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

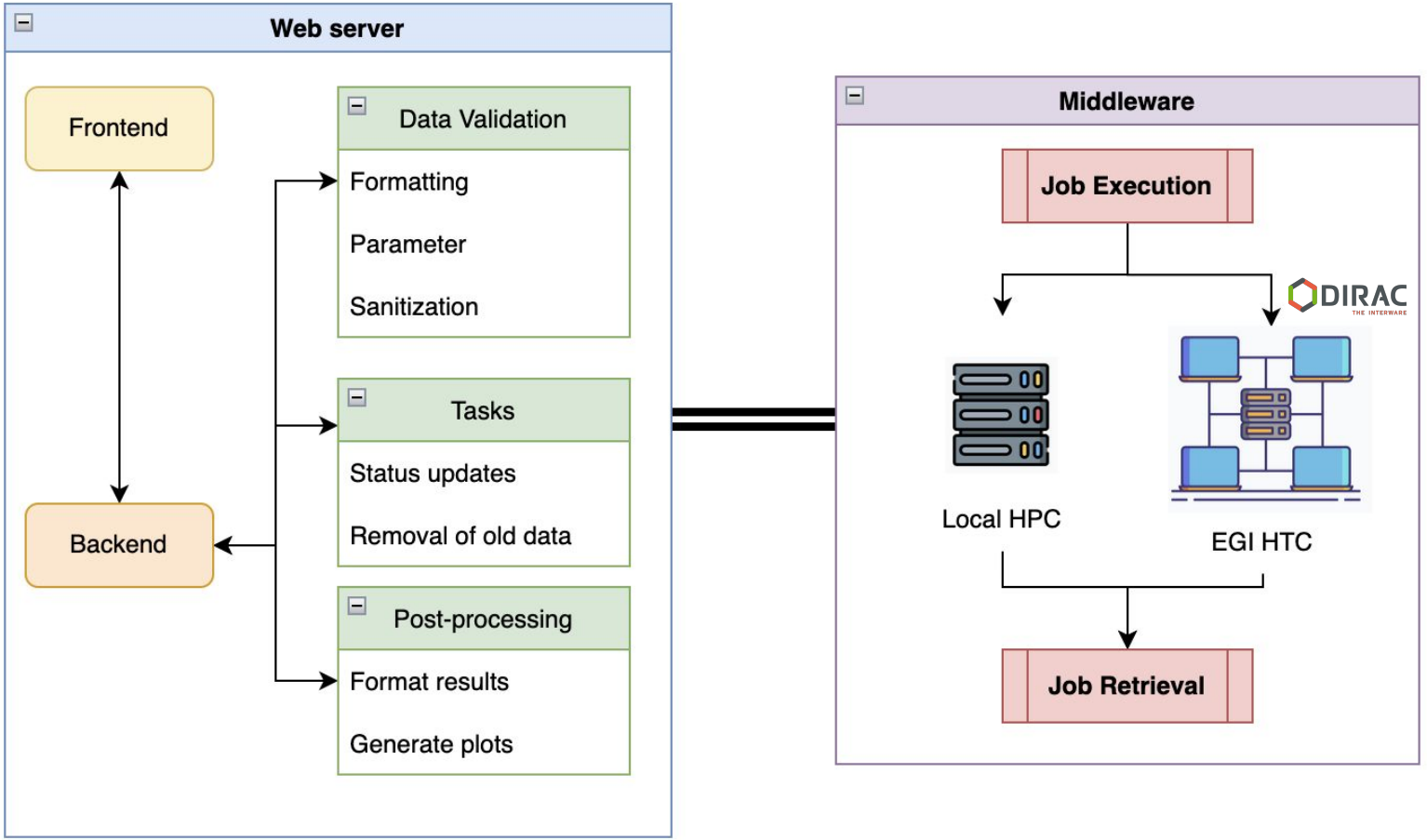
EOSC-WeNMR

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

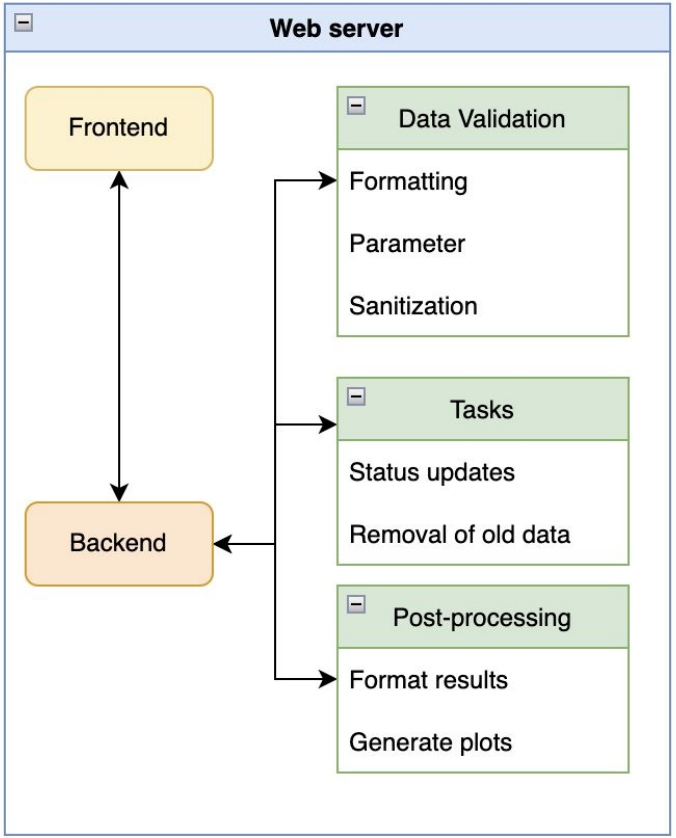
Under the Hood



