Pan-European digital assets supporting research communities

WeNMR – A worldwide e-Infrastructure for NMR and Structural Biology

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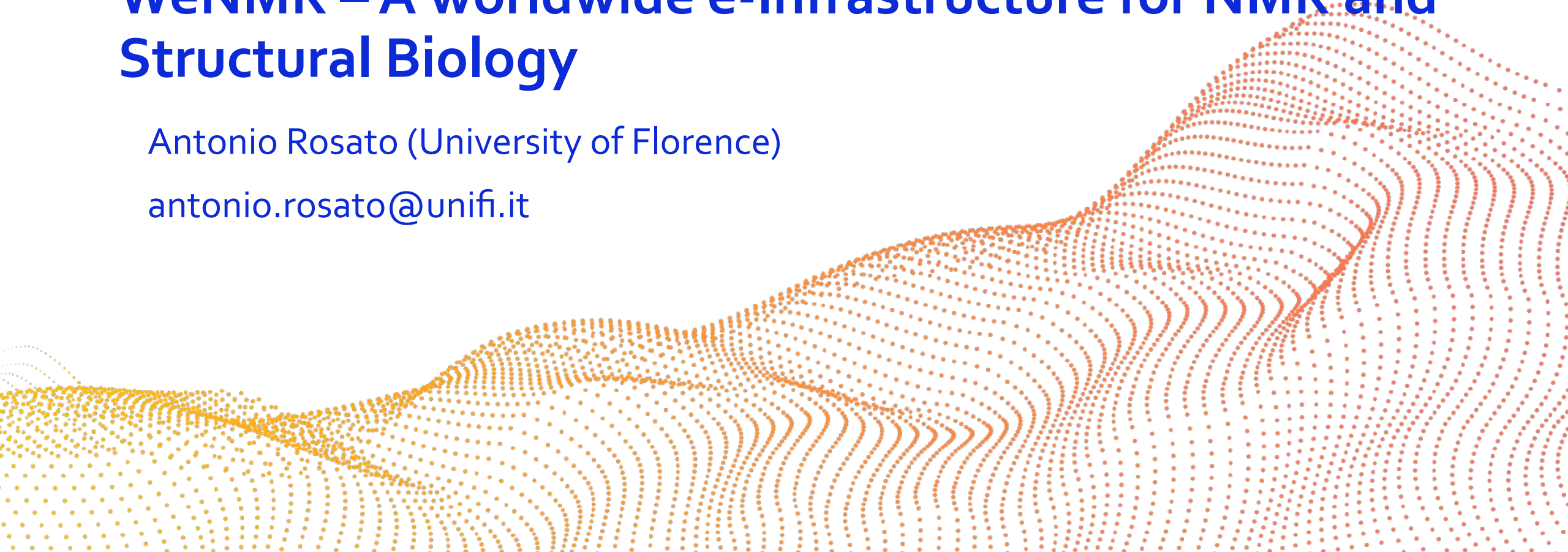
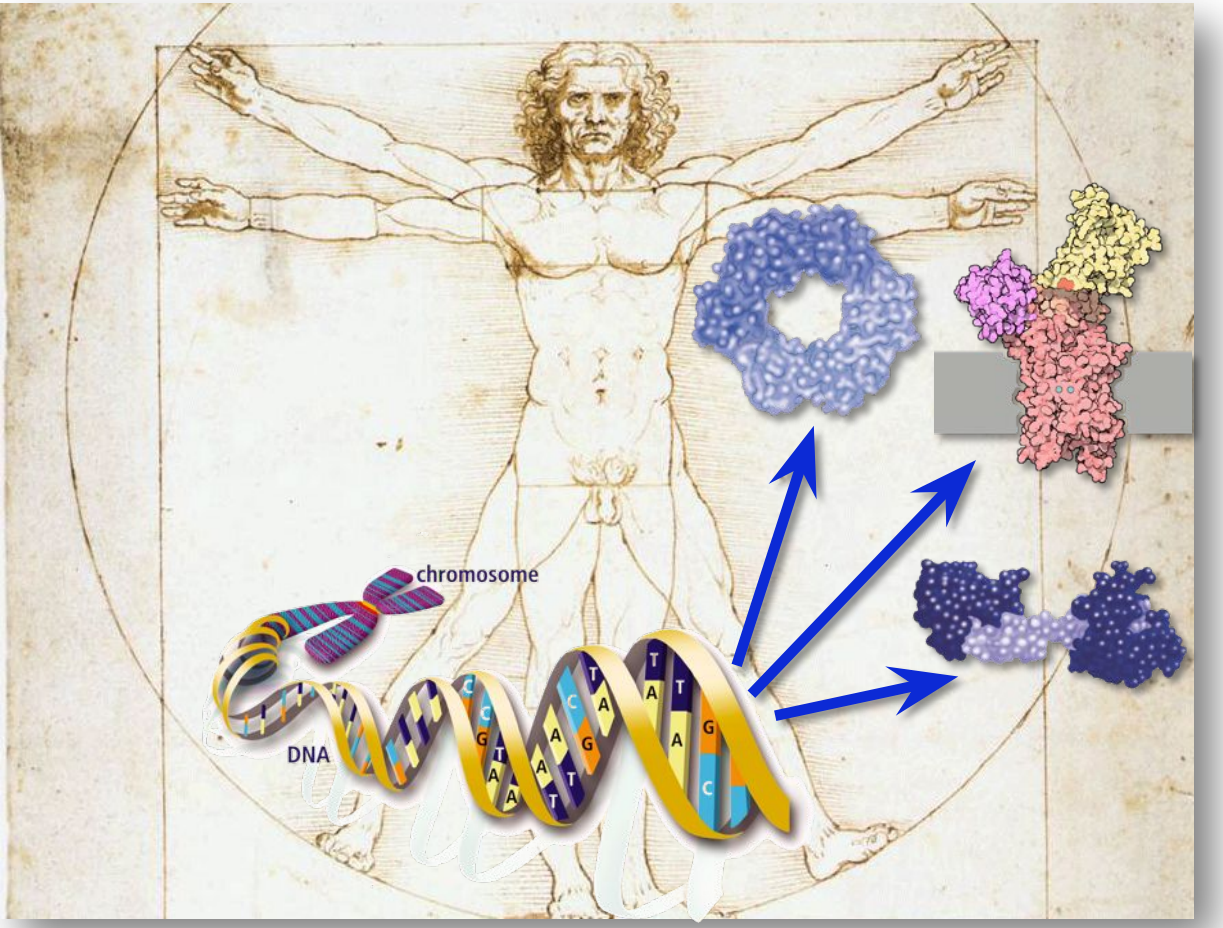
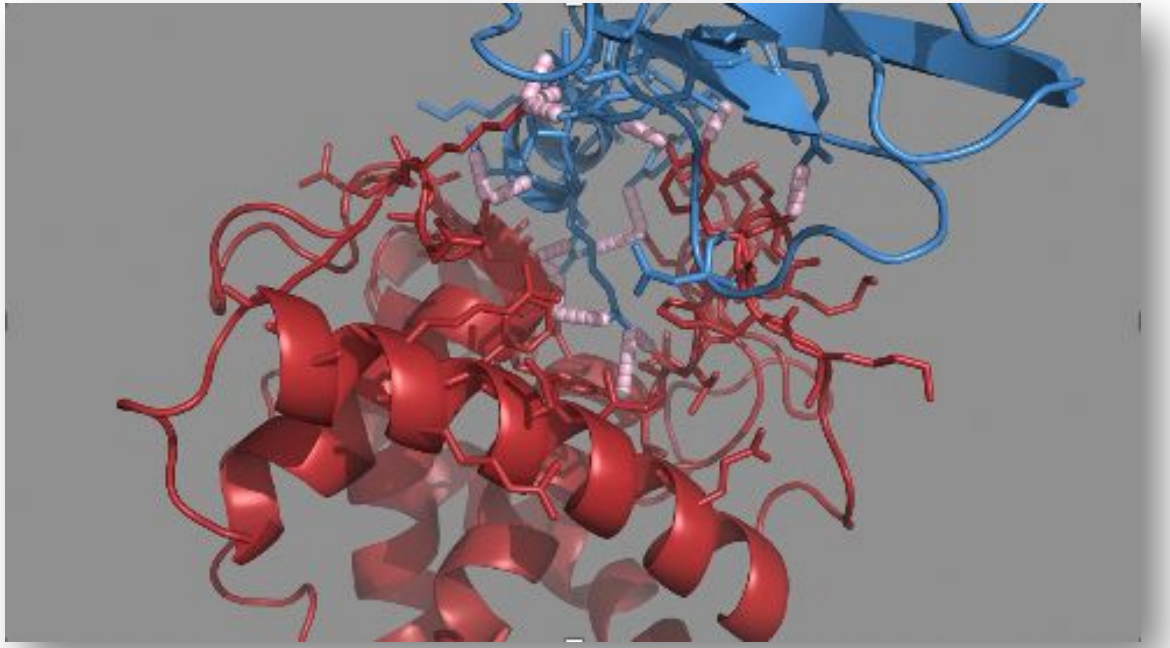


