

Pan-European digital assets supporting research communities

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

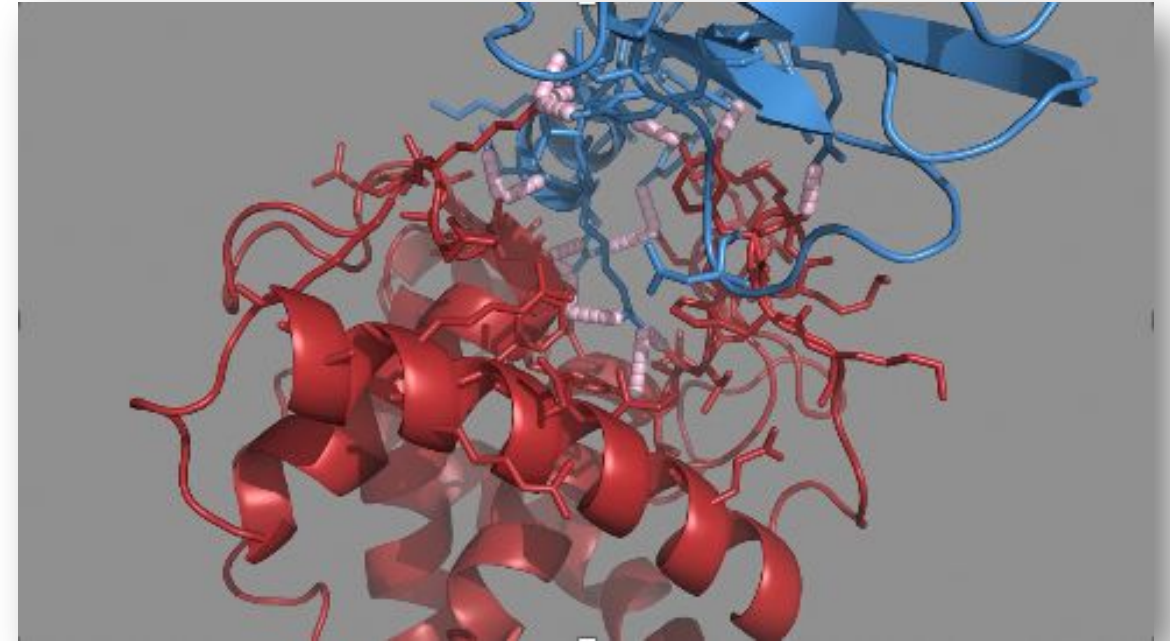
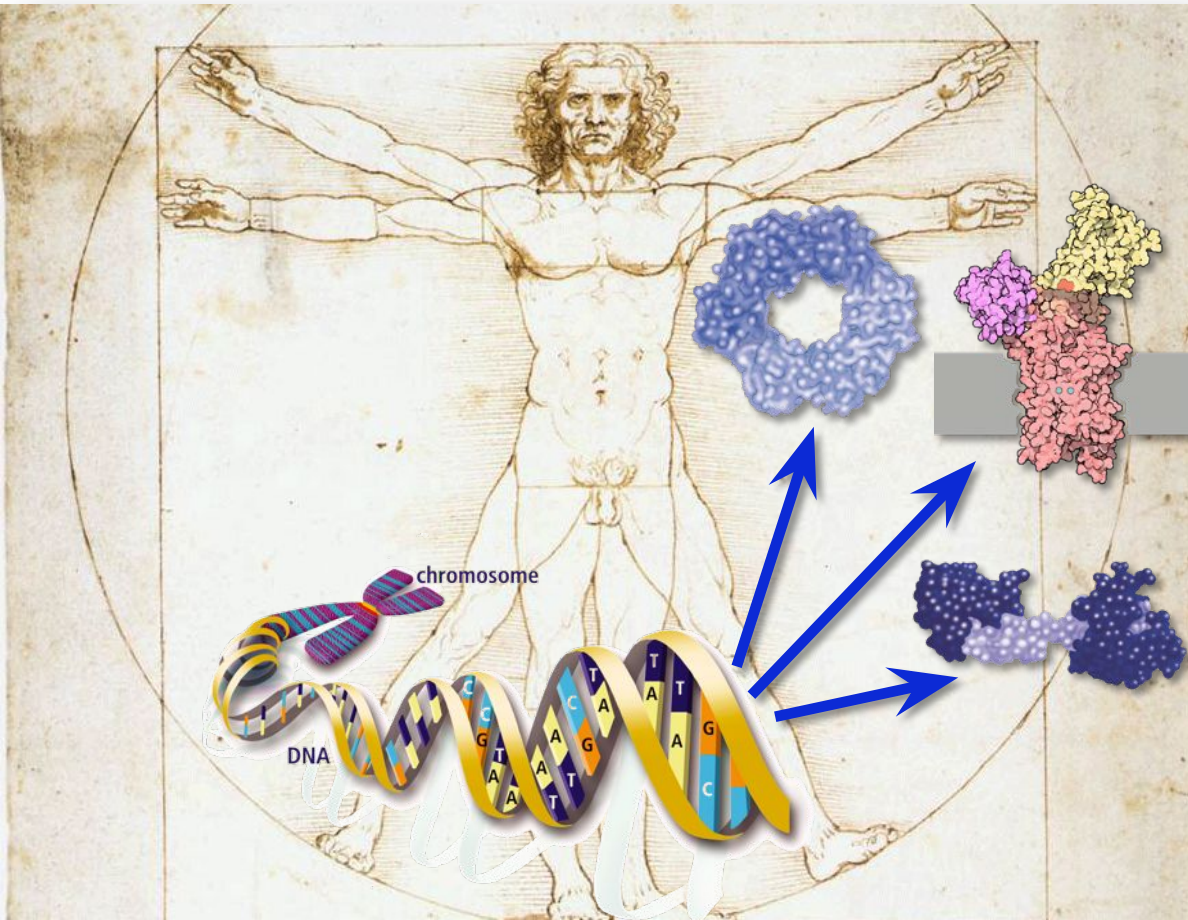
Antonio Rosato (University of Florence)

