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@EGI_eInfra

Scientific Computing 2021-2030

*Achievements and future opportunities
for Europe-Asia collaboration*

Tiziana Ferrari / Director, EGI Foundation
ISGC 2021 – 25 March 2021



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is partly funded by the European Commission
under H2020 Framework Programme

Collaborations for Excellence in Science

*Science is borderless and so are
infrastructures for advanced computing*

The EGI Federation

The European infrastructure for advanced Computing for Research

Vision

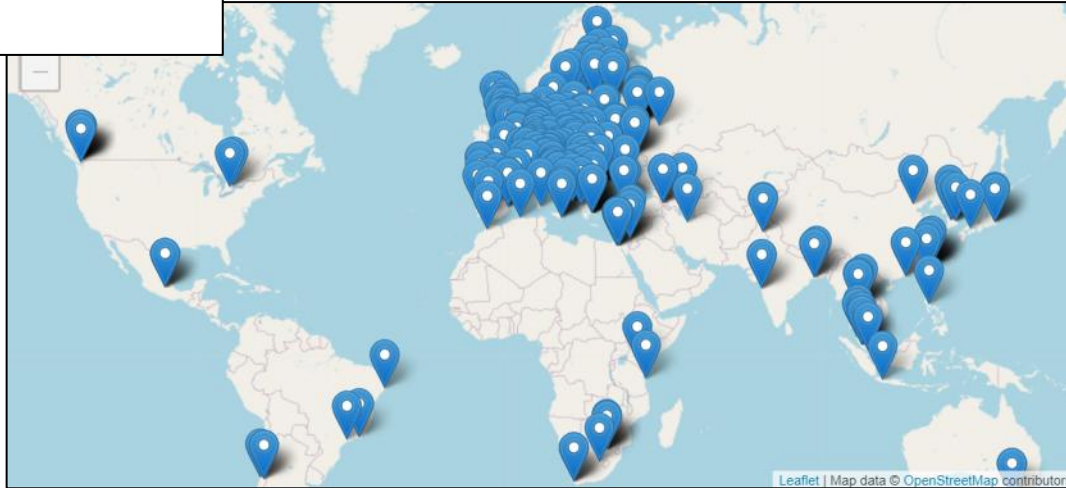
**All researchers have seamless access to
services, resources and expertise
to collaborate and conduct
world-class research and innovation**

Mission of the EGI Federation

**Deliver open solutions
for advanced computing and data analytics**

Memorandum of Understanding between EGI.eu and ASGC

Resource Infrastructure Provider MoU



**>1.3 Million
computing
cores**

**> 1 Exabyte
Data**

**Facilities
from 5
Continents**

April 2013

EGI Council participants

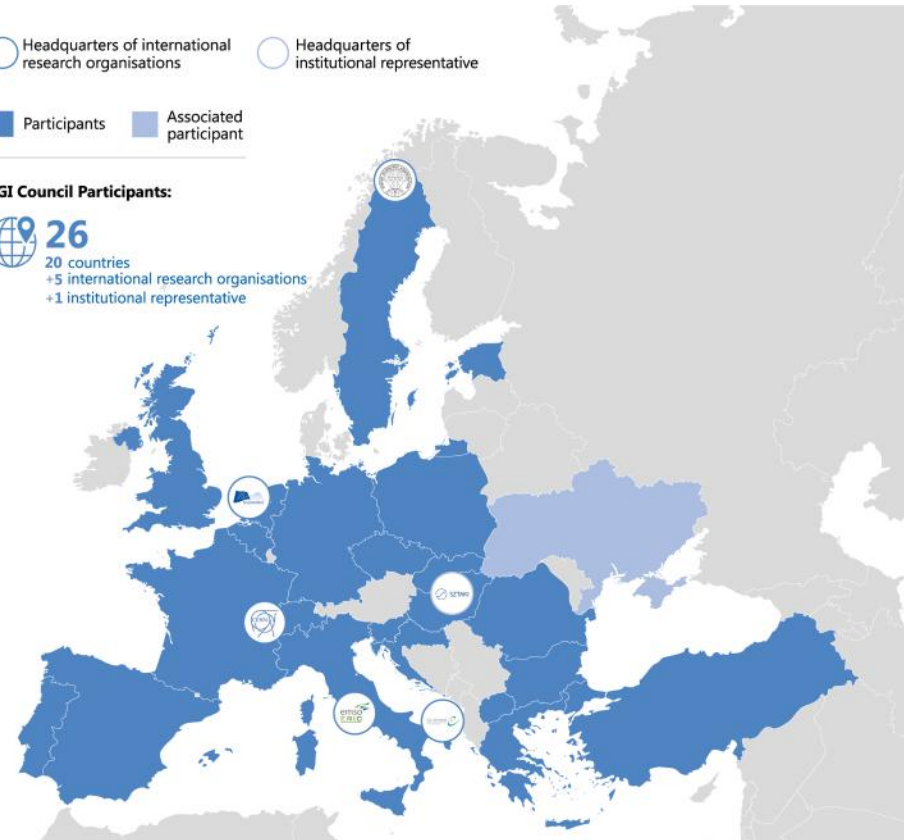
Belgium BELSPO's website	Bulgaria IICT's website	Croatia SRCE's website
Czech Republic Metacentrum's website	Estonia EENet's website	France France Grilles' website
Greece GRNET's website	Germany NGI-DE's website	Republic of North Macedonia MARGI's website
Italy INFN's website	Netherlands SURF's website	Poland Cyfronet's website
Portugal FCT's website	Romania IFIN-HH's website	Slovakia IISAS' website
Slovenia ARNES' website	Spain CSIC's website	Switzerland EnhancerR's website
Turkey ULAKBIM's website	United Kingdom Jisc's website	International CERN's website
International EISCAT's website	International EMSO's website	International IS-ENES website
International SeaDataNet website	Organisation SZTAKI's website	

○ Headquarters of international research organisations
○ Headquarters of institutional representative

■ Participants
■ Associated participant

EGI Council Participants:

26
20 countries
+5 international research organisations
+1 institutional representative



www.egi.eu/about/egi-council

Federation services

Security



Check-in

Login with your own credentials



Attribute Management

Manage memberships and groups in communities and virtual organisations

Coordination



Operations Coordination and support

Coordinate activities to ensure seamless operations



Community Coordination

A joint approach to user engagement



ITSM Coordination

Ensures professional service management for EGI IT services



Technical Coordination

Progress and innovation through collaboration



Strategy and Policy Development

One federation, one vision, one strategy



Project Management and Planning

A joint approach to planning and management



Security Coordination

Enhance local security for a safer global infrastructure



Communications

Share your successes at a larger scale

Operations



Marketplace

Expose your services to a broader audience



Accounting

Track and report the usage of your services



Collaboration Tools

IT tools for better coordination



Configuration Database

Manage the configuration information of federated e-infrastructure assets and their functional relations



Operational Tools

Integrate resources and operations in a federated ecosystem



Validated Software and Repository

Benefit from a repository of high-quality software validated for the EGI infrastructure



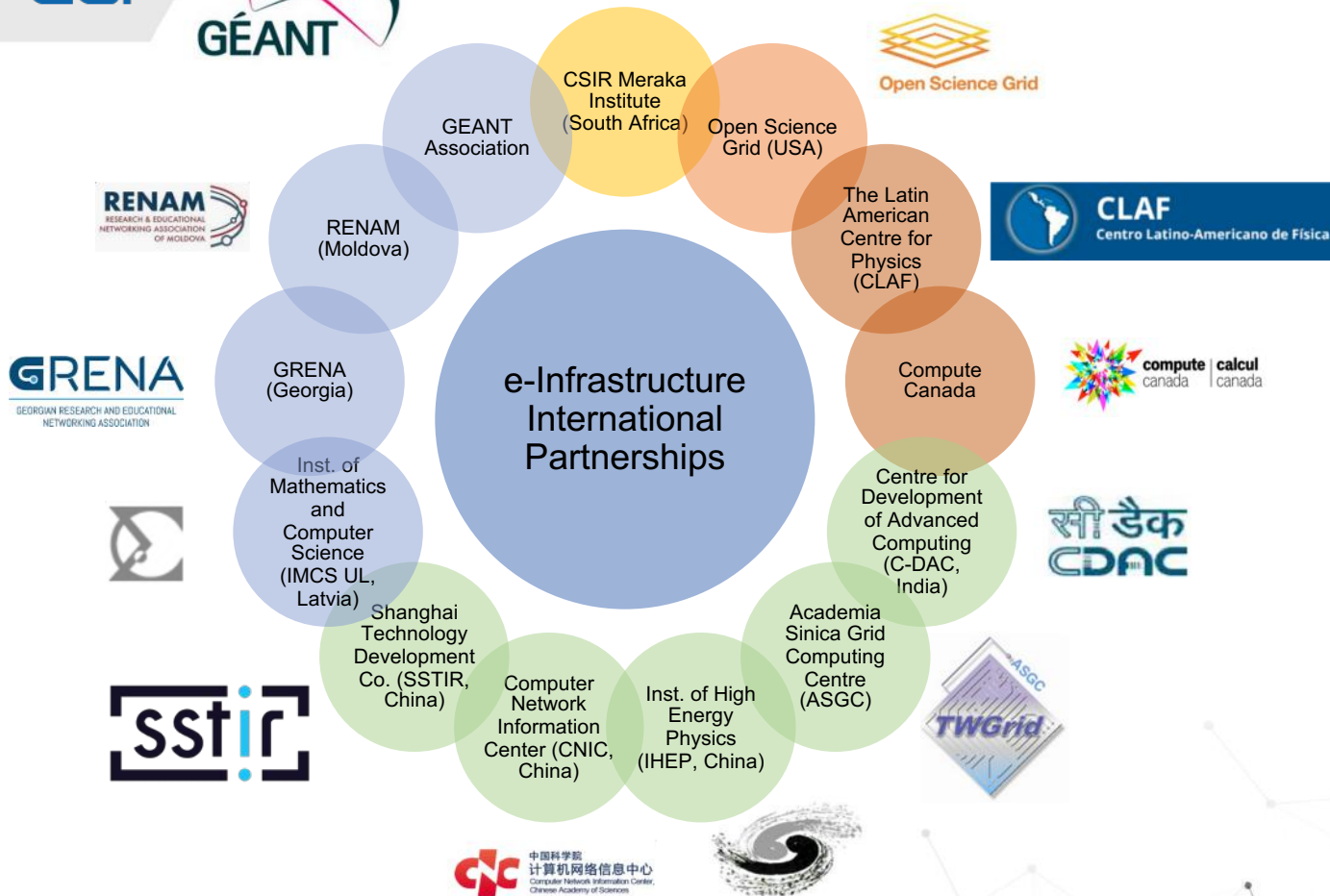
Service Monitoring

Monitor the performance of IT services



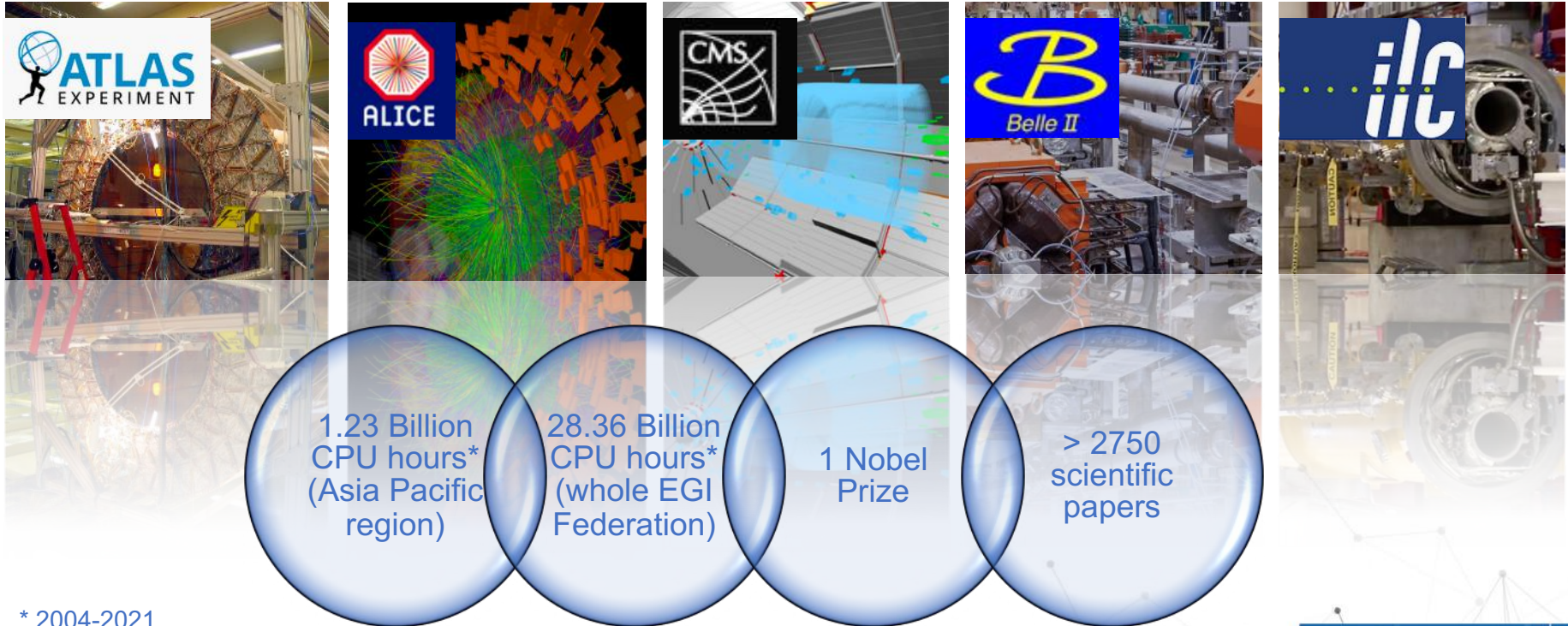
Helpdesk

Your point of contact to ask for support at EGI

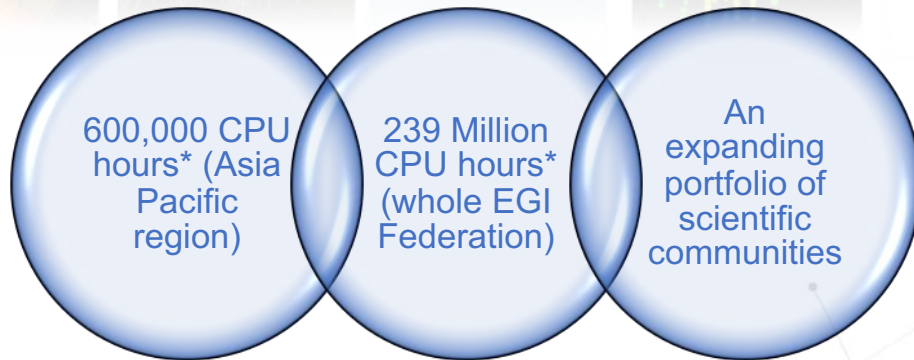
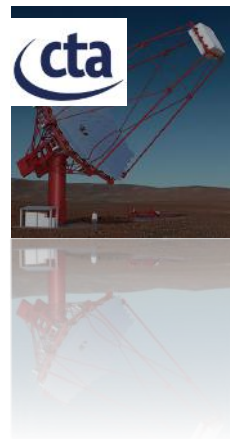
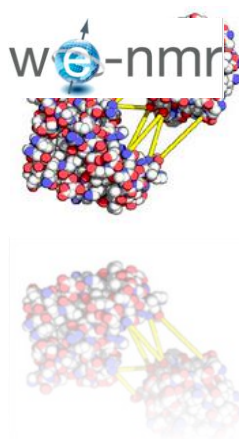
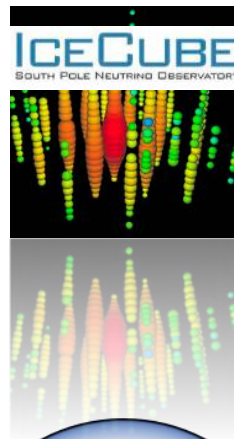


Advanced computing for international science

From High energy physics - a strong foundation of European-Asian collaboration since 2004