Domain: life sciences / structural biology

Understand life at a molecular level





Main use cases:

- Disease-causing mutations
- Engineer better molecules for material, health or food applications
- Obtain a starting point for drug design to combat disease

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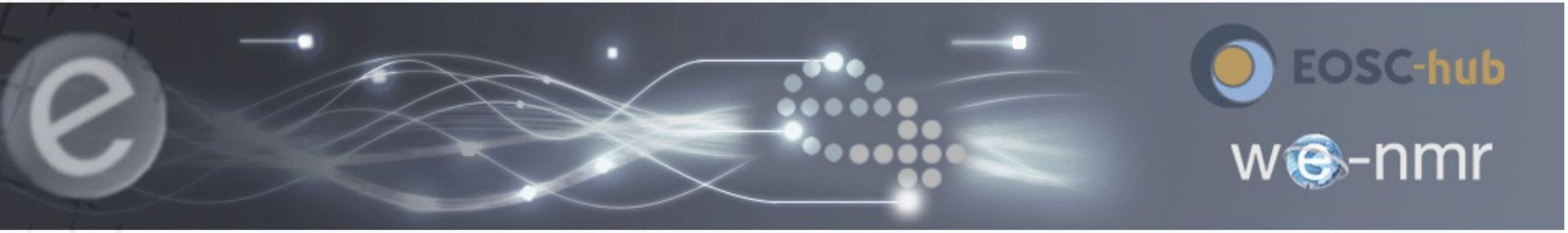
WENMR | A WORLDWIDE E-INFRASTRUCTURE FOR NMR AND STRUCTURAL BIOLOGY

ABOUT NEWS EOSC-HUB SERVICES SUPPORT TUTORIALS



we-nmr

WeNMR is a worldwide e-Infrastructure for NMR and structural biology

- Email
- Facebook
- LinkedIn
- Github
- Youtube

WeNMR is a Virtual Research Community supported by EGI. WeNMR aims at bringing together complementary research teams in the structural biology and life science area into a virtual research community at a worldwide level and provide them with a platform integrating and streamlining the computational approaches necessary for data analysis and modelling.

This is a new re-design of the WeNMR entry. At the moment, WeNMR is operating as a thematic service in the EOSC-hub project.

The old registration system has been discontinued, but we are working to provide a new one soon.

www.wenmr.eu

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WeNMR & EOSC

EUROPEAN OPEN SCIENCE CLOUD

Security & Operations 0
Sharing & Discovery 7
Training & Support 0
Other 0

FILTERS

Research steps

Find or choose from the list below

- Process and Analyse 5
- Access Research Infrastructures 1
- Access Training Material 1
- Access Computing and Storage Resources 0
- Discover Research Outputs 0

Show 4 more

Scientific Domains

Find or choose from the list below

- Natural Sciences 7
  - Biological Sciences 7
  - Chemical Sciences 0
  - Computer & Information Sciences 0
  - Earth & Related Environmental Sciences 0
  - Mathematics 0
  - Other Natural Sciences 0

ketplace

Providers › A Worldwide e-Inf

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ABOUT DETAILS

OPEN ACCESS

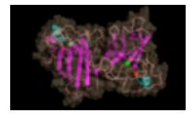
AMBER-based Portal Server for NMR structures (AMPS-NMR)

APSfNs(

Web portal for the refinement of Nuclear Magnetic Resonance (NMR) structures of macromolecules

Organisation: A Worldwide e-Infrastructure for Structural Biology
Provided by: Magnetic Resonance Center of the University of Florence - CERM, Interuniversity consortium CIRMMP, Instruct-ERIC
Scientific domain: Biological Sciences, Other Medical Sciences

Add to comparison Add to favourites



OPEN ACCESS

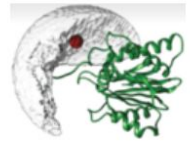
DisVis web portal

DisVis web portal

Visualisation of interaction space between two molecules

Organisation: A Worldwide e-Infrastructure for Structural Biology
Provided by: Bijvoet Centre - Utrecht University, Instruct-ERIC
Scientific domain: Biological Sciences, Other Medical Sciences

Add to comparison Add to favourites



FULLY OPEN ACCESS

FANTEN (Finding Anisotropy TENsor)

F(AT

FANTEN for the analysis of magnetic anisotropy-induced NMR data

Organisation: A Worldwide e-Infrastructure for Structural Biology
Provided by: Magnetic Resonance Center of the University of Florence - CERM, Interuniversity consortium CIRMMP, Instruct-ERIC

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https://marketplace.eosc-portal.eu/providers/eosc.wenmr

