

Structural Biology in the Clouds: The HADDOCK/WeNMR-EOSC Ecosystem

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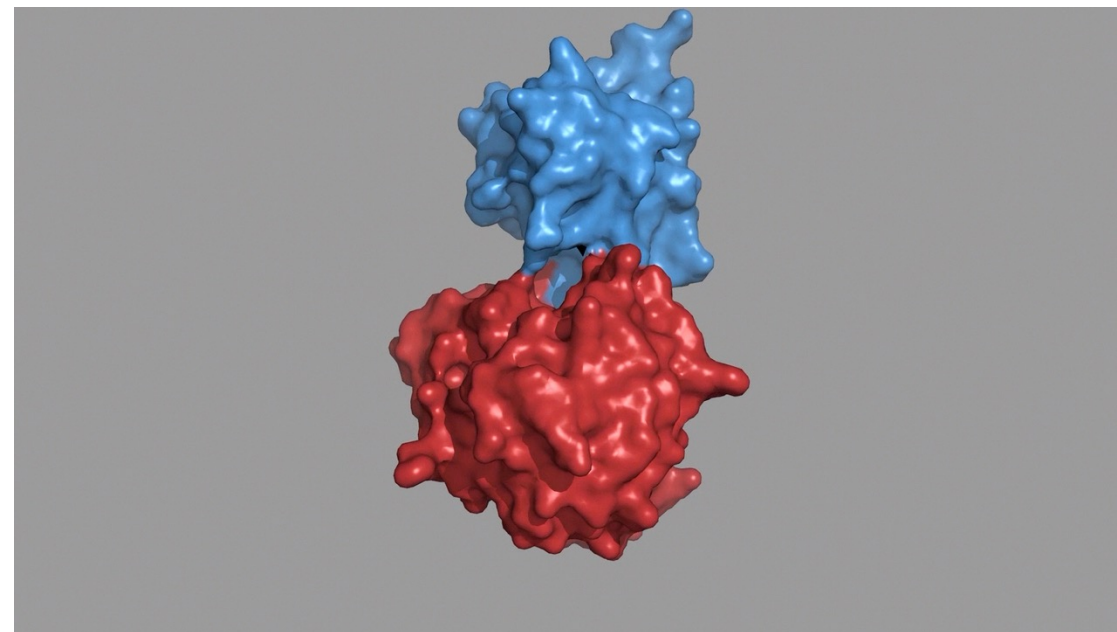
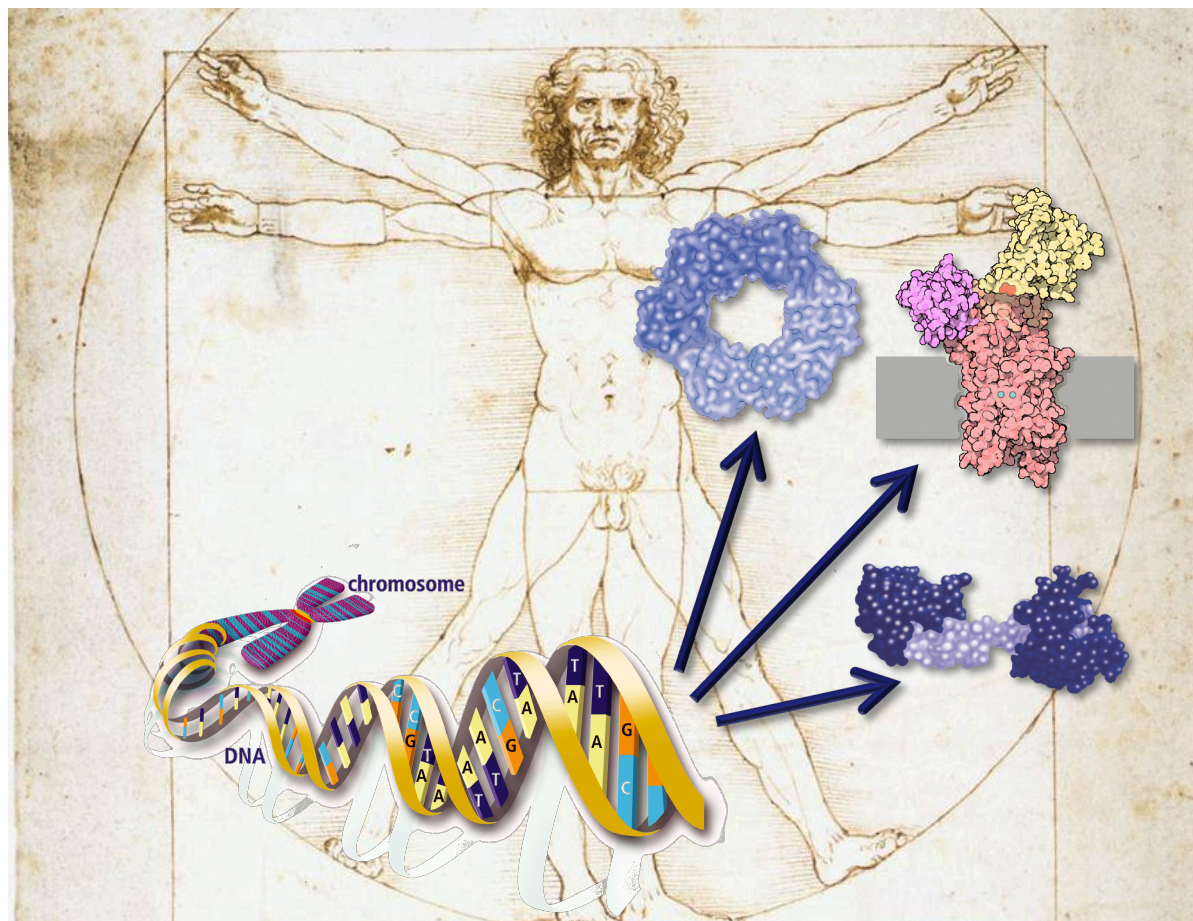
The Netherlands

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 [@br_jimenez](https://twitter.com/br_jimenez)

- Domain and background of the scientific community
- Community and Impact
- Challenges and solutions
- Supporting COVID-19 research
- Future perspectives

Understanding life at the 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



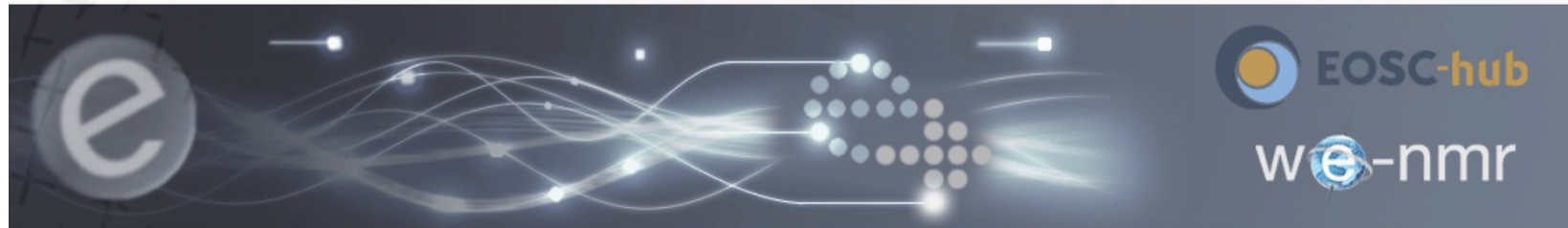
Virtual Research Community

>11 years of serving this research community

**Made possible via HTC resources provided by
FP7 and H2020 e-Infrastructure projects over
the years**

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



HADDOCK 2.4
@Bonvinlab


WELCOME TO THE UTRECHT BIOMOLECULAR INTERACTION WEB PORTAL >>>

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

HADDOCK distinguishes itself from ab-initio docking methods in the fact that it encodes in its protein interfaces in ambiguous interaction restraints (AIRs) to drive the docking process using unambiguous distance restraints (e.g. from MS cross-links) and supports a variety of other restraints including residual dipolar couplings, pseudo contact shifts and cryo-EM maps. HADDOCK can deal with a large class of modeling problems including protein-protein, protein-ligand, and protein-nucleic acid complexes, including multi-bodies (N>2) assemblies.

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

Login via [learn more ...](#)

 [Check-In](#)

OR

Email or User Name

Password

Login ☐ Keep me logged in

New user? [Register](#)

Forgot your password? [Reset](#)

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](#)

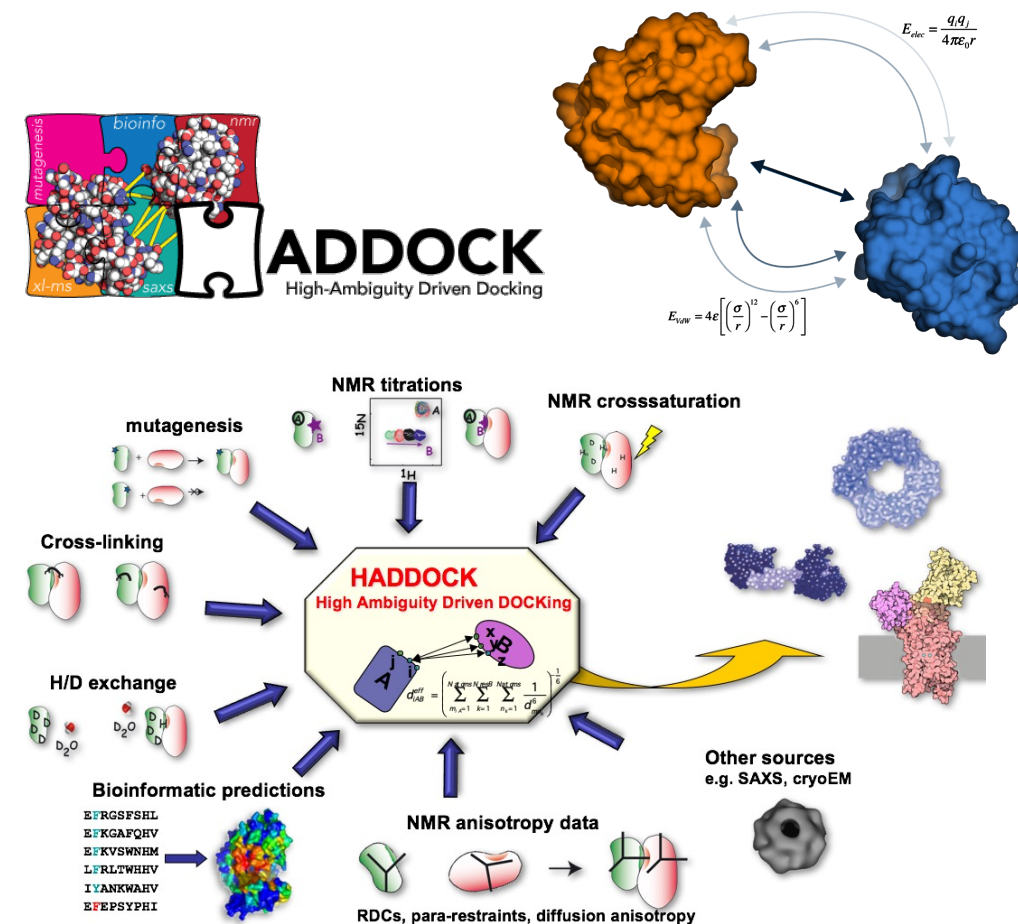
HADDOCK is used for **excellent science** and so far it has been cited more than 5000 times!

