

WeNMR under the hood

How to operate a complex
collection of scientific web
services



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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

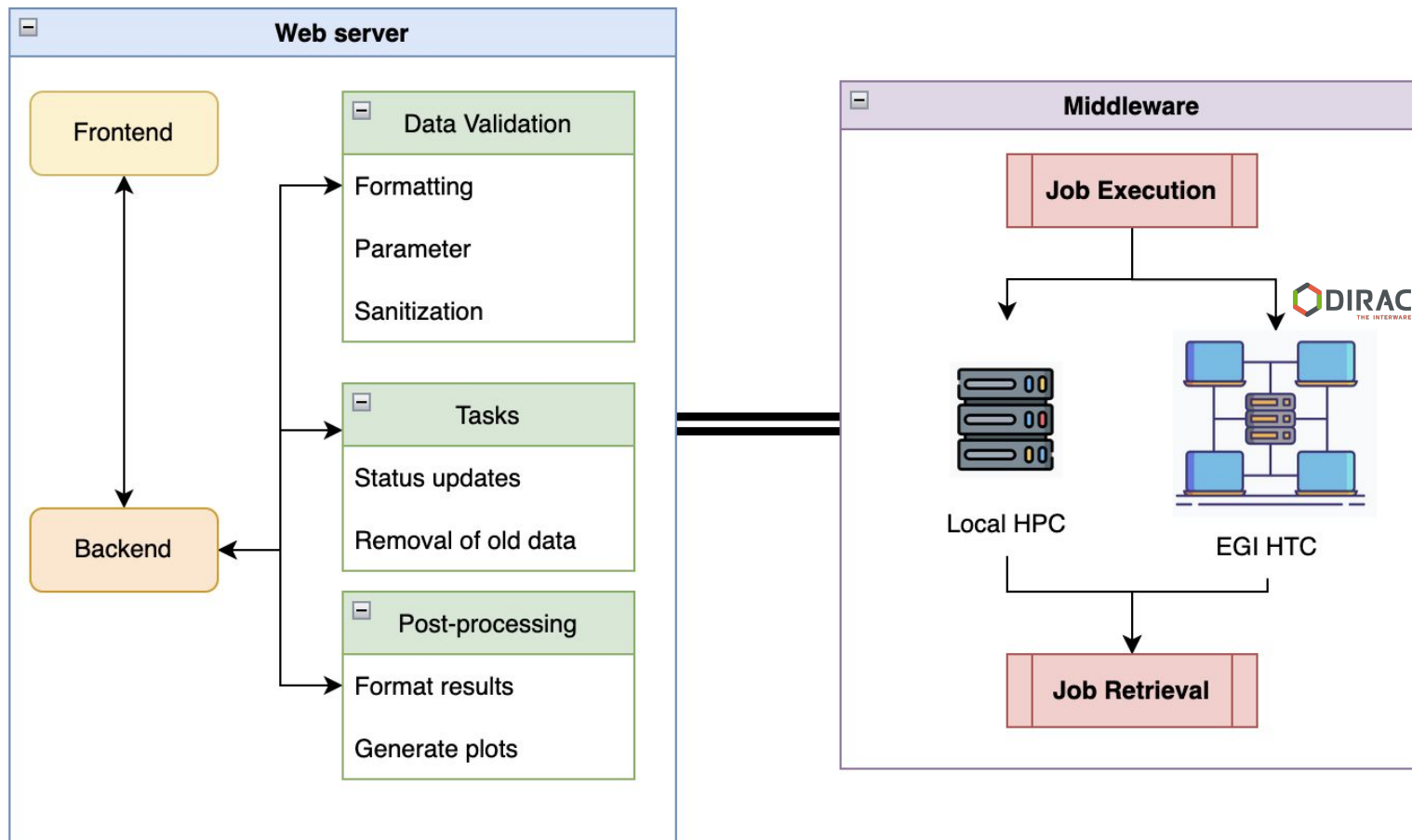
Computational methods developed by the academic groups are instrumentalized into applications and served as web services to the life sciences community

