Bringing together open source scientific software development for HPC and beginners

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In the scope of the National Research Data Infrastructure Germany (NFDI) [1] we develop and maintain a knowledge-base with guides and best practices about scientific software development – available at https://nfdi4ing.pages.rwth-aachen.de/knowledge-base/.

With the knowledge-base we pursue the goal to make sustainable software development possible for everybody. Most importantly, we want to encourage people without strong computer science background to apply fundamental best practices, e.g., version control, from the start. We believe this is necessary since many engineers – and not computer scientists – write scientific code. Starting from version control, the topics range to fully automated experiments using CI/CD workflows. Many of the existing examples concern OpenFOAM development due to the knowledge-base’s heritage in TU Darmstadt’s CRC 1194 [2]. Since then, we also are working with the Lehrstuhl für Hydromechanik und Hydroystemmodellierung (LH²) [3] as well as with the Institute of Wasserbau [4] and the Institute of Fluidsystemtechnik [5] at TU Darmstadt.

While curating the content, which we maintain in a Gitlab repository using the HUGO website generator, we realized that one of the most important additions that we provide is an actively maintained and simple glossary. Especially for people not yet very familiar with the technologies used, the pure number of terms can be intimidating and confusing. Our glossary helps by providing brief explanations of relevant terms used throughout the articles. An addition for which we modified the actual HUGO template is that we provide a taxonomy of articles rather than a pure folder structure to ease the navigation.

The knowledge-base is an on-going effort in which we appreciate feedback and contributions. In the presentation, we will take a closer look on the different materials provided for people developing software, people using software, and how people can actively contribute to the knowledge base through our peer-review process and material creation.

[3] Chair for Hydromechanik und Hydroystemmodellierung at University of Stuttgart https://www.iws.uni-stuttgart.de/lh2/