

Keywords:

#Data, #OpenScience, #StructuralBiology, #Haddock, #WeNMR, #ResearchObjects, #EOSCinPractice

Empowering Global Collaboration in Structural Biology and Life Sciences

Unifying Research Teams and Streamlining Computational Approaches for Advanced Data Analysis and Modelling

The Project Involved



WeNMR is a Virtual Research Community which aims at bringing together complementary research teams in the structural biology and life science areas into a virtual research community at a worldwide level and providing them with a platform integrating and streamlining the computational approaches necessary for data analysis and modelling.

The Research Community

WeNMR serves a community of structural and computational biologists and life scientists distributed worldwide, covering over 135 countries. Researchers using WeNMR portals range from bachelor and master students through PhD students and post-doctoral researchers to advanced researchers. The majority of users are in academia and non-profit organisation, with some also coming from industry (pharma and biotech).

The Challenge

Structural biology is a field that focuses on understanding the intricate details of biological macromolecules at the atomic level, including their structural and dynamic properties. This knowledge is essential for understanding the majority of cellular processes and has various applications in fields like health and food sciences. The WeNMR initiative aims to provide valuable tools to the structural biology community while ensuring their accessibility in a user-friendly, efficient, and cost-effective manner. The challenge is to execute these tools in a distributed environment that optimizes their utilization, thus benefiting the wider scientific community.

Alexandre Bonvin

Scientific Director of the Bijvoet Centre for Biomolecular Research and Computational Structural professor at Utrecht University



"EOSC had a pivotal role in distributing the computational load by providing services that enabled job execution and computation. Furthermore, EOSC services facilitated user registration and authentication mechanisms, making it possible for researchers to access the tools provided by WeNMR."

EOSC service or tool used

Since 2009, WeNMR has collaborated with EGI, benefitting from a dedicated Competence Centre involving user experts in the scientific domain, resource centres, and the NGIs, the technology providers of the EGI, set up to further support the community needs. This activity allows the scientific communities to use High-Throughput Computing and Online Storage services to develop portals for life and brain scientists worldwide, also accessible on the EOSC Marketplace. EGI provided WeNMR with technical support to extend COVID-19-related research in the US using the computing resources provided by Open Science Grid. Additional consultancy and technical support were also offered to integrate the EGI Workload Manager in the WeNMR portals to facilitate the distribution of computing jobs.

Useful tips & tricks

EOSC services and tools have been implemented and refined over many years, in most cases in the context of European e-Infrastructure projects in which EGI was a partner or coordinator. Close collaboration with EGI experts over the years has been key to the smooth operation of WeNMR services. WeNMR services are described in the following publication: R. Vargas Honorato, P.I. Koukos, B. Jimenez-Garcia, A. Tsaregorodtsev, M. Verlato, A. Giachetti, A. Rosato and A.M.J.J. Bonvin. Structural biology in the clouds: The WeNMR-EOSC Ecosystem. *Frontiers Mol. Biosci.* 8, fmolb.2021.729513 (2021).



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Benefits and impact

The HADDOCK service, one of the services provided by WeNMR, has attracted an increasing worldwide community of users with exponential growth since 2008. The impact is only expected to grow in the coming years. In a recent survey (2022) on the users who submitted jobs since 2020 (~7,500, ~660 responses collected), 27% of users indicated they used HADDOCK for education and 95% for research. This indicates that the training of next generation scientists in using modern e-Science EOSC solutions results in them using those later on in their research. The impact on research is also evident from the responses, with 56% indicating they used WeNMR tools in disease/health-related research, 34% for drug and antibody design and 22% for COVID-19-related research.

Why do I need EOSC?

To achieve its goal, the WeNMR initiative developed a services suite comprising a front-end and a backend web page consisting of different software and scripts. EOSC had a pivotal role in distributing the computational load by providing services that enabled job execution and computation. Furthermore, EOSC services facilitated user registration and authentication mechanisms, making it possible for researchers to access the tools provided by WeNMR.

Across disciplines

WeNMR services are mostly used in disease/health-related research, but also find applications in food and material research, and have also become embedded in various educational programmes.

Useful material related to this story



wenmr.eu

Limitations and future improvements

WeNMR is working on making its services independent from the underlying hardware and operating system and easily deployable, for example, in EOSC cloud resources. This is an area where, with the support of EGI, WeNMR hopes to automate such deployments and scale up the services when needed.



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