

# WeNMR under the hood

How to operate a complex collection of scientific web services



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[bonvinlab.org](http://bonvinlab.org)

# Overview

EOSC-WeNMR

Under the hood

Development and Operation

Worldwide Usage

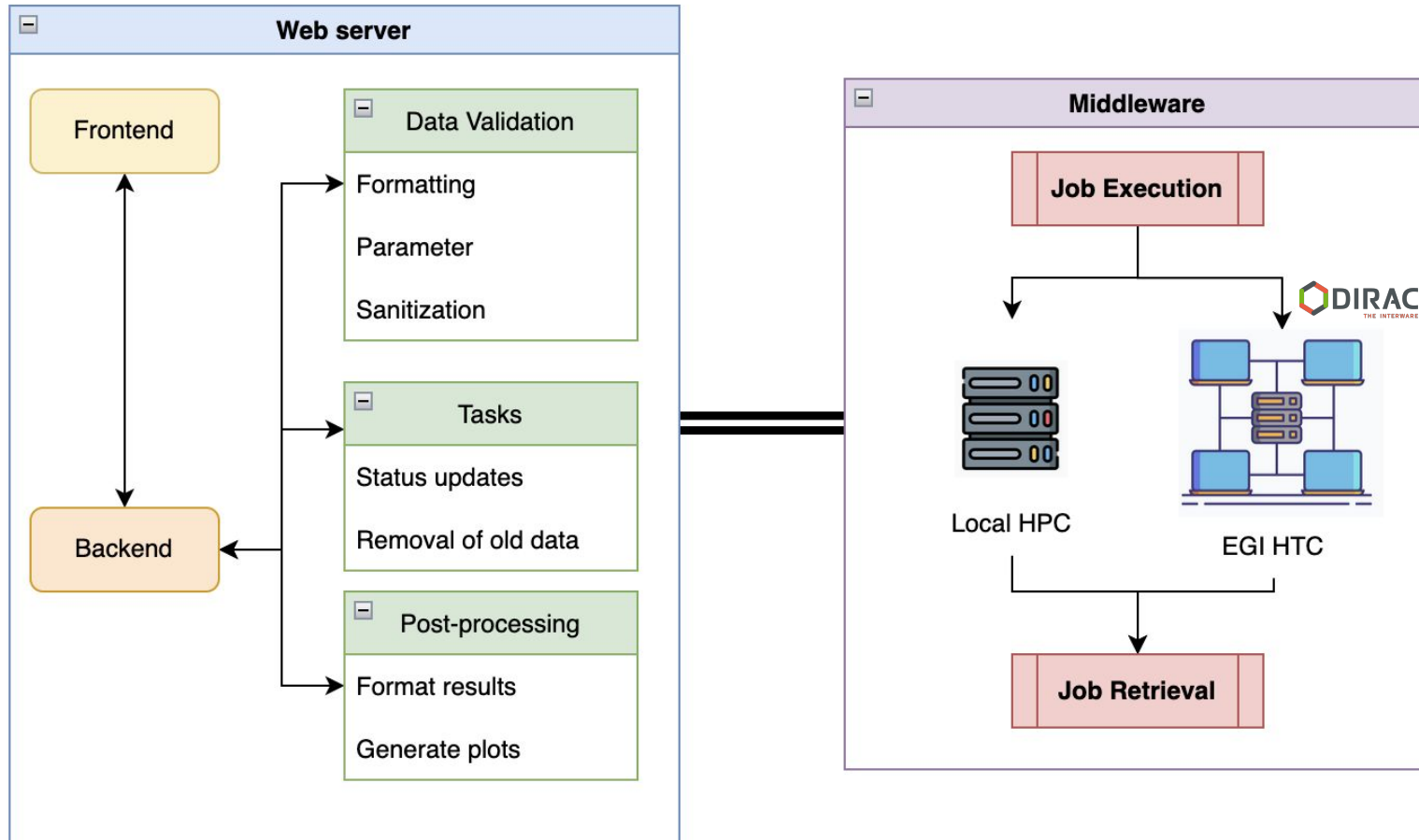
**WeNMR** is a worldwide e-infrastructure for Nuclear Magnetic Resonance (NMR) and Structural Biology

