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Design of a Workflow Description for Documentation and Integration of FAIR Computational Experiments

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Numerical algorithms and computational tools are essential for managing and analyzing complex data processing tasks. With increasing meta-data awareness and parameter driven simulations, the demand for reliable and automated workflows to reproduce computational experiments across platforms has grown.

In general, computational workflows describe the complex multi-step methods that are used for data collection, data preparation, predictive modeling, and simulation in various engineering applications. They are characterized through their input-output relation such that the associated meta-data can be used interchangeably and redundantly.

In this regard, we develop a prototypical CSE workflow that abstracts the multi-layered components from computational experiments. As a case study, we incorporate the time-dependent Stokes-Darcy solver [1] into our workflow, and execute the coupled system of free flow adjacent to a permeable porous media via the monolithic block-preconditioning scheme implemented entirely in the DuMux framework. Within this example, we focus on solver approaches for the coupled problem, and determine the run time and memory behavior of the system. Moreover, the workflow adheres to FAIR principles, such that abstracted components are Findable, Accessible, Interoperable, and Reusable [2]. Lastly, we discuss how the CSE workflow description presented here as a part of the MaRDI consortium serves as a scientific tool for research data management in numerical mathematics.

References:

[1] Schmalfuss, J., Reithmueller C., Altenbernd M., Weishaupt K., Goeddke D., "Partitioned Coupling vs. Monolithic Block-Preconditioning Approaches for Solving Stokes-Darcy Systems." *arXiv preprint* arXiv:2108.13229 (2021).

[2] Carole G., Sarah C-B., Stian S-R., Daniel G., Yolanda G., Michael R. C., Kristian P., Daniel S., FAIR Computational Workflows. *Data Intelligence* 2020; 2 (1-2): 108–121.

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Sitzung Einordnung: Contributed Talks