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Semi-structured Knowledge Models and Web Service Driven Integration for Online Execution, Visualization and Sharing of Water Sustainability Models

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Abstract The wide variety in descriptions, implementations, and accessibility of scientific models poses a huge challenge for model interoperability. Model interoperability is key in the automation of tasks including model integration, seamless access to distributed models, data reuse and repurpose. Current approaches for model interoperability include the creation of generic standards and vocabularies to describe models, their inputs and outputs. These domain-agnostic standards often do not provide the fine-grained level required to describe a specific domain or task, and extending such standards requires a considerable amount of effort and time that is deviated from the purpose of producing scientific breakthrough and results. This paper presents a semi-structured, knowledge-based framework implemented with a service-driven architecture: The Sustainable Water through Integrated Modelling Framework (SWIM). SWIM is part of an ongoing effort to expose water sustainability models on the Web with the goal of enabling stakeholder engagement and participatory modelling. SWIM is a science-driven platform, leveraged by the technology advances on service-oriented architectures (SOA), schemaless database managers (NoSQL) and widely used Web-based frontend frameworks. The SWIM semi-structured knowledge model is flexible enough to adapt on-the-go as the underlying water sustainability models grow in complexity. SWIM fosters the sharing and reuse of data and models generated in the system by providing the descriptions of models, inputs, and outputs of each run using relevant metadata mapped to widely-used standards with JSON-LD, a JSON extension for linked data.

***Keywords**:* Service-oriented; model integration; linked data; environmental modelling; SWIM

1 INTRODUCTION

Scientists working on environmental problems are increasingly expected to engage stakeholders outside of academia in order to ensure that research findings will be more comprehensive, address issues that are timely, relevant, and salient, and generate results that can potentially have broader societal impact (Hamilton et al., 2015; Laniak et al., 2013a). Participatory modelling with stakeholders has not yet become commonplace, but interest is growing and there are emerging models for how to do so more effectively (Belete et al., 2017; Hamilton et al., 2015; Jakeman et al., 2006; Laniak et al., 2013a; Pennington et al., 2018; Voinov et al., 2016; Voinov and Bousquet, 2010). A best practice is to meet with stakeholders regularly throughout the modelling process, enabling them to have input into how the models are constructed and the kinds of questions the models can address, as well as early access to model results. In most cases, the modelling work itself is carried out by the modellers in between stakeholder meetings, since most models are complex and time consuming to construct, calibrate, validate, and run. Especially when modelling decades into the future, it can be difficult for stakeholders to envision the capabilities of any given model and the kinds of output it might generate. In addition, it is often not until stakeholders have seen results that they are able to articulate their questions. This lengthens the timeline for modelling with stakeholders.

In this paper, we describe the **S**ustainable **W**ater through **I**ntegrated **M**odelling Framework (SWIM), which enables stakeholders to access an online interface for water sustainability models. SWIM currently provides models that represent the socio-environmental water system in a simpler form so that stakeholders may run computational experiments in real time. This feature enables stakeholders to rapidly generate a variety of outputs based on different input scenarios (e.g. future climate, urbanization, economic, and technology scenarios), and consider what scenarios are of most interest to them. These scenarios can further become the baseline for more complex, time consuming, spatially-explicit models. SWIM provides an online framework that is transparent and easy to grasp by stakeholders who are neither trained nor have experience in modelling. SWIM followed a bottom-up, science-driven design process to create a seamless, easy-to-use framework that facilitates creating, integrating and sharing scientific models with stakeholders, with a particular emphasis on stakeholders who are not tech-savvy or interested in the science behind the models, but want to use the models for decision-making in their specific context.

