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

EOSC-WeNMR

WeNMR is a worldwide e-infrastructure for Nuclear Magnetic Resonance (NMR) and Structural Biology
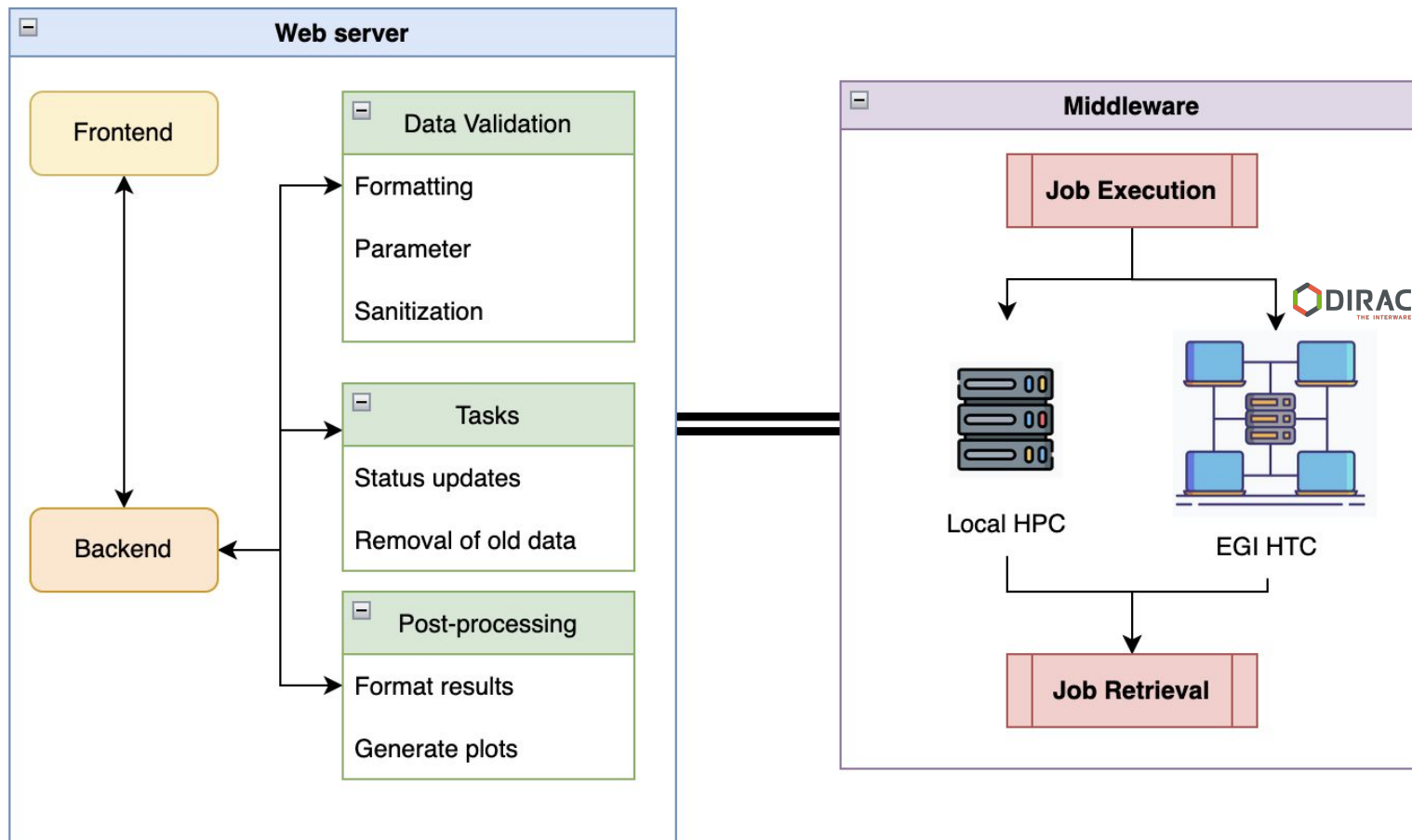
Computational methods developed by the academic groups are instrumentalized into applications and served as web services to the life sciences community

