 50 million hours of European supercomputing time since 2005, POLYRES used large-scale computer simulations, powered by DEISA, to study membrane folding, a process crucial to the transport of vital proteins through our bodies. A *Nature* magazine cover story, this breakthrough showed that in the presence of proteins, sections of the cell membrane can deform and eventually fold in on themselves, enveloping the proteins to create tiny packages perfect for delivery through the body.

This research has significant consequences for our understanding of nutrient transport, cell signalling, drug interactions and the behaviour of viruses in living cells.



Nature 447, 461-464(24 May 2007)



"Access to world-class supercomputer resources, such as those PRACE will provide, is mandatory to achieve scientific breakthroughs. An outstanding example, ranked as one of the top ten scientific results in 2008 by *Science*, is the calculation of the hadron masses on JUGENE, currently the most powerful supercomputer in Europe and one of the PRACE prototype systems." *Thomas Lippert, Juelich Supercomputing Centre*



"GÉANT plays a key role in shaping worldwide research and education. The network enables the best minds across Europe and the world to work together on ground-breaking research activities that were previously impossible or inefficient due to limited and poor quality data connections." *Dai Davies, DANTE*



"EGEE is driven by the needs of its users, now numbering more than 10,000 researchers in over 200 virtual communities. With these users in mind, we're focused on achieving smooth transition to a fully sustainable European grid infrastructure through the European Grid Initiative." *Bob Jones, Enabling Grids for E-sciencE*



"E-infrastructures are essential to global science. One example is the EVALSO project, which aims to connect telescopes in Chile to international e-infrastructures such as GEANT in Europe, RedCLARA in Latin-America and REUNA in Chile. This new infrastructure will greatly enhance access to astronomical data and reduce the cost of research and time losses." *Sandra Jaque, REUNA*



"DEISA has had a pioneering role in the development of supercomputing services on a European scale. Our services are organized in European expert teams, thus creating the essential technical and operational building blocks for a persistent European high performance computing ecosystem." *Hermann Lederer, Rechenzentrum Garching (RZG), Max Planck Society Institute for Plasmaphysics*



"As national infrastructures in the United States, the Open Science Grid, and our partners in TeraGrid, appreciate strong collaborators in Europe to deliver the worldwide systems needed by our scientific and scholarly communities. Revolutionary technologies and collaboratories are required to solve global issues of climate, energy, and fiscal stability; this vision depends on each worldwide partner to support their computational infrastructures." *Ruth Pordes, Open Science Grid*

For more information:

ICT infrastructures for e-Science (EC communication) ***www.tr.im/j2b7***

ALICE2 (América Latina Interconectada Con Europa) ***alice2.redclara.net***

DEISA (Distributed European Infrastructure for Supercomputing Applications) - www.deisa.org

EGEE (Enabling Grids for E-sciencE) - www.eu-egee.org

EGI (European Grid Initiative) - web.eu-egi.eu

e-Infrastructure Reflection Group - www.e-irg.eu

EVALSO (Enabling Virtual Access to Latin-American Southern Observatories) - www.evalso.eu

GÉANT (Gigabit European Academic Network) ***www.geant.net***

Open Science Grid - www.opensciencegrid.org

PRACE (Partnership for Advanced Computing in Europe) ***www.prace-project.eu***

TeraGrid - www.teragrid.org

iSGTW (International Science Grid This Week) ***www.isgtw.org***

GridBriefing 3: European Grid Initiative: towards a sustainable long-term European grid infrastructure ***www.gridtalk.org/briefings/whatisegi.pdf***

GridTalk - www.gridtalk-project.eu

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