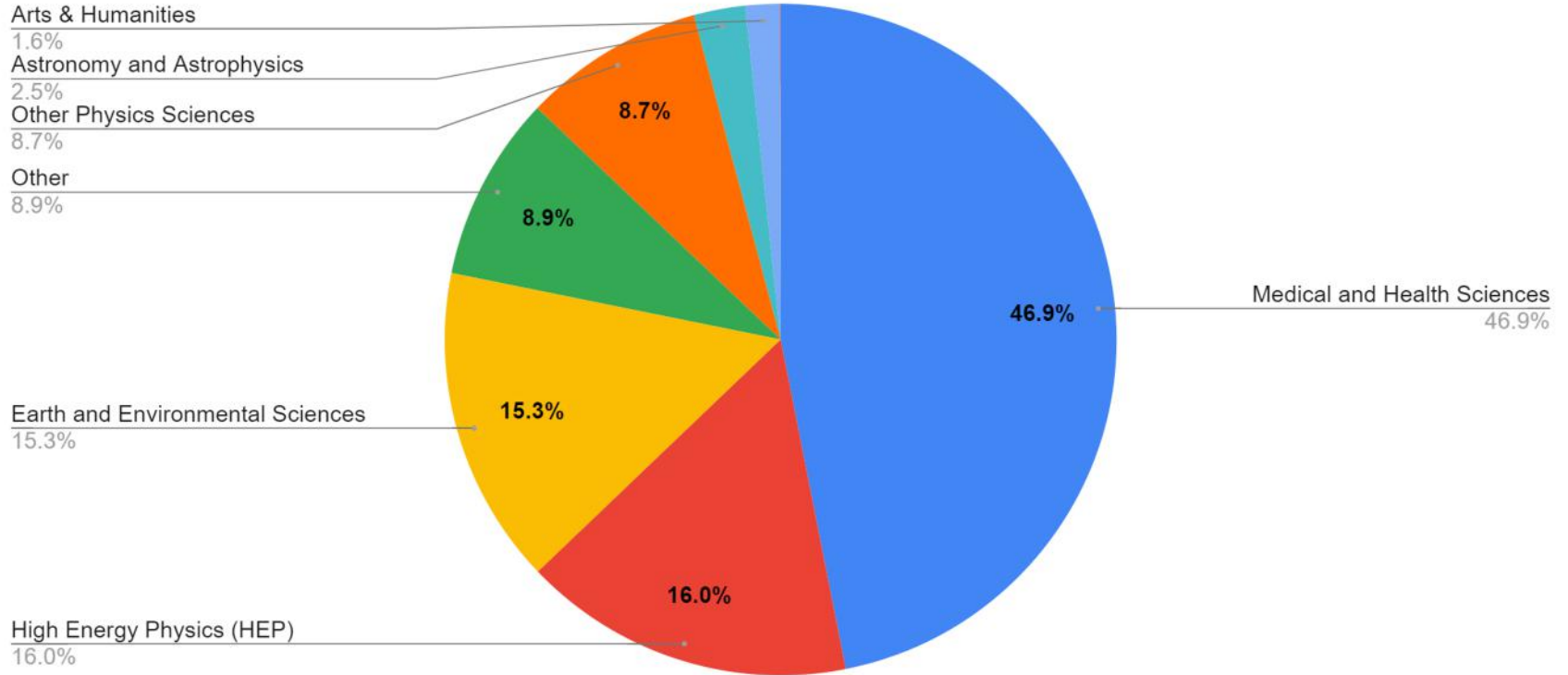


... to Photon and Neutron Science, Astronomy, Astrophysics, Space Science and Biology



* 2004-2021

EGI scientific disciplines (2020)



EGI Community project portfolio 2020-2021



Health and
Medicine

Photon and
Neutron
Sciences

Social
Sciences

Data-driven
innovation and
AI

StarwAI



Energy and
Manufacturing



Earth
Observation



Policy
management

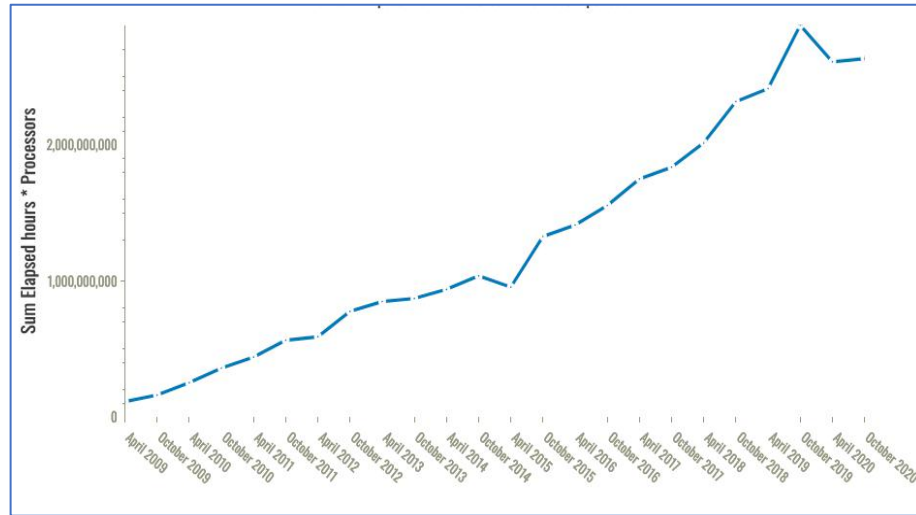


DECIDO

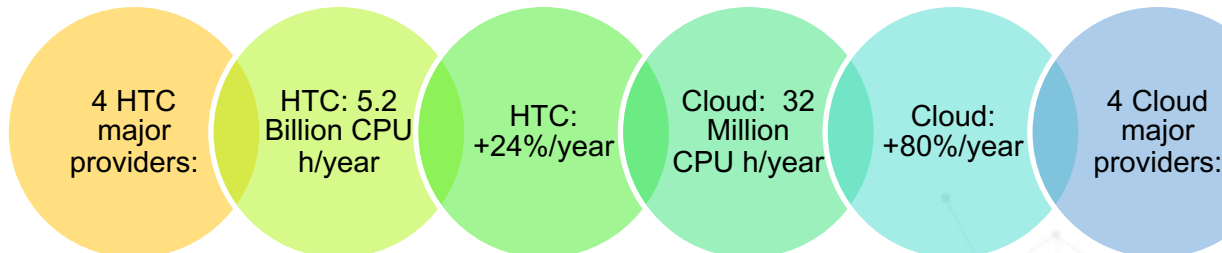
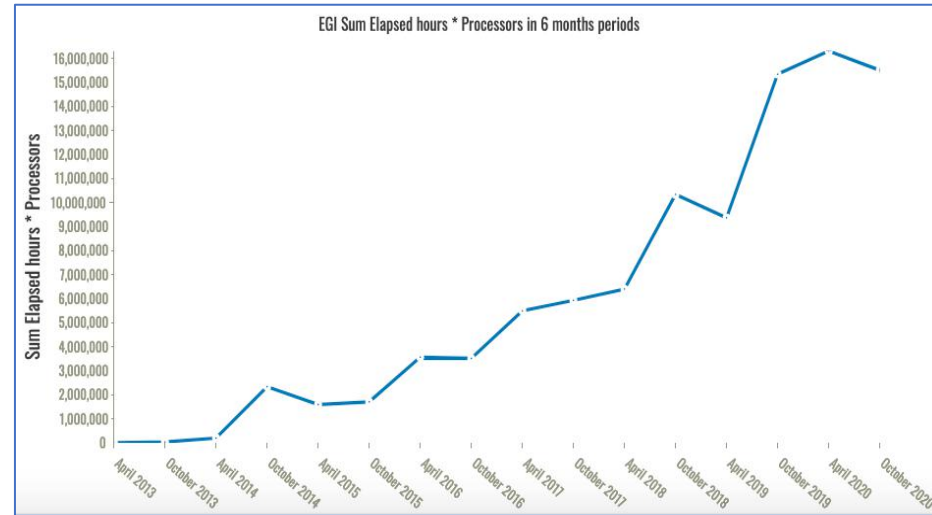


EGI Federation – Usage trends (2020)

High Throughput Computing



Cloud Computing



From Open infrastructures to Open Science

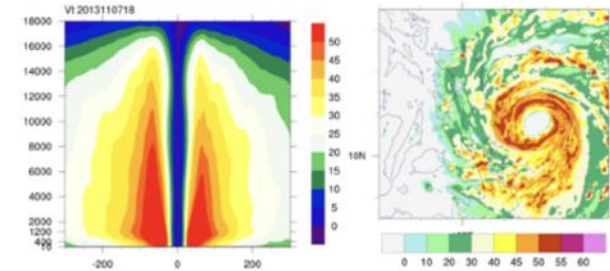
Innovation to expand from to new scientific collaborations and address societal challenges