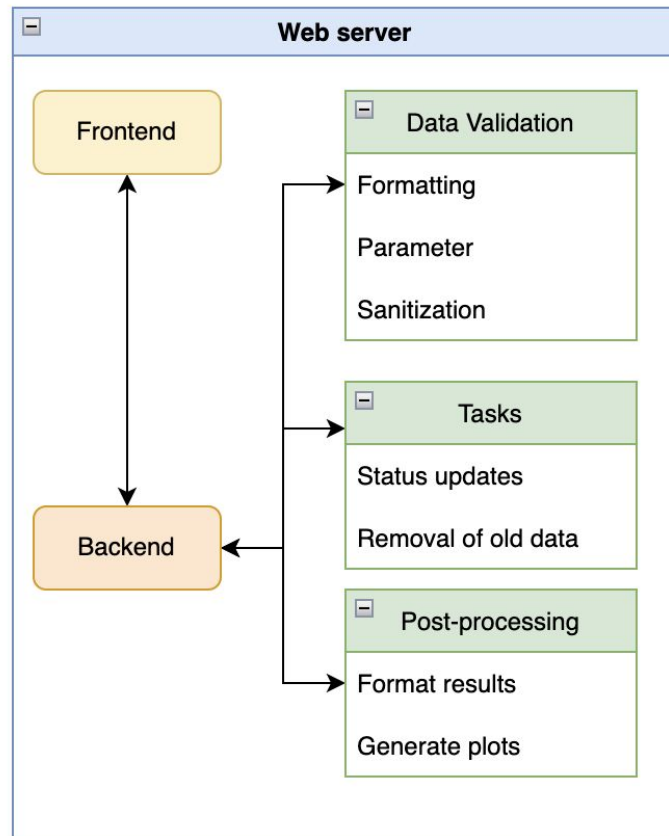**wenmr.eu**

bonvinlab.org

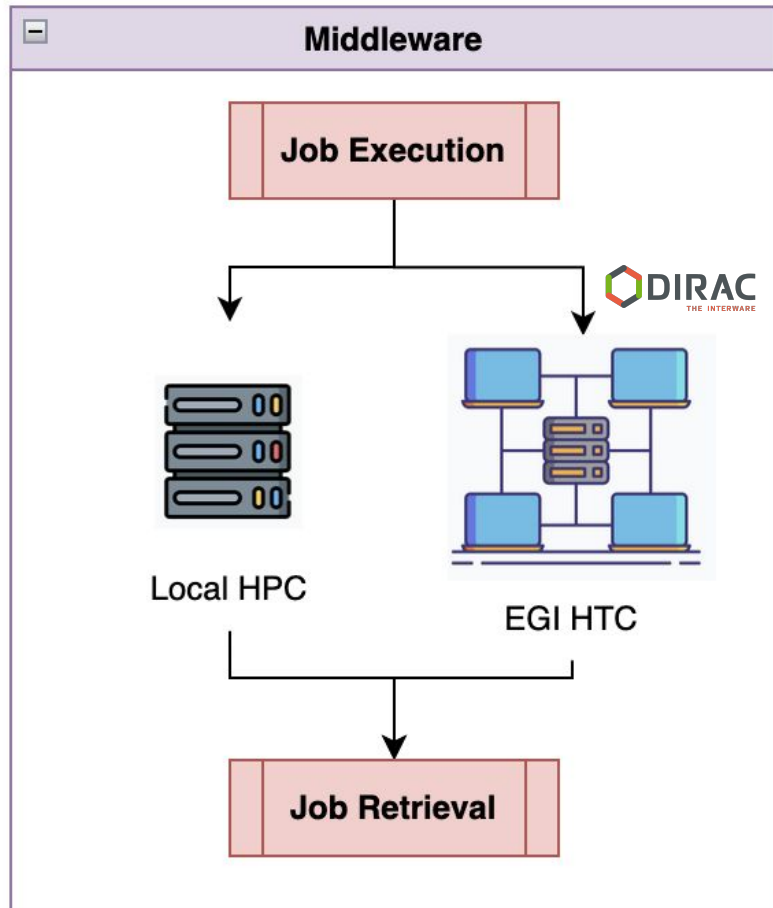Universiteit Utrecht

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

Development and Operation

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