Computational methods developed by the academic groups are instrumentalized into applications and served as web services to the life sciences community

[wenmr.eu](http://wenmr.eu)

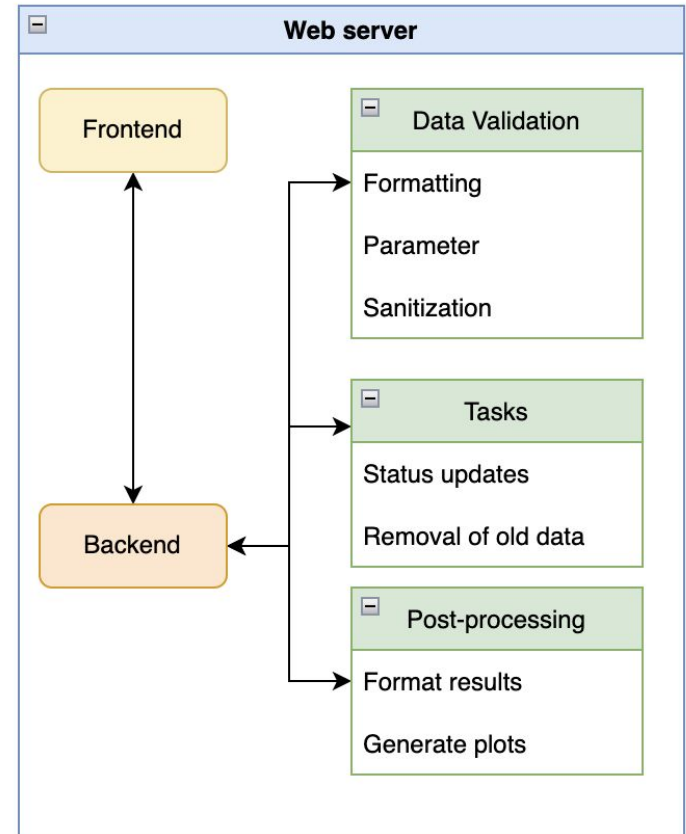


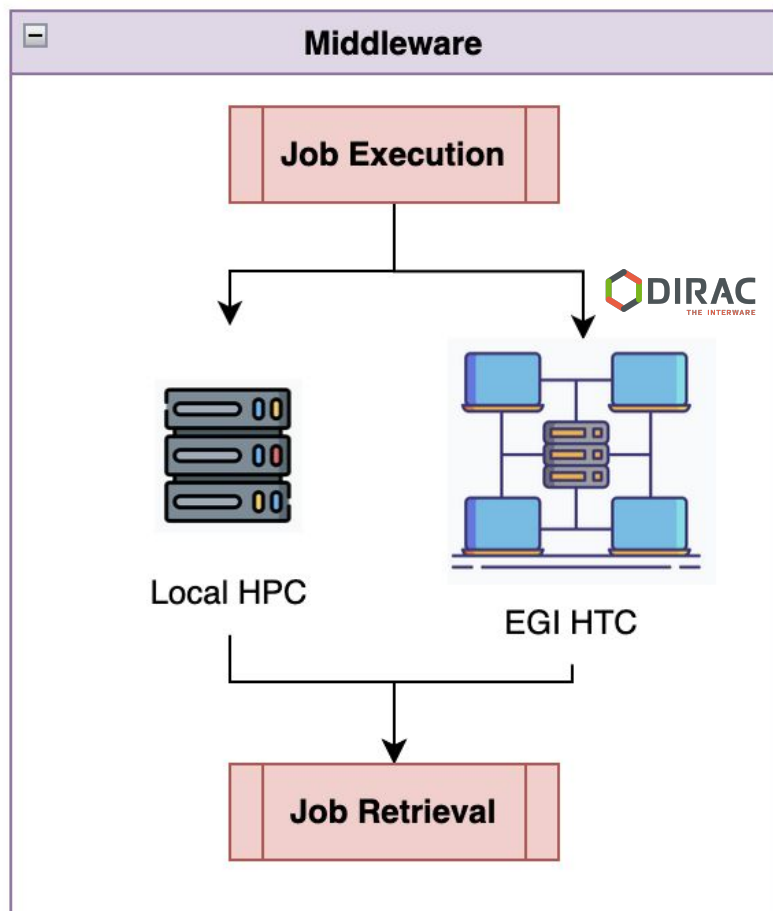
The screenshot shows the homepage of the EOSC-WeNMR portal. The header features the text "EOSC-WeNMR portal" and "@Bonvinlab" on a blue background with abstract light patterns. Below the header is a navigation menu with links to various software tools: HADDOCK2.2, HADDOCK2.4, DISVIS, CPORT, POWERFIT, PRODIGY, SPOTON, PROABC2, WHISCY, PDBTOOLS, FANDAS, GENTBL, EOSC marketplace, and a "Login" button. A welcome message reads: "WELCOME TO THE UTRECHT BIOMOLECULAR INTERACTION WEB PORTAL >>". A paragraph of text states: "The Utrecht Biomolecular Interactions software portal provides access to software tools developed in the Computational Structural Biology group / NMR Research Group of Utrecht University with a main focus on the characterization of biomolecular interactions. Please note that this site is in active development." A "Research" section follows, containing text about the group's focus on developing reliable bioinformatic and computational approaches to predict, model, and dissect biomolecular interactions at the atomic level. It also describes a holistic approach to integrating experimental data with computational methods for a comprehensive description of structural and dynamic landscapes. To the right of this text is an image of several colorful 3D molecular models.