(1) Scientific software as a service

Use case: Environmental science and disaster mitigation



- *Goals*
 - Capacity building for hazard risk analysis
 - Enhance the knowledge of hazard risk reduction
 - Improve accuracy and efficiency of hazard risk simulation
- *Provide scientific applications as a service*
 - iCOMCOT portal for tsunami simulations
 - WRF portal for weather prediction
- *Implement scientific case studies*
 - 18 case studies of 6 types of hazards in 8 partner countries
 - Collaborations with data providers (e.g. Sentinel Asia, Himawari Satellite Mirror Sites)
- *Exploit federated capacity and resources*
 - Infrastructure federation: Use distributed compute resources for simulations
 - Semantic/data federation: Share data based on FAIR principles
- *Organise events*
 - CRADR Workshops in Feb, Mar, May 2021; Training in April (TH)
 - Joint workshop or APAN WG meetings: Aug/Sep 2021 @APAN52 (ID)

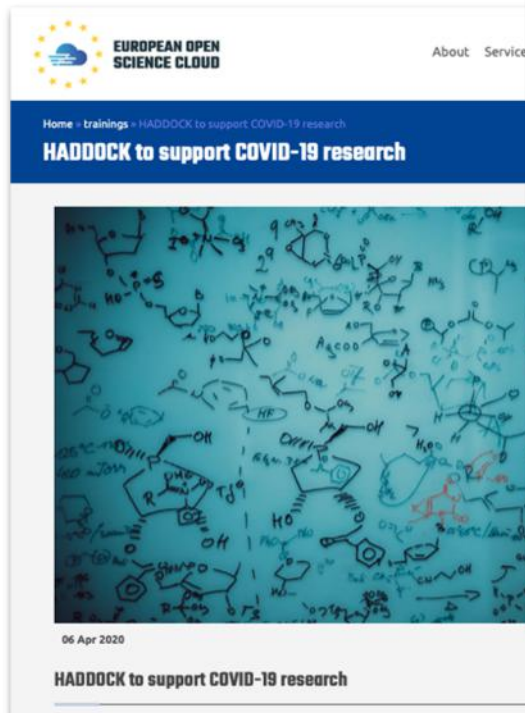


(1) Scientific software as a service (cont)

Use case: Modelling of various Sars-Cov2 - human protein interactions

<https://wenmr.science.uu.nl/>

- Screening of approved drugs against the protease with HADDOCK
- Docking of ~2,000 approved drugs run on EGI Federation/OSG HTC resources in ~3 ½ days

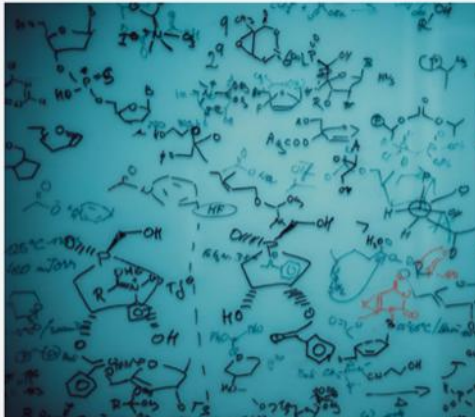


EUROPEAN OPEN SCIENCE CLOUD

About Services

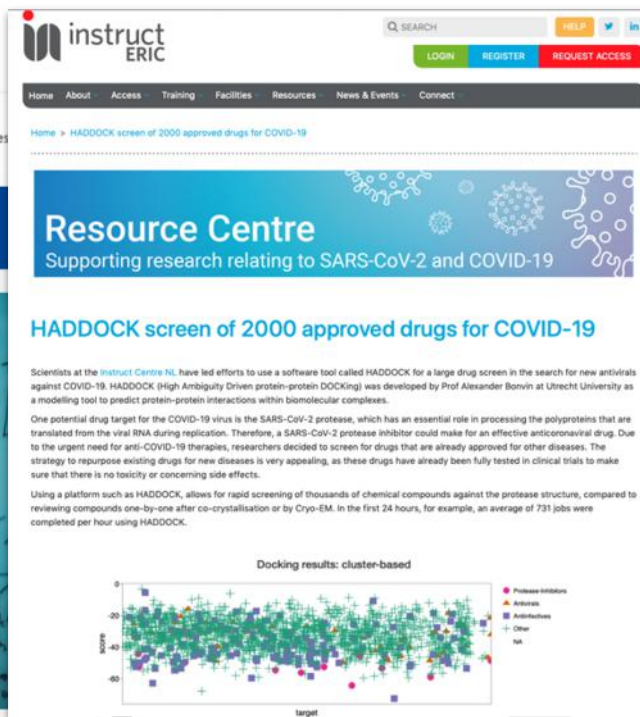
Home » trainings » HADDOCK to support COVID-19 research

HADDOCK to support COVID-19 research



06 Apr 2020

HADDOCK to support COVID-19 research



instruct ERIC

SEARCH LOGIN REGISTER REQUEST ACCESS

Home About Access Training Facilities Resources News & Events Connect

Home » HADDOCK screen of 2000 approved drugs for COVID-19

Resource Centre

Supporting research relating to SARS-CoV-2 and COVID-19


HADDOCK screen of 2000 approved drugs for COVID-19

Scientists at the [Instruct Centre NL](#) have led efforts to use a software tool called HADDOCK for a large drug screen in the search for new antivirals against COVID-19. HADDOCK (High Ambiguity Driven protein-protein DOCKing) was developed by Prof Alexander Bonvin at Utrecht University as a modeling tool to predict protein-protein interactions within biomolecular complexes.

One potential drug target for the COVID-19 virus is the SARS-CoV-2 protease, which has an essential role in processing the polyproteins that are translated from the viral RNA during replication. Therefore, a SARS-CoV-2 protease inhibitor could make for an effective antiviral drug. Due to the urgent need for anti-COVID-19 therapies, researchers decided to screen for drugs that are already approved for other diseases. The strategy to repurpose existing drugs for new diseases is very appealing, as these drugs have already been fully tested in clinical trials to make sure that there is no toxicity or concerning side effects.

