A Metadata-Driven Management System for Numerical Modeling

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***Abstract*— Research in hydroinformatics extensively studies approaches on reducing the complexity of modeling processes. Input data, the CFD-processing and visualization of results are combined in various ways into so-called integrated modeling frameworks or management systems. Community Modeling Systems (CMS) provide users with a concentrated view on data handling and coupling resources and models, in particular. Unfortunately, most web-based hydroinformatics environments lack consistent, standardized documentation of the modeling process. A reusability or reproducibility outside a CMS is only given for single elements like standardized webservices or metadata descriptions for datasets. Using elements of Spatial Data Infrastructures (SDIs), we propose a concept for a metadata-driven architecture for Computational Fluid Dynamics simulations and to integrate model descriptions into SDIs. We illustrate the abilities of such a metadata-based system with two use cases an extensive outlook.**

Keywords—metadata; data management system; spatial data infrastructures

I. Motivation

Within the science of hydroinformatics, information technology methods and tools are applied on problems from the water domain [1]. A central concern is the reduction of complex workflows along with handling an increasing data volume. Modeling processes require constantly more processing power producing more and more data to store; data comes from and goes into distributed environments for different users. Consequently, Internet technologies more and more become part of numerical modeling. To cope with the increasing demands, Community Modeling Systems (CMS) have been or are under development to enable users to have a concentrated view on modeling processes. A major goal is to couple different models or model modules to archive an integrated and harmonized view on a domain or a special field of interest. Mostly different data sources are assembled and a user interface is designed.

Most CMS contain elements of Geographic Information Systems (GIS). GIS as a collective of hardware, software, data and applications manage, model, and analyze spatial data for in multi-user environments [2]. Input-output routines for spatial data, or geodata, and visualization capabilities always are part of a GIS. With the rise of online computing, more and more of those characteristics move to web-based platforms into so-called WebGIS. While the handling in WebGIS stays similar, the infrastructure of data allocation changes towards distributed sources: standardized webservices supply users with data. The access to Spatial Data Infrastructures (SDIs) via a geoportals, which effectively have similar capabilities as WebGIS, represent the online version of a GIS with arbitrary distributed sources and are seen as a way to publish and disseminate spatial data not only to expert users but also to a broad public. Within an SDI, metadata for webservices and datasets build the backbone for data exchange: Metadata is used as documentation by the producer of data and users in an SDI searches on these documentations only and not on the data itself. Elements of the metadata are standardized to enable machine-processing and distribution between different metadata catalogues.

Most CMS use standards for webservices or data formats, which are useful in SDIs as well. However, only certain parts of a modeling process can be integrated in a SDIs so far, those are usually input data and output data. The model core used for processing usually stays named only, described with free text or in a non-standardized structure. A complete description of the modeling process from input data over processing details to output data is missing [3]. The integration of such a scenario into an SDI has several benefits:

- Quality control: Modeling systems are used, when forecasts are made or pure measurement data alone is insufficient to make trustful decisions. Measured data can only be used with metadata on methods and confidence, forecasts gain with the quantification of uncertainties: How can a model result be assessed, how seriously can the results be taken be stakeholders or decision makers if there is no documentation on the processing? The European Water Framework Directive even suggests the usage of modeled data to solve extensive problems [4]. Consequently, closing the gap in the documentation would help to ease stakeholders' doubts on scientific results.
- Reproducibility: If modeled results are scientifically used, scientists need to know the details of a previous model run when reusing results. When decisions are made for large public projects such as deepening of navigation channels or the construction of a harbor, modeling results also have to be legally accounted for.

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- Sharing: Sharing and propagation of a models run becomes much simpler when using a common format. While a documentation or protocol of a model run can be produced by each owner, sharing requires non-proprietary exchange formats.

We propose a concept for a metadata-based modeling system, where metadata takes the role of a protocol and at the same time is able to be published in an SDI. The metadata set is standardized with ISO 19115 – Geographic Information Metadata [5], which core elements form the minimal exchange quantity between metadata systems in most SDIs. We address the issue of updating the history between a modeling system and a metadata set. Two use cases show the relevance and abilities of the approach and conclude with options for the further usage of such a system.