[See our tutorials](#)

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

[Get Help](#)

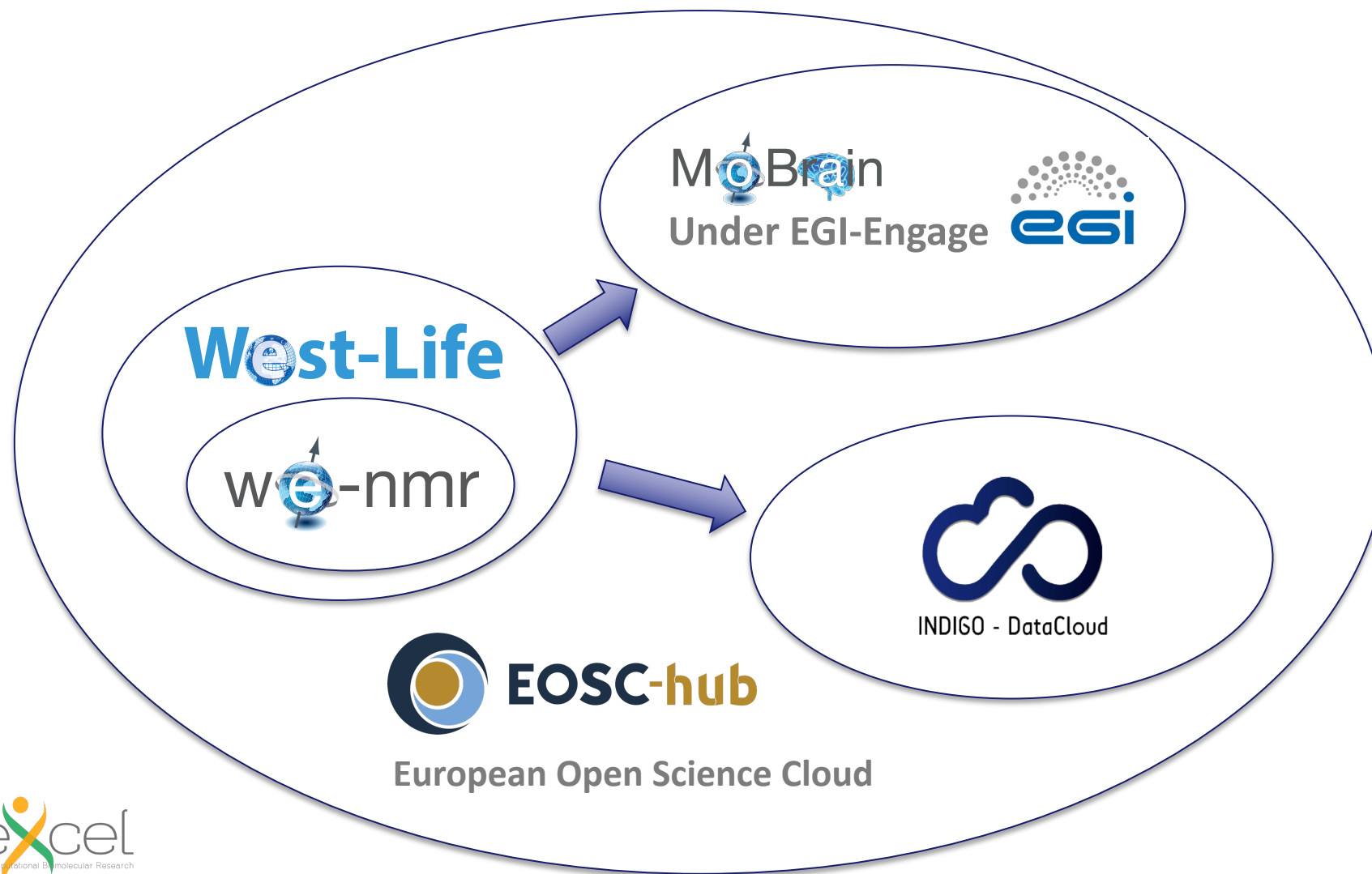
<https://wenmr.science.uu.nl/haddock2.4/>



Dominguez, Boelens & Bonvin. JACS 125, 173 (2003).

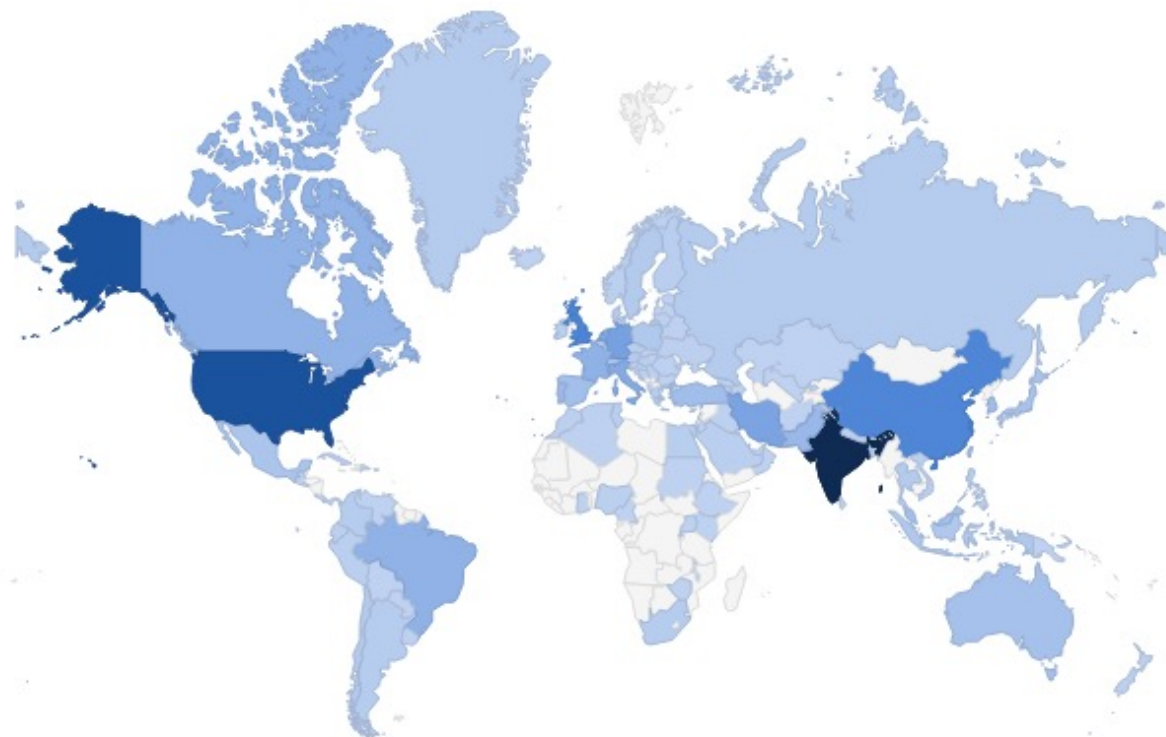
De Vries *et al.* Nature Prot. 2010

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

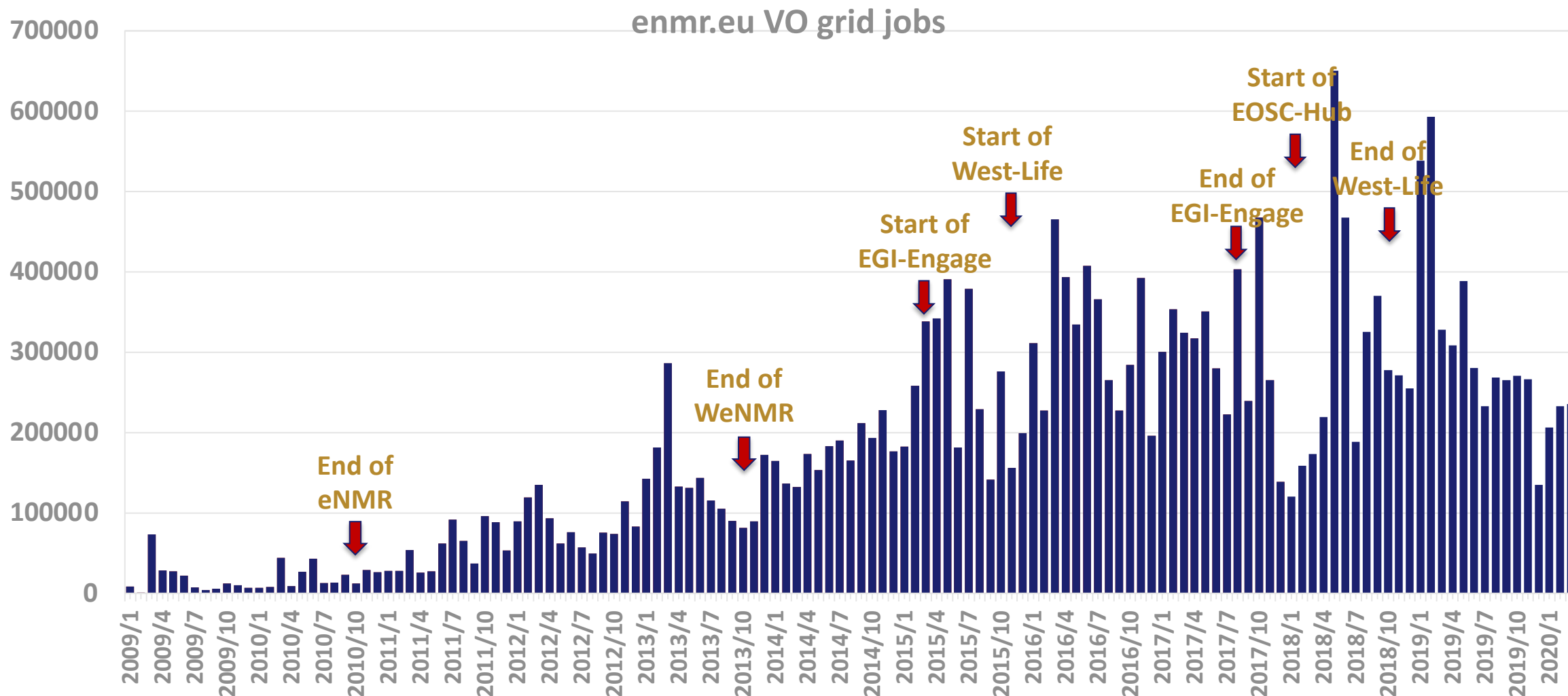


- ~ 22,000 registered users
- > 120 countries reached
- Both researchers and students
- Sustained growth of the community

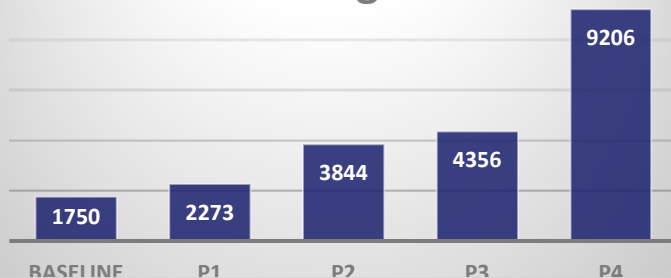
https://wenmr.science.uu.nl/user_map



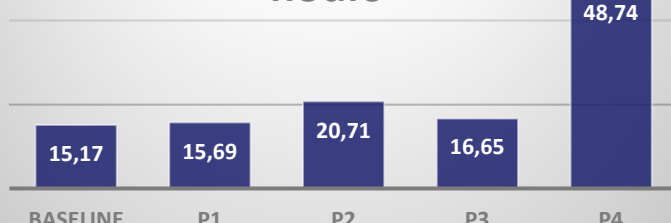
	Country	All_Users ▼	HADDOCK	DISVIS	POWERFIT	SPOTON
1	Total Users	21,924	21,126	3,073	2,445	2,803
2	EU Users	4,589	4,345	652	456	510
3	India	4,549	4,445	605	532	601
4	United States	3,174	3,054	421	298	371
5	United Kingdom	1,327	1,272	148	124	127



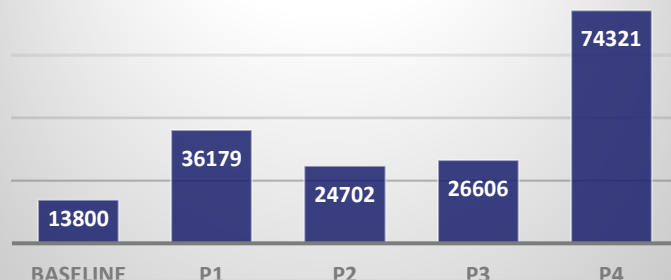
new user registrations



HS06 CPU wall time in million hours

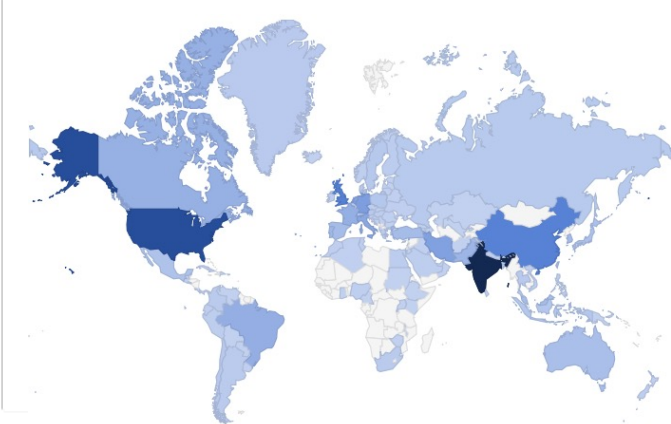


user submissions

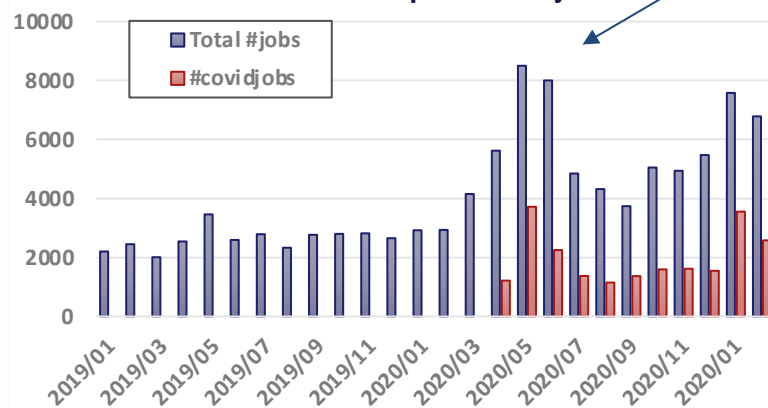


- Steady increase in number of users over the duration of the project
- Worldwide impact
- Relevance of the WeNMR services for COVID-related research made clear by the huge increase in usage over the last period
- ~80% of submissions run on EOSC HTC resources

