

# Automation of Workflows for Numerical Simulation Data and Metadata

*Freitag, 9. Juni 2023 09:15 (15 Minuten)*

Recording the workflow of numerical simulations and their postprocessing is an important component of quality management as it, e.g., makes the CFD result files reproducible. It has been implemented in an existing workflow in coastal engineering and has proven its worth in practical application.

The data history recording is achieved by saving the following information as character variables together with the actual results in CF-compliant NetCDF files:

- content of the steering files
- parameterization of simulation and postprocessing
- name of initial and boundary datasets
- name and version of the used simulation and analysis programs

Each program inherits this information from its predecessor, adds its own information, e.g., its steering file, and writes both old and new information in its result file. As a consequence, a researcher can, by downloading just the result file of the last program in the processing chain, access the recorded metadata of the whole chain.

In order to make use of these data, a second automated workflow has been established to archive the results and store the metadata in a Metadata Information System (<https://datenrepository.baw.de>). A Java-based post-processor has been extended to evaluate the above mentioned NetCDF files and convert the information into ISO compliant files in XML format. The postprocessor starts copying the numerical results into a long-term storage via a REST interface and, in case of a successful copy, imports the XML metadata into the Metadata Information System (MIS) via a CSW-T interface. The MIS offers interactive search and download links to the long-term storage.

Both workflows follow the FAIR principles, e.g., by making numerical results and their metadata available to the public. The automation eliminates the error-prone manual editing and processing, relieves the user and assures quality.

**Hauptautor:** Herr SCHADE, Peter (Bundesanstalt für Wasserbau)

**Co-Autoren:** Dr. KÖSTERS, Frank (Bundesanstalt für Wasserbau); Herr ARIF, Mohammad Shafi (Bundesanstalt für Wasserbau)

**Vortragende(r):** Herr SCHADE, Peter (Bundesanstalt für Wasserbau)

**Sitzung Einordnung:** Talks