II. LINKING SDIS AND NUMERICAL MODELING

Spatial Data Infrastructures and numerical modeling as part of engineering already have some overlapping characteristics (Fig. 1). Input and output data can possibly be found in both worlds, although modeling results are likely to be processed towards a presentation and therefore are more likely to be found in SDIs. As mentioned before, modeling applications or, on a larger level, CMS and GIS have a lot of features in common. Barely anything in common with the respective other side have model engines and elaborated data products such as data products for reporting or maps. As the glue in between the so far separated items we propose metadata, incorporating the relevant parts from engineering and geographic information science.

In the following, we will shortly describe the relevant elements from both worlds and previous work on how they can be connected.

A. Numerical Modeling

Scientifically speaking, a model can be seen as a hypothesis on the structure and behavior of the real world. In the water engineering domain, simple models might just consist of one equation like the forecast for the temperature at one location, based on previous measurements. In computational fluid dynamics (CFD), numerical models forecast and hindcast not only more parameters but also more locations, the space in between those locations, continuous or discrete time steps, or the interaction between the parameters, as for example the movement of tides in the ocean. As being a hypothesis, the results of the model should be able to be verified of falsified, although an exact image of nature is impossible [6]. Thus an adequate documentation for sharing results with other experts points in the right direction.

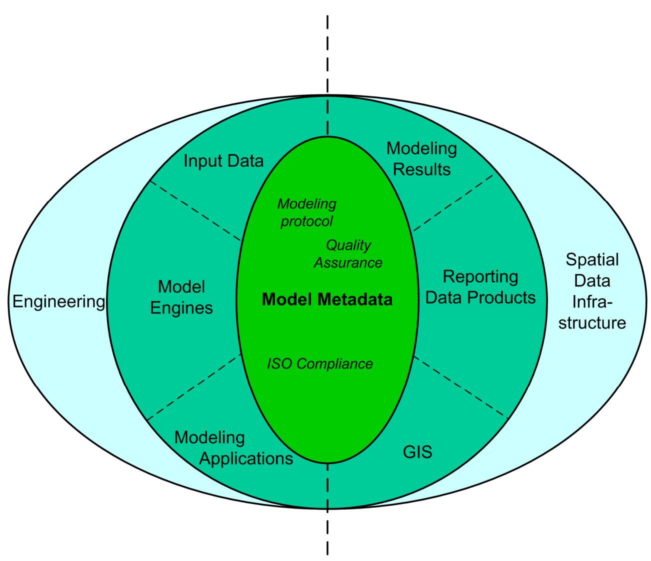

Fig. 1. Relationship between Engineering and Spatial Data Infrastructures.

When interacting with models, we have to differentiate the term ‘model’ [7]: A model of an abstracted world always consists of data that goes into a modeling engine and of data coming out of the modeling engine, the results are naturally restricted by the input data. The term ‘model’ however is used in two ways: To describe the ‘model engine’ (or ‘model core’) which contains the capabilities expressed in numerical equations with its valuations or to describe a complete model set up with input and output data, which we try to specify as ‘model scenario’ or ‘model run’. This explicitly includes all in- or outcoming data used as part of a particular model run, which might only use a part of the overall capabilities of the model core. In this paper, we aim to describe model scenarios as the base for modeling products.

B. Community Modeling Systems

Community Modeling Systems are usually developed to simplify the process of numerical modeling by providing an easier data access, guiding the modeler with a graphical user interface or visualizing the data and results and enable a coupling of models or model modules. CMS are generally large software projects, which require know-how with sufficient staff and technical equipment during the setup and later for maintenance. Therefore only larger organizations or companies start the development of such comprehensive systems. While smaller projects may focus on developing result-oriented prototypes, larger projects need to organize the data volume and apply standards as part of an effective and sustainable data management.