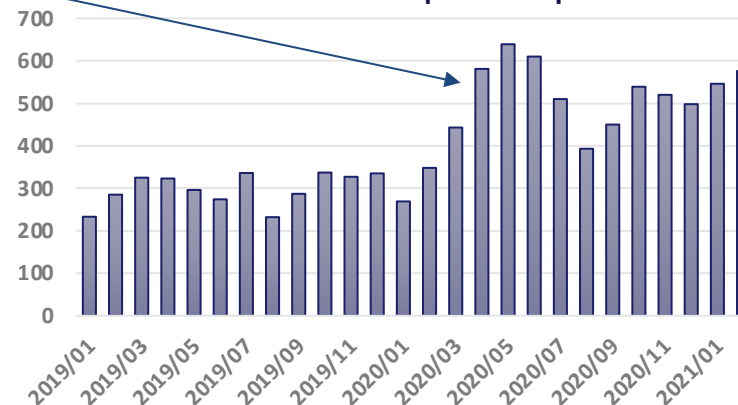
From 96 to 123 countries reached



HADDOCK server processed jobs



HADDOCK server unique users per month



A dramatic sky scene featuring a bright sun in the upper center, partially obscured by wispy clouds. A faint rainbow arches across the upper half of the image. The lower half is filled with a dense, textured layer of white, fluffy clouds. The overall color palette is dominated by deep blues, whites, and a hint of orange from the sun's glow.

Challenges and solutions

- **Attract users!**
 - **Offer them top of the line eScience solutions for their research ... which means top of the line software**



HADDOCK
e-NMR GRID-enabled web portal

Home HADDOCK Xplor-NIH AMBER CYANA CS-ROSETTA TALOS
FormatConverter 3D-DART eNMR-Grid eNMR-Wiki

WELCOME TO THE e-NMR WEB PORTAL >>>

HADDOCK (High Ambiguity Driven protein-protein DOCKing) is an information-driven flexible docking approach for the modeling of biomolecular complexes. HADDOCK distinguishes itself from other 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. HADDOCK can deal with a large class of modeling problems including protein-protein, protein-nucleic acids and protein-ligand complexes.

More information about HADDOCK can be found on the HADDOCK website

HADDOCK WEBSERVER

To use the HADDOCK eNMR GRID-enabled docking server you must:

- have registered for a GRID-enabled HADDOCK account
- have registered with the eNMR grid infrastructure.

Note: registration does require a valid grid certificate!!!

Xplor-NIH
e-NMR GRID-enabled web portal

WELCOME TO THE e-NMR WEB PORTAL >>>

This is the eNMR interface to the Xplor-NIH allowing you to run NMR structure calculations with NOE, J-coupling, and paramagnetic restraints on the eNMR grid infrastructure.

Logged as **Andres Giachetti** (from 150.217.145.84 Currently using 76.8 % of your MB)

You have a personal proxy certificate present in database. Please select "Copy the Proxy" menu

Your Certificate is actually set as: **Robot**

Parameters

1. Structure: 2. Structure:

Structures (psf)

1. Structure: 2. Structure:

Coordinates (pdb)

1. Structure: 2. Structure:

SERVICES

The eNMR web portal is an easy:

AMBER
e-NMR GRID-enabled web portal

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FormatConverter 3D-DART eNMR-Grid eNMR-Wiki

WELCOME TO THE GRID-ENABLED AMBER WEB PORTAL

INTRODUCTION TO AMBER WEB PORTAL

Amber (extremly 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 AMBER eNMR GRID-enabled Molecular Dynamics you have to register to enter grid infrastructure

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

CYANA
Web Portal

Home HADDOCK Xplor-NIH AMBER CYANA CS-ROSETTA TALOS
FormatConverter 3D-DART eNMR-Grid eNMR-Wiki

WELCOME TO CYANA WEB PORTAL

RECOMMENDED BROWSER: MOZILLA FIREFOX

Important information

To use this portal one needs a CYANA license, a valid Grid Certificate. For queries related to CYANA license please contact Prof. Dr. R. W. V. D. V. If you already have a CYANA license and a valid Grid Certificate, login credentials or regarding any other query with respect to

• Description of the portal

This service allows three types of Cyana structure calculations.

In the default case, calculations can be performed using conformational restraints that NMRs have already been assigned and converted to use automated assignment of NOEs is performed.

Manually assigned peaks can be used in the assigned peaks case.

Automated NOE/peaks list assignment can be done using the online calculation. The peak data are assigned NOE/peaks list in the form

CS-ROSETTA
e-NMR GRID-enabled web portal

Home HADDOCK Xplor-NIH AMBER CYANA CS-ROSETTA TALOS
FormatConverter 3D-DART eNMR-Grid eNMR-Wiki

WELCOME TO THE e-NMR WEB PORTAL >>>

CS-ROSETTA is a protocol which generates 3D models of proteins, using only the 13CA, 13CB, 13C', 15N, 1HA and 1HN NMR chemical shifts as input. Based on these parameters, CS-ROSETTA uses a SPARTA-based selection procedure to select a set of fragments from a fragment library (where the chemical shifts and the 3D structure of the fragments are known). The fragments are assembled using the ROSETTA protocol. The generated models are ranked based on the difference between the back-calculated chemical shifts of the generated models and the input chemical shifts. For more information see our online web portal manual and tutorial and/or email the CS-Rosetta home page at: <http://open.mdb.uh.gu.se/Software/CSROSETTA/index.html>.

WEBSERVER USER MANUAL AND TUTORIAL

CCPN format converter
e-NMR web portal

WELCOME TO THE e-NMR WEB PORTAL >>>

This is the eNMR interface to the CCPN Format Converter allowing you to convert your NMR data into a target variety NMR formats.

TALOS
e-NMR (GRID-enabled) web portal

Home HADDOCK Xplor-NIH AMBER CYANA CS-ROSETTA TALOS
FormatConverter 3D-DART eNMR-Grid eNMR-Wiki

WELCOME TO THE e-NMR WEB PORTAL >>>

TALOS is, as the original program TALOS, a program which predicts torsion angles (phi and psi) for a given protein structure. It uses a large database of chemical shifts and the area of the Ramachandran map where the information is compared to information stored in a large database; currently 200 are the 13CA, 13CB, 13C', 15N, 1HA and 1HN NMR backbone chemical shifts of 1 BRB8 format.

TALOS is, as the original program TALOS, a program which predicts torsion angles (phi and psi) for a given protein structure. It uses a large database of chemical shifts and the area of the Ramachandran map where the information is compared to information stored in a large database; currently 200 are the 13CA, 13CB, 13C', 15N, 1HA and 1HN NMR backbone chemical shifts of 1 BRB8 format.

AnisoFIT
WeNMR GRID-enabled web portal

Home HADDOCK Xplor-NIH AMBER CYANA CS-ROSETTA TALOS
FormatConverter 3D-DART eNMR-Grid eNMR-Wiki

WELCOME TO ANISOFIT WEB PORTAL

PROFILE >>>

Supported browser:

AnisoFIT

Fitting of Pseudocontact Shifts and Residual Dipolar Couplings - The program allows users to fit pseudocontact shift and/or residual dipolar couplings measured for a protein against its structure. The calculation exploits the SIMPLEX minimization algorithm. As extensively documented in the literature, this procedure allows the determination of the magnetic susceptibility tensor anisotropy (for pseudocontact shifts) as well as residual dipolar couplings induced by the presence of a paramagnetic metal center) or of the anisotropy of the diffusion tensor (for residual dipolar couplings induced by the presence of orienting media in the protein solution).

This service has a value either as a preliminary step for protein structure refinement or determination using the aforementioned NMR data or as a tool to validate structural models such as those generated through homology modeling. At present, the interface accepts job files containing either a single structure or a bundle of structures. In the latter case, however, only the first model is used. Results are provided in a graphical as well as tabular, downloadable form.

Please quote the following references when reporting the use of this program:

Banci L, Bertini I, Breni RL, Cremonesi HA, Gray RB, Luchinat C, Turano P, J. Biol. Inorg. Chem. (1996) 1, 117-126.

Banci L, Bertini I, Huber JO, Luchinat C, Rosato A, J. Am. Chem. Soc. (1998) 120, 12803-12809.

MARS
Web Portal

Home HADDOCK Xplor-NIH AMBER CYANA CS-ROSETTA TALOS
FormatConverter 3D-DART eNMR-Grid eNMR-Wiki

WELCOME TO MARS WEB PORTAL

ABOUT THE PORTAL (RECOMMENDED BROWSER: MOZILLA FIREFOX)

- Contact Us / Feedback
- Tutorial on MARS

MARS is a program for robust automatic backbone assignment of 13C/15N labeled proteins. MARS simultaneously optimizes the local and global quality of assignment to minimize propagation of initial assignment errors and to extract reliable assignments. It can be applied independent of the assignment complexity, it does not require tight thresholds for establishing sequential connectivity or detailed adjustment of these thresholds, it can work with a wide variety of NMR experiments and it is robust against missing chemical shift information.

Compared to other currently available programs MARS is applicable to proteins above 15 kDa using only Ca and Cb chemical shift information with connectivity thresholds as high as 0.5 ppm and it is applicable to proteins with very

3DDART
e-NMR (GRID-enabled) web portal

Home HADDOCK Xplor-NIH AMBER CYANA CS-ROSETTA TALOS
FormatConverter 3D-DART eNMR-Grid eNMR-Wiki

WELCOME TO THE e-NMR WEB PORTAL >>>

When using 3D-DART please cite the following article:

M. van Dijk and A.M.J.J. Bonvin (2009) "3D-DART: a DNA structure modeling server" *Nucleic Acids Res.* 37 (Web Server Issue):W235-W239 (doi:10.1093/nar/gkp287)

For an explanation of the various options and access to sample data please consult the help pages and the **help link** available at the bottom right corner of every dialog

Antechamber
GRID-enabled web portal

Home HADDOCK Xplor-NIH AMBER CYANA CS-ROSETTA TALOS
FormatConverter 3D-DART eNMR-Grid eNMR-Wiki