antonio.rosato@unifi.it



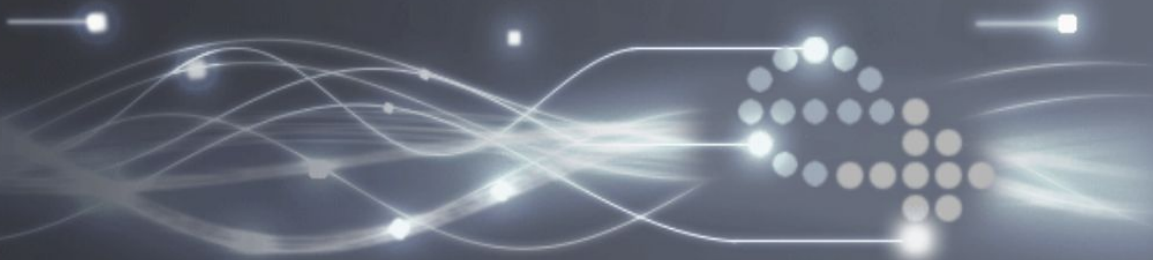
Domain: life sciences / structural biology

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



*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

WeNMR & EOSC



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

FILTERS

Research steps

Find or choose from the list below

<input type="checkbox"/> Process and Analyse	5
<input type="checkbox"/> Access Research Infrastructures	1
<input type="checkbox"/> Access Training Material	1
<input type="checkbox"/> Access Computing and Storage	0
Resources	
<input type="checkbox"/> Discover Research Outputs	0

Show 4 more

Scientific Domains

Find or choose from the list below

<input type="checkbox"/> Natural Sciences	7
<input type="checkbox"/> Biological Sciences	7
<input type="checkbox"/> Chemical Sciences	0
<input type="checkbox"/> Computer & Information Sciences	0
<input type="checkbox"/> Earth & Related Environmental Sciences	0
<input type="checkbox"/> Mathematics	0
<input type="checkbox"/> Other Natural Sciences	0