## Web

- FLASK framework, PostgreSQL, NGINX
- Provides user-friendly “smart” forms for user input
- Focus on **usability**, tight feedback loop with the community via [ask.bioexcel.eu](https://ask.bioexcel.eu)
- User authentication
- Data validation & pre/post-processing
- *Server side execution of services with low footprint*





## Middleware

- Heterogenous service execution workflow
- Decoupled from web framework
- Job execution with in-house dedicated HPC
- SLURM/TORQUE
- Access to EGI Grid with **DIRAC** via **WeNMR Virtual Organization**
- Middle layer as a collection *in-house* shell scripts

## Code development

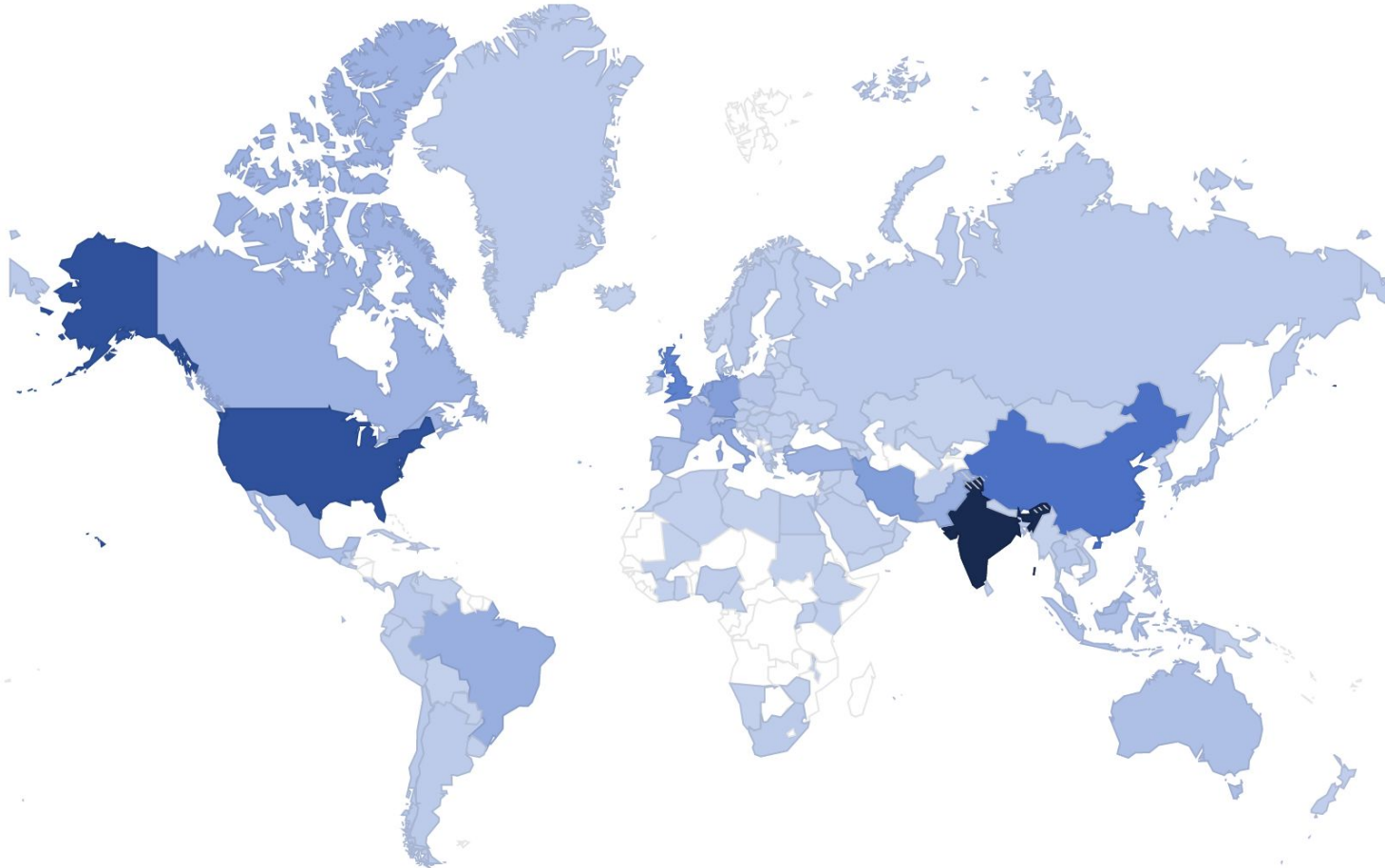
- Version control in GitHub
- Moved all services to a single monorepo
- Dedicated runner for continuous integration
- Continuous deployment currently being implemented with webhooks & dockerhub

## Deployment

- Via docker-compose in dedicated resources
- Planned migration to Kubernetes for high availability deployment

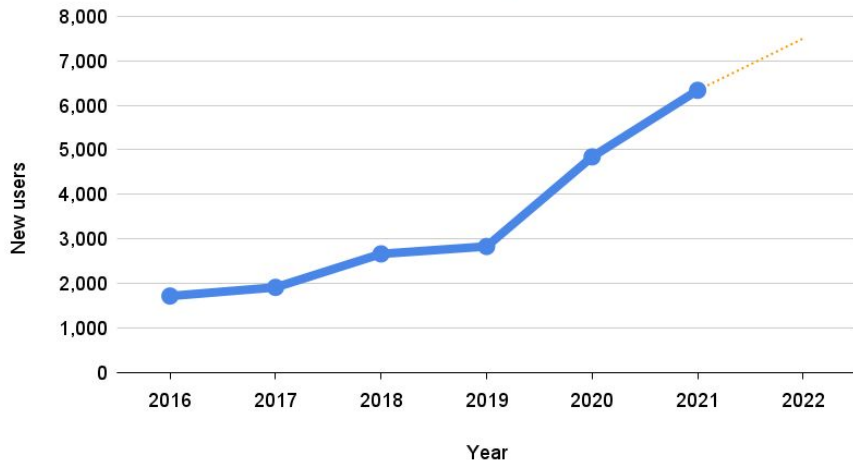
# Worldwide User Map

The HADDOCK web portal is being used by **31779 users** across **136 countries!**





New HADDOCK Users per Year



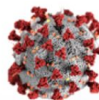
## Worldwide Impact and Usage:



31,770+ users & 456,720+ submissions

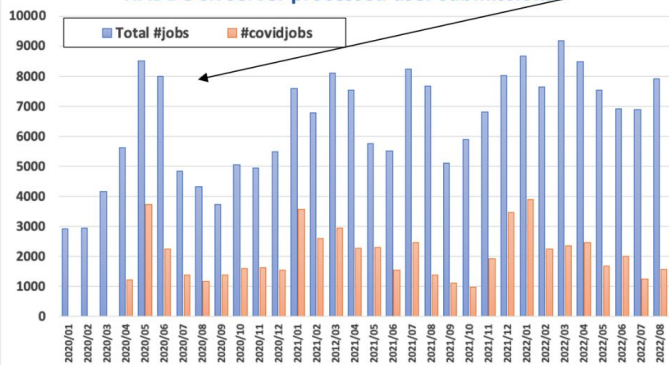
## COVID-19 Support:

- Additional EOSC HTC dedicated resources to support COVID-19 research
- ~30% of all simulations since April 2020 are COVID-19-related

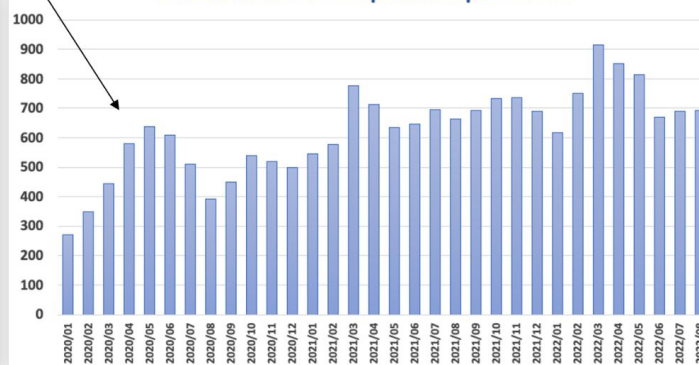


COVID19 effect

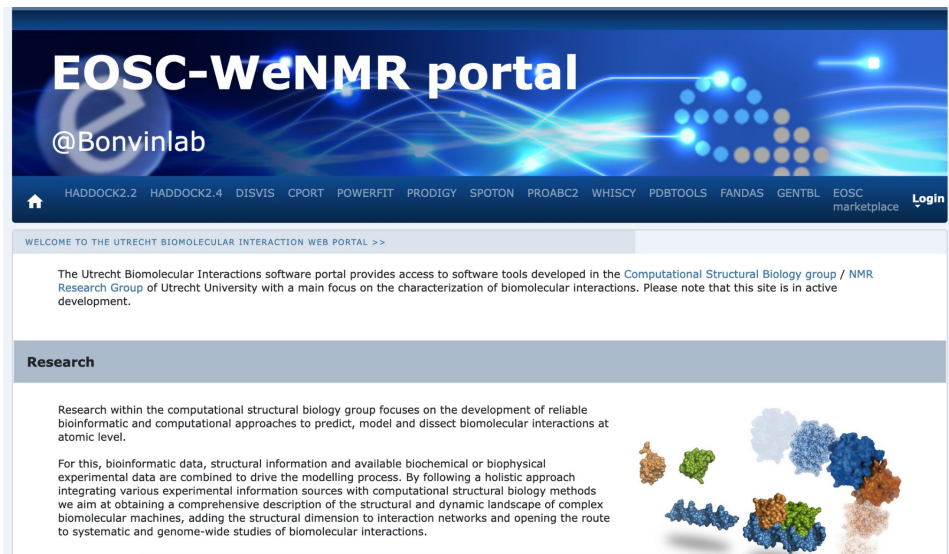
HADDOCK server processed user submissions



HADDOCK server unique users per month



[wenmr.science.uu.nl](http://wenmr.science.uu.nl)



**EOSC-WeNMR portal**  
@Bonvinlab

HADDOCK2.2 HADDOCK2.4 DISVIS CPORT POWERFIT PRODIGY SPOTON PROABC2 WHISCY PDBTOOLS FANDAS GENTBL EOSC marketplace Login

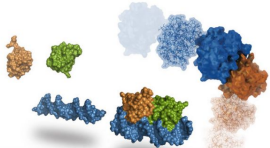
WELCOME TO THE UTRECHT BIOMOLECULAR INTERACTION WEB PORTAL >>

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**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.




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