WELCOME TO THE e-NMR WEB PORTAL >>>

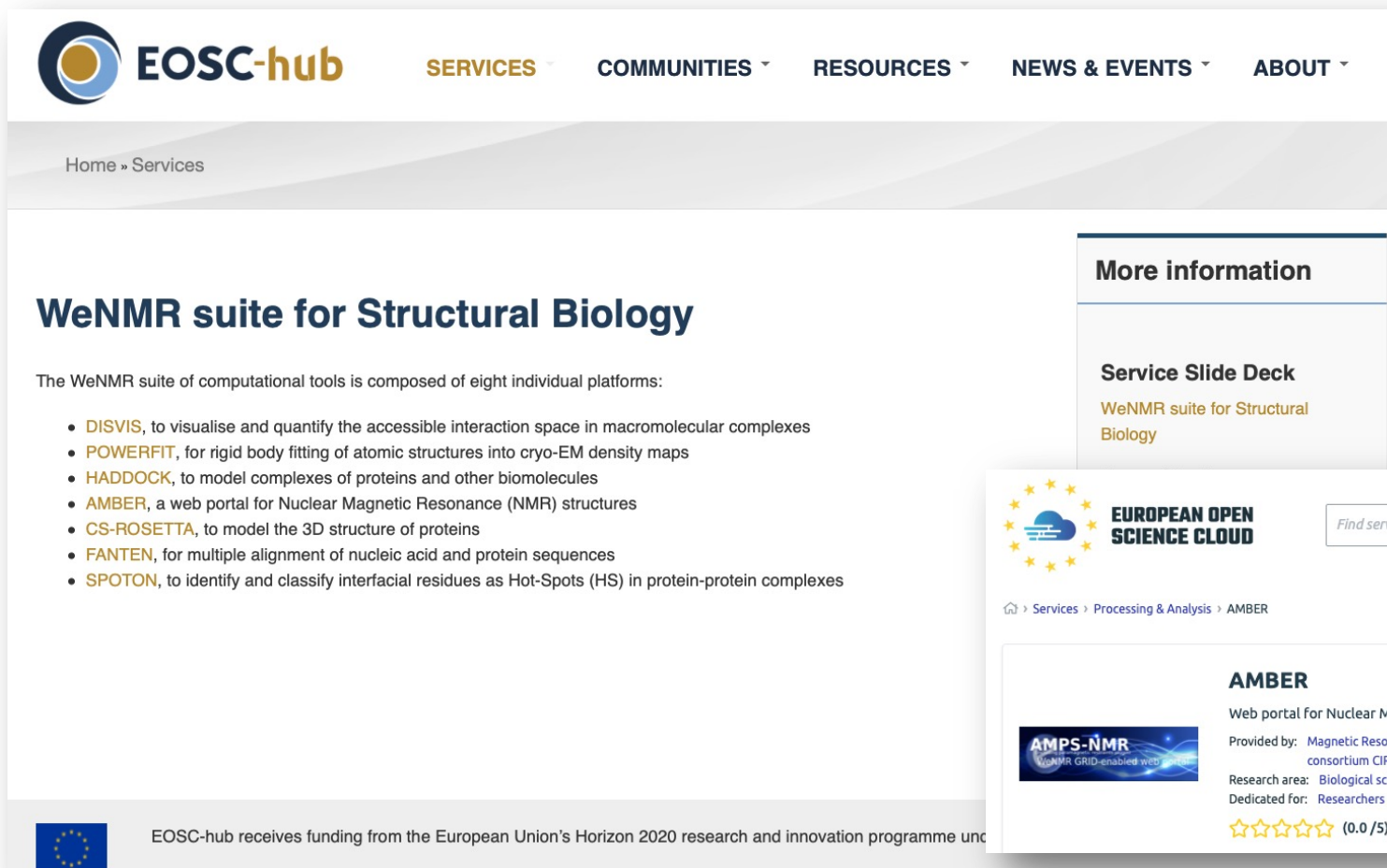
The most common use of the **Antechamber** program suite is to prepare input files for LEaP, starting from a three-dimensional structure, as found in a PDB file. The antechamber suite automates the process of developing a charge distribution and assigning atom types, and partially automates the process of developing parameters for the various combinations of atom types found in a given molecule. Antechamber can automatically generate input force field parameters for most organic molecules, thereby allowing users to use AMBER, also through AMPS-NMR web portal, to refine the structure of protein-ligand adducts.

Setup input

You can upload residue (.pdb or .mol2 file):

Type*: File*: Charge:

Rename residue: MOL



EOSC-hub SERVICES COMMUNITIES RESOURCES NEWS & EVENTS ABOUT

Home » Services

WeNMR suite for Structural Biology

The WeNMR suite of computational tools is composed of eight individual platforms:

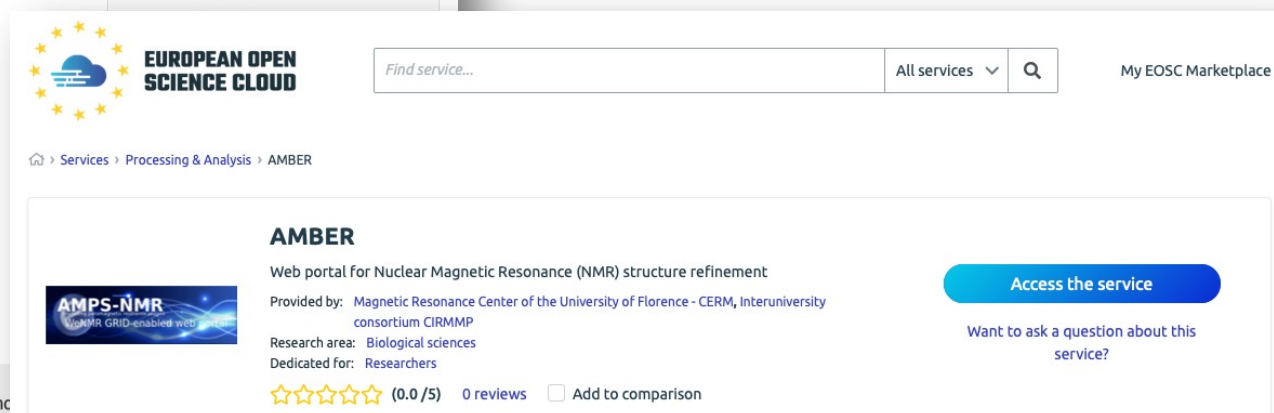
- **DISVIS**, to visualise and quantify the accessible interaction space in macromolecular complexes
- **POWERFIT**, for rigid body fitting of atomic structures into cryo-EM density maps
- **HADDOCK**, to model complexes of proteins and other biomolecules
- **AMBER**, a web portal for Nuclear Magnetic Resonance (NMR) structures
- **CS-ROSETTA**, to model the 3D structure of proteins
- **FANTEN**, for multiple alignment of nucleic acid and protein sequences
- **SPOTON**, to identify and classify interfacial residues as Hot-Spots (HS) in protein-protein complexes

More information

Service Slide Deck
WeNMR suite for Structural Biology

EOSC-hub receives funding from the European Union's Horizon 2020 research and innovation programme under

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



EUROPEAN OPEN SCIENCE CLOUD

Find service... All services 🔍 My EOSC Marketplace

Services > Processing & Analysis > AMBER

AMBER

Web portal for Nuclear Magnetic Resonance (NMR) structure refinement

Provided by: Magnetic Resonance Center of the University of Florence - CERM, Interuniversity consortium CIRMMP

Research area: Biological sciences

Dedicated for: Researchers

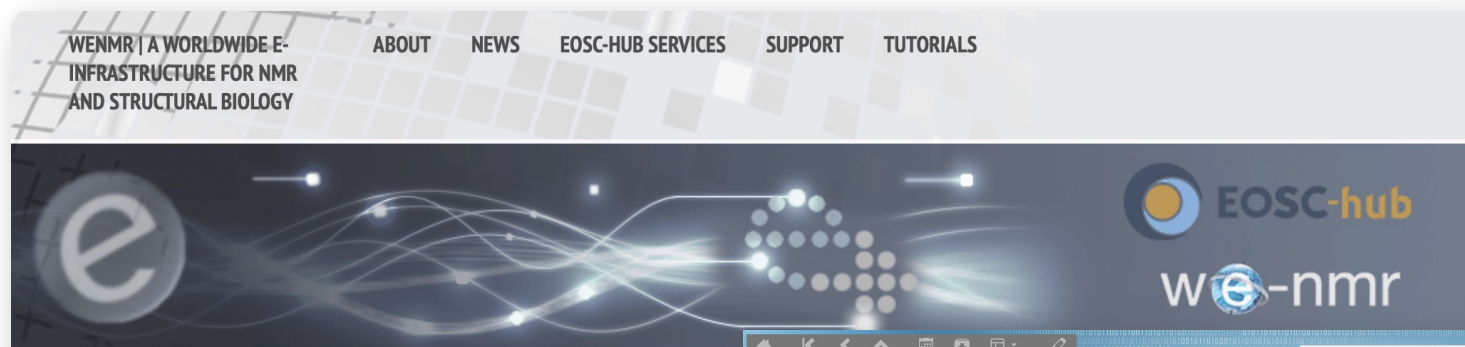
⭐⭐⭐⭐⭐ (0.0 / 5) 0 reviews ☐ Add to comparison

Access the service

Want to ask a question about this service?

<https://www.eosc-hub.eu>

- **Attract users!**
 - Offer them top of the line eScience solutions for their research ... which means top of the line software
 - Provide them training, tutorials and support



- **Support center**
- **Tutorials**
- **YouTube channel**
- **Many workshops ...**

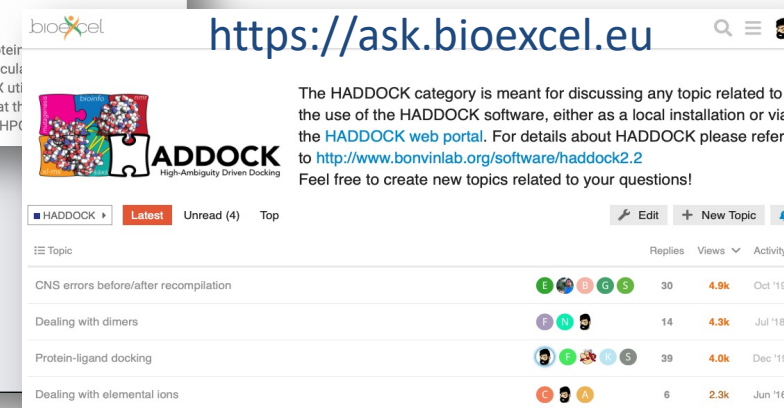


WeNMR Tutorials

We provide here a number of link portals.

Table of contents

- **Online tutorials**
 - [3D-DART](#)
 - [CS-ROSETTA](#)
 - [DISVIS](#)
 - [HADDOCK](#)
 - [POWERFIT](#)
 - [RMD-AMBER](#)
 - [RMD with RDC's](#)
 - [RMD including disulfide bonds](#)
 - [SPOTON](#)
- **Online lectures**



- **Attract users!**
 - Offer them top of the line eScience solutions for their research ... which means top of the line software
 - Provide them training, tutorials and support
 - Make their life easier

- SSO Integration with European Open Science Cloud EGI CheckIn



EOSC-WeNMR portals
@Bonvinlab

Navigation bar: HADDOCK2.2 HADDOCK2.4 CPORT DISVIS POWERFIT PRODIGY SPOTON CS_ROSETTA3 PROABC2 WHISCY PDBTOOLS EOSC marketplace **Login**

WELCOME TO THE UTRECHT BIOMOLECULAR INTERACTION WEB PORTAL >>

The Utrecht Biomolecular Interactions software portal provides access to software tools developed in the Computational Structural Biology group at Utrecht University with a main focus on the characterization of biomolecular interactions. Please note that this site is in active development.

Research

Research within the computational structural biology group focuses on the development of reliable bioinformatic and computational approaches to predict, model and dissect biomolecular interactions at atomic level.

For this, bioinformatic data, structural information and available biochemical or biophysical experimental data are combined to drive the modelling process. By following a holistic approach integrating various experimental information sources with computational structural biology methods we aim at obtaining a comprehensive description of the structural and dynamic landscape of complex biomolecular machines, adding the structural dimension to interaction networks and opening the route to systematic and genome-wide studies of biomolecular interactions.

