



# A Worldwide e-Infrastructure for NMR and structural biology

Contract n°: RI-261572  
Project type: CP-CSA  
Duration: 36 months  
Total budget: 2'434'000 €  
EC Funding: 2'150'000 €

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UNIVERSITY OF  
CAMBRIDGE

EMBL

SpronkNMR

NL

DE

IT

IT

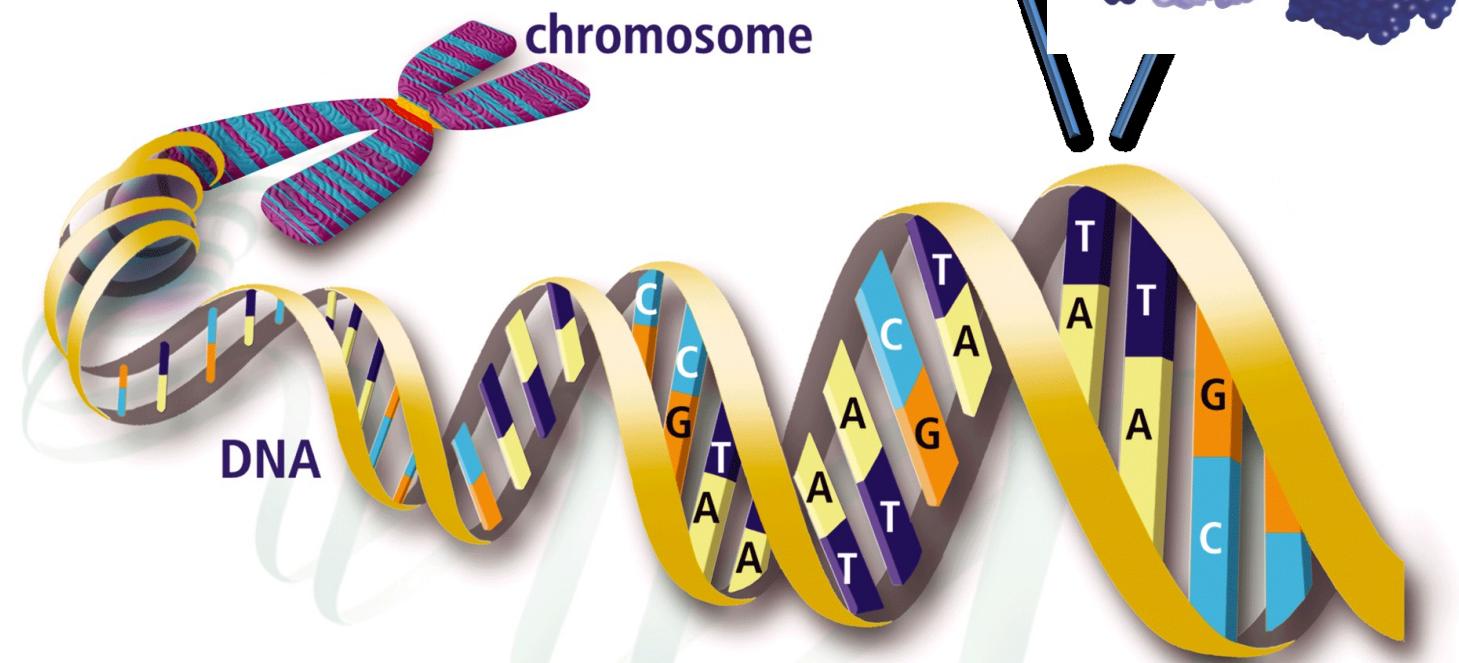
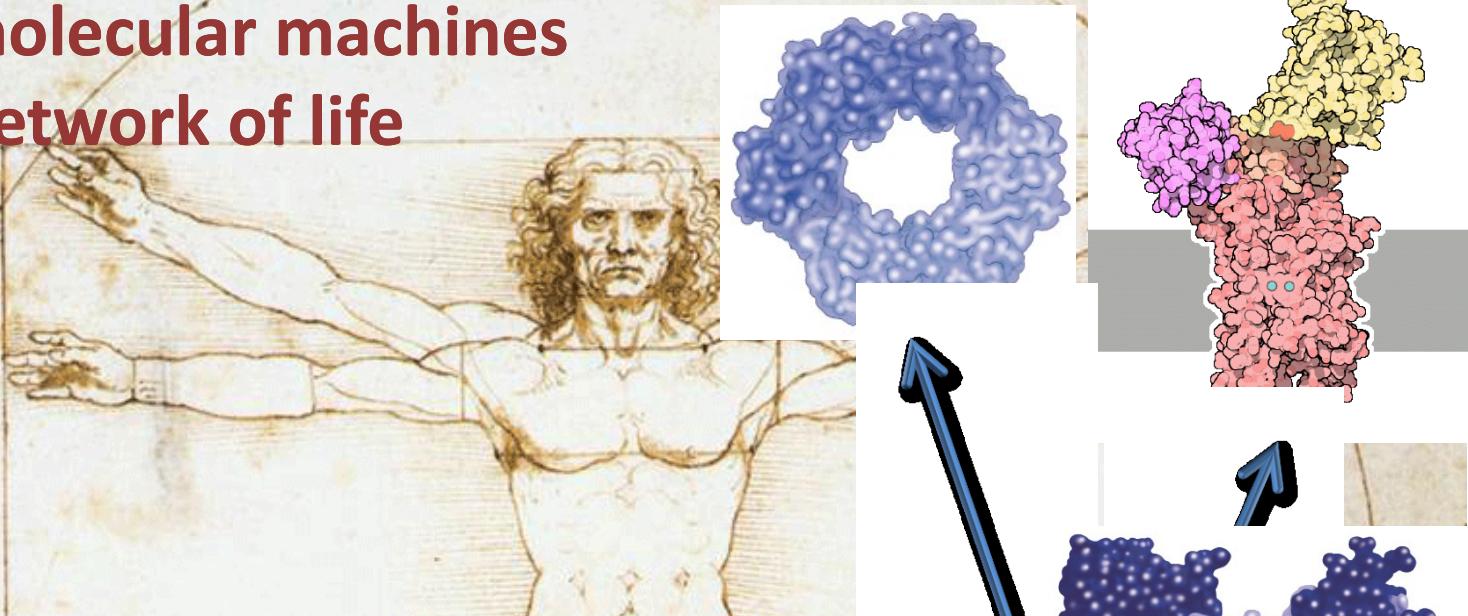