Providers > A Worldwide e-Inf



ABOUT

DETAILS

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

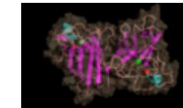
APSFNs(

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

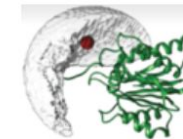
DisVis web portal

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

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

FULLY OPEN ACCESS



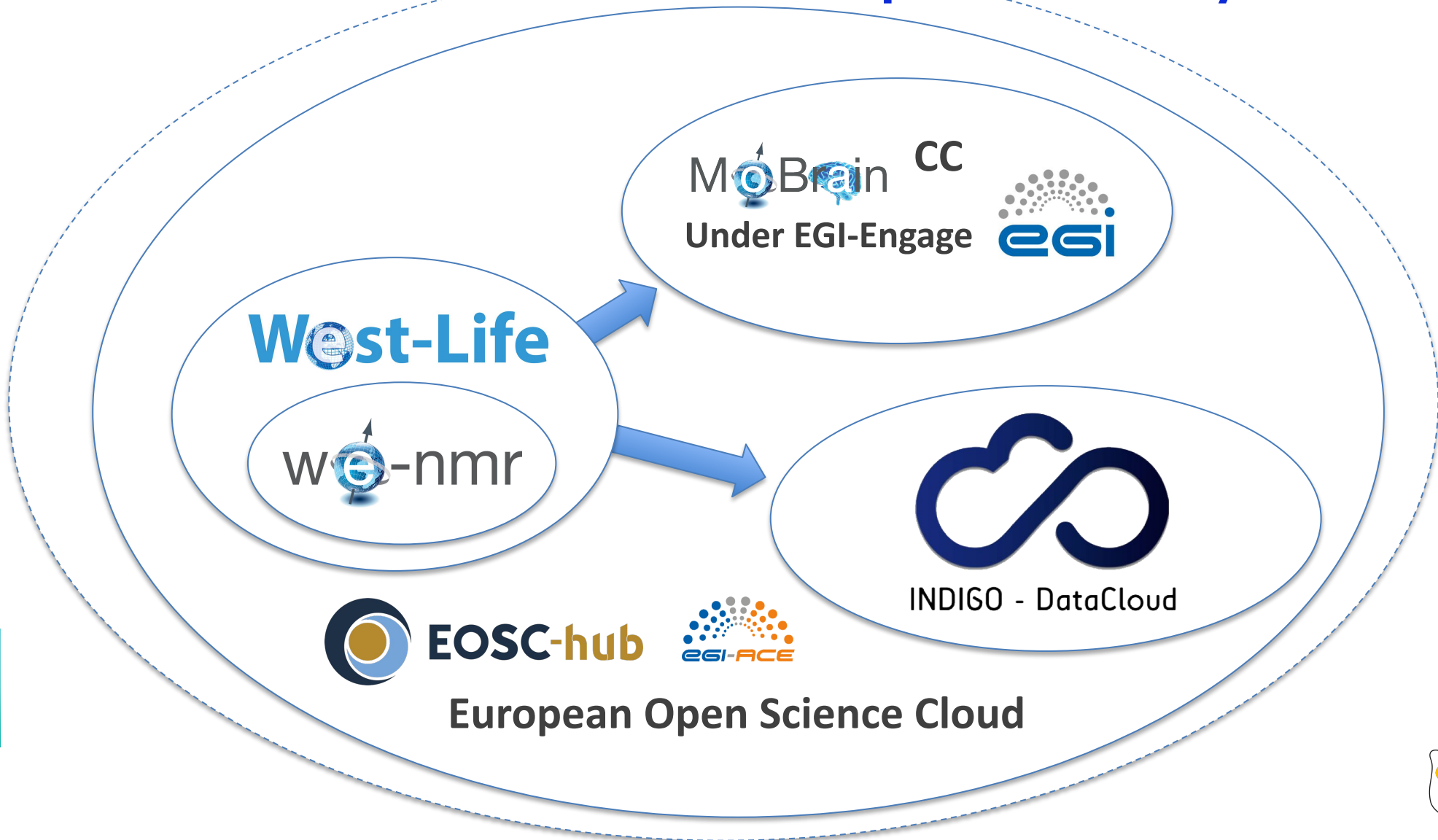
marketplace



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

How did we get there?