Login via [learn more ...](#)

 **Check-In**

OR

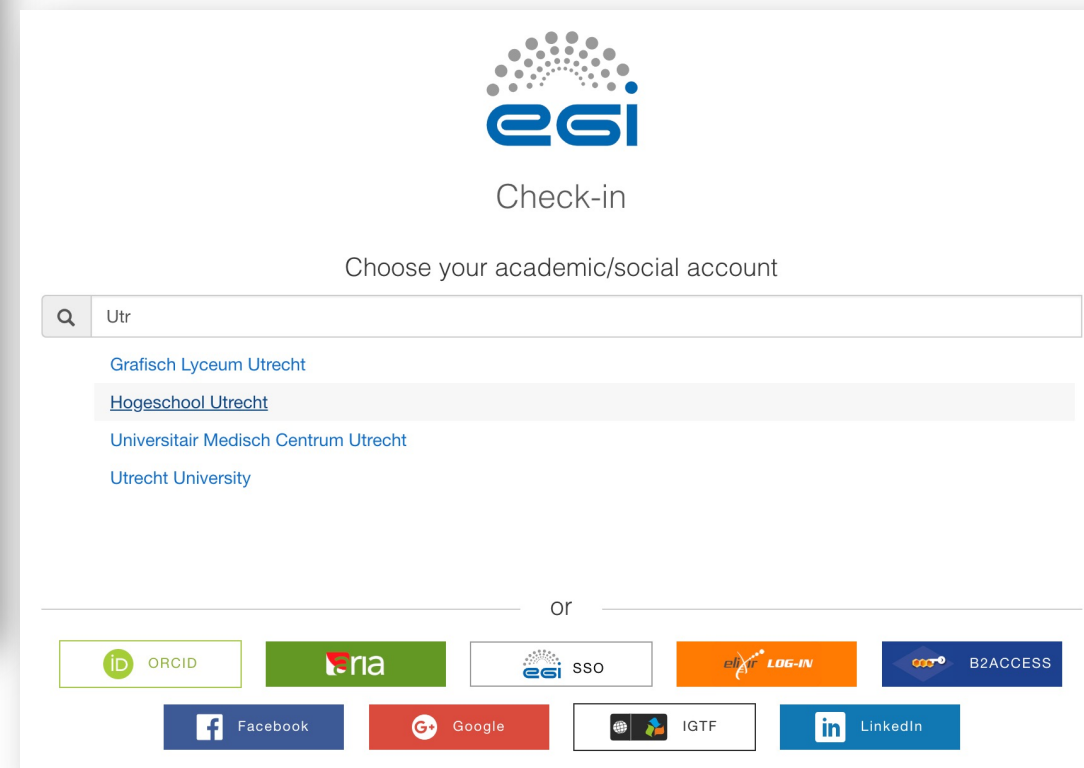
Email or User Name


Password

Login ☐ Keep me logged in

New user? [Register](#)

Forgot your password? [Reset](#)









Check-in





Choose your academic/social account

Search: Utr

- [Grafisch Lyceum Utrecht](#)
- [Hogeschool Utrecht](#)
- [Universitair Medisch Centrum Utrecht](#)
- [Utrecht University](#)

or

 ORCID
  Inra
  EGI SSO
  ELIXIR LOG-IN
  B2ACCESS

 Facebook
  Google
  IGTF
  LinkedIn

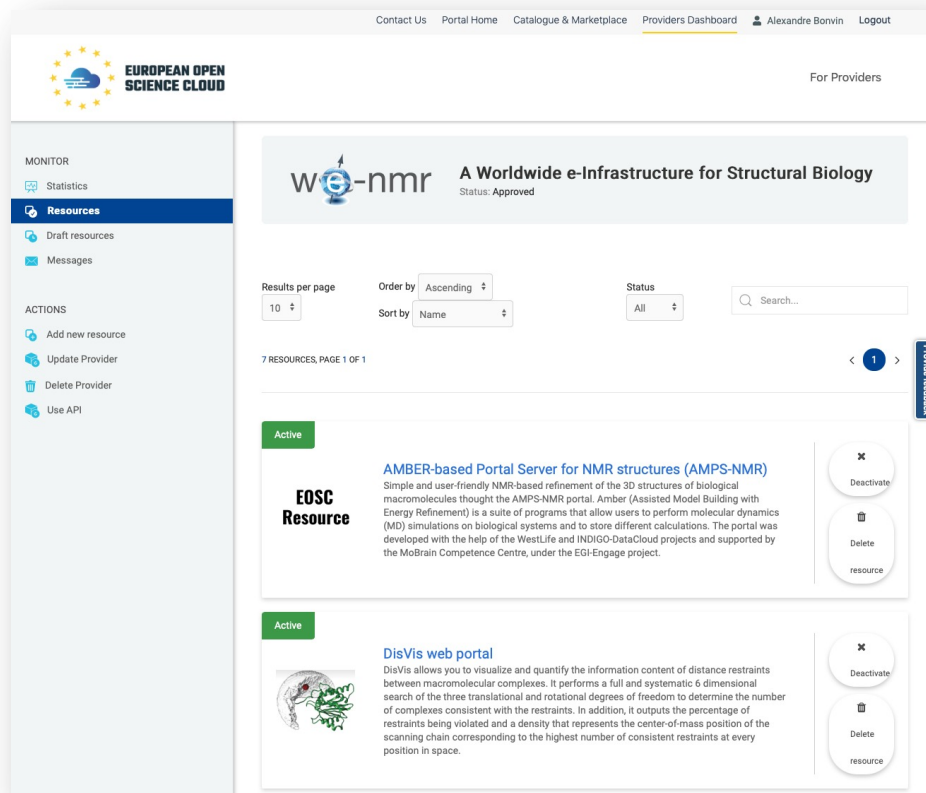
- Keep monitoring user satisfaction and get input from users

- User satisfaction ratings

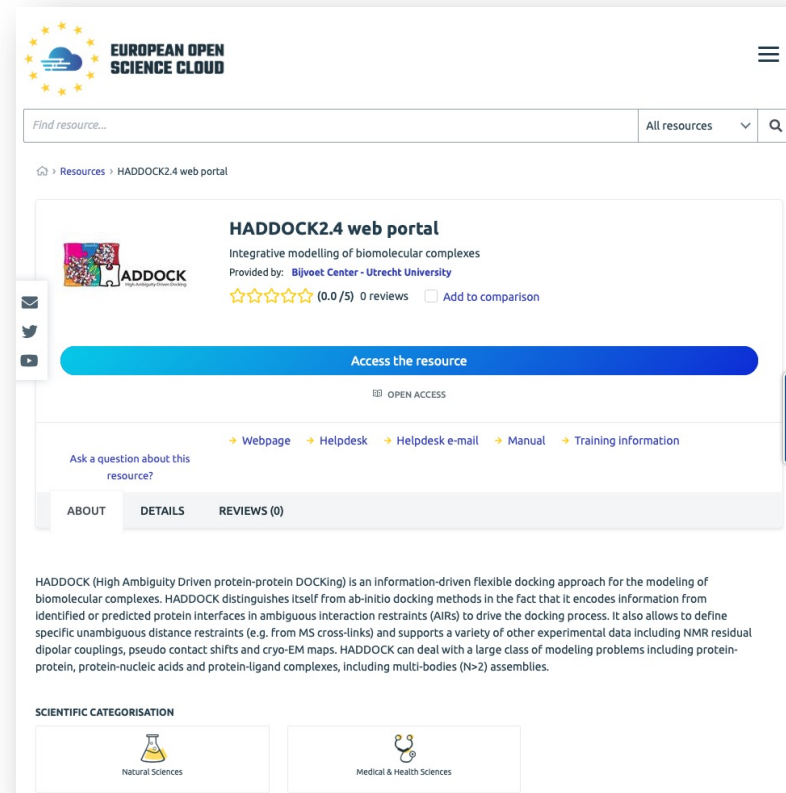


- CS-ROSETTA3: 5.0 (from 5 respondent)
- DISVIS: 4.8 (from 38 respondents)
- HADDOCK: 4.9 (from 3263 respondents)
- HADDOCK2.4: 4.9 (from 103 respondents)
- POWERFIT: 4.8 (from 14 respondents)
- PRODIGY: 4.7 (from 792 respondents)
- SPOTON: 4.7 (from 74 respondents)

Integrated in EOSC marketplace and in full operation from day 1



This screenshot shows the 'Providers Dashboard' for the 'we-nmr' resource in the EOSC marketplace. The interface includes a sidebar with navigation options like 'MONITOR', 'Resources', 'Draft resources', and 'Messages'. The main content area displays a list of resources, with 'we-nmr' highlighted as 'A Worldwide e-Infrastructure for Structural Biology' with a status of 'Approved'. Below this, there are filters for 'Results per page' (10), 'Order by' (Ascending), 'Sort by' (Name), and 'Status' (All). A search bar is also present. The list shows two resources: 'EOSC Resource' and 'DisVis web portal', each with an 'Active' status and a 'Delete resource' button.



This screenshot shows the 'HADDOCK2.4 web portal' resource page. The header includes the 'EUROPEAN OPEN SCIENCE CLOUD' logo and a search bar. The resource is titled 'HADDOCK2.4 web portal' and is described as 'Integrative modelling of biomolecular complexes'. It is provided by 'Bijvoet Center - Utrecht University'. The page shows a rating of 0.0/5 with 0 reviews and an 'Add to comparison' button. A large blue button labeled 'Access the resource' is prominent. Below this, there are links for 'Webpage', 'Helpdesk', 'Helpdesk e-mail', 'Manual', and 'Training information'. The page also includes a 'Provide feedback' button and a 'SCIENTIFIC CATEGORISATION' section with icons for 'Natural Sciences' and 'Medical & Health Sciences'.

- **Attract users!**
- **Access to e-Infrastructure**

- The WeNMR services have been in production since >11 years under various projects (eNMR, WeNMR, EGI-Engage, West-Life, EOSC-Hub)
- Access to resources formalized through a SLA agreement valid until 6/2023
 - 53 million CPU hours (opportunistic access)
 - 412 cloud CPU cores
 - 59 TB storage

“The FP7 WeNMR (project# 261572), H2020 West-Life (project# 675858), the EOSC-hub (project# 777536) and the EGI-ACE (project# 101017567) European e-Infrastructure projects are acknowledged for the use of their web portals, which make use of the EGI infrastructure with the dedicated support of CESNET-MCC, INFN-PADOVA-STACKE, INFN-LNL-2, NCG-INGRID-PT, TW-NCHC, CESGA, IFCA-LCG2, UA-BITP, SURFsara and NIKHEF, and the additional support of the national GRID Initiatives of Belgium, France, Italy, Germany, the Netherlands, Poland, Portugal, Spain, UK, Taiwan and the US Open Science Grid.”

<https://documents.egi.eu/document/2751>

EGI Document 2751-v30

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VO SLA WeNMR and VO OLAs WeNMR (Former Mobrain)

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Document type:
 Internal document

Submitted by:
 Unknown

Updated by:
[Giuseppe La Rocca](#)

Document Created:
 16 Feb 2016, 16:43

Contents Revised:
 18 Jan 2021, 17:03

Metadata Revised:
 18 Jan 2021, 17:03

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

Files in Document:

- [EGI VO WeNMR OLA CESGA - FINAL.pdf](#) (187.7 kB)
- [EGI VO WeNMR OLA CESNET-MCC - FINAL.pdf](#) (191.4 kB)
- [EGI VO WeNMR OLA IFCA-LCG2 - FINAL.pdf](#) (190.7 kB)
- [EGI VO WeNMR OLA INFN-LNL-2 - FINAL.pdf](#) (190.8 kB)
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- [EGI VO WeNMR OLA UA-BITP - FINAL.pdf](#) (188.2 kB)
- [EGI VO WeNMR SLA - FINAL.pdf](#) (263.2 kB)

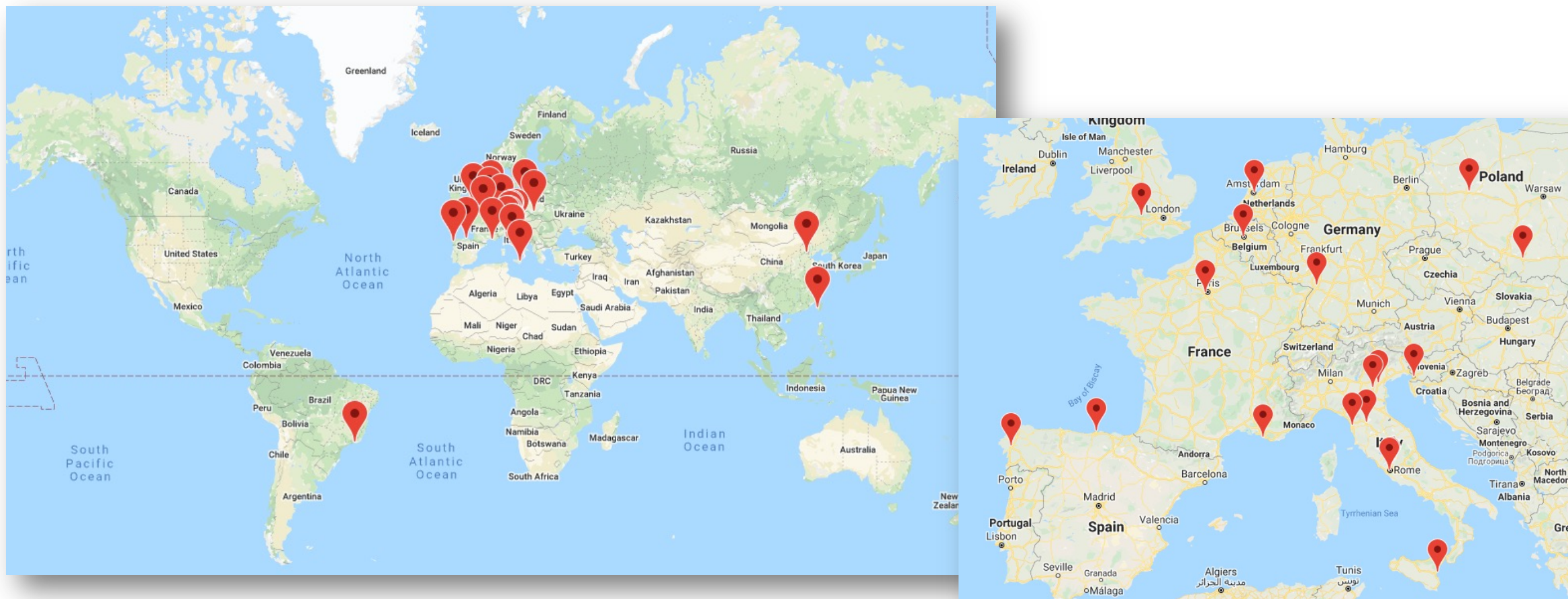
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Other Versions:

- [EGI-doc-2751-v29](#)
18 Jan 2021, 17:03
- [EGI-doc-2751-v28](#)
18 Jan 2021, 16:56
- [EGI-doc-2751-v27](#)
15 Jan 2021, 11:34
- [EGI-doc-2751-v26](#)
13 Jan 2021, 16:13

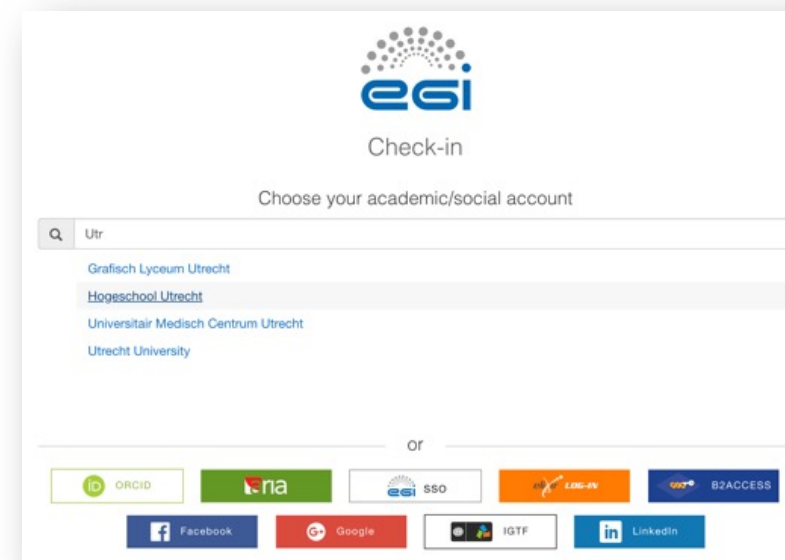


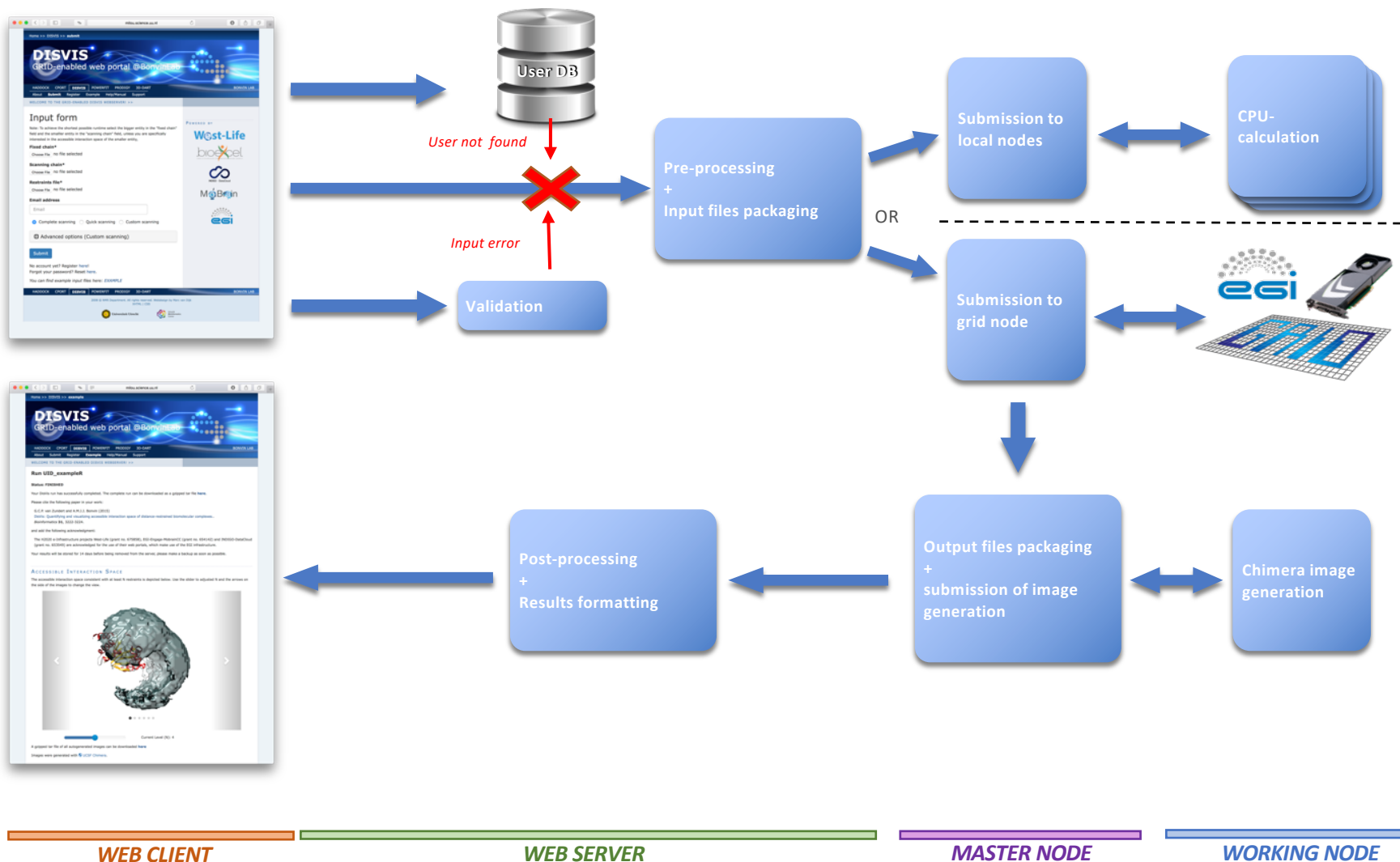
World-wide (excl. OSG) April 2020:
> 500'000 CPU cores from 22 sites

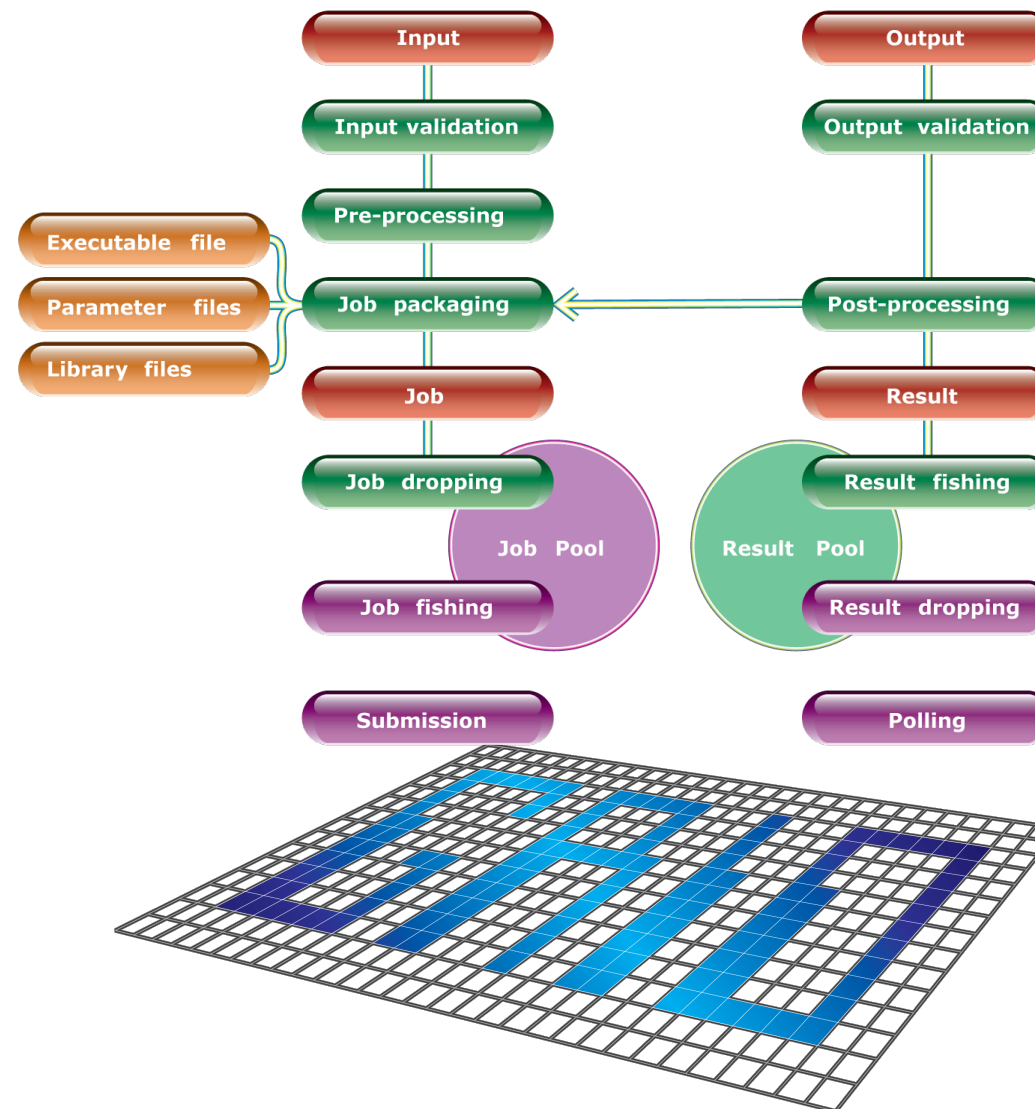
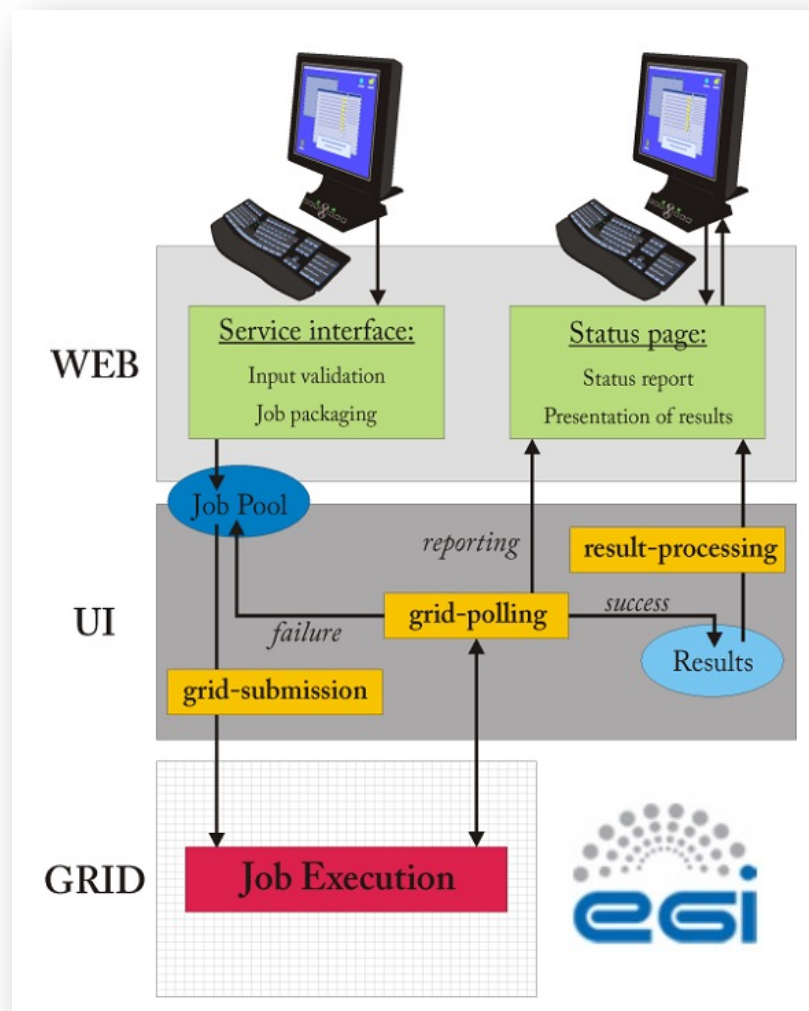
- **Attract users!**
- **Access to e-Infrastructure**
- **Develop software and maintain and operate a complex infrastructure**