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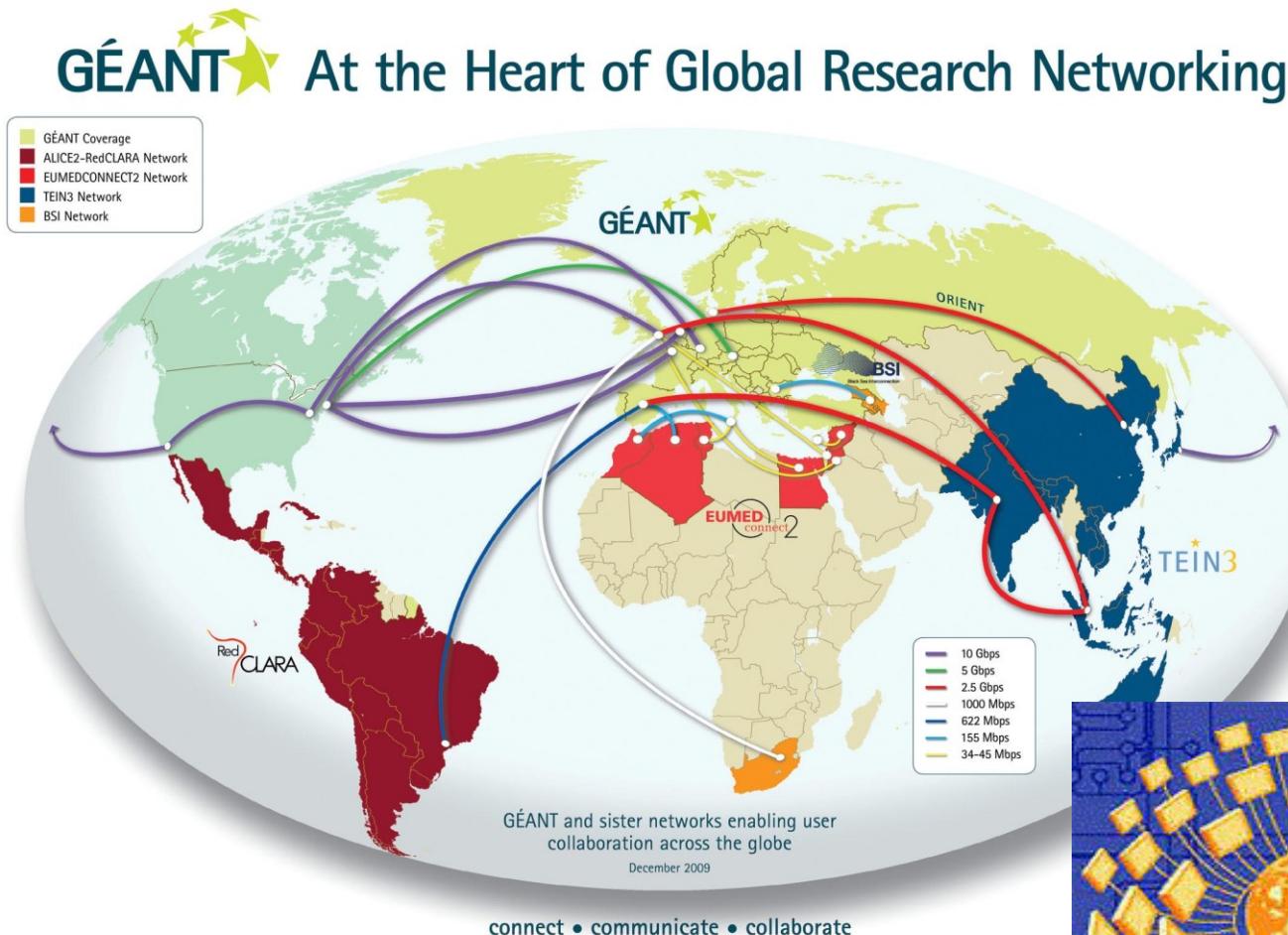
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# The molecular machines and network of life