There are a few examples of CMS, which started with different intentions and therefore realized different elements, also in terms of a standardized data management. The extensive CUASHI online Hydrologic Information System (HIS) set the main focus on sharing hydrological data, including databases, servers and client applications using web services as the connecting technique [8]. Users can discover, access and publish data in various ways. Combined with the Open Modeling Interface (OpenMI) it is possible to control and couple model processes in the graphical user interface of the HIS, the HydroDesktop [9]. Another CMS, the free and open source initiative OpenEarth, provides and hosts tools and environmental data [10]. An emphasis lies on models and their coupling using the netCDF format. The INTAMAP (Interoperability and Automated Mapping) [11] research project funded by the European Union focused on the interoperable use of web processing services and other services put forward by the Open Geospatial Consortium, with the aim of developing an integrated environment with corresponding tools. The BASINS system[1] is a multi-purpose environmental analysis system and provides extensive metadata for the offered datasets. However, there is little focus on the history or lineage of the dataset.

C. Spatial Data Infrastructures

A Spatial Data Infrastructure is a distributed structure consisting of geodata, metadata, geodata webservices, network services and –technology. Major geodata webservices are developed under the administration of the OpenGeoSpatial Consortium (OGC)[2]. Well known are the Web Mapping Service (WMS) [13] for displaying geodata or the Web Feature Service (WFS) [14] for accessing vector-based geodata. On the non-technological side, there are agreements on usage, access as well as mechanisms and processes for coordination and (quality) control. The overall goal is to make geodata available in an interoperable way. Therefore an SDI comprises technological standards as well as organizational conventions [12].

Several SDIs have been developed primarily to make data from state-owned agencies available to the public. Large examples are the National Spatial Data Infrastructure of the United States [15] or the European INSPIRE framework directive [16], both providing the technical and organizational requirements for a US-wide, or European-wide SDI, respectively. Its views focus on data sets, web services and how both can be disseminated efficiently in a service-oriented architecture (SOA) based on above mentioned standards. In Europe, the member states implement the directive by formulating guidelines for its data providing agencies.

Numerical modeling is seen as one data source among others, documentation standards do not differ from those of field or monitoring data. However, even in European Directives as the Marine Strategy Framework Directive the usage of modeling as a tool to generate and improve results is suggested [4].

D. Metadata

Metadata present the core element to exchange information in an SDI. Users search for data and webservices on the descriptions of data, which has been preprocessed from XML to human-readable format by a geoportal or another kind of client. The ISO 191xx family standardizes general information, spatial and temporal extent, quality and more properties of geodatasets and -services. ISO 19115 – Geographic Information - Metadata [5] assumes a central role as being the de-facto standard for geodatasets in SDIs worldwide. It contains a large number of elements; it is quite common to use the "recommended core" subset of those elements, which ensures the interoperability between different metadata systems.

Metadata information systems (MIS) such as GeoNetWork[3] or NOKIS, the German North Sea and Baltic Sea Coastal Information System [17], commonly contain a database, a user interface for saving and editing metadatasets and a user management module. An additional crucial role in an MIS plays the OGC Catalogue Service Web Standard (CSW) [18] for editing, inserting, and exchanging metadatasets. The CSW enables filtering metadatasets based on the requirements of the receiving MIS, for example only datasets containing a pre-defined keyword. The catalogue service also is able to edit elements within an existing metadataset.

Numerical models are not explicitly covered in the ISO 19115. However, extensions can be defined for domain-specific data making the ISO a variable base for well adapted metadata profiles. A few approaches towards a metadata profile for documenting modeling scenarios have been made to create standardized and machine-readable descriptions. The Content Standard for Computational Models [19] was the first concept for a holistic documentation of numerical model runs, including input- and output data for complete model scenarios. Crosier et al. [20] further elaborated the approach into a framework for sharing environmental models. It was updated and refined to sharpen the proposed profile and to perform a mapping with the IAHR Validations documents and the current ISO version by Wosniok and Lehfeldt [21].

Other approaches go further towards an all-embracing design of model metadata, but omit interoperability and therefore the path towards the integration into an SDI. Islam and Piasecki [22] proposed a metadata structure based on an ontology in the Web Ontology Language (OWL) as a step towards the semantic web. However, OWL is not yet compatible with today's SDIs. Another approach was made in the ECOBAS project[4] to document the modeling process; however the structure is relatively closed in itself. The concept of the model web [23] as a web of connected and exchanging models has been subject of a few large projects but an SDI-compatible metadata profile has not been developed yet. Granell et al. [24] describe the usage of webservices in the model web, but a discussion on metadata is omitted.

