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Structural biology in the clouds: The HADDOCK/WeNMR-EOSC Ecosystem

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Structural biology aims at characterizing the structural (atomic coordinates) and dynamic (fluctuation of atomic coordinates over time) properties of biological macromolecules. Gaining insight into 3D structures of biomolecules is critical for understanding the vast majority of cellular processes, with direct application in health and food sciences.

Since 2010, the **WeNMR** project (www.wenmr.eu) has implemented numerous web-based services to facilitate the use of advanced computational tools by researchers in the field, using the HTC infrastructure provided by EGI. These services have been further developed in subsequent initiatives under H2020 projects are a now operating as Thematic Services in the EOSC-Hub project (www.eosc-portal.eu), with the **HADDOCK** portal (haddock.science.uu.nl) sending >10 millions of jobs and using ~4000 CPU-years per year.

We will summarize 11 years of successful use of e-infrastructure solutions to serve a large worldwide community of users (>18'000 to date), providing them with user-friendly, web-based solutions that allow to run complex workflows in structural biology. We will in particular share our experience operating and deploying those services from the provider point of view with a focus on sustainability and easy of deployment of the services, making use of containerization technologies.

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