# The network of science...



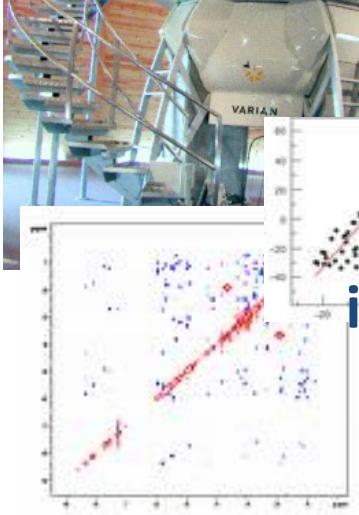
## GRID resources



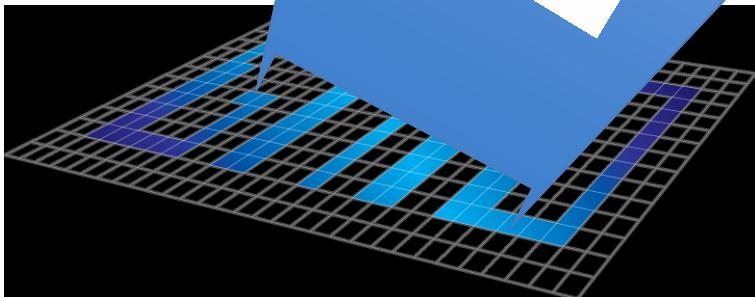
e-infrastructure

# Exploiting GRID resources in structural biology...

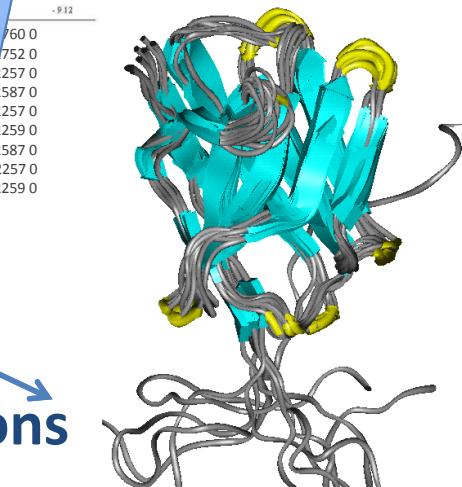
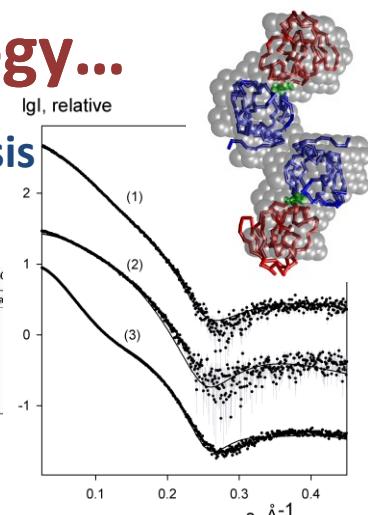
## NMR data collection and processing



Data  
interpretat



## SAXS data analysis



Computations

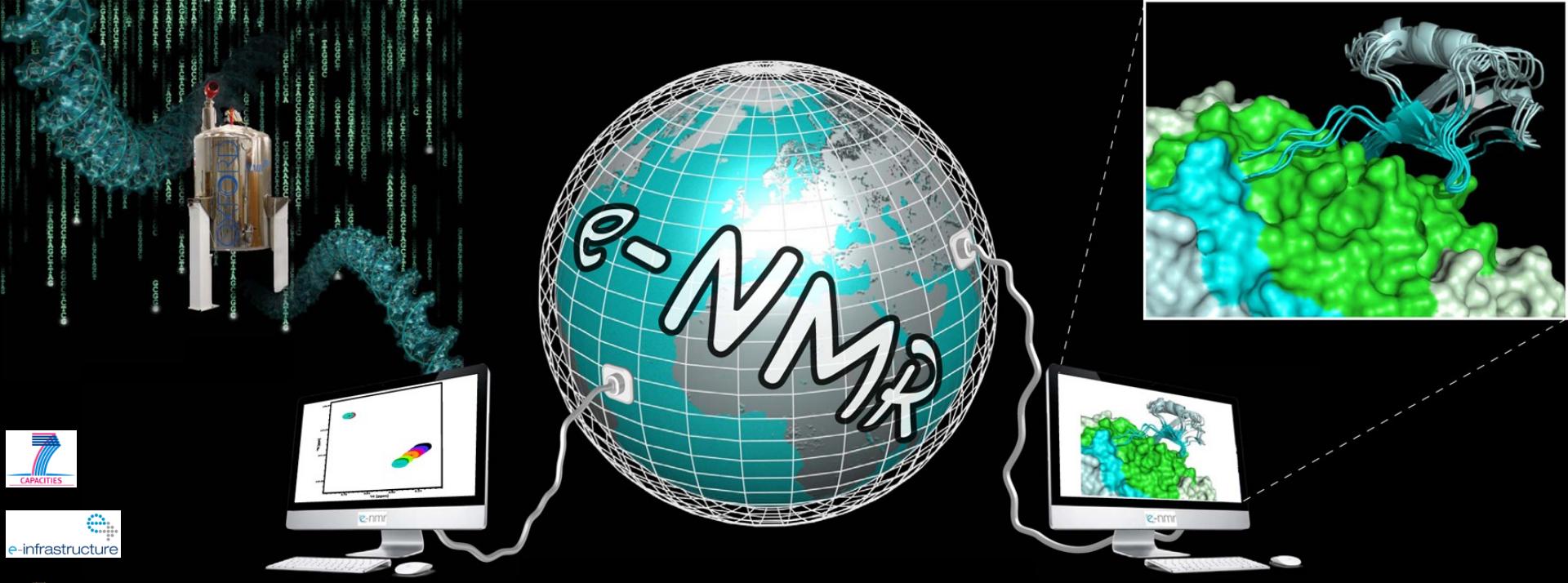
Structure, dynamics & interactions  
→ impact on research and health:  
- origin of disease  
- design of new experiments  
- drug design...



