Contribution ID: **31** Type: **Oral Presentation**

Customizable Integrative Modelling Workflows with HADDOCK3

Monday, 21 March 2022 14:30 (30 minutes)

HADDOCK3 is a ground-up rework of our well-established flagship software for integrative modelling with as main goals improved extensibility, modularization, testability and documentation in order to allow a high degree of customization. The core routines of HADDOCK have been modularized and the underlying python interface adapted so that these core modules, as well as new ones, including third party software, can be organized in different manners to generate custom workflows. This modularity is the most significant contrast with the previous HADDOCK2.x version which is running a fixed workflow. In HADDOCK3, users and developers can create their own project-specific modules that can be easily integrated into the HADDOCK machinery to best suit their research goals. This redesign directly benefits our efforts towards exascale computing in the context of the BioExcel Center of Excellence (https://www.bioexcel.eu) . We divided the new Python-shell architecture managing HADDOCK3 functionalities into independent building blocks, such as: non-variable physical parameters, command-line interfaces, plug-ins, the CNS code for the actual simulations, and most importantly, the functional modules configuring for each calculation stage. We can manage each of these blocks and blocks' pieces independently, adding or removing them without breaking the remaining of the software. To achieve this pipelining capacity, we have developed a dedicated input/output system that homogenizes the I/O interfaces of the modules. Thus, the only requirement to assemble two modules is that the output of the first conceptually (scientifically) matches the input of the next module. This new modular version of HADDOCK is available as an open-source repository at https://github.com/haddocking/haddock3

Primary authors: HONORATO, Rodrigo (Utrecht University); CORREIA TEIXEIRA, Joao Miguel (Utrecht University); BONVIN, Alexandre M.J.J. (Utrecht University)

Presenter: HONORATO, Rodrigo (Utrecht University)

Session Classification: Health & Life Science Applications

Track Classification: Track 2: Health & Life Sciences (including Pandemic Preparedness Applications)