Contribution ID: **19** Type: **Lightning talk**

WeNMR activities in the EOSC-Hub

Wednesday, 10 October 2018 16:40 (5 minutes)

Structural biology deals with the characterization of the structural (atomic coordinates) and dynamic (fluctuation of atomic coordinates over time) properties of biological macromolecules and adducts thereof. Since 2010, the WeNMR project has implemented numerous web-based services to facilitate the use of advanced computational tools by researchers in the field, using the grid computational infrastructure provided by EGI [1]. These services have been further developed in subsequent initiatives, such as the West-Life VRC (www.west-life.eu). In particular, the latter project developed implementation of a cloud storage solution, called VirtualFolder [2], which allows the user to connect to her/his account on B2DROP or on public clouds. This solution has been implemented in several thematic portals in order to allow input data to be downloaded from and calculation results to be uploaded to the users cloud storage. Regarding AAI, the thematic portals are transitioning, also in response to the GDPR, to the EGI SSO or other systems that are compatible with it. Finally, all the thematic portals that send calculations to the grid infrastructure are now making use of DIRAC [3].

[1] Wassenaar TA, et al. WeNMR: Structural biology on the Grid. J. Grid. Computing 10:743-767, 2012

[2] https://portal.west-life.eu/virtualfolder/

[3] https://github.com/DIRACGrid/DIRAC

Type of abstract

Lightning Talk

Summary

The WeNMR thematic portals provide a variety of user-friendly solutions for researchers working in Structural Biology. Within the EOSC-Hub initiative, our thematic portals are implementing a number of state-of-the-art solutions to enhance their compatibility with the infrastructure, improve usability and development and remove legacy solutions. The new solutions address aspects from cloud storage to AAI.

Primary authors: BONVIN, Alexandre (eNMR/WeNMR (via Dutch NGI)); ROSATO, Antonio (CIRMMP); Dr VERLATO, Marco (INFN)

Presenter: ROSATO, Antonio (CIRMMP)

Session Classification: Lightning Talks

Track Classification: Lightning Talks