The e-Infrastructure landscape over the years

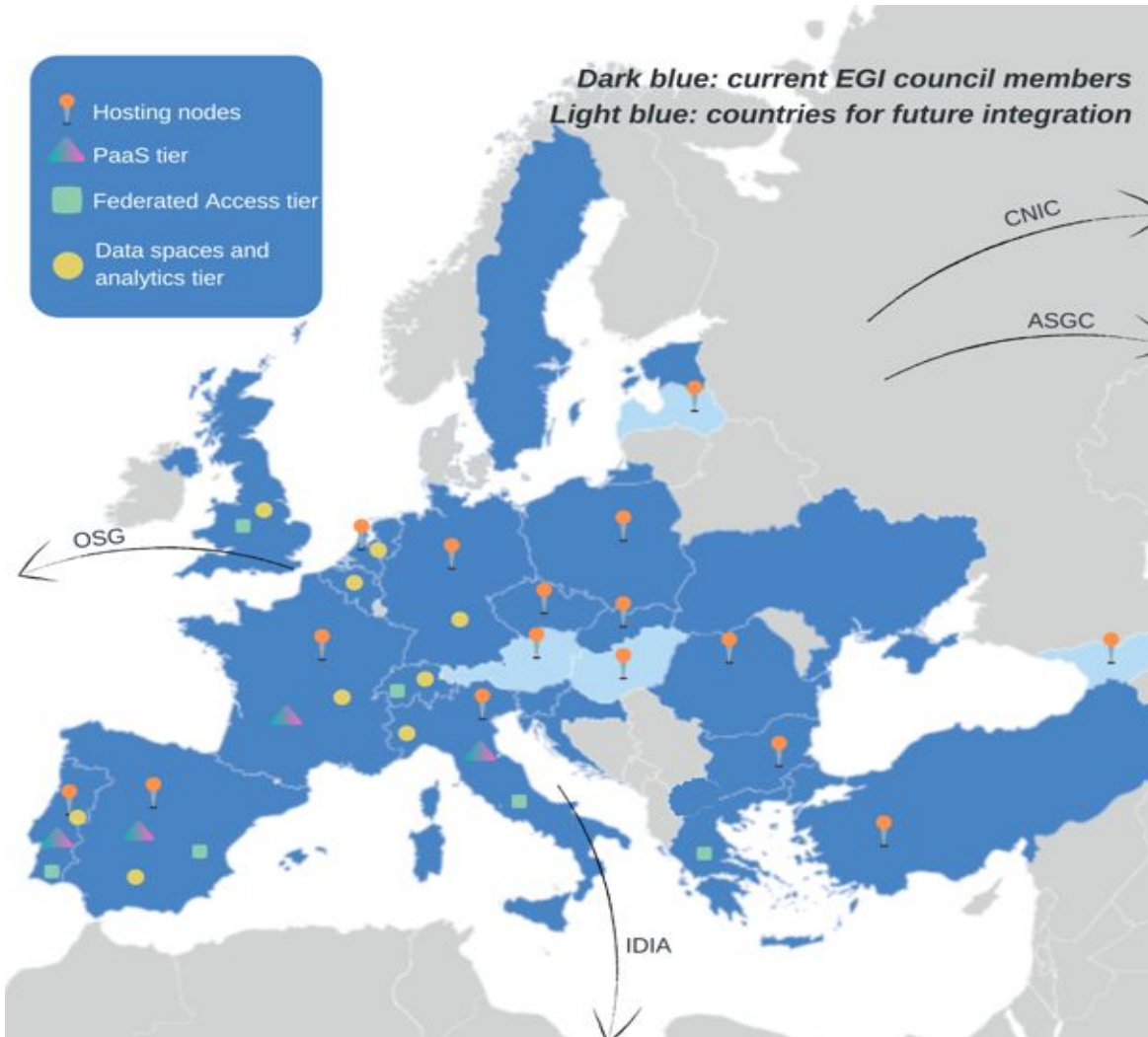


EGI-ACE Mission



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

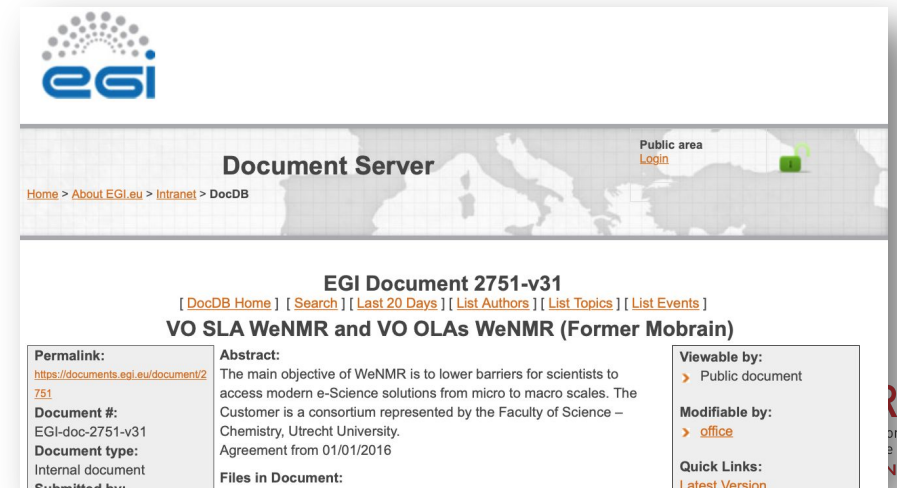
- 1472 PMs, 48 FTEs
- **49% Virtual Access** (35 services, 38 providers)

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



The screenshot displays the EGI Document Server interface. At the top left is the EGI logo. The main header reads "Document Server" with a "Public area Login" link on the right. Below the header is a breadcrumb trail: "Home > About EGI.eu > Intranet > DocDB". The main content area features the title "EGI Document 2751-v31" and a list of navigation links: "[DocDB Home] [Search] [Last 20 Days] [List Authors] [List Topics] [List Events]". Below this is the document title "VO SLA WeNMR and VO OLAs WeNMR (Former Mobraint)". A table-like structure provides document metadata:

Permalink: https://documents.egi.eu/document/2751	Abstract: The main objective of WeNMR is to lower barriers for scientists to access modern e-Science solutions from micro to macro scales. The Customer is a consortium represented by the Faculty of Science – Chemistry, Utrecht University. Agreement from 01/01/2016	Viewable by: > Public document
Document #: EGI-doc-2751-v31	Files in Document:	Modifiable by: > office
Document type: Internal document		Quick Links: Latest Version
Submitted by:		

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

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

AMPS-NMR
(including paramagnetic restraints plugin)
WeNMR GRID-enabled web portal

WELCOME TO AMPS-NMR WEB PORTAL

AMBER-BASED PORTAL SERVER FOR NMR STRUCTURES (AMPS-NMR)

Amber (acronym to Assisted Model Building with Energy Refinement) is a suite of programs that allow users to perform molecular dynamics (MD) simulations on biological systems. This web portal makes available the entire functionality of AMBER, in particular (but not only) using NMR-derived information as restraints for MD.

To use AMPS-NMR you have to register on the NMR services website.

You can access a trial version of the service using username *guest* and password *guest*.

NB: the trial version is available only for NMR services.

we-nmr
West-Life
e-infrastructure

Access to AMPS-NMR:

Username:

Password:

RedirectIAM

AMPS-NMR
(including paramagnetic restraints plugin)
WeNMR GRID-enabled web portal

WELCOME ANTONIO ROSATO

My Account Amber Jobs Projects Logout

structure upload constraint specification sander submit calculation

Choose mode view: basic extended

Choose section view: control ewald wt debug

General minimization and dynamics parameters

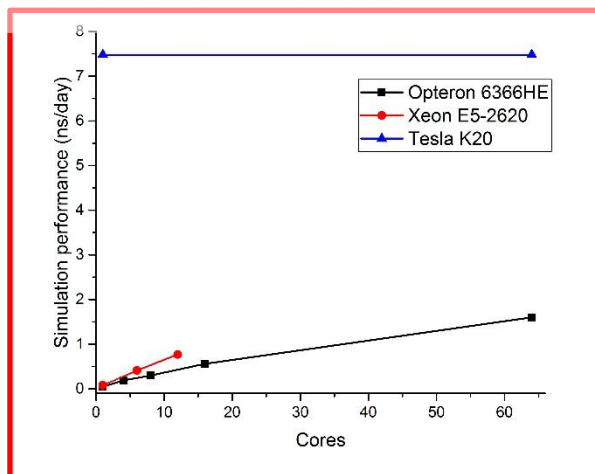
MIN

- Nature and format of the input
- Nature and format of the output
- Frozen or restrained atoms
- Energy minimization
- Molecular dynamics
- Temperature regulation
- Pressure regulation
- SHAKE bond length constraints
- Potential function parameters