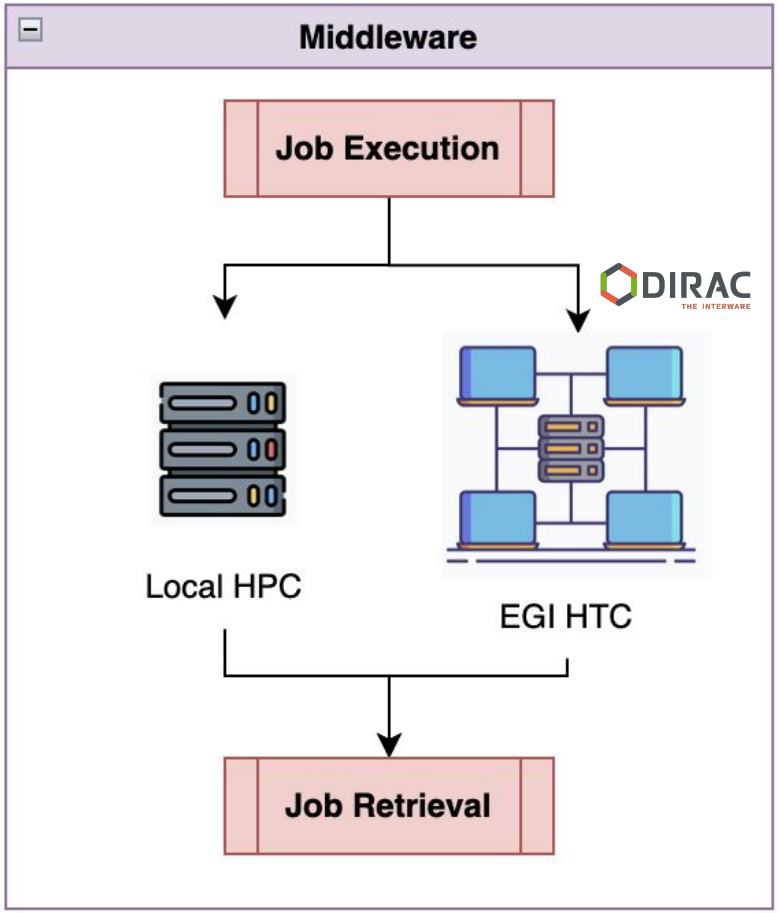
Under the hood

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 *in-house* shell scripts

Development and Operation

Code development

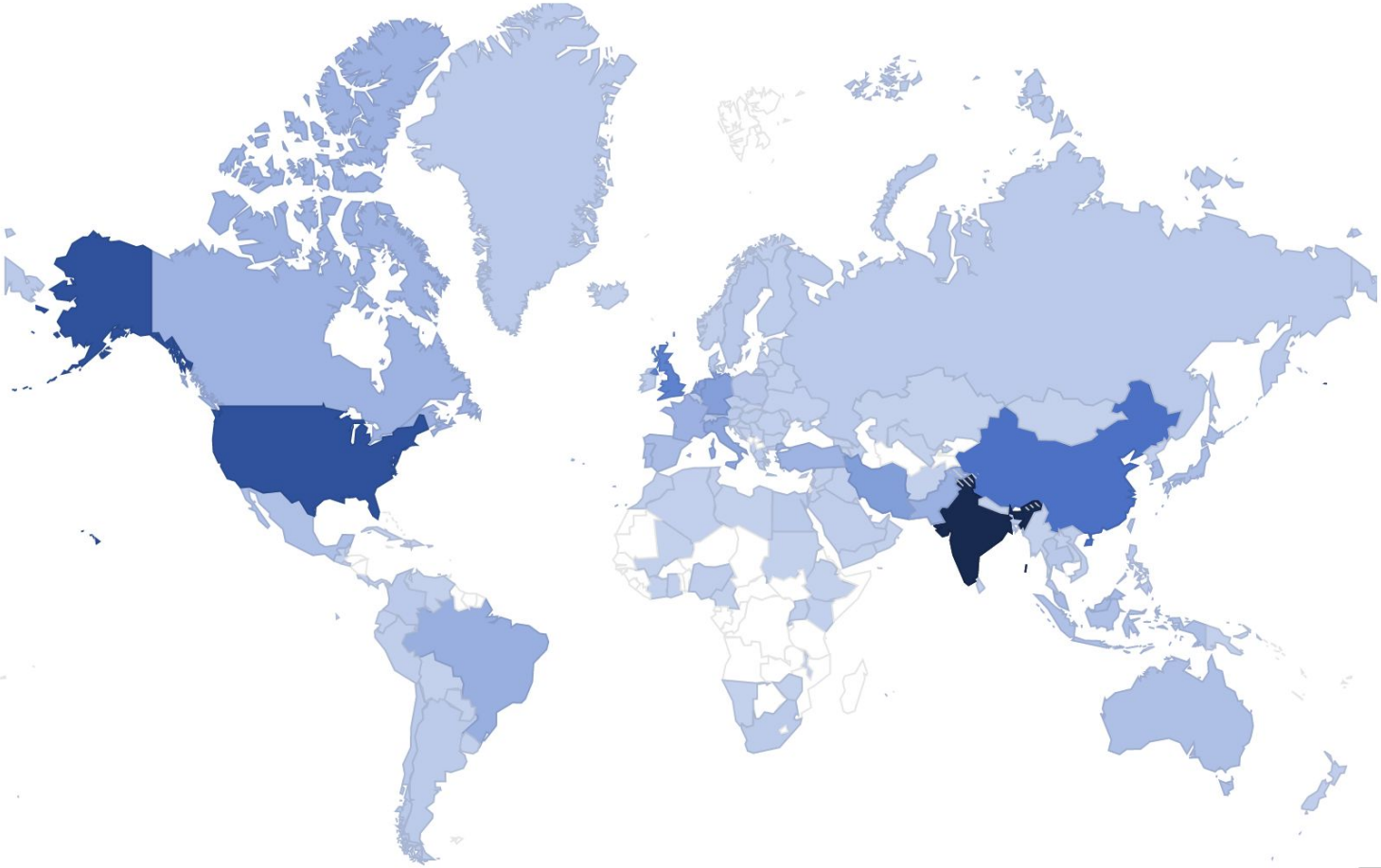
- Version control in GitHub
- Moved all services to a single monorepo
- Dedicated runner for continuous integration
- Continuous deployment currently being implemented with webhooks & dockerhub

