A worldwide e-Infrastructure for NMR and Structural Biology

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About

WeNMR is a Virtual Research Community (VRC) supported by EGI. WeNMR aims at bringing together complementary research teams in the structural biology and life science area into a virtual research community at a worldwide level and provide them with a platform integrating and streamlining the computational approaches necessary for data analysis and modelling.

The WeNMR VRC is represented by the University of Utrecht (UoU), CIRMMP-Florence, INFN-Padova and the consortium partners.

The Challenge

WeNMR provides biomedical scientists with a portfolio of portals for the study of molecular forces and biomolecular interactions to improve drug design, treatments and diagnostics. From a technical perspective, 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.

The operation of the WeNMR VRC has been in production for 10 years under various projects including: eNMR, WeNMR, EGI-Engage, West-Life and EOSC-hub. Starting from January 2021, the operation of the VRC will continue in the EGI-ACE project.

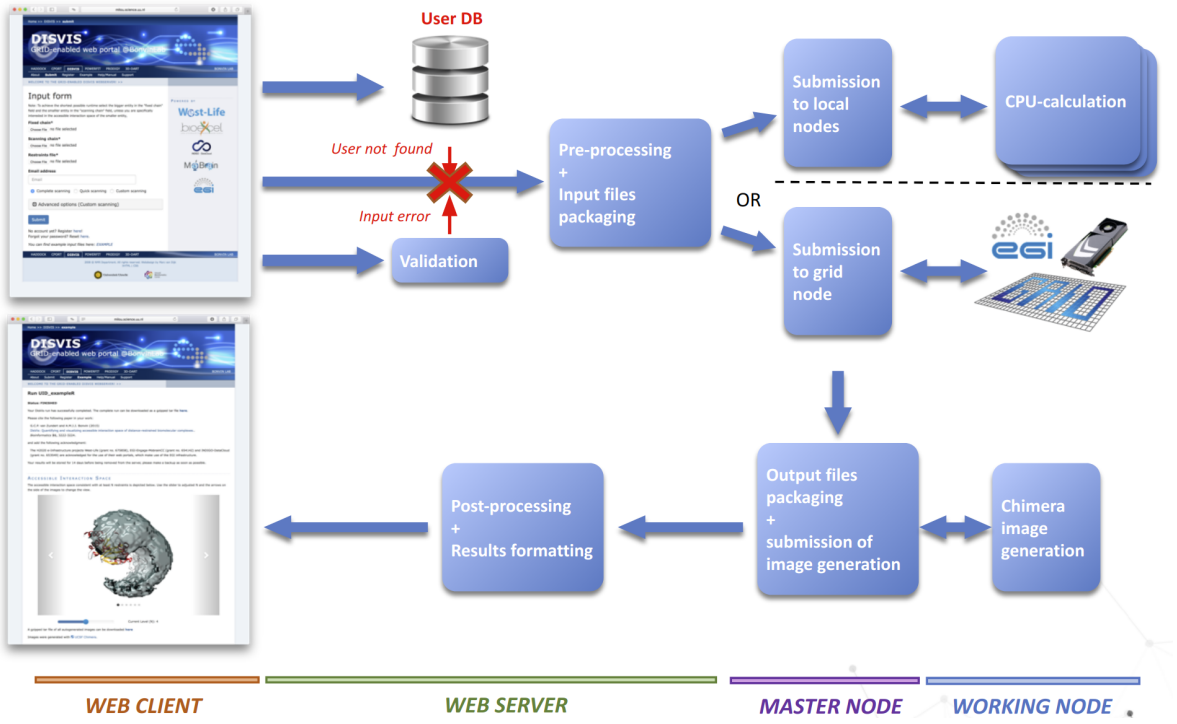
The WeNMR thematic services operated under EOSC-hub consist of eight individual platforms:

- AMPS-NMR, a web portal for Nuclear Magnetic Resonance (NMR) structures.
- DISVIS, to visualise and quantify the accessible interaction space in macromolecular complexes.
- FANTEN, for multiple alignment of nucleic acid and protein sequences.
- HADDOCK2.2, to model complexes of proteins and other biomolecules.
- HADDOCK2.4, to model complexes of proteins and other biomolecules.
- POWERFIT, for rigid body fitting of atomic structures into cryo-EM density maps.
- SPOTON, to predict Hot-Spots at protein-protein interfaces.

