

# Expanding an Ontology with semantically linked CFD-Simulation Data by Segmentation into reusable Concepts

Mittwoch, 26. Oktober 2022 15:40 (25 Minuten)

Computational-Fluid-Dynamics (CFD) simulation and other numerical simulation tools generate a rich variety of complex (meta-)data, which are inherently difficult to store in a FAIR manner (Findable-Accessible-Interoperable-Reusable). As the amount of data generated by such simulations is one of the major challenges, meta-data, e.g. the simulation settings and major output variables, offers the possibility of restoring, revising, and re-evaluating existing simulations. However, due to the linked nature of the parameters of such simulations, classifying and storing metadata in a standardized manner is difficult. Ontologies are key to the FAIRness of such data, as they inherently classify the data and are capable of reasoning and querying.

As storing large amounts of linked data in ontologies comes with its challenges, a segmentation method is introduced for data condensation and pre-classification. The method proposed here uses nested python dictionaries in the form of JSON files and populates an existing ontology with respective simulation data. Those nested dictionaries represent the linked structure of the setting options and are either given or can be generated from existing simulations (e.g. the CFX command language from ANSYS). These dictionaries are segmented into sub-dictionaries, representing main concepts, which are then archived and related between different simulation dictionaries to pre-classify the data. The population of the ontology is performed via the above-mentioned sub-dictionaries. This condenses the data by linking and reusing concepts between multiple simulations.

While this method is generic in its concept, the workflow has already been performed by converting the results of simulations into meta-data, populating an ontology with such data, and evaluating the results. Important steps in the workflow are already solved, such as the population of arbitrarily named entities that occur throughout the dictionaries, the multiplicity of concepts, varying linkages, and renaming into semantically aligned classes.

As the number of manual inputs is minimized, which are required to populate the ontology with the given data, a non-expert operable and FAIRer storage was achieved.

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**Sitzung Einordnung:** Contributed Talks