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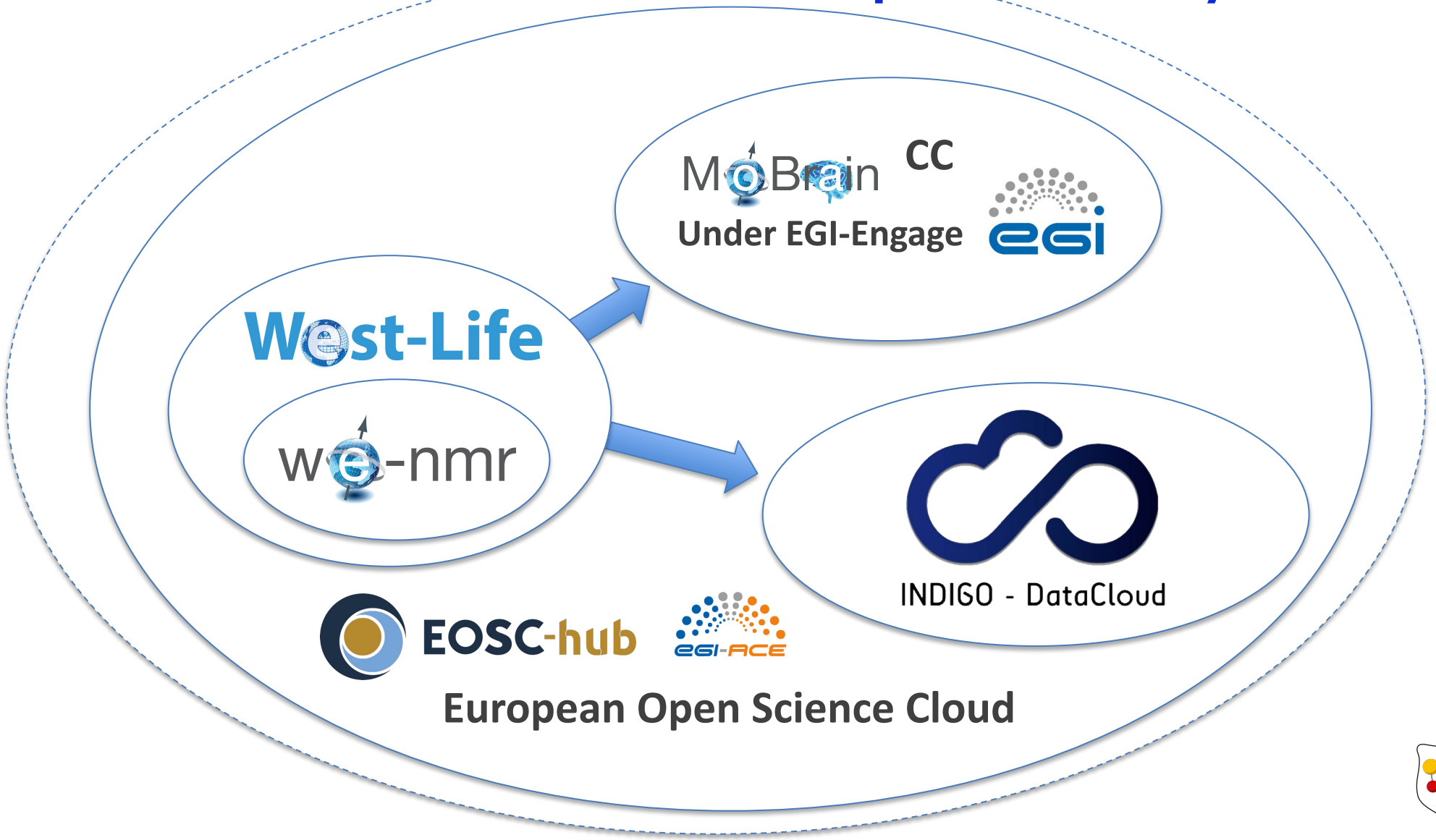
How did we get there?

The e-Infrastructure landscape over the years



instruct ERIC
EUROPEAN RESEARCH INFRASTRUCTURE CONSORTIUM

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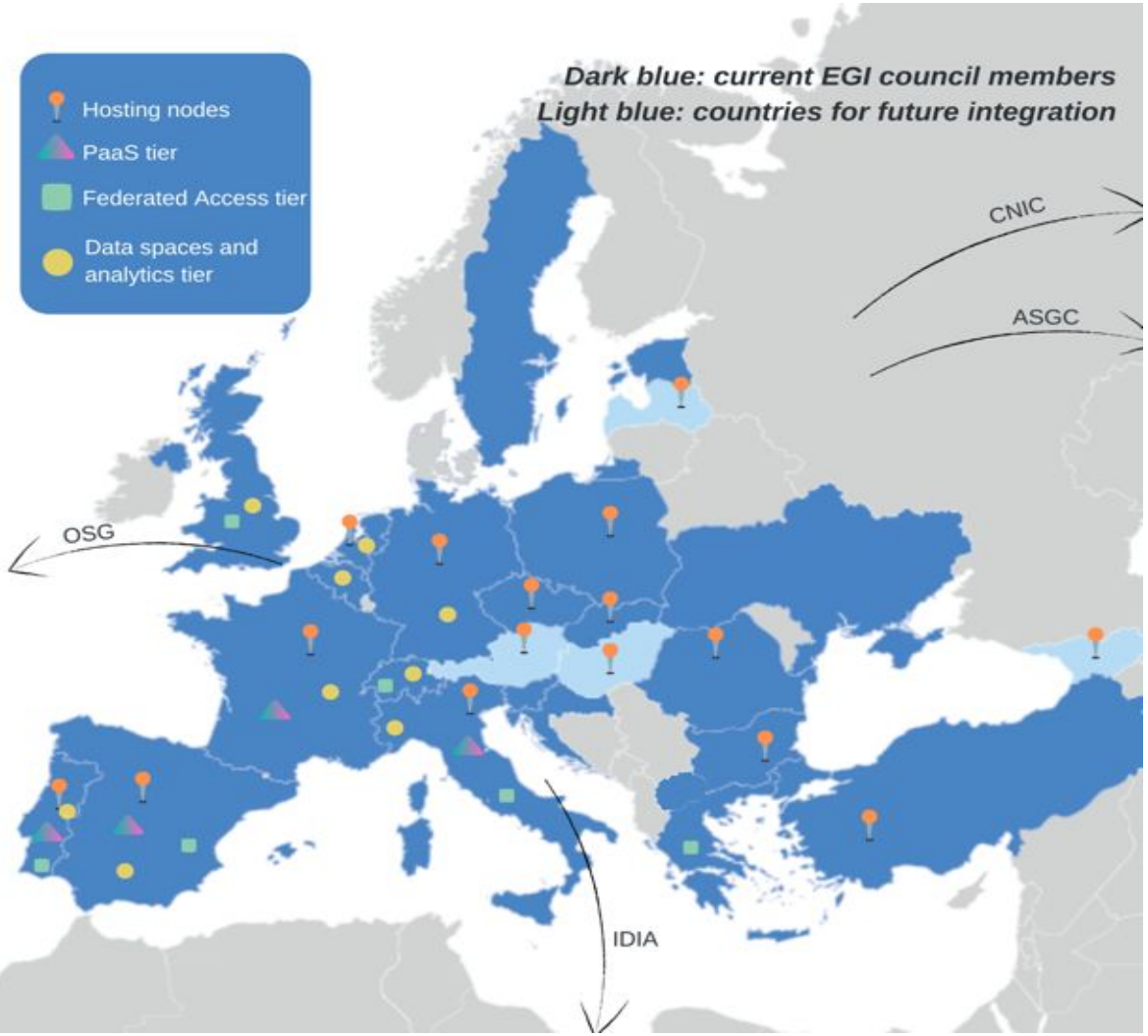
EGI-ACE Mission

Implement the **Compute Platform of the EOSC** and contribute to the **EOSC Data Commons** by delivering integrated computing, platforms, data spaces and tools as an integrated solution that is **aligned with** major European cloud federation projects and HPC initiatives.

