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
Under the hood

Web server
- Frontend
  - Data Validation
    - Formatting
    - Parameter
    - Sanitization
  - Tasks
    - Status updates
    - Removal of old data
  - Post-processing
    - Format results
    - Generate plots
- Backend

Middleware
- Job Execution
- Local HPC
- EGI HTC
- Job Retrieval
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 across 136 countries!
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
Thanks!

wenmr.science.uu.nl