# Main objectives

- Operate and further develop a user-friendly **e-Science gateway for the NMR and SAXS communities**
- Establish a **virtual research platform** for (interaction with) the user community
- **Provide support** to software developers, users and other e-Infrastructure projects
- **Foster the adoption and use of e-Infrastructure** in a wide range of flanking disciplines within the life sciences
- **Operate and consolidate the eNMR Grid infrastructure** and to extend it to interoperate with other **worldwide Grid initiatives**
- Develop a model to ensure **sustainability** of the project





## eNMR platform operational and well used!

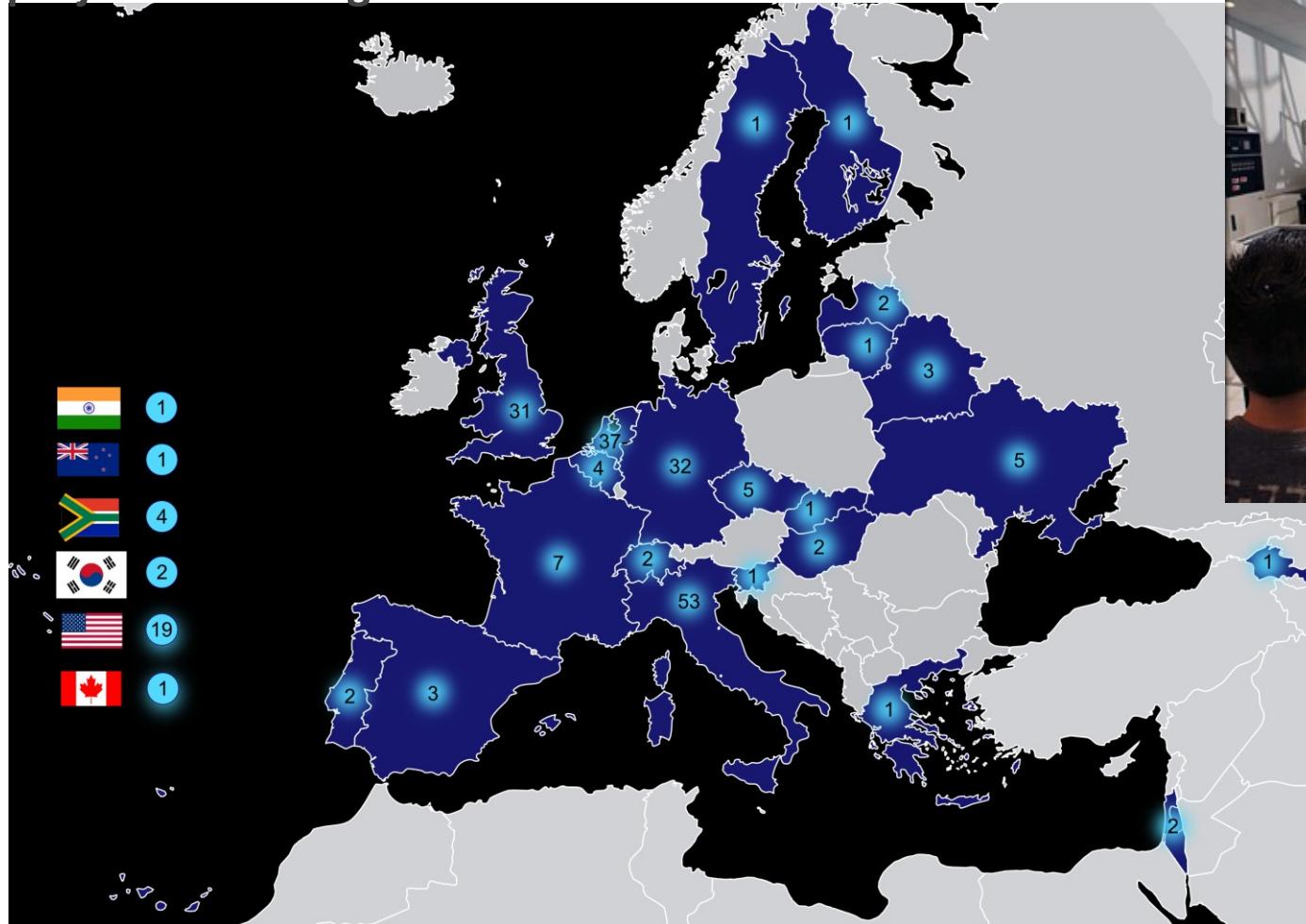
- **2<sup>nd</sup> largest VO in the life sciences**
- Over 225 registered users and growing
- >16000 CPUs
- >350 CPU years over the last 12 months
- **20% of Life Sciences on the Grid**
- User-friendly access to e-Infrastructure via web portals