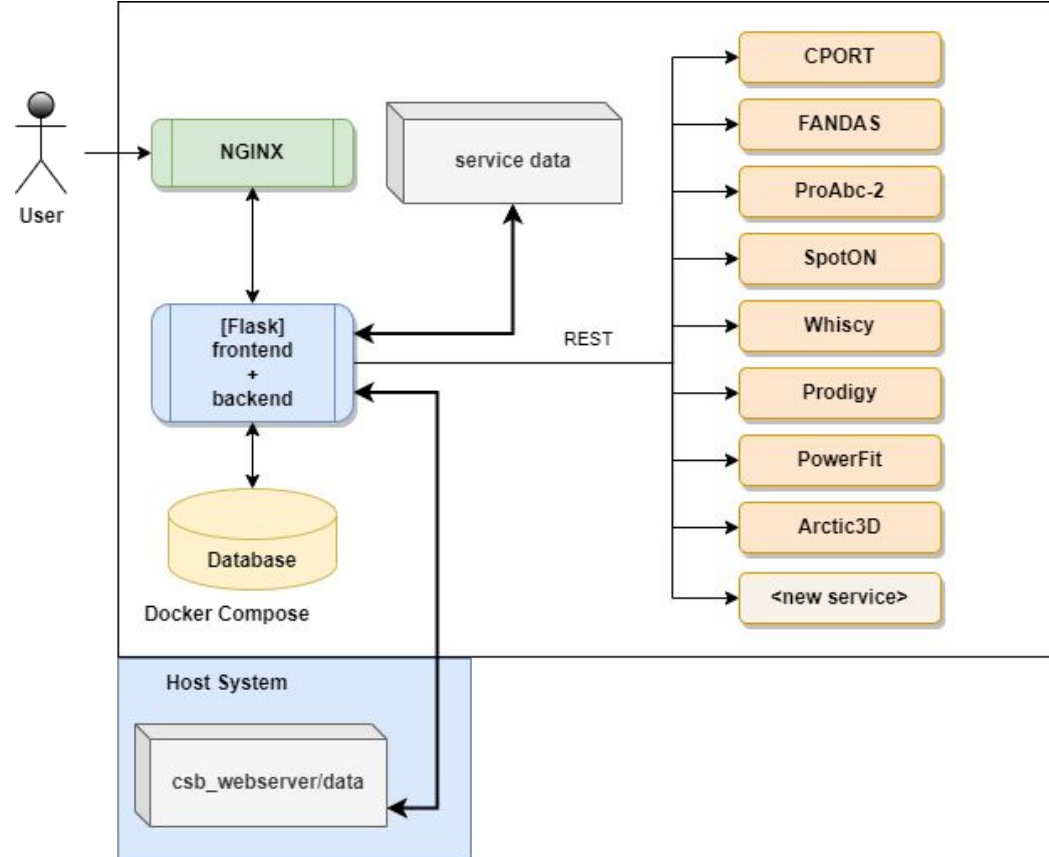
- Via docker-compose in dedicated resources

Development and Operation

Microservices

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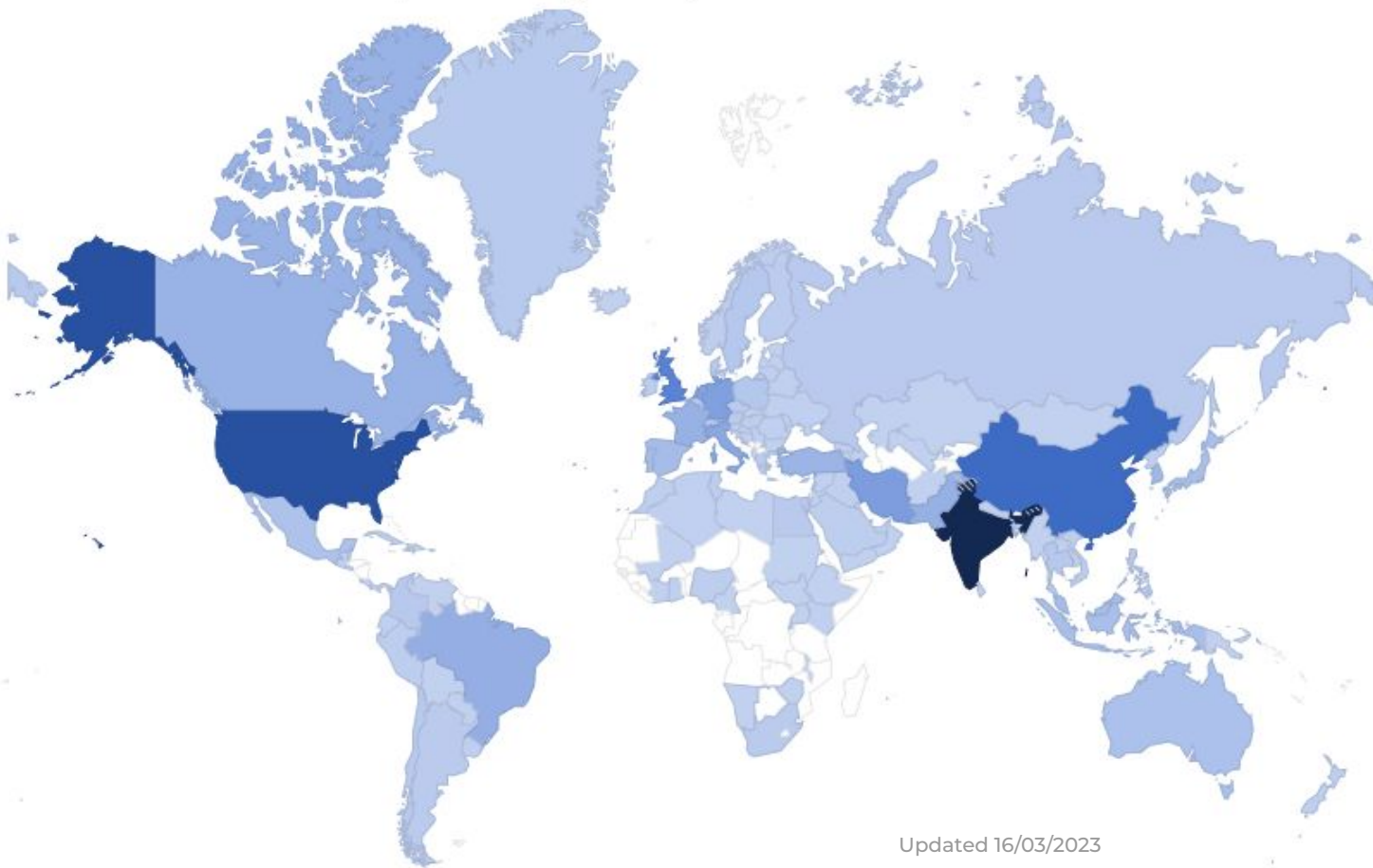- Enabling standardized REST endpoints
- Off-site deployment