Project Overview



EGI Advanced Computing for EOSC
Grant agreement ID: 101017567

Budget

- Total budget: € 12,009,988
- EC budget: € 8,000,000

Consortium

- Coordinator - Stichting EGI
- 33 Partners, 23 third parties

Effort

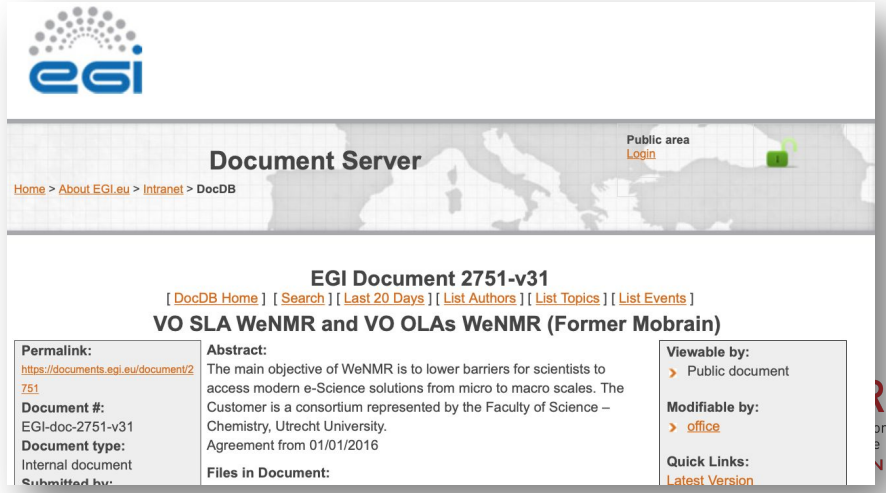
- 1472 PMs, 48 FTEs
- **49% Virtual Access** (35 services, 38 providers)

Duration

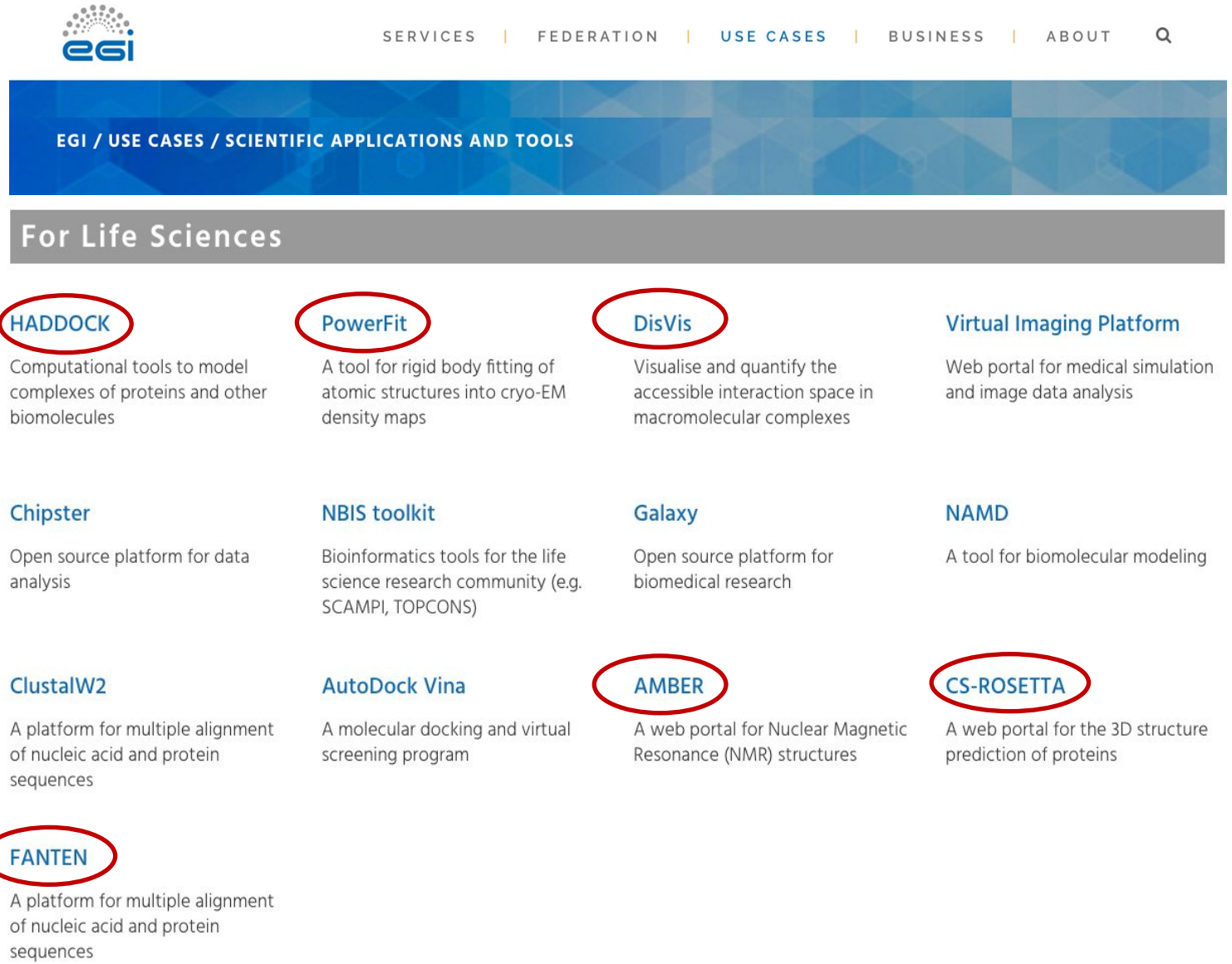
- Jan 2021 - June 2023 (30 months)

Why registering in EOSC?