[www.enmr.eu](http://www.enmr.eu)



# Users distribution

The project leverages on EU-NMR (FP6), EAST-NMR, and the new BioNMR (FP7) Research Infrastructures projects to enlarge its users basis



Linked to  
Instruct (ESFRI)

# User-friendly access to Grid resources via web portal

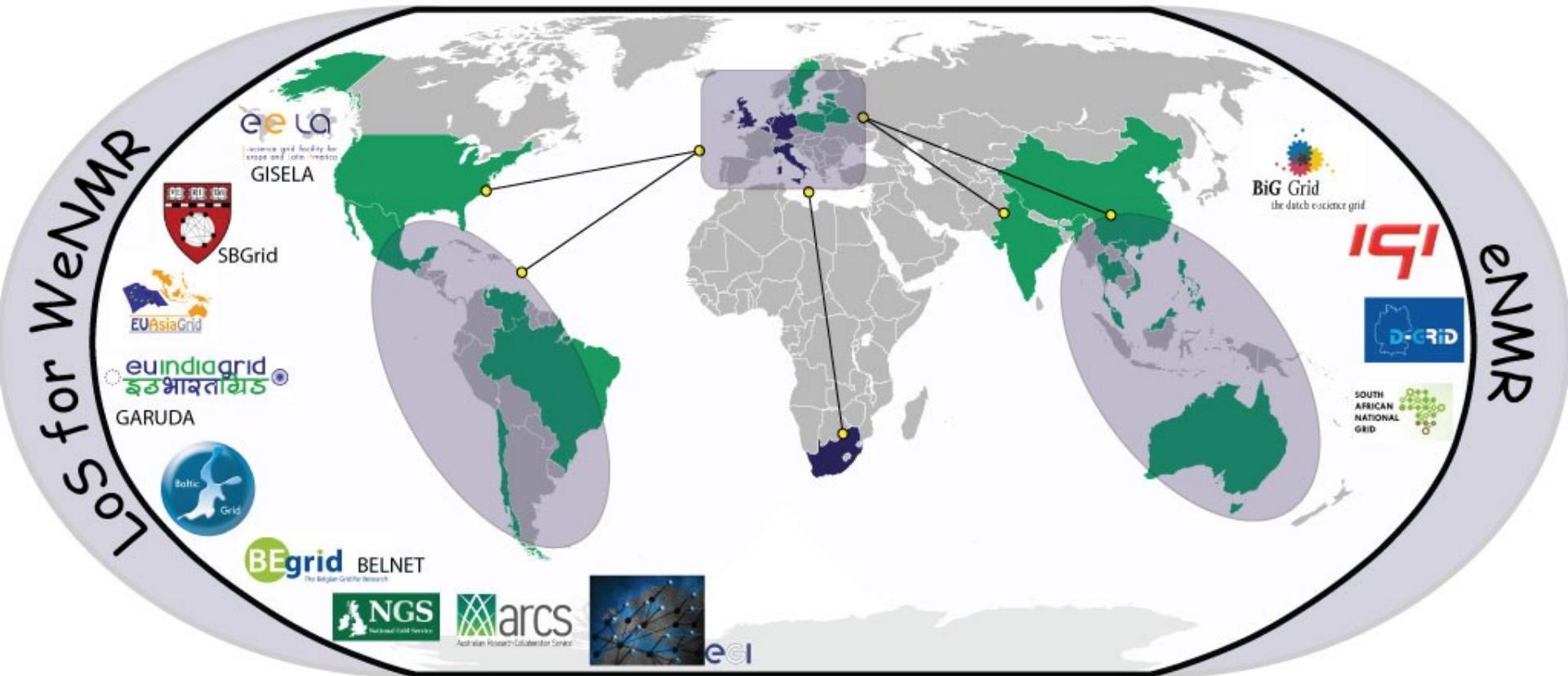
The screenshot shows the e-NMR web portal homepage. The header features the "e-NMR" logo and the text "NMR computational infrastructure". Below the header is a navigation bar with links to various tools: Home, HADDOCK, Xplor-NIH, AMBER, CYANA, CS-ROSETTA, TALOS+, AutoAssign, MARS, MDD, RSS, FormatConverter, 3D-DART, eNMR-Grid, and eNMR Wiki. The main content area has two columns. The left column is titled "WELCOME TO THE E-NMR WEB PORTAL >>" and contains text about the project's aim to unify NMR computational infrastructure in system biology, funded by the European Union. It also describes how NMR plays a role in life sciences and structural biology. The right column is titled "PROFILE >>" and displays logos for "e-nmr" and "e-infrastructure".

e-NMR aims at deploying and unifying the NMR computational infrastructure in system biology, a project funded under the 7th framework program of the European Union (Contract no. 213010 - e-NMR).