wenmr.eu



The screenshot shows the EOSC-WeNMR portal website. The header features the title "EOSC-WeNMR portal" and the handle "@Bonvinlab". Below the header is a navigation bar 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. The main content area includes a welcome message and a description of the portal's purpose: "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." Below this is a "Research" section with text describing the group's focus on developing reliable bioinformatic and computational approaches to predict, model, and dissect biomolecular interactions at the atomic level. To the right of the text is a 3D molecular model showing several protein structures in different colors (blue, green, orange, red) interacting with each other.

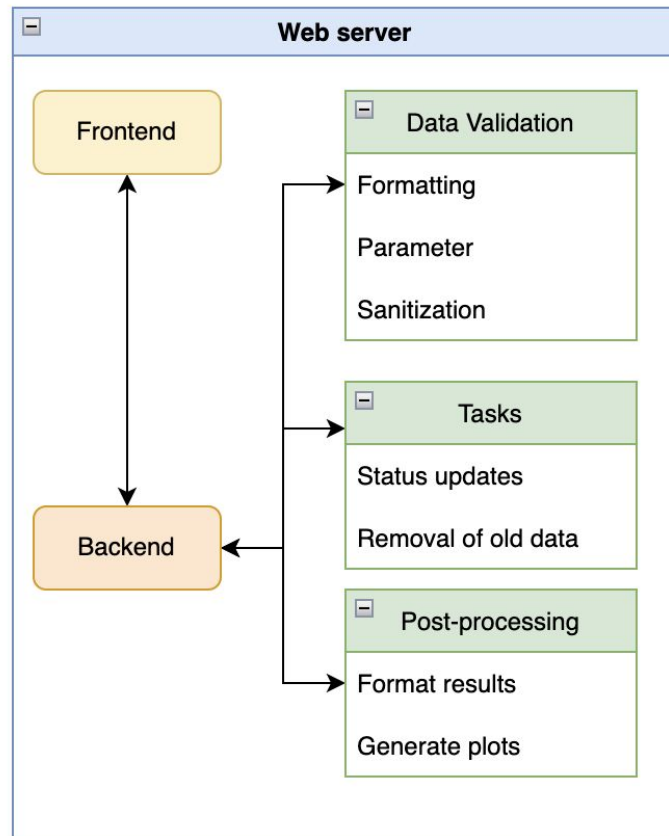
Under the hood



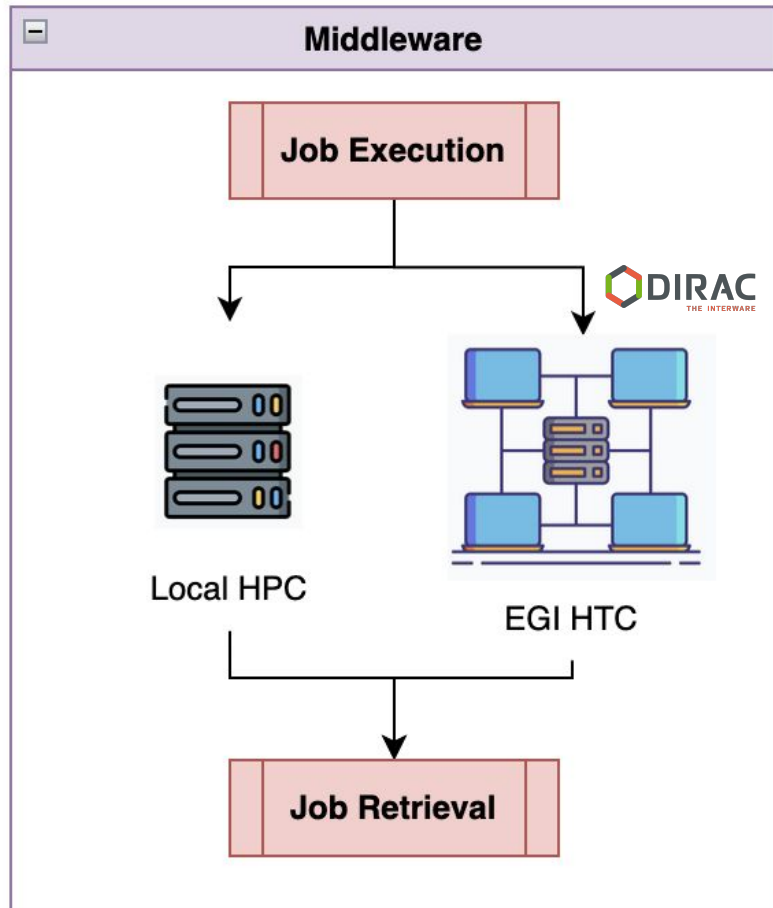
Under the hood

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
- User authentication
- Data validation & pre/post-processing
- *Server side execution of services with low footprint*



Under the hood



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 of *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

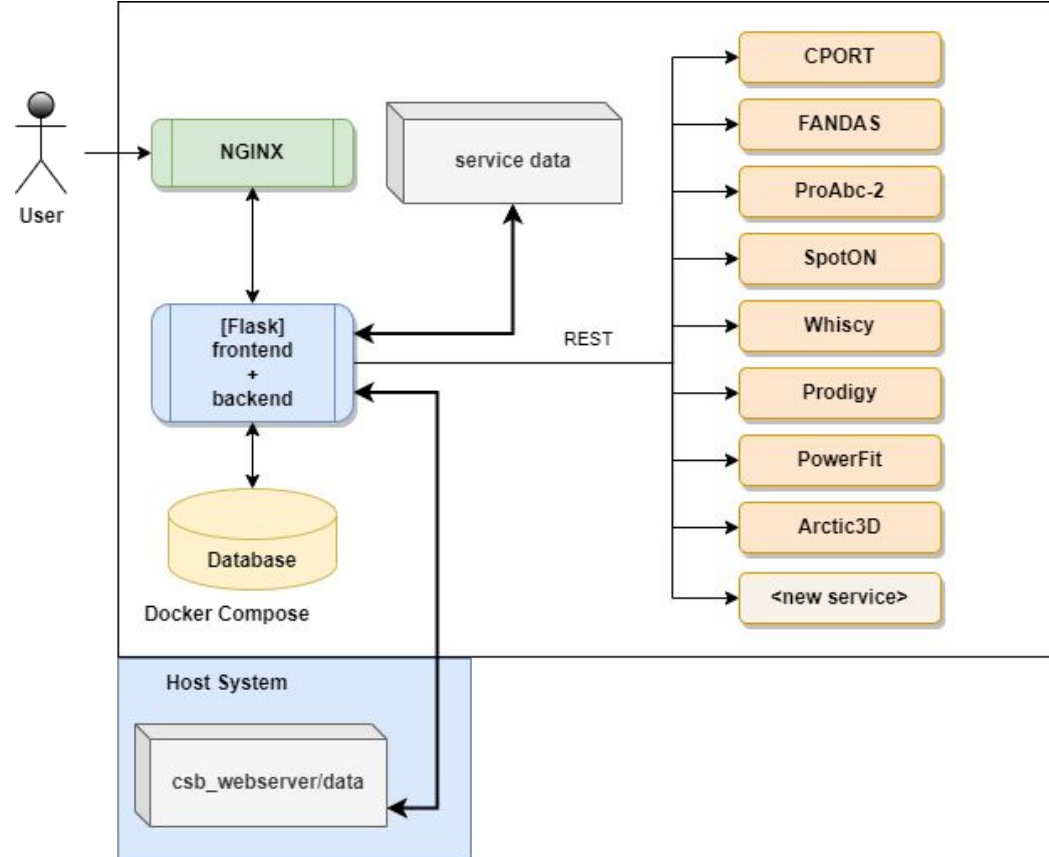
Development and Operation

Microservices

- Ongoing
- Containerization of tools
- Enabling standardized REST endpoints
- Off-site deployment

