JUPYTER: GOD OF HUMAN-CENTRIC SCIENTIFIC COMPUTING

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Scientific computing became nowadays important in all academic disciplines, including arts and humanities. It is not always meant to be a typical "number crunching", where lengthy calculation jobs are being sent to a HPC facility for processing and then the received results are evaluated and used further, possibly to prepare even more calculation jobs and so on. Such an approach, although still common in many areas of research, seems to be ineffective and hardly reproducible exactly if necessary. Quite often it is also necessary to write some extra computer code dedicated to a particular task. It is very easy to loose track which piece of code belongs to which task without keeping precise notes. A “computational notebook”, as introduced in many computer algebra systems, offers a remedy to such problems, providing also a natural human interface to work with code and data, but usually only within a single dedicated computational system. Recently, the Jupyter notebook interface [1], together with the respective free and open-source software developed around [2], became a *de facto* standard for interactive computing and sharing the results in a reproducible way. Jupyter notebooks are designed as programming language agnostic and based on open standards, without limitations to a particular environment.

Since the last year, in order to provide unified interactive access and management for students and research groups, more and more computing facilities at our Alma Mater were organized with Jupyter-based software. Jupyter Hub servers are used for spawning individual single-user Jupyter Notebook or Jupyter Lab instances, each with full access to the user assigned computational resources, and at the web browser level. This contribution summarizes our efforts in making scientific computing more human-centric, with Jupyter help.

References:

[1] T.Kluyver & al.: “Jupyter Notebooks—a publishing format for reproducible computational workflows”, pp. 87-90, in: “Positioning and Power in Academic Publishing: Players, Agents and Agendas”, F. Loizides and B. Schmidt (Eds.), IOS Press, Amsterdam (2016).

[2] Project Jupyter: <http://jupyter.org/>