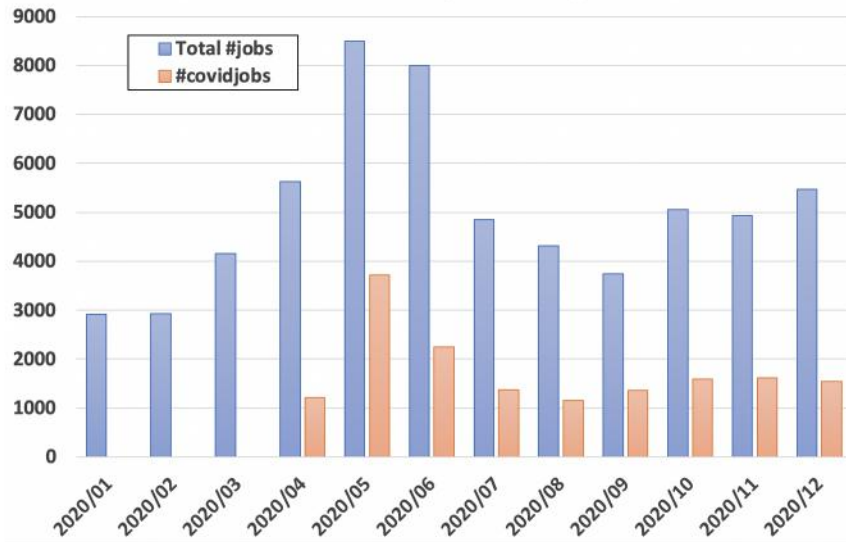
Using a platform such as HADDOCK, allows for rapid screening of thousands of chemical compounds against the protease structure, compared to reviewing compounds one-by-one after co-crystallisation or by Cryo-EM. In the first 24 hours, for example, an average of 731 jobs were completed per hour using HADDOCK.

Docking results: cluster-based

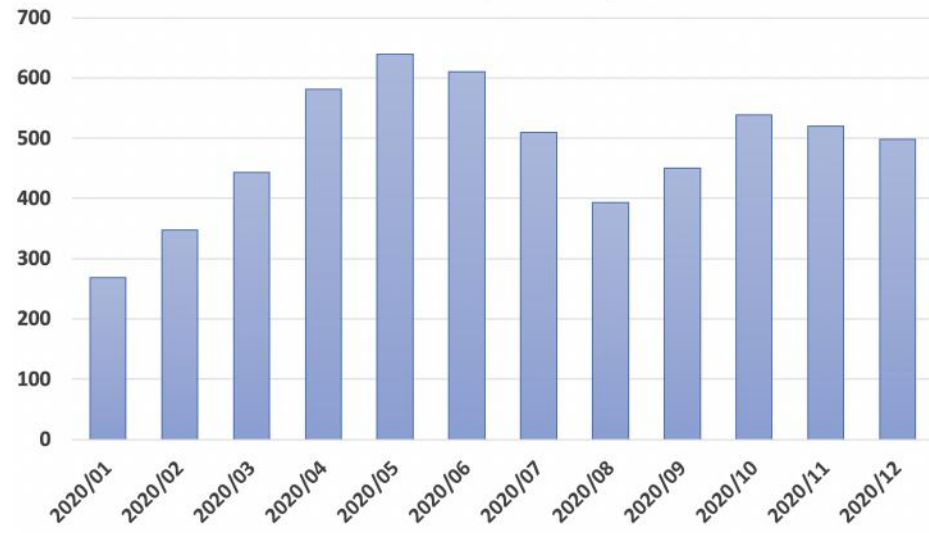


(1) Scientific software as a service (cont)

HADDOCK server processed jobs



HADDOCK server unique users per month



On average **~550 active users per months**, **11,000 simulations related to COVID-19** (the equivalent of **~1.5 million HTC jobs**, **~2.7 million CPU hours**) on the EGI and OSC grid resources over the months of April to Sept. 2020

(1) Scientific software as a service (cont)

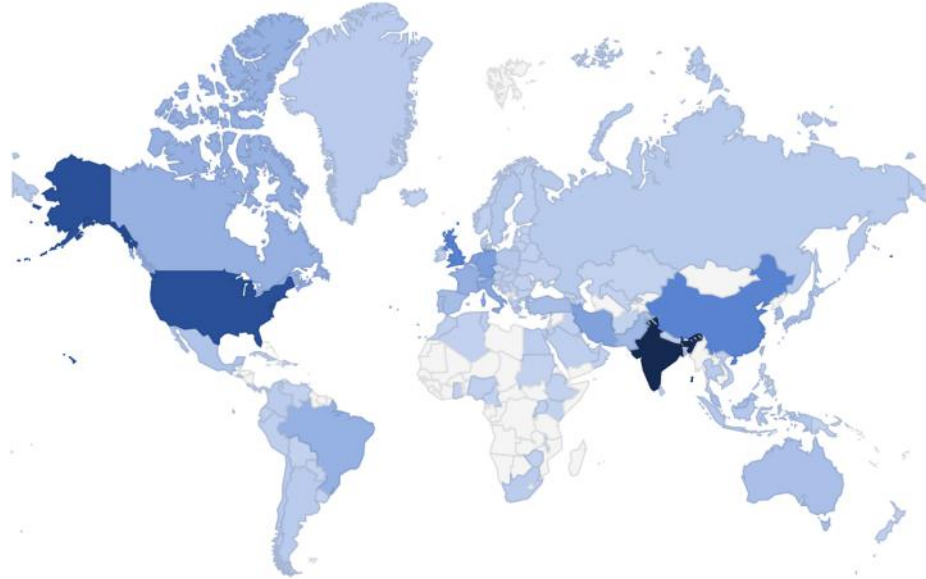
International user community

> **21,000** Registered users

> **110** Countries reached

Both researchers and students

Sustained growth of the communities



	Country	All_Users ▼	HADDOCK	DISVIS	POWERFIT	SPOTON
1	Total Users	21,306	20,526	2,934	2,324	2,668
2	India	4,444	4,345	577	507	575
3	EU Users	4,432	4,191	628	437	482
4	United States	3,109	2,992	407	283	356
5	United Kingdom	1,277	1,222	138	115	117