In a previous paper [3] we illustrated special characteristics in metadata of a model run. Sections of a metadata set should encompass:

- The underlying digital evaluation model 'carrying' the model on a structured or unstructured grid.
- The start values: The first set up for the parameters a model scenario.
- The boundary values: Steering incoming parameters from the borders of the modeling area, for example the currents in or out of a water body.
- Driving model parameters: modules or physical parameters defining capabilities of the model, including level of details as for example the number of vertical layers in the water column.

We will further elaborate on versioning of a model run in section III A., as this plays a crucial role in metadata-driven modeling systems.

[1] http://water.epa.gov/scitech/datait/models/basins/index.cfm

[2] http://www.opengeospatial.com

[3] http://geonetwork-opensource.org/

[4] http://www.ecobas.org

III. Structure of a Metadata-Driven Modeling System

We identified several similar elements between the concepts and implementation of Spatial Data Infrastructures and Community Modeling Systems. Most modeling frameworks use standardized technology; standardized components such as netCDF or OGC web services are well-known and widely accepted. Nevertheless most are more or less stand-alone systems. We want to use metadata to open CMS their way into SDIs.

As pointed out above, there is no standardized scripting or history format which would capture the relevant steps of a modeling process that at the same time could save the complete process in an interoperable way. In Fig. 2, the role of metadata in our concept is depicted. A central metadataset accompanies the modeling process. The metadataset is created when the modeling process is run by the modeler the first time: The model specific metadata elements are written into the metadataset, along with the references to metadata of input datasets. The metadata for input datasets can be saved locally or remote, in the last case accessed via the CSW-interface. Within the metadatasets, the links to the actual data can again point to local or remote data stores, repositories or, in case of webservices, to webservers. If the modeler chooses to edit the model run and starts it again under different conditions, this step will be saved in the metadataset as well. We further elaborate on this mechanism in the next section.

The central modeling process happens within a modeling system, which per se is independent of the metadata catalogue and can contain other software elements such as an elaborated user interface. For our concept, we focused on the modeling process itself, the steering and configuration of a model scenario. The modeling software needs an extension which grabs the relevant model metadata from configuration files and writes this information via a CSW-interface into the model metadataset. This requires some manual work, as each model has its own specific configuration format. This part can hardly be standardized; however, libraries for communicating with the MIS can support the implementation.

Most of the elements can be retrieved automatically reducing error-proneness and workload for the modeler. Nevertheless, metadata elements like title, abstract or purpose