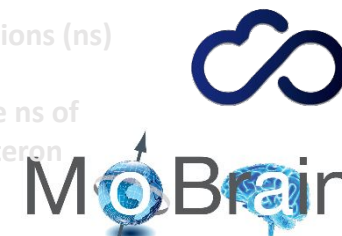
- rem_vacuo_pcs.xml
- restrainedMD.xml
- restrainedMD_PCS.xml
- GPUrestrainedMD.xml
- GPUrestrainedMD.xml
- GPUrestrainedMD.xml
- restrainedMDwithRDC.xml
- min_vacuum.xml
- min_vacuo_restrained.xml

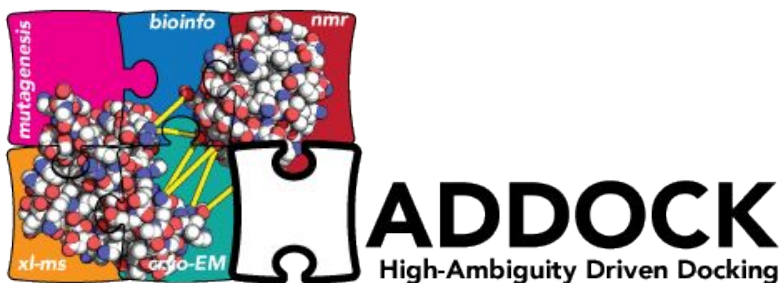
reset all

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

HADDOCK 2.4
@Bonvinlab


WELCOME TO THE UTRECHT BIOMOLECULAR INTERACTION WEB PORTAL >>

Welcome! **HADDOCK** (High Ambiguity Driven protein-protein **DOCK**ing) is an information-driven flexible docking approach for the modeling of biomolecular complexes.

HADDOCK distinguishes itself from ab-initio docking methods in the fact that it encodes information from identified or predicted protein interfaces in ambiguous interaction restraints (AIRs) to drive the docking process. It also allows to define specific unambiguous distance restraints (e.g. from MS cross-links) and supports a variety of other experimental data including NMR residual dipolar couplings, pseudo contact shifts and cryo-EM maps.

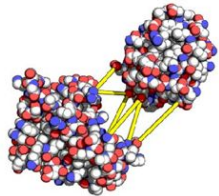
HADDOCK can deal with a large class of modeling problems including protein-protein, protein-nucleic acids and protein-ligand complexes, including multi-bodies (N>2) assemblies.

HADDOCK is one of the **flagship software** in the EU H2020 **BioExcel** Center of Excellence for Biomolecular Research.



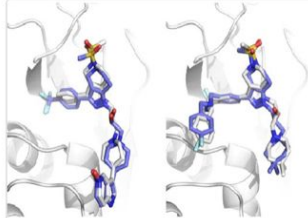
New to HADDOCK? To use the HADDOCK docking server you must have registered for an account.

[Register](#)




Our server is **easier than ever** to use.
Try our new submission interface!

[Submit a new job](#)



HADDOCK is used for **excellent science** and so far it has been cited more than **5000 times!**

[See our tutorials](#)



Looking for support or **questions about HADDOCK's usage?** Check our BioExcel forum!