(2) Bring new solutions to common users

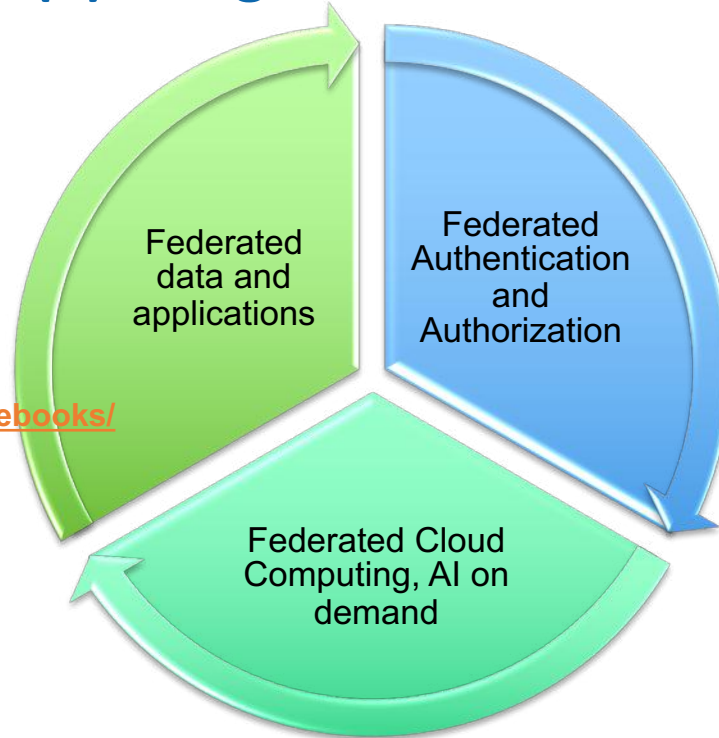
Applications



Create interactive documents with live code, visualisations and text

Notebooks





<https://www.egi.eu/services/notebooks/>




Login with your own credentials

Check-in

<https://www.egi.eu/services/check-in/>

 <p>Run virtual machines on demand with complete control over computing resources</p> <p>Cloud Compute</p>	 <p>Run Docker containers in a lightweight virtualised environment</p> <p>Cloud Container Compute</p>	 <p>Execute thousands of computational tasks to analyse large datasets</p> <p>High-Throughput Compute</p>	 <p>Manage computing workloads in an efficient way</p> <p>Workload Manager</p>
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<https://www.egi.eu/services/cloud-compute/>

Service Portfolio

Data Spaces and Analytics

Data and thematic data analytics and processing tools

Platforms

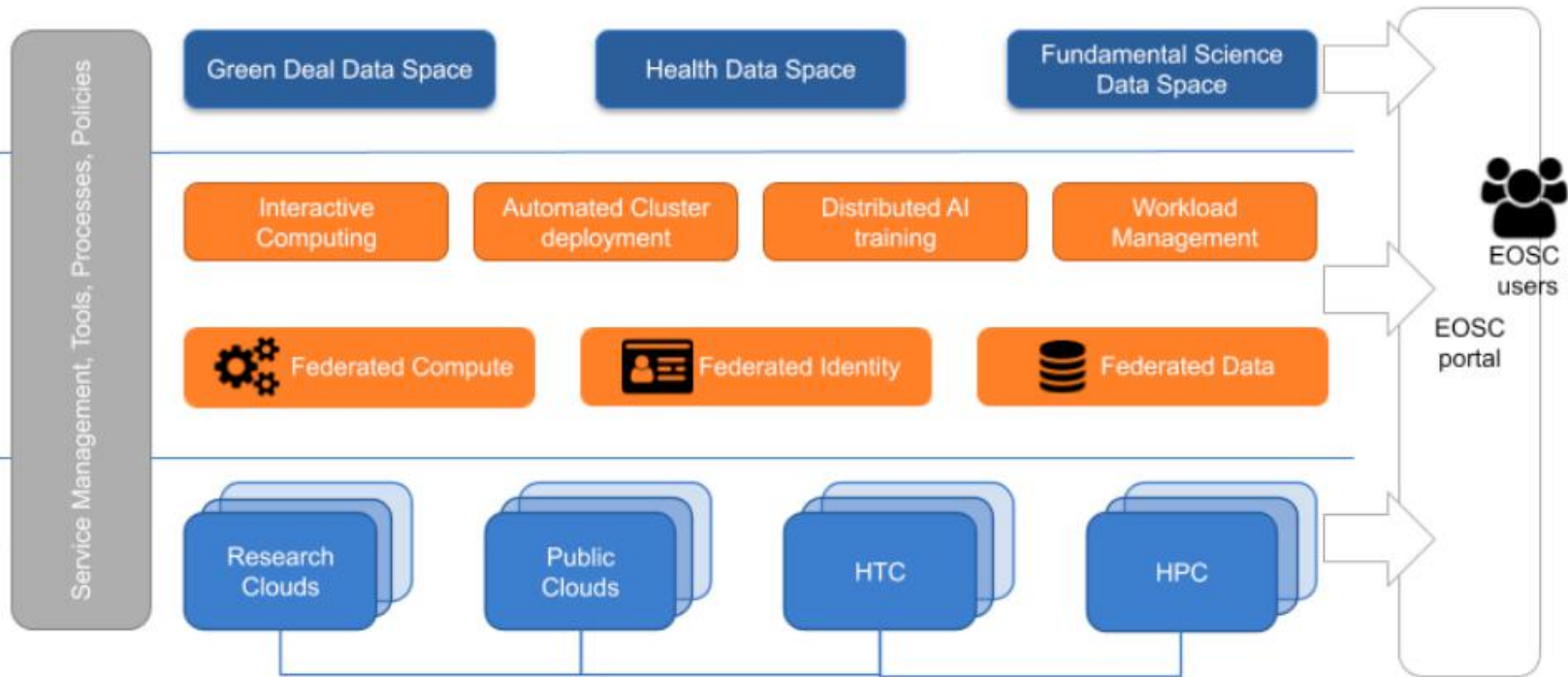
generic added-value platform level services