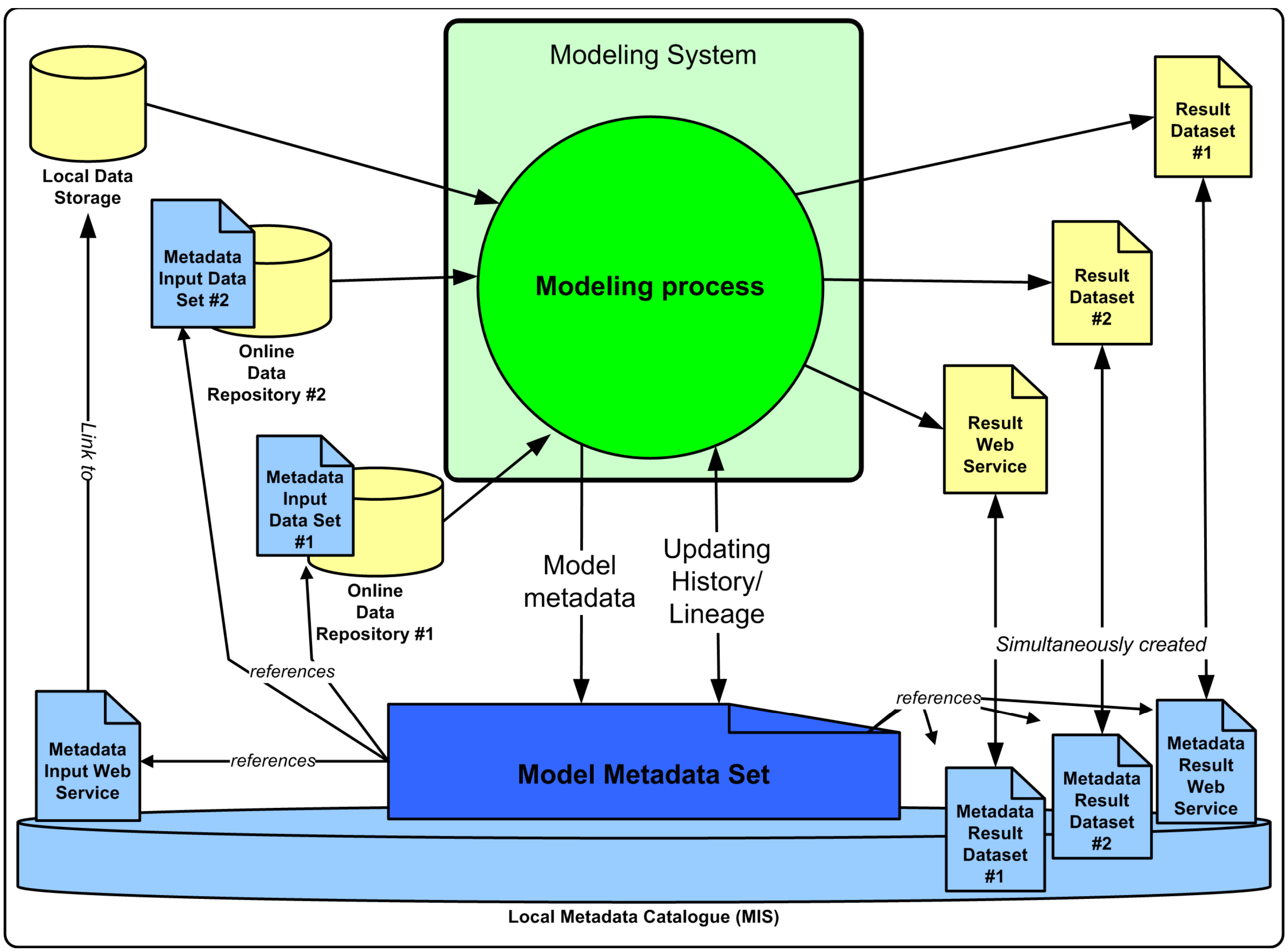

Fig. 2. The role of metadata in the modeling process

need to be filled, either by providing suitable input fields as part of a mini-GUI in the modeling system or directly in the MIS. The latter would require the modeler to directly access the MIS, the first requires more implementation work in the modeling system. Either way, the concept minimized the effort of creating metadata for the operator of the model.

A. *Versioning*

When simulating complex scenarios, more than one model run is performed to archive the best or a different result. Usually several runs are made, each time changing parameters or the modeling time frame. This versioning characteristic when performing simulations using numerical models needs to be reflected in the concept of a metadata-based modeling system: Each step needs to be noted to give outstanding modelers the opportunity what has been performed. Methods of how such a history is kept vary, most organizations modeling climate change or weather scenarios use their own, proprietary solutions tailored on their specific data management. In our concept, parts of the metadata will have to be added with every variation of a model run. There are nearly unlimited possibilities on how a model run could look like, considering there are three major categories of model specific metadata elements (start values, boundary values and driving model parameters) which can be split into several sub-elements. Further, these sub-elements are not only binary values (use/ do not use), but also floating numbers or other models as for example for wind fields.

Within the earth science community different options for persistent identifiers are debated to identify and track changes [25]. Duerr et al. [26] discussed different identifiers towards their ability to identify, locate and cite items or datasets in such environments, with the result that every option has its shortcomings but specifically that none of the examined options were able address scientific datasets as a whole. Universally Unique Identifiers (UUIDs) however were detected to be the most suitable to identify unique items. UUIDs are already known as being used in ISO 19115 metadatasets for giving a dataset a unique identificator within MIS. Unlike URLs or DOIs, UUIDs itself are not able to locate items. This drawback comes only in effect for remote MIS, where it can be compensated with the by wrapping UUIDs in URLs using the CSW-standard. Although this makes handling of identifiers within a metadata-driven system more complex, the fact that UUIDs are a known and established in metadata and SDIs counterbalances the complications. Consequently, we use UUIDs for our concept, where the references are either realized by UUIDs directly or by UUIDs wrapped in CSW-URLs. Each UUID identifies a step in the history of the simulation, which is added, possibly with the help of the CSW, to the ISO 19115 element 'lineage'. To encapsulate the complexity, referencing to other models would be done using UUIDs as well, similar to input datasets.