2 TECHNICAL CHALLENGES, REQUIREMENTS AND DESIGN DECISIONS

There are a plethora of scientific models available for different aspects of water systems (Black et al., 2014; Graveline, 2016; Horne et al., 2016; Swain et al., 2015). Each model was designed and developed to solve a particular problem, from a given perspective, and to address a question at a particular time and place. Models are simplifications of reality, and how reality is abstracted depends on the question that is being addressed, the information available at the time, and the mental models of the modeller (Jones et al., 2011). It is only in recent years that scientists have sought to model water systems in more comprehensive, unified ways. Hence, although there are many relevant models to choose from, they were not designed for integration and even when technical issues such as data formats, programming language, and software platform can be overcome, their integration may not make sense scientifically (Voinov and Shugart, 2013). Yet it is imperative that we develop methods for overcoming these issues in order to generate systems-level understanding of water sustainability (Rogers et al., 2013).

The creation of scientific models that enable a better understanding of water sustainability in a specific area or context restriction faces the challenge of integrating heterogeneous data, available in in different formats and from decoupled sources, e.g., climate data, urban data, agricultural data. In addition, these data were created for a different purpose. Data quality, bias, and scale, model assumptions and parameters, are just a few of the critical issues in assessing the appropriateness of a given dataset or a model for reuse when answering a specific question (Laniak et al., 2013a). Once appropriate data and tools are identified, there remains an often-monumental task of syntactically transforming data into formats that can be ingested by a given model (Michener and Jones, 2012). The learning curve required to use different tools, the need of coding skills, and limited documentation contribute to the challenge of interoperability between scientific tools (Gil et al., 2007). In our work we use the definition of interoperability from (Wilkinson et al., 2016) "the ability of data or tools from non-cooperating resources to integrate or work together with minimal effort".

SWIM leverages our experience within the automated retrieval and manipulation of data for the generation of biodiversity models (Villanueva-Rosales et al., 2015) in the Earth, Life and Semantic Web (ELSEWeb) project. ELSEWeb enables interoperability between data and model providers with the automated retrieval and manipulation of data to be ingested by a model. ELSEWeb and SWIM follow the GEO Model Web principles for the creation of cyberinfrastructure: open access, minimal barriers to entry, service-driven, and scalability (Nativi et al., 2013). SWIM uses the World Wide Web as a platform to expose data and models using Web Services, and standard Web languages and protocols to find, retrieve and integrate data and models. The design of SWIM was driven by an interdisciplinary community of researchers and stakeholders with expertise in areas that include Economy, Hydrology, Participatory Analysis, Earth Science, Computer Science, and Civil Engineering. This community identified the need of having a shared vocabulary, which is used as metadata for annotating data and currently found in SWIM glossary. SWIM's semantic vocabulary is used for: i) guiding the integration of data with different resolutions, ii) describing the science behind the models exposed in SWIM, iii) clearly identifying the processes for data manipulation, and iv) the generation of a provenance trace. Additional requirements were gathered in a survey of potential users (Rajkarnikar Tamrakar, 2017). The evolution of SWIM was driven by the increase in complexity of the bucket model created by the modelling team. The bucket model combines hydrologic biophysical models (Loucks and Beek, 2017) with an economic optimization model (Ward Frank A. and Becker Nir, 2015) and it's implemented in the General Algebraic Modelling System (GAMS Development Corp., 2017). Although the interface or frontend of SWIM has been designed with the bucket model in mind, the workflows and tools at the backend have been directed to accommodate additional models and data sources with minimal effort.

3 SYSTEM ARCHITECTURE

3.1 General Overview

SWIM is composed of: i) two database repositories, ii) a Web-based user interface, and iii) a self-contained Model Distributor service that encloses API interaction with The General Algebraic Modelling System (GAMS). MongoDB holds the core data and data model specification of the system, details are explained in section 3.3 of this paper. The MySQL database repository is used for handling user registration and authentication into the system. The graphical interface allows users to interact with the bucket model by creating modelling scenarios. Finally, the Model Distributor resides as a backend application, it embodies communication and interaction with offline third-party modelling software – it is exposed to the Web as a RESTful Web service. A general architectural diagram of the system is presented in Figure 1.