The **WeNMR services** are based on:

- A web page front end to the service exposed to the user
- Back end consisting of a variety of software and scripts
- Make use of the **DIRAC4EGI/EGI workload** service for distributing compute jobs and of some **gLite** components in some cases
- Make use of the **HTC EGI resources (grid, cloud, GPGPUs)** of EOSC-Hub to distribute the computations
- User registration and authentication mechanisms connected to **EGI Check-in**
- Some portals use the **INDIGO-Datacloud udocker** solution







- **DIRAC4EGI allows for simplified and efficient job submission and monitoring**

- No root access required
- Only DIRAC software installation required
- You can already benefit from it to transform your laptop into an HTC server



<http://diracgrid.org>



Andrei
Tsaregorodtsev

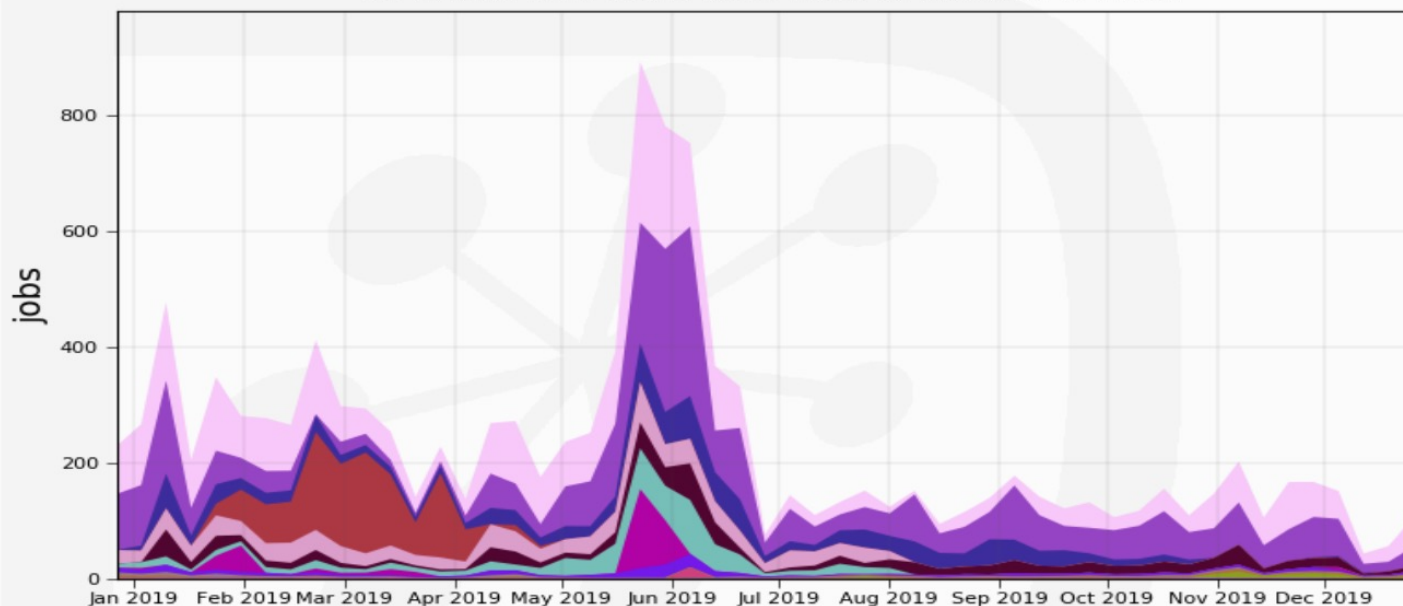


Ricardo
Graciani

```
JobName = "dirac-xxx";  
CPUTime = 100000;  
Executable = "dirac-xxx.sh";  
StdOutput = "dirac-xxx.out";  
StdError = "dirac-xxx.err";  
InputSandbox = {"dirac-xxx.sh", "dirac-xxx.tar.gz"};  
OutputSandbox = {"dirac-xxx.out", "dirac-xxx.err", "dirac-xxx-result.tar.gz"};
```

- **Very efficient submission, high job throughput** (used for our servers since 2015)

Running jobs by Site
52 Weeks from Week 51 of 2018 to Week 51 of 2019

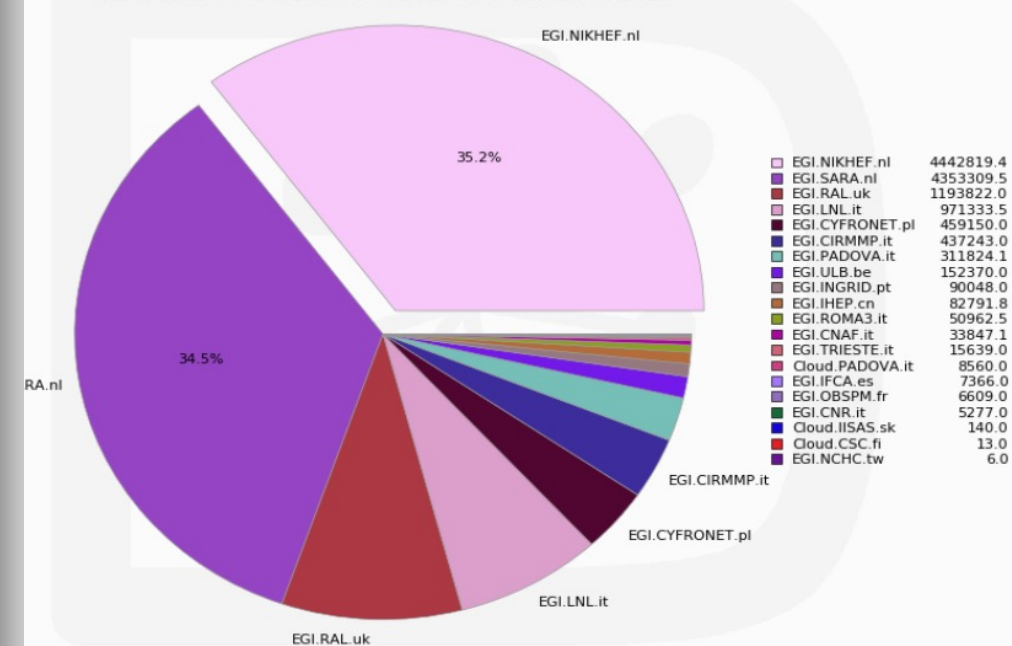


Max: 892, Min: 42.7, Average: 231, Current: 105

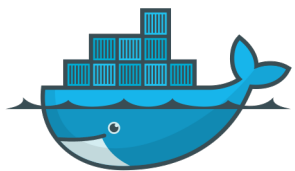
EGI.NIKHEF.nl	27.9%	EGI.CYFRONET.pl	6.7%	EGI.IHEP.cn	0.7%	EGI.TRIESTE.it	0.0%
EGI.SARA.nl	27.3%	EGI.PADOVA.it	5.3%	EGI.ROMA3.it	0.4%	EGI.CNR.it	0.0%
EGI.CIRMMMP.it	9.2%	EGI.CNAF.it	2.6%	Cloud.PADOVA.it	0.2%	Cloud.IISAS.sk	0.0%
EGI.RAL.uk	8.9%	EGI.ULB.be	2.2%	EGI.OBSPM.fr	0.1%	Cloud.CSC.fi	0.0%
EGI.LNL.it	7.6%	EGI.INGRID.pt	0.8%	EGI.IFCA.es	0.0%	EGI.NCHC.tw	0.0%

Generated on 2020-04-22 12:57:01 UTC

Total Number of Jobs by Site
52 Weeks from Week 00 of 2019 to Week 52 of 2019

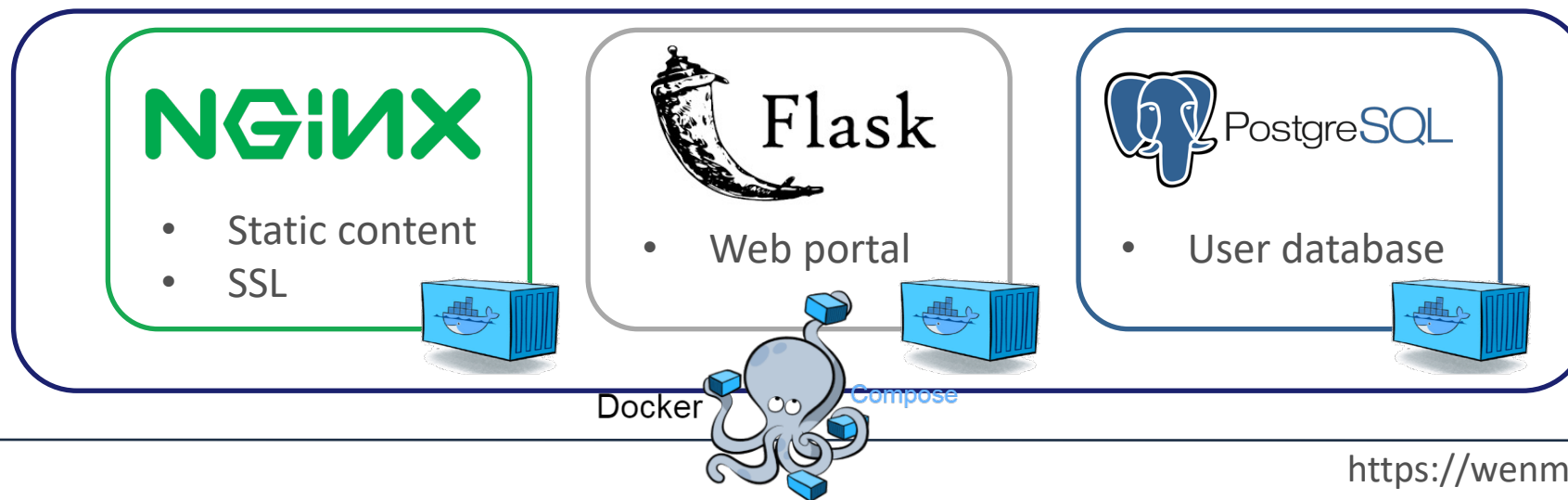


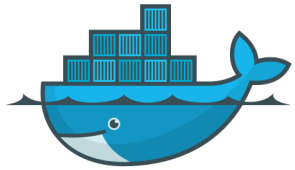
Generated on 2020-04-22 12:58:25 UTC



Migration from local provisioning to provisioning via docker-compose

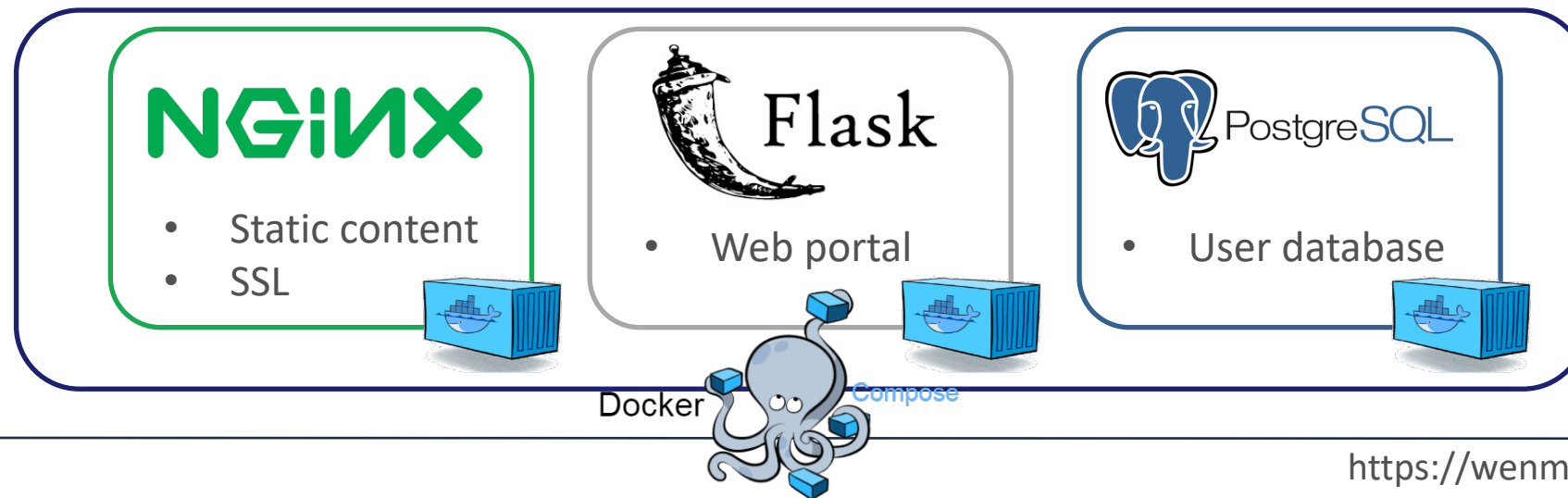
- Improves portability and development
- Separation of the different components
- Important configuration stored in docker compose file
- Easy to switch between development/production configuration
- Easy scaling by deploying to a docker swarm
- Used in HelixNebula pilot project