More details: https://bianca.science.uu.nl/

Architecture

The high-level architecture of the WeNMR services suite is shown in the figure below:



Expertise & Support from EGI

Starting from 2016, WeNMR signed an SLA (Service Level Agreement) with seven EGI data centres allowing the scientific communities to use High-Throughput Computing and Online Storage services needed to develop portals for life and brain scientists worldwide. Over the years, this collaboration agreement has been further extended. More specifically, a dedicated Competence Centre across the NGIs, involving user experts in the scientific domain, resource centres, and technology providers of the EGI Collaboration was set-up with the goal to further support the community needs. In the context of the EGI-ACE project, the agreement has been recently renewed until June 2023 in order to provide access to:

- 60 millions CPU hours (opportunistic access)
- 540 vCPU cores, up to 1.3TB of RAM and 8TB of block storage

EGI services used by WeNMR

The WeNMR services suite are based on:

- A web page front end to the service exposed to the user.
- A backend consisting of a variety of software and scripts.
- The EGI Workload Manager service for distributing compute jobs and of some gLite components in some cases.
- The EGI computing and storage resources such as the EGI High-Throughput Compute and the EGI Online Storage to distribute the computations.
- User registration and authentication mechanisms connected to EGI Check-In.

- The INDIGO-Datacloud udocker solution (some portals).

Modelling of various Sars-Cov2 human protein interactions

In 2020, as part of the EGI call for COVID-19 related projects, EGI contributed to port the HADDOCK in the EGI cloud resources operated by the providers supporting the WeNMR SLA and the resources provided by Open Science Grid (OSG). HADDOCK is an integrative platform for the modeling of biomolecular complexes. It supports a large variety of input data and it is also a core software in the BioExcel Center of Excellence to support COVID-19 researchers. Thanks to the cooperation already established between EGI, the Open Science Grid (OSG) and various high energy physics sites that committed to support COVID-19 related research, the HADDOCK platform was able to more than double its processing capacity, serving **on average ~550 active users per months**, **11,000 simulations related to COVID-19** (the equivalent of **~1.5 million HTC jobs**, **~2.7 million CPU hours**) on the EGI and OSC grid resources over the months of April to September 2020.

WeNMR in numbers

Users in the EGI Operations Portal

A total of **392** active users are registered in the EGI Operations Portal.

Number of users accessing the services

The scientific community is composed by: **>21,000** researchers and students registered across **>110** countries. The breakdown of the users accessing the WeNMR services suite is available here.

Usage of the EGI computing resources

Over the last 5 years WeNMR consumed more than **17 millions** of (HTC) and **3.5 millions** of (Cloud) CPU hours. For more updated usage, please check the metrics reported in the EGI Accounting Portal.

Resource providers supporting WeNMR

More than **32** HTC providers of the EGI Federation are supporting the WeNMR VRC. In addition, a Service Level Agreement with **10** providers was agreed with WeNMR:

- CESNET-MCC, Czech Republic,
- INFN-PADOVA-STACK and INFN-LNL-2, Italy,
- CESGA and IFCA-LCG2, Spain,
- NCG-INGRID-LP, Portugal,
- TW-NCHC, Taiwan,
- NIKHEF-PROD, SARA-Matrix, The Netherlands, and
- UA-BITP, Ukraine

For further details, about the collaboration agreement between EGI and WeNMR, please check the EGI documents repository.

Publications

The list of publications submitted by WeNMR can be found in Google Scholar, or in the OpenAIRE dashboard.

WeNMR Tutorials

A link to tutorials illustrating the use of various WeNMR portals are available here.

More information about WeNMR

Website: https://www.wenmr.eu/about/
EGI news:
https://www.egi.eu/news/egi-mobrain-collaboration-an-sla-for-better-research/
INSTRUCT:
https://instruct-eric.eu/haddock-screen-of-2000-approved-drugs-for-covid19
WeNMR in EOSC
The WeNMR services suite is published in the EOSC Marketplace.