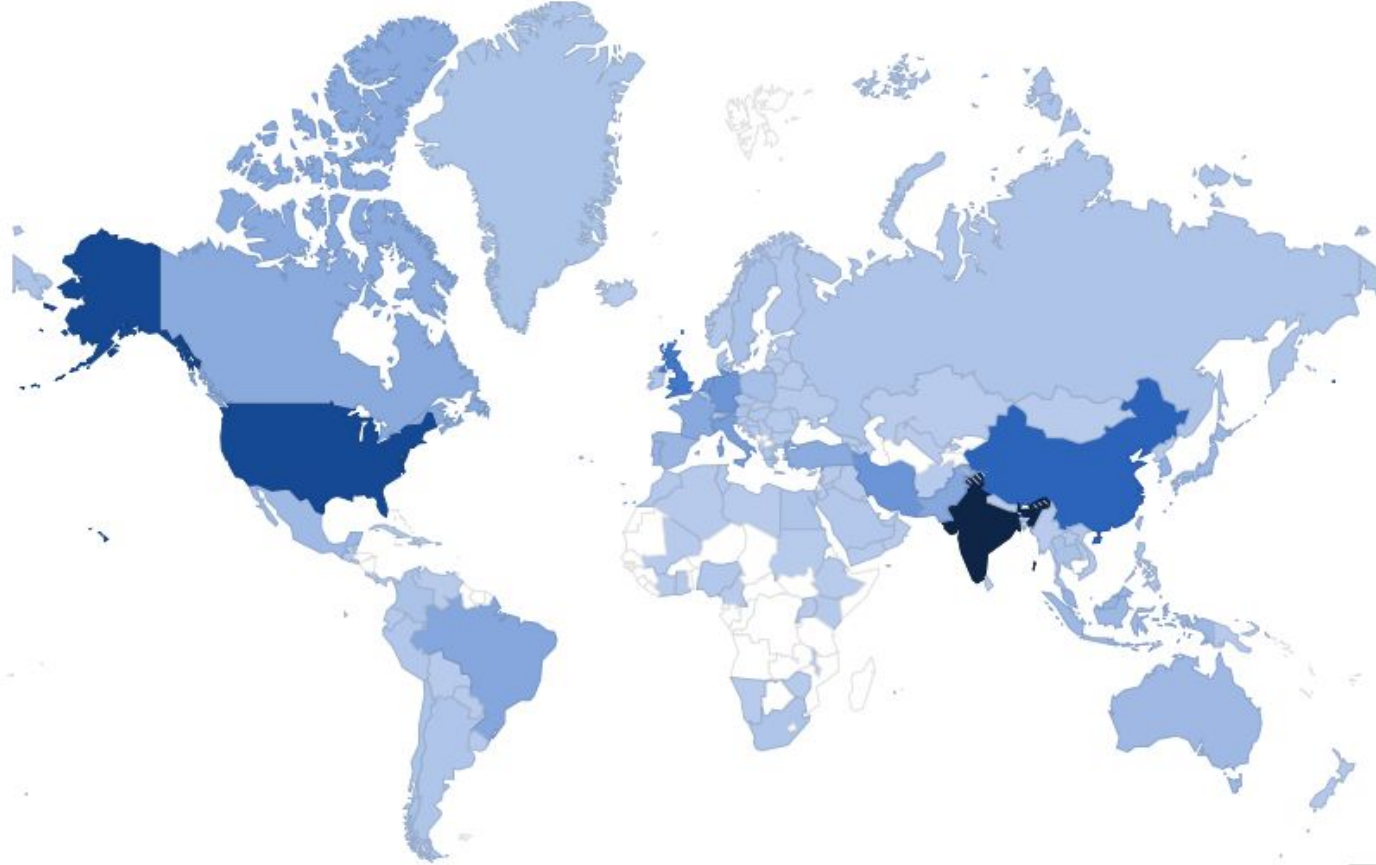
[Get Help](#)

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



Worldwide User Map

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

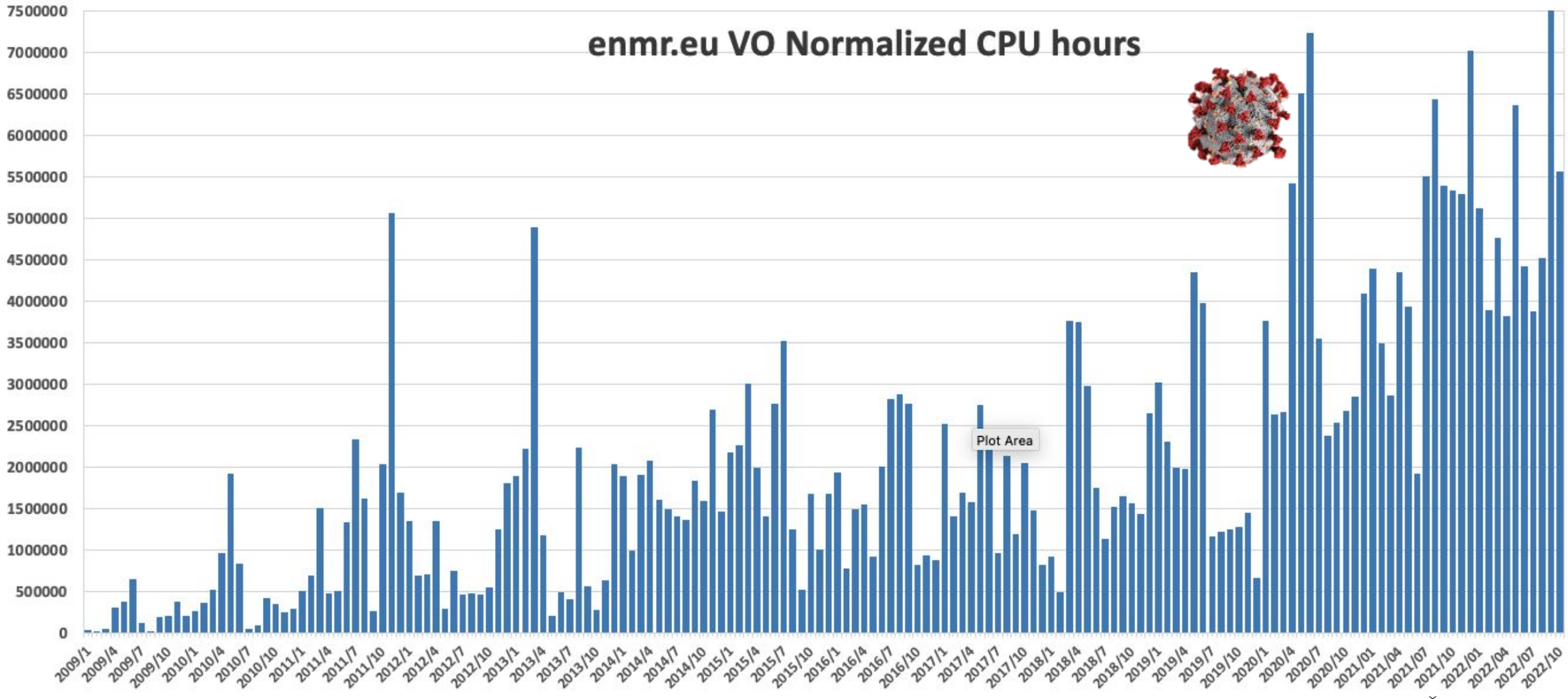


Show entries

Search:

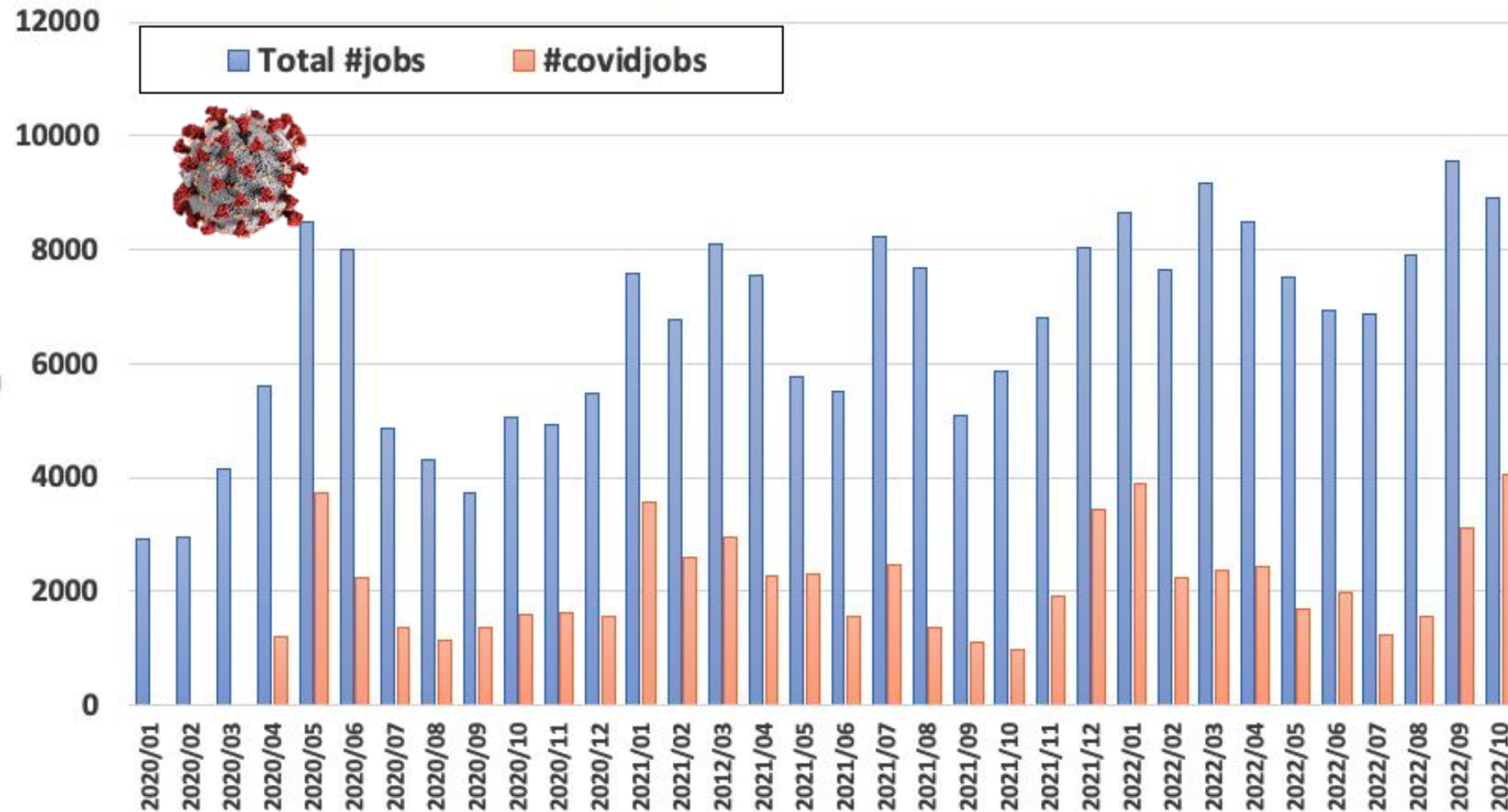
Country	Total	HADDOCK	DisVis	PowerFit	SpotON
Worldwide	33070	31476	5615	4628	5215
India	6619	6363	1164	1049	1153
Europe	6607	6255	1079	763	889
United States	4477	4275	720	540	640
China	2683	2499	509	460	498