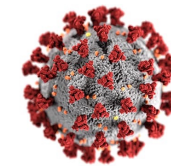
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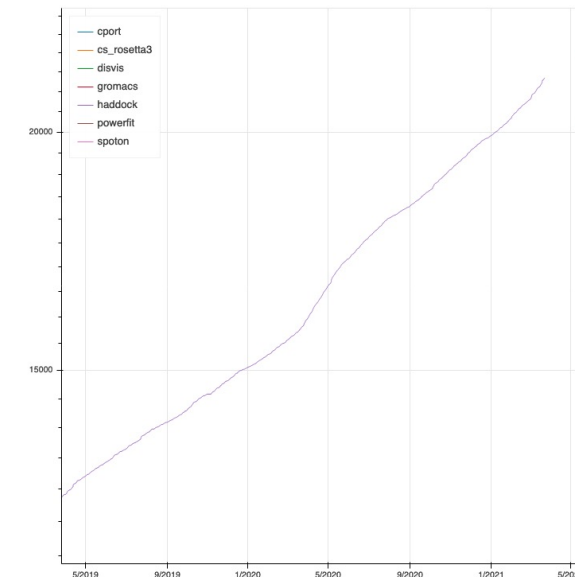
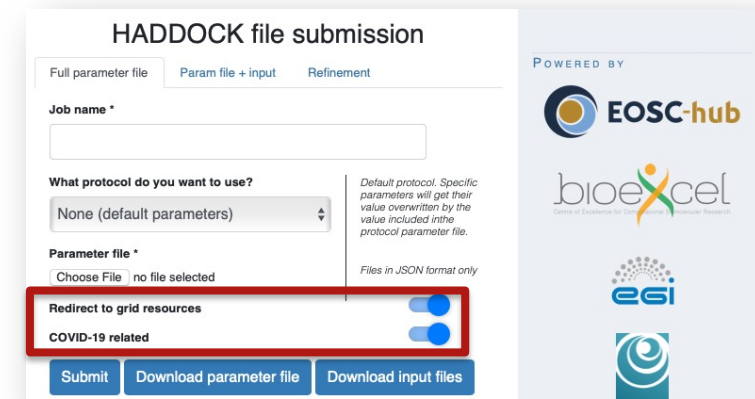


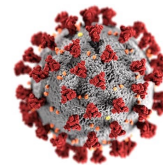


Supporting COVID-19 related
research



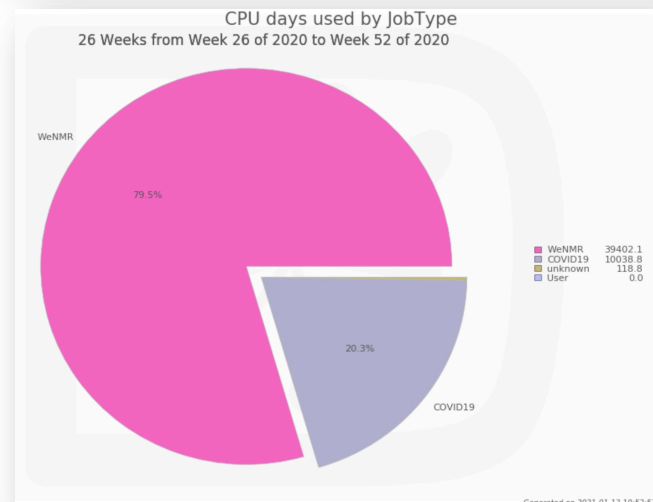
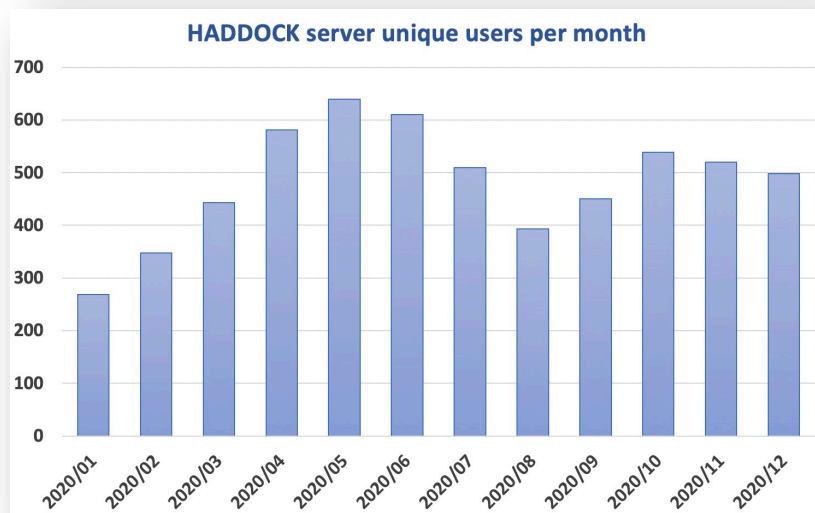
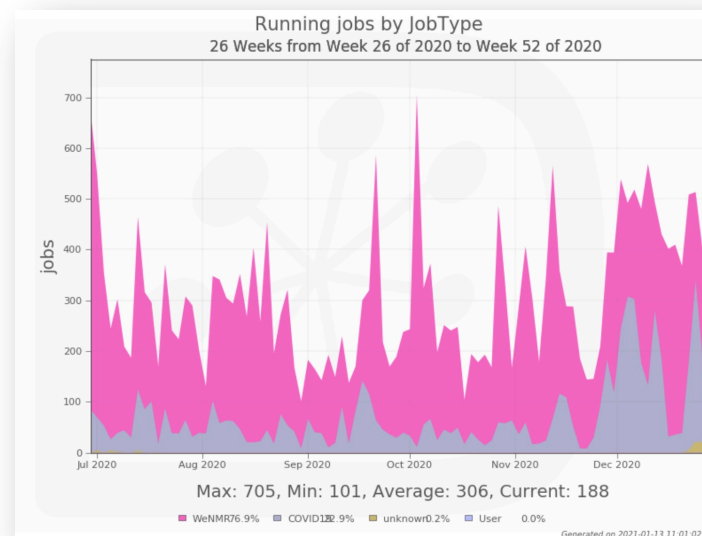
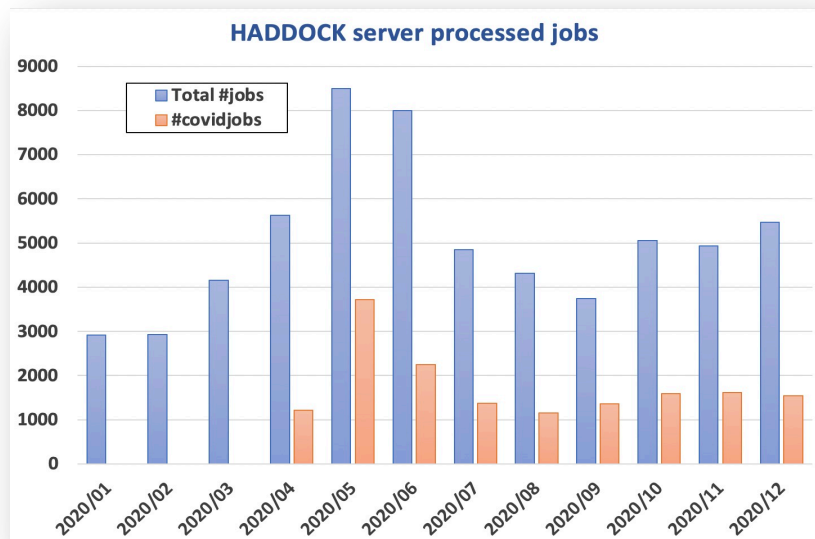
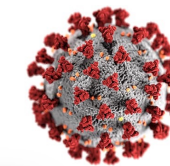
- HADDOCK can be used to model interactions between virus and human proteins and for drug screening
- Increased number of registrations since several weeks (months)
- We have doubled our processing capability by modifying the backend machinery managing the HADDOCK workflow
 - From ~95 docking runs per day to ~183 per day
- Users can now tag their submissions as COVID-related

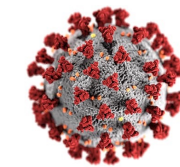





- **Via contacts between EGI and the US Open Science Grid, WeNMR has now access (via DIRAC4EGI) to the US HTC resources**
- **Via contacts with high energy physics (WLCG - Worldwide Large hadron collider Computing Grid), additional sites are now supporting WeNMR COVID-related jobs**
 - Centre de Physique des Particules de Marseille (CPPM)
 - Karlsruhe Institute of Technology
 - Spanish LHCb Tier2 (USC-LCG2) site
- **Mechanism in place in DIRAC4EGI to tag submissions as COVID and direct those to sites especially supporting this research (thanks to Andrei Tsaregorodtsev)**

```
Tag = {"COVID19"};  
JobType = "COVID19";
```

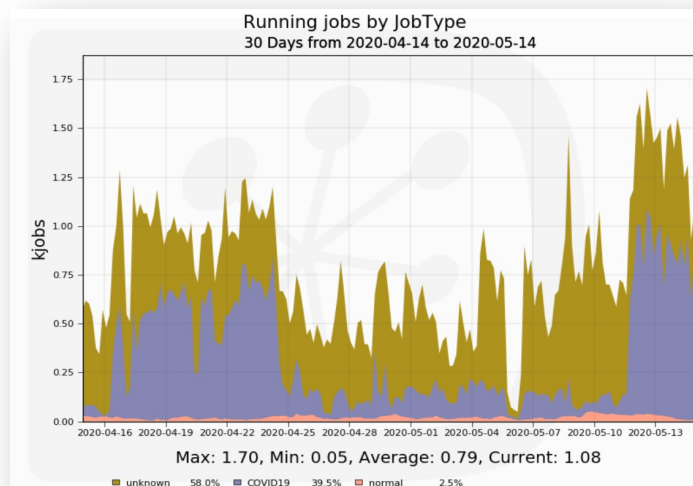




Modelling of various Sars-Cov2 – human protein interactions

Screening of approved drugs against the protease with HADDOCK

- Docking of ~2000 approved drugs run on EGI/EOSC/OSG HTC resources in ~ 3 1/2 days



See: bonvinlab.org/covid


<https://instruct-eric.eu/haddock-screen-of-2000-approved-drugs-for-covid19>

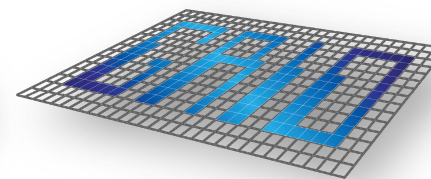


<https://www.eosc-portal.eu/news/haddock-support-covid-19-research>

A dramatic sky scene featuring a bright sun in the upper center, partially obscured by clouds. A faint rainbow arches across the upper half of the image. The lower half is filled with a dense, textured layer of white, fluffy clouds. The overall color palette is dominated by deep blues, whites, and yellows from the sun.

Future perspectives

- Keep operating state-of-the-art portals
- Keep ensuring a smooth operation
- Provide user support and training
- Adopt (when needed / makes sense) new solutions
- Keep monitoring user satisfaction 



- Harvest transparently both
- DIRAC4EGI can handle both without the additional burden of managing cloud VMs
- We still have much more grid than cloud resources
- Efforts within BioExcel to move HADDOCK toward Exascale (e.g. large-scale simulations on HPC resources, using singularity containers)
- Deployment of the HADDOCK portal in the FedCloud for COVID-19 specific projects

Acknowledgements



EUROPEAN OPEN
SCIENCE CLOUD