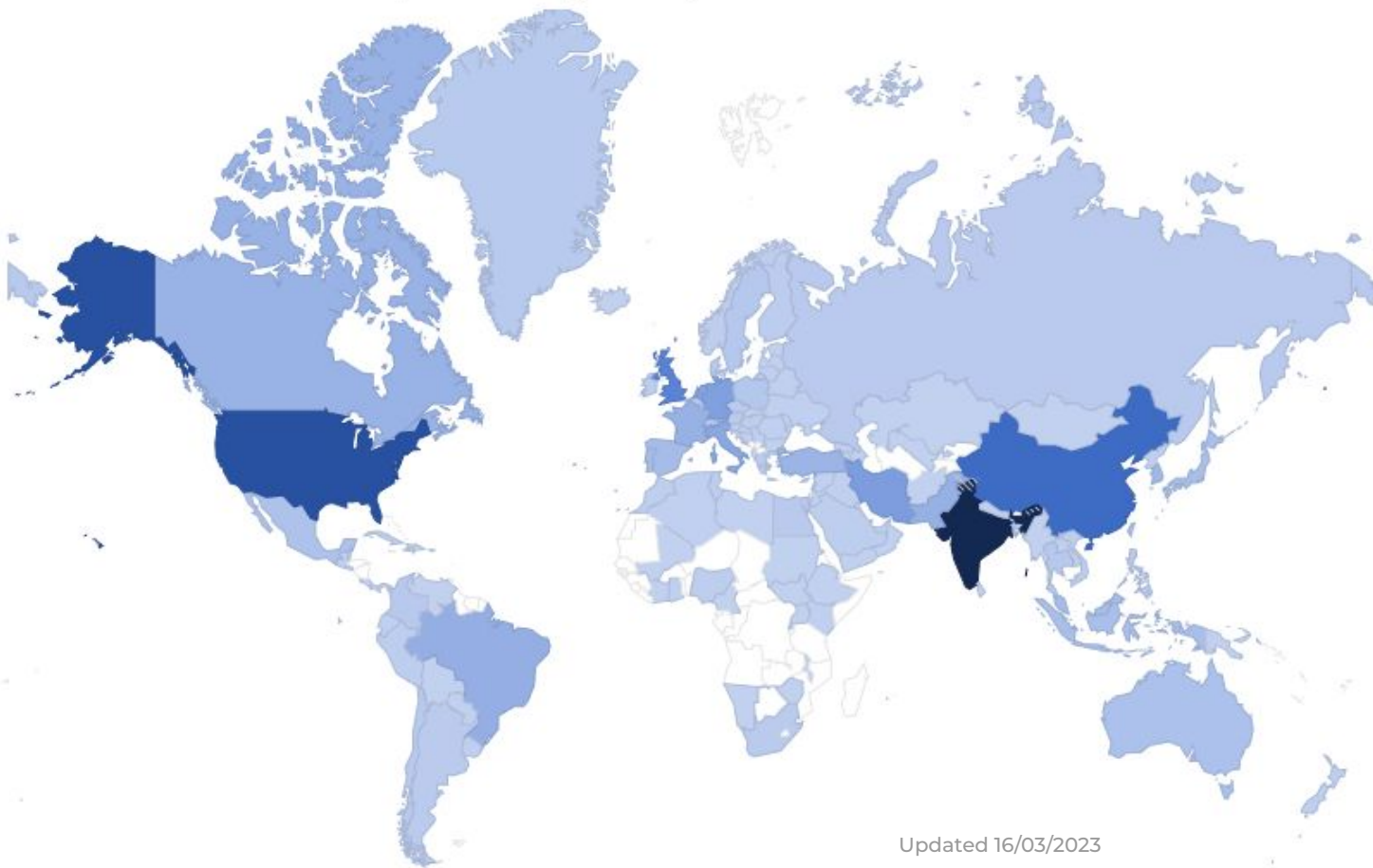
Scaling

- Migrating from Flask (Python) into React/Go

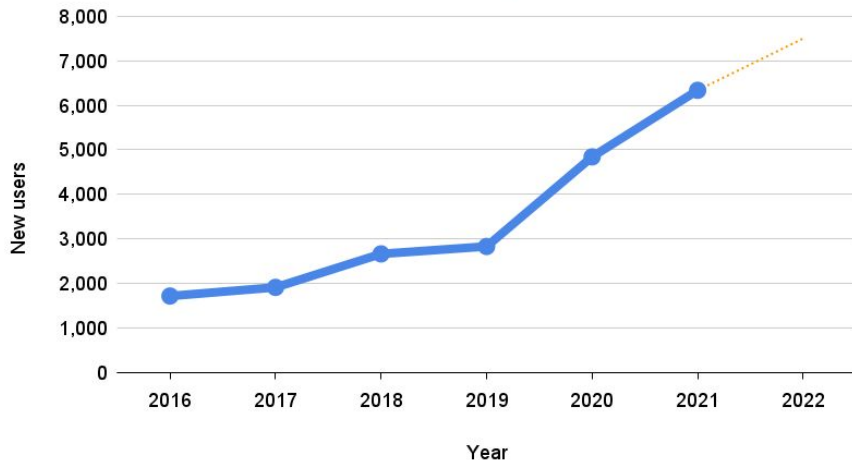


Worldwide User Map

The HADDOCK web portal is being used by **35004 users** across **136 countries**!



New HADDOCK Users per Year



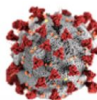
Worldwide Impact and Usage:



35,000+ users & 507,900+ submissions

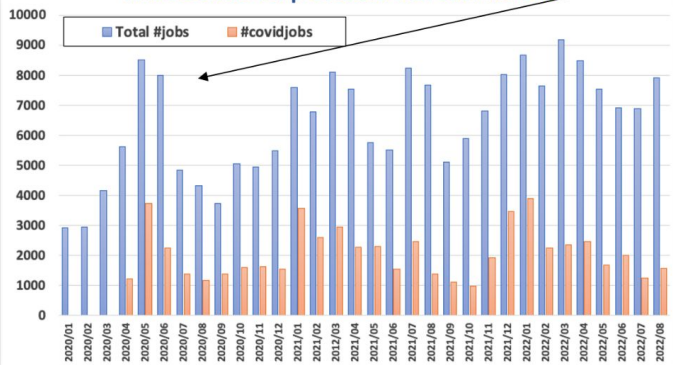
COVID-19 Support:

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

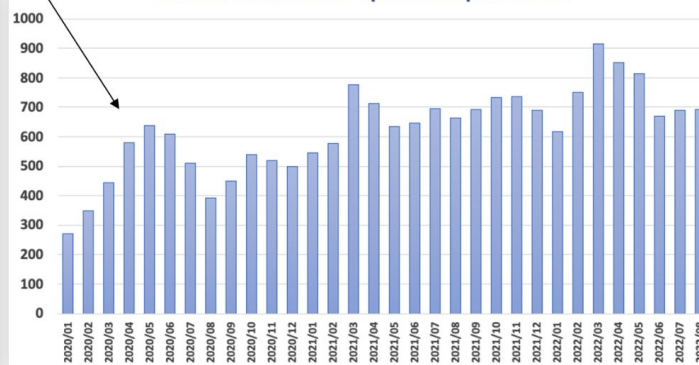


COVID19 effect

HADDOCK server processed user submissions



HADDOCK server unique users per month



wenmr.science.uu.nl



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 >>

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.

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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