- The WeNMR services have been in production since >10 years under various projects (eNMR, WeNMR, West-Life, EOSC-Hub, EGI-ACE)
- Thematic services under EOSC
- Access to resources formalized via EGI through a SLA agreement valid until 06/2023
  - 50+ million CPU hours (opportunistic access)
  - 500+ cloud CPU cores
  - ~60 TB storage



WeNMR services



SERVICES | FEDERATION | USE CASES | BUSINESS | ABOUT

EGI / USE CASES / SCIENTIFIC APPLICATIONS AND TOOLS

For Life Sciences

HADDOCK
Computational tools to model complexes of proteins and other biomolecules

PowerFit
A tool for rigid body fitting of atomic structures into cryo-EM density maps

DisVis
Visualise and quantify the accessible interaction space in macromolecular complexes

Virtual Imaging Platform
Web portal for medical simulation and image data analysis

Chipster
Open source platform for data analysis

NBIS toolkit
Bioinformatics tools for the life science research community (e.g. SCAMPI, TOPCONS)

Galaxy
Open source platform for biomedical research

NAMD
A tool for biomolecular modeling

ClustalW2
A platform for multiple alignment of nucleic acid and protein sequences

AutoDock Vina
A molecular docking and virtual screening program

AMBER
A web portal for Nuclear Magnetic Resonance (NMR) structures

CS-ROSETTA
A web portal for the 3D structure prediction of proteins

FANTEN
A platform for multiple alignment of nucleic acid and protein sequences

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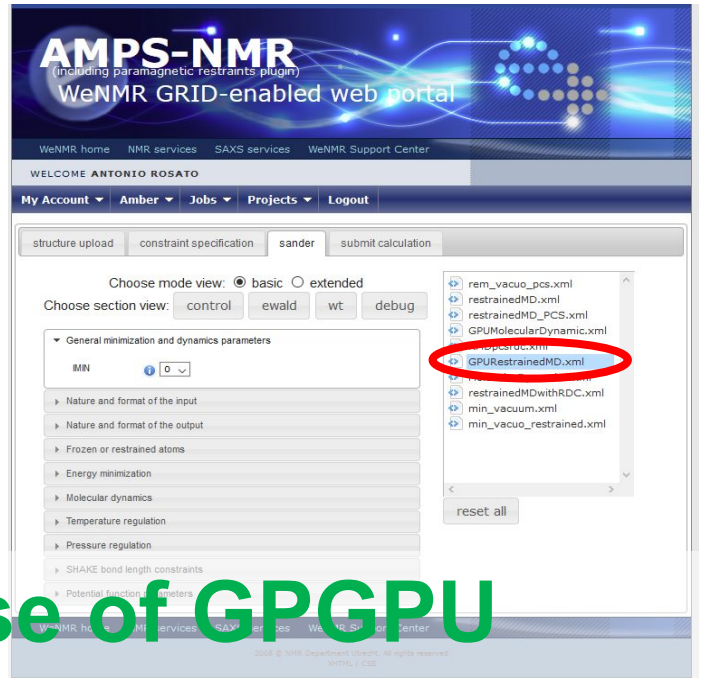
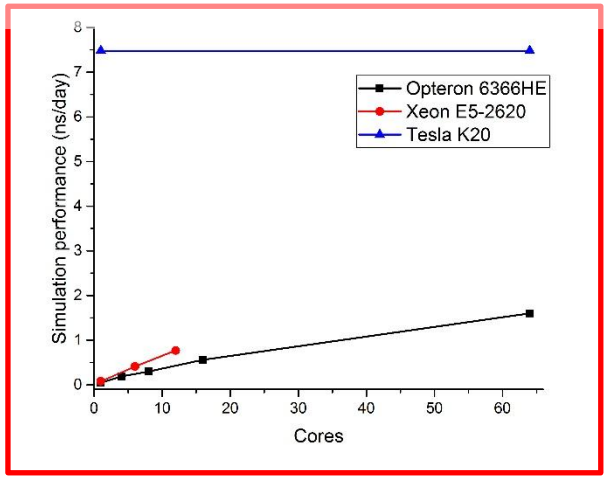
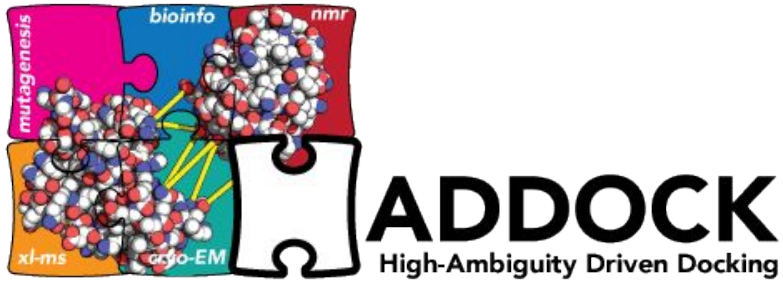
Enabling GPGPUs on the AMPS-NMR web portal for MD simulations using predefined protocols



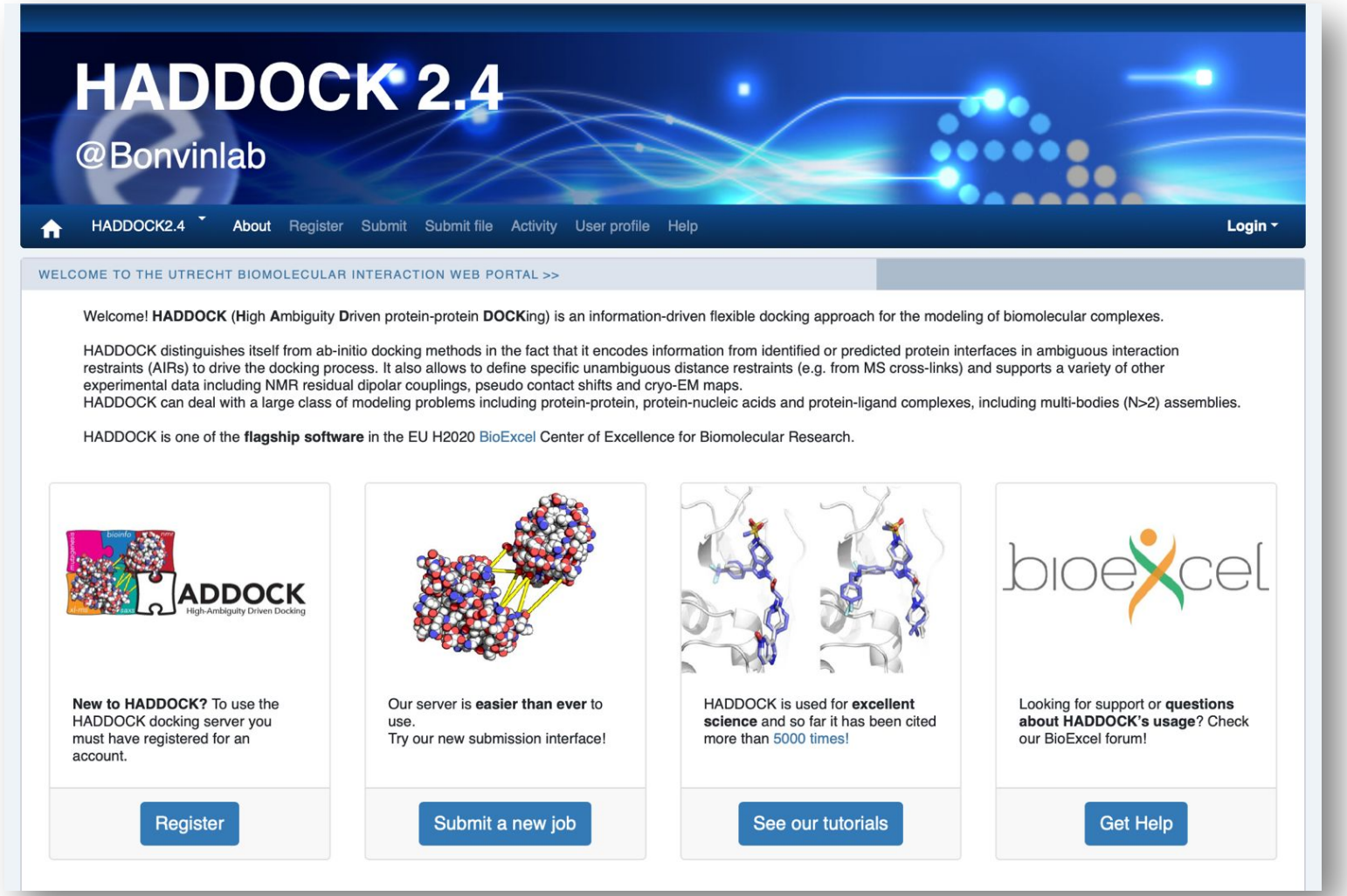
We pioneered the use of GPGPU resources in EGI



