

A Multi-Layered CSE Workflow Framework for FAIR Numerical Experiments

Tuesday 18 February 2025 15:30 (1h 15m)

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: Poster Presentations