NMR plays an important role in life sciences (biomolecular NMR), and structural biology in particular, at both European and international levels. Our main objective is to optimize and extend the use of the NMR Research Infrastructures of EU-NMR through the implementation of an e-Infrastructure in order to provide the biomolecular NMR user community with a platform integrating and streamlining the computational approaches necessary for NMR data analysis and structural modelling (e-NMR).

<http://www.enmr.eu/webportal>

# A global virtual research community



Web-nmr

The word cloud illustrates the following key themes:

- Research and e-Infrastructure:** Grid, research, sciences, activities, access, build, maintain, serve, user, portal, offered, NA, develop, international, user-friendly, gateway, growing, ranking, use, remote, existing, exchange, also.
- Community and Initiatives:** SAXS, communities, established, global, current, including, around, wide, public, eNMR, Europe, involving, extend, stakeholders, limited, extensive, developers, European, initiatives, interest, Service, deployed, variety.
- Structural Biology and Tools:** WeNMR, biology, large, year, teams, Networking, sustainability, objects, adaptive, increasing, offers, internationally, jointly, structural, provide, number, synchrotron, ensure, biological, virtual, life, users, initiatives, range, software, facilities, tools, secure, i.e., National, joint, activities, aim, knowledge, communication, generation, future, groups, general, EGI, instrumentation, operate, projects, line, consolidate, main, size, method, different, worldwide, services.