- We benchmarked calculations run on a very large protein system via the portal using different hardware configurations
- A single GPGPU card computes longer simulations (ns) per day (*wall time*)
- Energy consumption *(dynamic power)* per one ns of simulated time is about 8% of the 64 core Opteron system



- > 31500 registered users
- > 482000 served runs since June 2008
- > 60% on EOSC/EGI HTC resources (>80% for the 2.4 server!)



De Vries *et al.* Nature Prot. 2010

Van Zundert *et al.* J.Mol.Biol. 2016

https://wenmr.science.uu.nl

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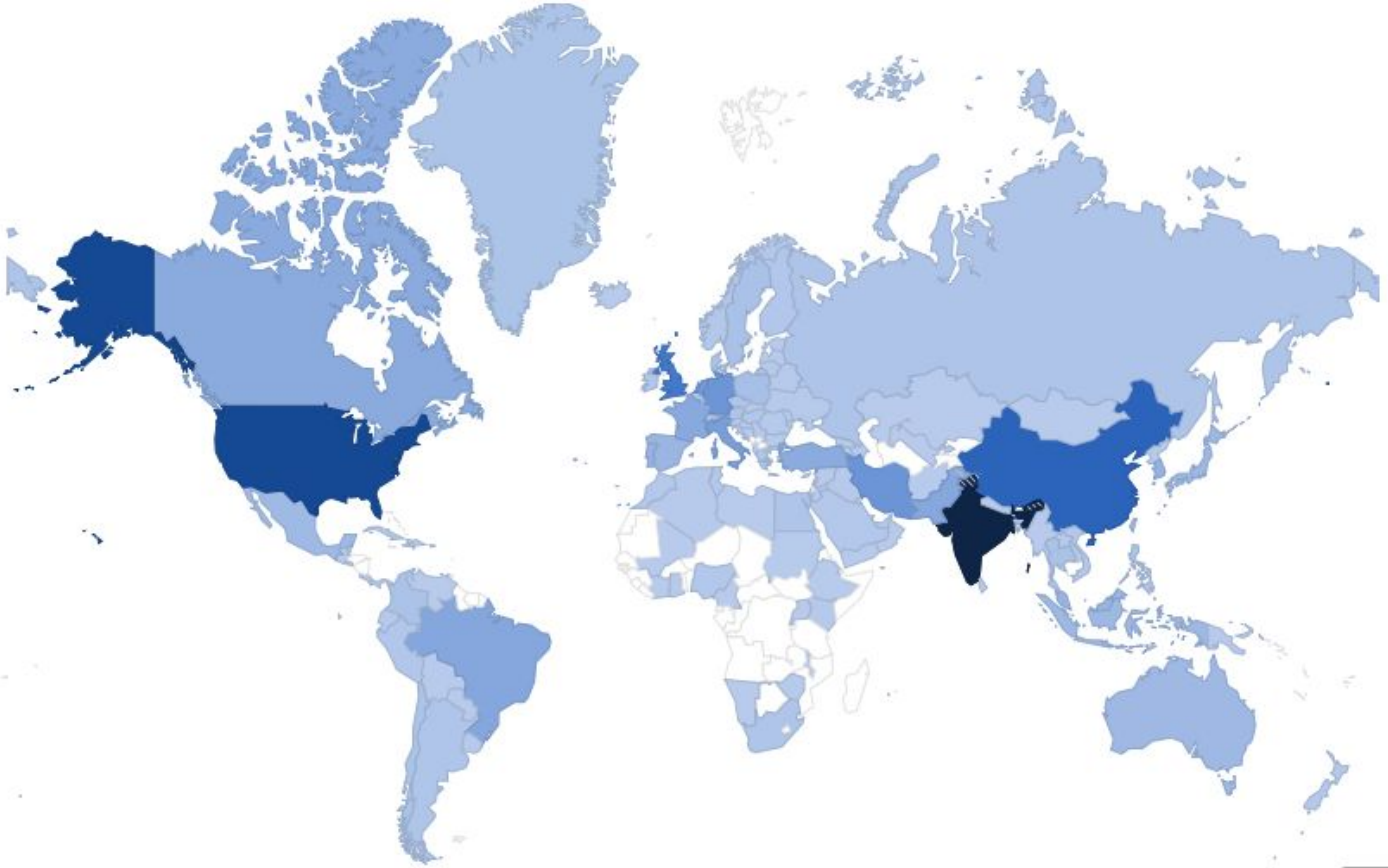
Worldwide User Map

The HADDOCK web portal is being used by **33070 users** accross **135 countries**!