Scaling

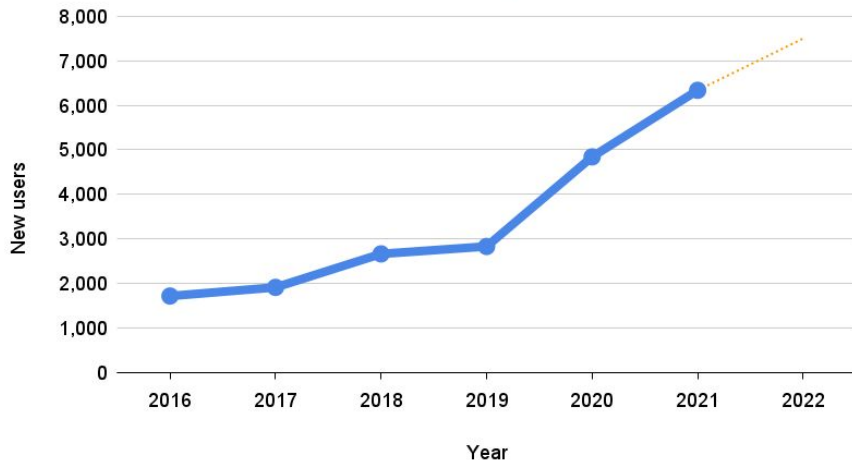- Migrating from Flask (Python) into React/Go

Worldwide User Map

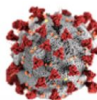The HADDOCK web portal is being used by **35004 users** accross **136 countries**!

Updated 16/03/2023

New HADDOCK Users per Year

Worldwide Impact and Usage:

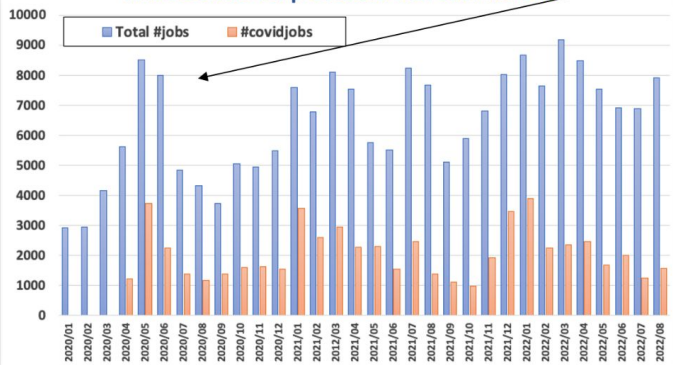35,000+ users & 507,900+ submissions

COVID-19 Support:

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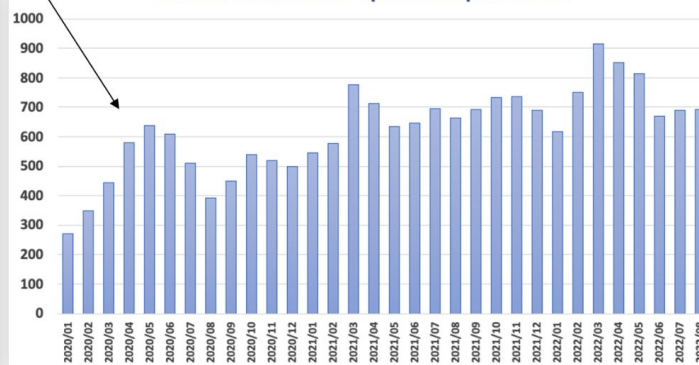- ~30% of all simulations since April 2020 are COVID-19-related

COVID19 effect

HADDOCK server processed user submissions

HADDOCK server unique users per month

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Thanks!

wenmr.science.uu.nl