

General Information

<i>i-Space Name</i>	EGI Foundation
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EGI is a publicly-funded federation of ~300 data and computing data centres spread across Europe and worldwide.

EGI has over 48,000 users from a wide range of fields. EGI provides access to over 650,000 logical CPUs and 500 PB of disk and tape storage.

EGI offers a wide range of services for compute, storage, data and support.

Over the last decade, EGI has built a federation of long-term distributed compute and storage infrastructures that support research and innovation. This international e-infrastructure has delivered unprecedented data analysis capabilities to more than 48,000 researchers from many disciplines. The federation brings together roughly 300 data and compute centres worldwide. EGI is coordinated by the EGI Foundation and funded through a combination of membership fees, national and EC funding and delivery of professional services such as training and consultancy. Today, EGI provides both technical and human services, from integrated and secure distributed high-throughput and cloud computing, storage and data resources to consultancy, support and co-development. The research supported by EGI is diverse. Examples include the search for the Higgs boson at the Large Hadron Collider particle accelerator at CERN; finding new tools to diagnose and monitor diseases such as Alzheimer's, or the development of complex simulations to model climate change. EGI stimulates research and innovation by:

1. Ensuring uniform and reliable availability of resources to researchers on a local, national and European scale;
2. Enabling faster production of scientific results through collaboration across organisational and national boundaries;
3. Promoting open and collaborative science and ensuring open access to shared resources and expertise;
4. Allowing researchers to focus on their research rather than managing their e-infrastructure needs;
5. Providing effective use of resources in different administrative domains to ensure the most effective return on infrastructure investments;
6. Facilitating the innovation and sharing of solutions by building a thriving ecosystem through community events and collaborative services.

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Platform and Services Information

Platform(s) & Service(s)

Resource	Value
High-Throughput Compute cores	650000
Cloud Compute cores	6600
Online Storage	285PB
Archive Storage	280PB

Provided Services

Today, EGI provides both technical and human services, from integrated and secure distributed high-throughput computing and cloud computing, storage and data resources to consultancy, support and co-development.

Selected Projects and/or Success Stories

Modelling bacterial iron piracy from plant proteins - The HADDOCK portal helps to show that bacteria have a special drawbridge to steal iron from plant proteins

Iron is an essential element for life. Mammals, for example, use it to carry oxygen in red blood cells, plants need it to transport electrons. Bacteria are not an exception and they also need iron to infect other organisms and survive.

The problem for bacteria is that iron is not readily available in their environment. Animal and plant cells tend to 'hide' their iron inside proteins to prevent bacteria from getting it and stopping infections before they start. So bacteria had to escalate the evolutionary war and come up with mechanisms to get the iron they need.

Rhys Grinter, a microbiologist based at Monash University in Australia, investigated how *Pectobacterium* (the bacteria responsible for blackleg disease in potatoes or for slime flux in many species of trees) sources iron from the plants it infects.

He and his colleagues found that *Pectobacterium* cells have a receptor – dubbed FusA – specially adapted to grab the iron from ferredoxin proteins.

“Ferredoxin is a small iron-containing protein which plants use in a similar way to hemoglobin, but for transporting electrons rather than oxygen,” explains Grinter. “The fact that plants must produce this protein for their cells to function makes it a good target for *Pectobacterium* during infection.”

They first determined the molecular structure of FusA from Nuclear Magnetic Resonance (NMR) and X-ray crystallography data. Then the team used the HADDOCK docking tool to simulate how FusA binds to plant ferredoxins.

“HADDOCK consistently ranks at the top of protein prediction experiments and is one of the best programs available for molecular docking,” says Grinter. “This allowed us to place a high degree of confidence in its predictions and to present a credible representation of the FusA/ferredoxin complex for our paper.”

The team learned that FusA is a glove-like structure able to grab plant ferredoxins and squeeze them across the outer membrane of the bacteria.

“It’s very important for the bacteria that this opening of the hole in FusA is specific and temporary, because the bacterial membrane protects the cell from toxins and antibiotics which may be present in the environment,” says Grinter. “I kind of like to think of FusA as a drawbridge on a medieval castle, it can be specifically be opened and closed to allow ferredoxin to enter the cell.”

- HADDOCK and EGI

The thousands of computational tasks operated in the back-end of HADDOCK are powered by EGI’s High-Throughput Compute service. So far, HADDOCK has processed more than 130,000 submissions from over 8,000 scientists, which translates into about 8 million jobs per year on the EGI infrastructure. The computing resources required to enable HADDOCK are provided by the national e-Infrastructures of Belgium, France, Germany, Italy, the Netherlands, Poland, Portugal, Spain, UK, and other international organisations. Seven federated data centres have pledged 75 million hours of computing time and more than 50 TB storage capacity, ensuring the continuity of the HADDOCK services.