Impact: Resources usage



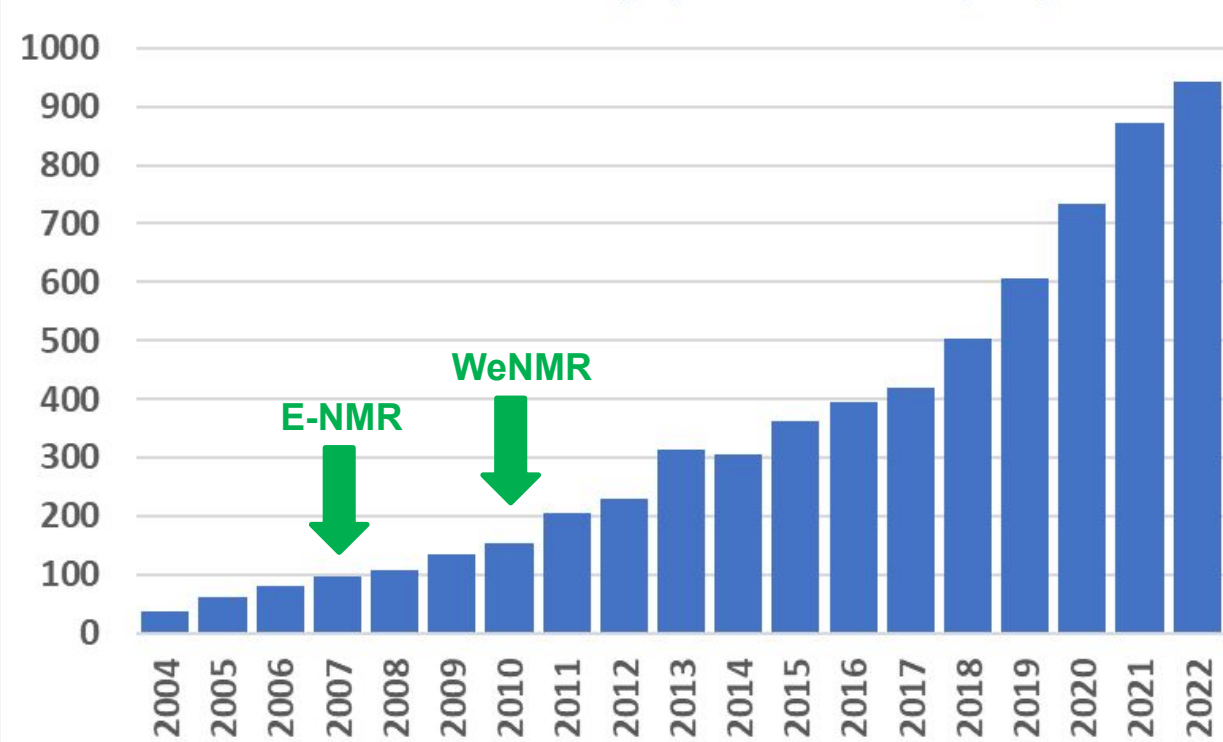
Impact: User submissions

HADDOCK server processed user submissions

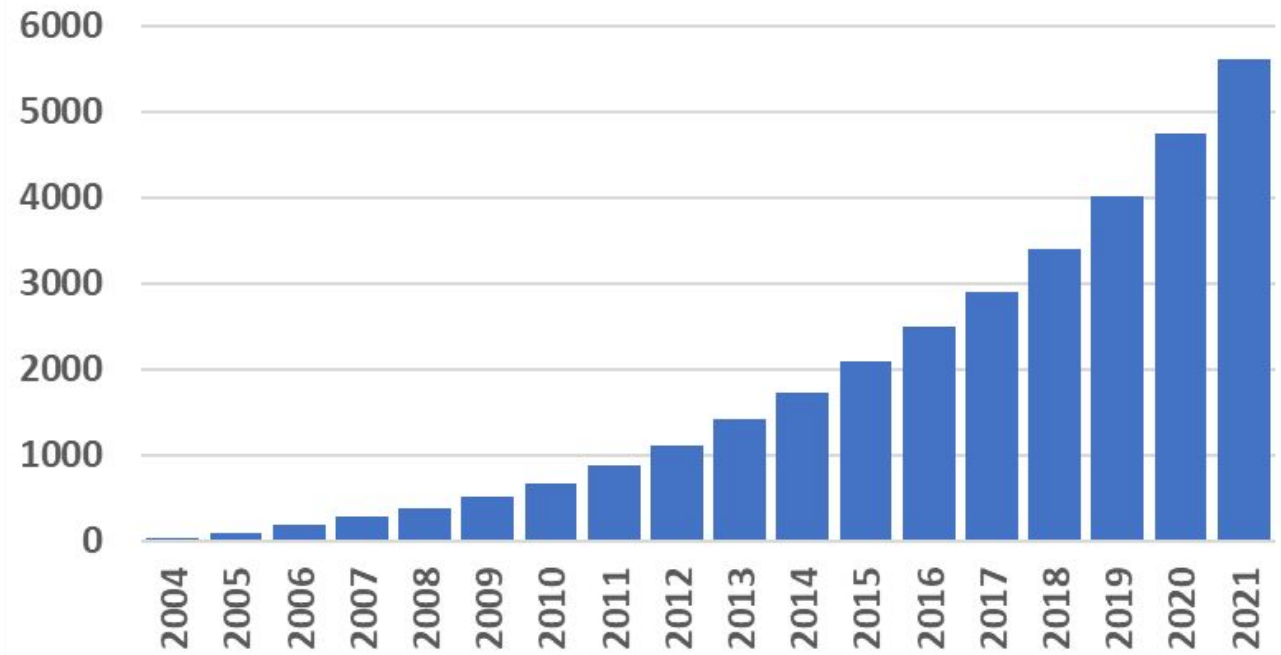


Impact: Citations of resources

WeNMR services-related papers - citations per year



WeNMR services-related papers
Cumulative citations since 2004



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)

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†