We also have to add that borders of when a simulation is called 'simulation run number x' or 'new simulation' are fluid and lie in the hands of the model operator. The history of a simulation could therefore be very short.

B. *Use Cases*

The relevance of the concept drawn above becomes easily visible when applying real world problems. We demonstrate two use cases, the first being a sensitivity study on the impact of wind changes on different parameters in the German Bight, the second showing the demand for detailed product histories in consistent bathymetries for data-based modeling. Both use cases origin from the AufMod project (‚Long-term analysis of morphosedimentary processes within the German Bight with integrated modeling') [27], an extensive project on morphodynamics and sediment flux in the German Bight using different numerical modeling systems.

1) *Sensitivity Study*

The German Bight as part of the North Sea is roughly shaped in a 90° angle opened towards the North-West. This is also the most common wind direction which is why wind has a critical impact on the coast especially in extreme weather events. To identify the impact of wind in the German Bight 12 simulation runs have been made to derive changes of 22 tidal characteristic values. Examples are high and low tide, flood and ebb duration, bottom friction and other values relevant for analyzing tide or morphodynamic attributes. Eight simulation runs have been performed with wind eight directions of North, North-East, East until North-West at a wind speed of 12.5 m/s, three runs with wind direction West at a wind speed of 0, 6 and 25 m/s and one run without wind but covering the complete year of 2006 instead for 2 days (21st of August – 23rd of August 2006) for all other runs.

Setting this study in our concept, the granularity of metadata has to be chosen by the modeler. In this use case, with the large number of 222 single results (22 characteristic values times 11 simulation runs), it is hardly recommendable to create a metadataset for each dataset. We propose to split up the sensitivity study in 22 metadata sets, one for each characteristic value, as we think a user would first search for a characteristic value. Other options would be to create one metadata set for each of the 12 simulation runs, for each wind direction or even just a single metadataset for the complete study, although this would cover a large amount of data.

Inserted into the concept drawn above, each of the 22 model metadatasets would have 12 history steps, one for each of the 12 simulation runs. Except for the name of characteristic and the history, the metadatasets would be similar. Input and output datasets can be referenced using the data source given in model steering files. In case of output files this might be a proprietary format, which could, as part of the postprocessing, be transformed into more shareable formats or into webservices.

2) *Consistent Bathymetries*

The German Bight is an economically densely used area, the biggest part of German imports from oversea are handled via the estuaries Elbe, Weser and Ems. These transport channels are regularly monitored and gauged for depth to ensure a secure passage way. Due to the high effort of regular measurements, large areas of the German Bight are examined only on demand, for example when constructing offshore wind parks, or as part of research projects. Consequently, the quality of the available bathymetry is spatially and temporally inconsistent, which is a requirement for long term studies on the tidal system in the German Bight.

As part of the AufMod project, a consistent bathymetry dataset of the German Bight was processed based on datasets from several distinct monitoring activities by different institutions over 30 years [28]. The dataset was compiled of all available data to yearly bathymetries from 1982 to 2012. This means for some areas, especially far off the coast, the last measurement could have been several years ago and additionally of a different quality in terms of method or precision. Therefore the publicly available datasets[5] are limited from the 20 meter depth line, as the data below is too fuzzy. To advise the user of the data, each year is provided with confidence datasets on the quality (fuzziness) of the measured data and on the temporal distance to the next measurement.

Again, there are different options to model the metadata granularity; either use one metadataset to describe the complete dataset or to split it up. Here, the year would be the sorting criteria. In this case, we decide for one metadataset, as the data is internally directly connected. The important step is to connect the yearly bathymetries with the two respective confidence datasets. This is archived by referencing to files within the lineage of the dataset.

