Contribution ID: **9** Type: **Talk**

A concrete CSE workflow framework for FAIR numerical experiments: A multi-layered approach

Wednesday 16 October 2024 17:00 (30 minutes)

Numerical algorithms and computational tools are essential for managing and analyzing complex data processing tasks. As meta-data and parameter-driven simulations have become more prevalent, the need for automated workflows to reproduce computational experiments across platforms has
significantly increased. In general, a computational workflow is defined as a step-by-step description for accomplishing a scientific objective. Characterized through their input-output relation, computational workflows are designed such that the associated meta-data can be used
interchangeably and redundantly. In the present work, we develop a computational framework, namely, MaRDIFlow, that focuses on the abstraction of meta-data while negating the underlying dependencies through multi-layered descriptions. Notably, by allowing the complete range between abstract descriptions and concrete numerical realizations (or even plain input-output data) of the tasks to serve equivalently and possibly redundantly in the definition of the workflows, we provide
the lowest possible barrier for findable, accessible, interoperable and reusable (i.e. FAIR) workflow definitions. We showcase minimum working examples and how they are systematically incorporated into our workflow framework.

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Session Classification: Contributed