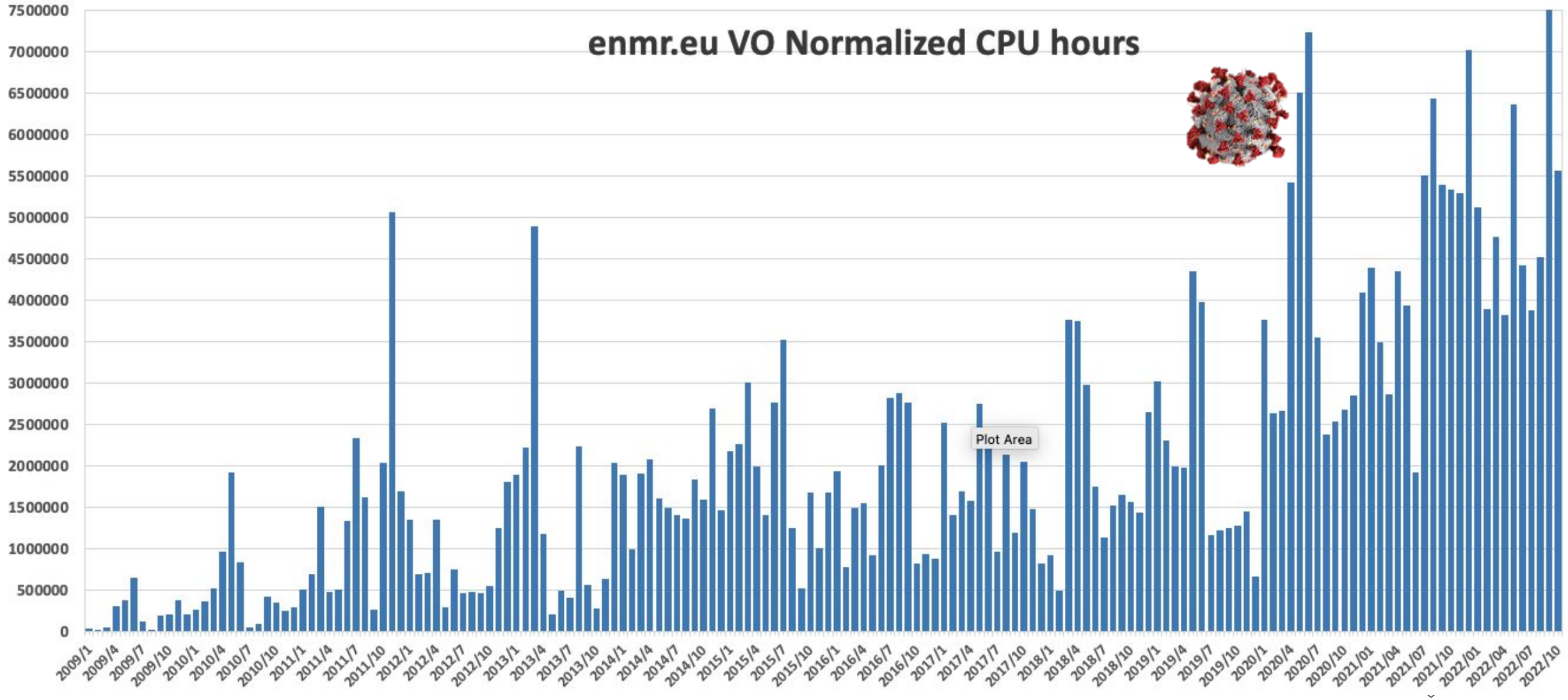


Show 50 entries

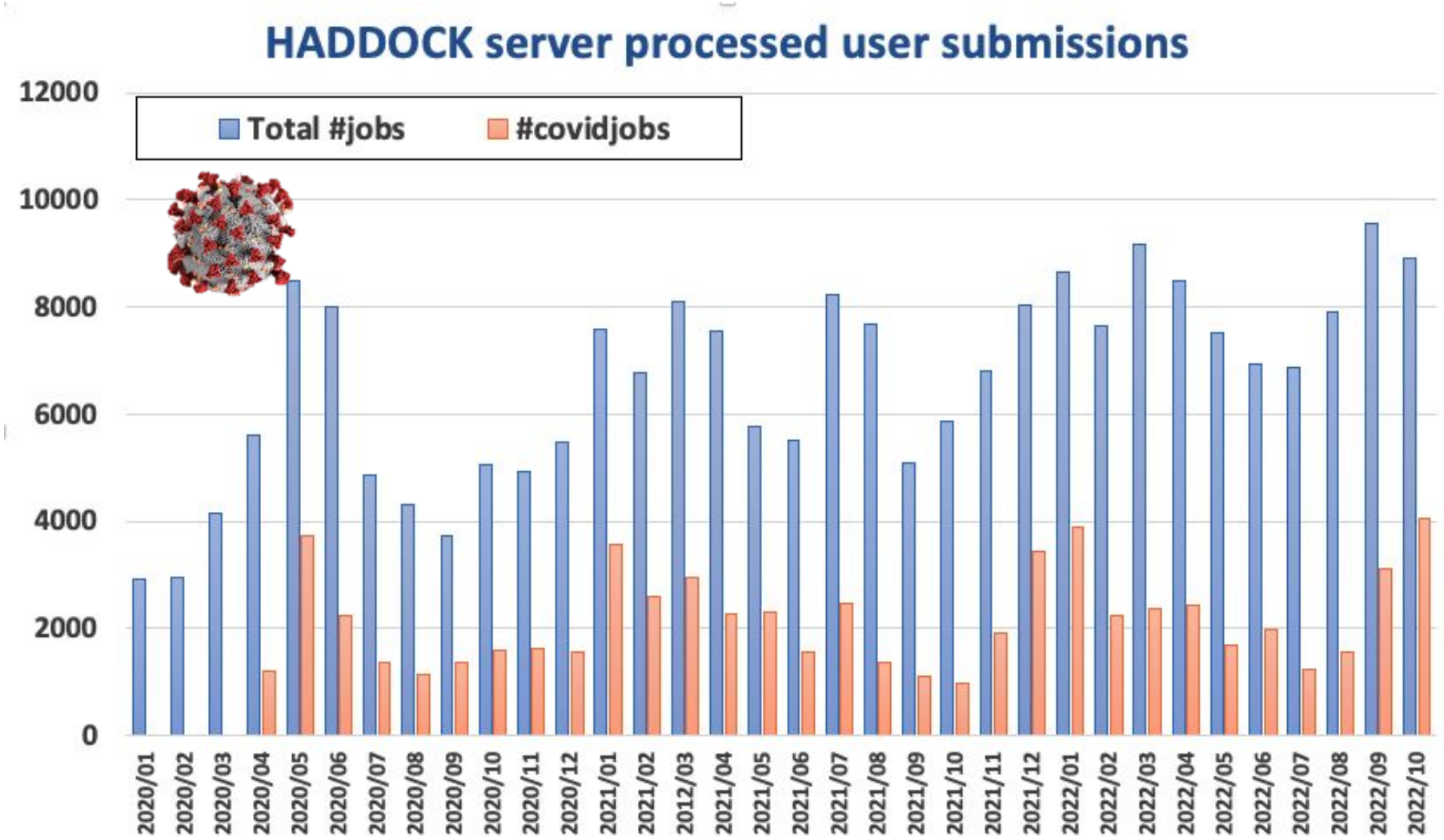
Search:

Country	Total	HADDOCK	DisVis	PowerFit	SpotON
Worldwide	33070	31476	5615	4628	5215
India	6619	6363	1164	1049	1153
Europe	6607	6255	1079	763	889
United States	4477	4275	720	540	640
China	2683	2499	509	460	498