IV. Options for Postprocessing

The integration of model runs into SDIs using standardized metadata opens the path towards further analysis. Being part of SDIs implicitly means to have different model run descriptions saved in metadata information systems which are available to the public and connected over interoperable interfaces to other MIS. The detailed descriptions offer further options for investigating internal model structures and different post-processing opportunities.

A. Model Core Analysis

Adding model runs from different model cores automatically creates a database of model cores and their capabilities. An application of the extensive descriptions would be the use as a repostory for supporting the recommendation of model cores for certain problem statements as part of a CMS, without the need to be an expert for every modeling system available. Searching on the model descriptions for keywords such as ‘morphodynamic’ or ‘run off’ could already give hints on model cores to use. Using the model core descriptions, even a coarse categorization of model cores becomes possible.

The definition of a model is very broad and even within domains such as CFD the possibilities to get an overview on available modeling systems and their capabilities are scarce. Additionally, modeling systems like Delft-3d or Telemac have modules to simulate certain tasks such as Telemac-Sisyphe for morphodynamics or Delft-3d Swan for waves, preventing universal statements such as ‘model xy is able to realize…’. There are always conditions attached. However, a general categorization is possible. An example gives the US Federal Emergency Management Agency (FEMA) by allocating 60 accepted models under the conditions of the "National Flood Insurance Program"[6]. They are further distinguished as coastal models, hydraulic models or hydrologic models, which again have up to three subcategories. For coastal models coastal storm surges, coastal wave heights, and coastal wave effects are listed.

Metadata descriptions of model purposes can be of more use. As part of the KLIWAS project[7] (‘Impacts of climate change on waterways and navigation - Searching for options of adaptation’), different modeling systems used to investigate climate change impact scenarios have been described in metadatasets[8]. The purposes have been archived within the keywords, but although the ISO 19115 is applied detailed information on the models are only expressed in free text: Keywords such as ‘run off’, ‘precipitation’, ‘snow’ or ‘soil moisture’ give general hints. Those broad categories and manual keywords could be refined with more and standardized metadata elements, optimally collected automatically.

B. Processing with Webservices

Central elements of SDIs are OGC webservices for distributing, displaying and allocating geodata. The development of some webservices such as Web Mapping Service of Web Feature Services have been consolidated, others are still under discussion such as the Web Processing Service (WPS) [29]. The WPS offers a container for starting spatial processes online, from simple transforming or merging processes to theoretically large modeling workflows. However, large processes pose not fully resolved issues with extensive requirement of resources, process chaining or uncertainty communication [30]. Nevertheless, geospatial standards in service-oriented architecture support the interoperable coupling of data sources, workflows, and modeling systems in online-based modeling systems [24].

Coupling the simulation software and the MIS can be eased with a WPS. One or more WPS could be implemented to perform tasks such as retrieving data from model steering files, transforming data formats and orchestrating the communication between a MIS and the modeling system with the CSW-standard. A direct application simplified by the concept proposed in this paper would be the validation of numerical models. The comparison of modeled data against the measured, real-world data could automatically be triggered after a model run: The sources of model input data and the results are already in one dataset. Several elements belong to such a task such as handling differences in temporal time steps, interpolating over spatial distances between measured and modeled points plus the handling of different input and output

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5 downloadable at http://www.mdi-de.org

6 http://www.fema.gov/national-flood-insurance-program-flood-hazard-mapping/numerical-models-meeting-minimum-requirements

7 http://www.kliwas.de/KLIWAS/EN/Home/homepage_node.html;jsessionid=D3832E47F8465BE1DEF2B01BA205B0DB.live2053

8 https://geoportal.bafg.de/portal/Start.do

formats.

V. Conclusion

Combining and extending previous ideas and methods, we propose a new concept of a metadata-driven infrastructure for Computational Fluid Dynamics simulations. A metadata set accompanies the modeling process which documents all user and machine triggered actions, starting with the selection of input data sets over processing parameters to the selection of output formats. This means a significant improvement of quality assurances with respect to the lineage of simulation results. Full traceability can be achieved for the modeling process. The possible searching for single steps of the modeling process leads to transparent data products, for example for assessment studies. In addition, by complying with the ISO as an international standard, the exchange of such metadata is possible on machine to machine basis and enables the inclusion in most SDIs which offering further possibilities for an online postprocessing.

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