Deployment

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

Worldwide User Map

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



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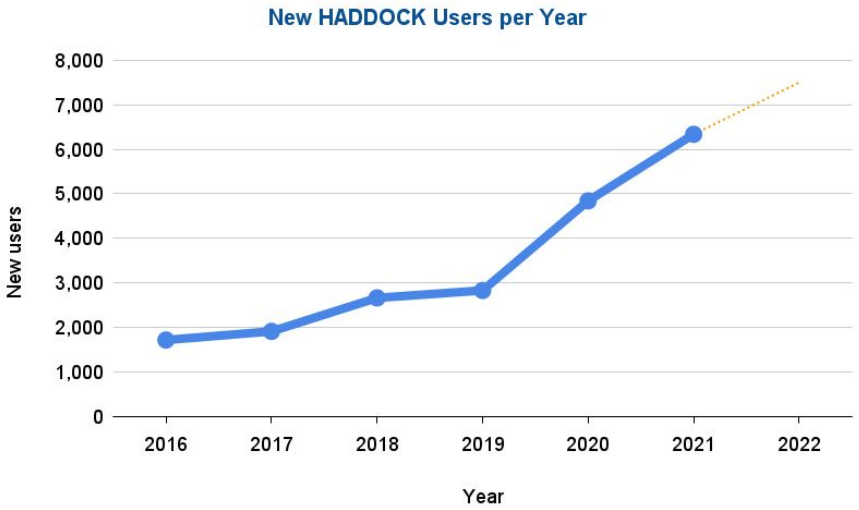
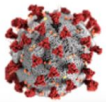


Worldwide Impact and Usage:

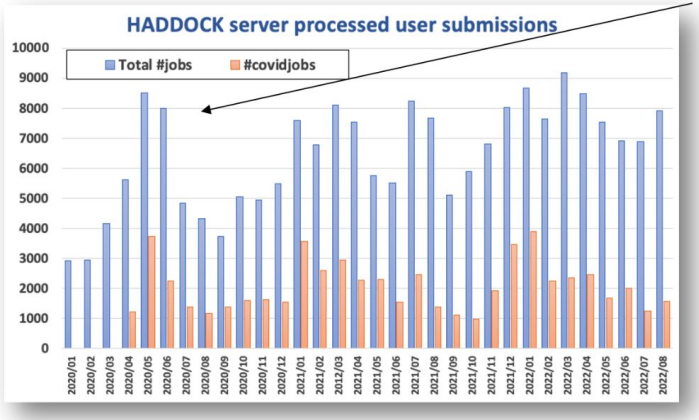
31,770+ users & 456,720+ submissions

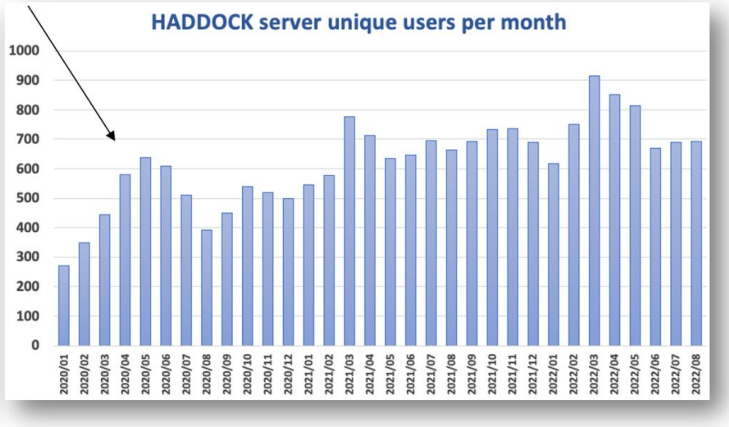
COVID-19 Support:

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



COVID19 effect





Thanks!

wenmr.science.uu.nl