Impact: Resources usage



Impact: User submissions



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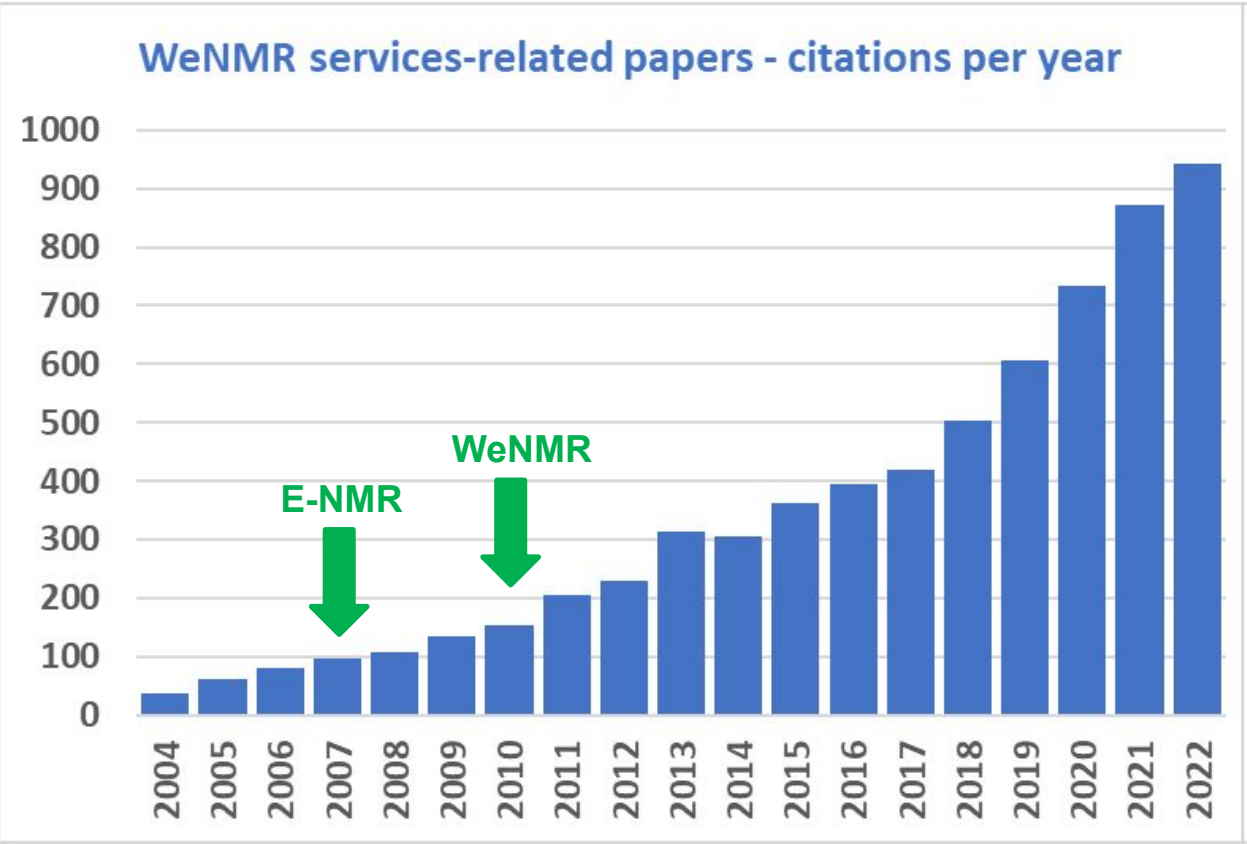
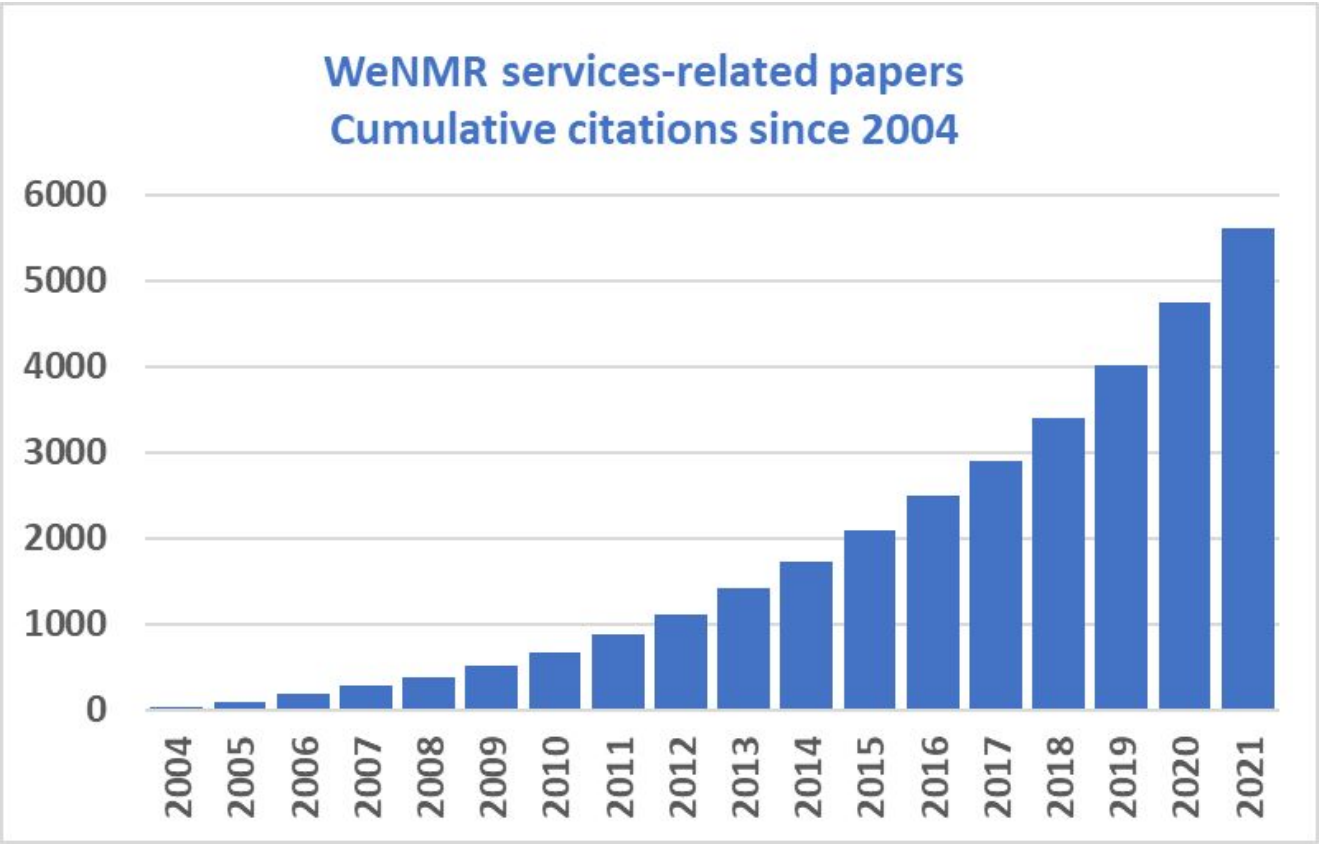
Impact: Citations of resources





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In summary

- A long history of providing services to a worldwide user community
- A long history of using EU e-Infrastructure (HTC)
- WeNMR well-established thematic service provider
- Natural transition into EOSC
- Main benefits:
  - Ensuring access to computational resources
  - Strong network that helps sustainability (e.g. via EU projects)

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Acknowledgments

- The core WeNMR team
  - Alexandre Bonvin (U. Utrecht)
  - Marco Verlato (INFN Padua)

- The Florence team
  - Andrea Giachetti
  - Enrico Morelli
  - Vincenzo Laveglia
  - Lucio Ferella
  - Ivano Bertini†

CIRMMP FIRENZE

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