Federated Access

Federation-wide management of data and computing

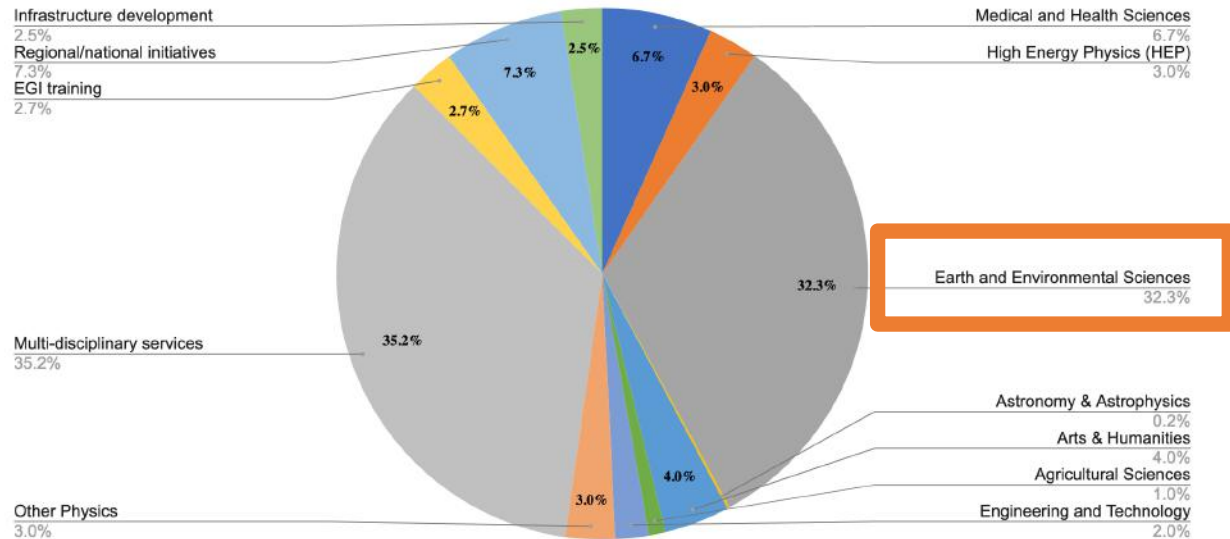
Federated Resources

Compute and storage facilities



A success story: Federated Cloud Computing

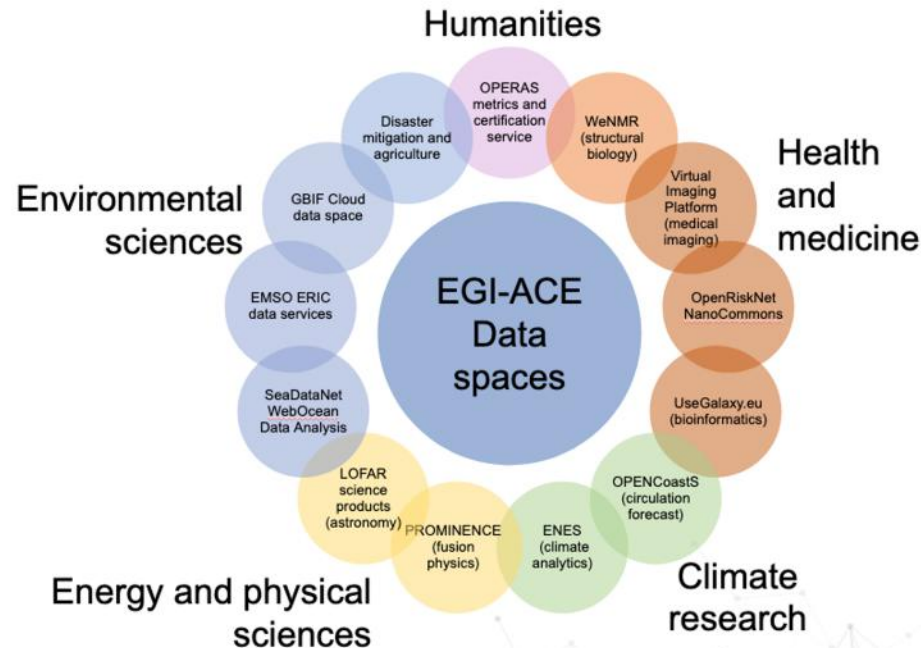
Users by discipline (2020)



Cloud providers

(3) Deliver Data as a Service

Data Spaces of the EGI-ACE project



1st Call for international use cases

Deadline: 15th of April

<http://go.egi.eu/open-call>

EGI-ACE Call for Use Cases



The EGI-ACE Horizon 2020 project delivers the 'EOSC Compute Platform', a distributed federated compute infrastructure that serves users of the [European Open Science Cloud](#) (EOSC). EGI-ACE (EGI Advanced Computing for EOSC) builds on the pan-european EGI e-infrastructure federation and provides various types of infrastructures, platforms and software services from publicly funded compute centres, commercial service providers and research communities with pan-European relevance.

With this call for use cases the EGI-ACE project offers access to infrastructure and platform services, dedicated user support and training. The services, support and training are sponsored by the European Commission and various national funding agencies and are free to access to the use cases that will be selected through the call.



Who should apply

The target audience of this call are international researchers, research projects, communities and infrastructures, as well as national research groups who need services and support for:

- Large-scale data processing, scientific analysis, visualisation
- Hosting data analysis platforms and applications in the cloud to offer them for international use cases
- Federate and make accessible community-specific compute services in EOSC

Applications for the call are welcomed from academic or industrial researchers at any level, from postgraduate students to the most senior researchers, who are working on or support non-proprietary research in any discipline where access to compute facilities is beneficial. Projects and research infrastructures that do not have access to similar facilities are particularly encouraged to apply. Applicants must be working in a research institute based in an eligible country (i.e. any EU member state or Associated State), OR must be submitted on behalf of a research project/experiment/collaboration that includes partners from eligible countries.

Note that applicants are NOT eligible for visits to the centres involved in this action.



The offering



Timeline



Submit use case



Contact

- International collaborations in scientific computing are key enablers of scientific excellence
 - Human networks for coordinated support, training consultancy
 - Access to shared compute and storage infrastructures
- Demand for innovative scientific computing services is increasing
 - Opportunities for joint innovation
 - Many opportunities to increase collaboration in domains such as Health and Medicine and Environmental Science
- Scientific computing needs integrated infrastructure, data and scientific software provisioning
- Submit your scientific use case! <http://go.egi.eu/open-call>