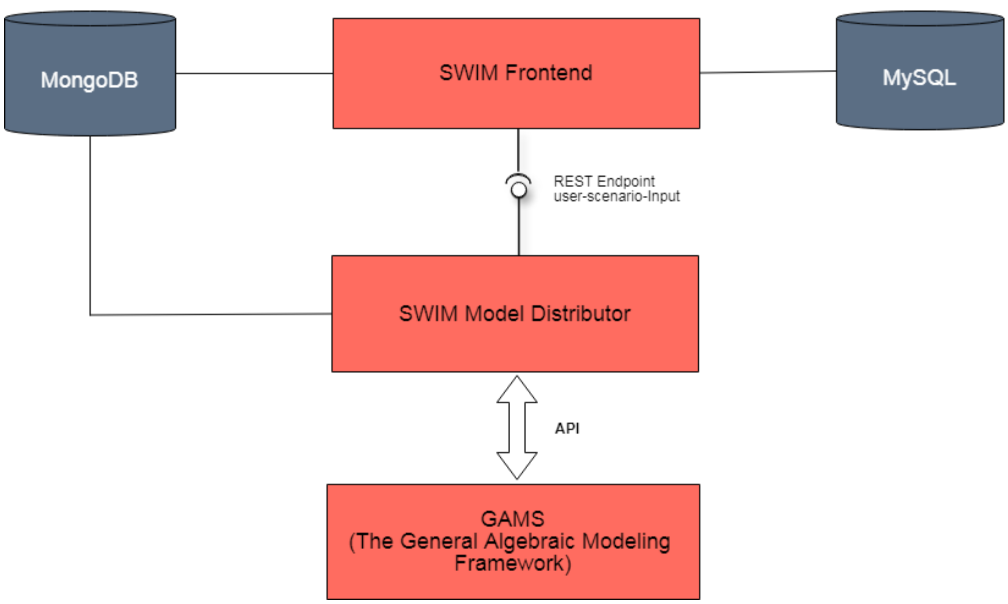

Figure 1. General Architectural Diagram of SWIM

3.2 Data Model

The SWIM data model is implemented with the use of MongoDB, a document database platform that stores data in flexible, JSON-like documents (MongoDB, Inc., 2007). Documents can contain one or more fields, including: arrays, binary data and sub-documents. Fields can also vary from document to document. Additionally, documents can map naturally to objects in modern languages, which allows developers to be extremely productive. Transparent object-document mapping in both backend and frontend modules are handled by programming MongoDB libraries such as Morphia and CIMongo respectively.

The rationale to use a semi-structured schema in SWIM includes: i) the schema facilitates rapid evolution of the data model as data requirements change, ii) a single data field can take many forms as it is not bound to a specific data type, iii) documents can be extended or reduced at the application level, and iv) documents can be semantically annotated with JSON-LD without affecting the functionality of the underlying application. Input data into the models can come in a wide variety of forms. In our initial use case covering the bucket model, data can be captured as single value, 2-D matrices, and multidimensional matrices. The flexibility of the value fields (paramDefaultValue and paramValue) accommodates all these different forms without explicit modifications of the database schema. The value information stored is handled at the application level depending on the content of additional metadata fields E.G. *structDimension* and *dataType*.

Documents in MongoDB are grouped as collections, where the SWIM database is composed of the following: i) *model-base*, ii) *model-meta*, iii) *output*, iv) *parameter*, v) *provschema* and vi) *userscenario*. The *model-base* is a JSON template that is used by the SWIM Interface, it is composed of the minimal metadata required for a scenario specification. The *model-meta* collection stores metadata information about each model registered in the system. The *parameter* collection stores a list of model inputs, it includes metadata used for backend processing such as: upper and lower bounds, structure type, default source, label and description, among other fields. The *output* collection stores metadata of available output variables generated by the registered models, fields include: name, label, units, description and category. All of the described collections can easily be extended to include additional fields for their underlying documents. Depending on the registered models selected for a single run, the SWIM frontend puts together a *userscenario* document composed of extending the model-base to incorporate model inputs, settings, sets and outputs in the form of subdocuments. The *userscenario* is consumed by the Model Distributor service for model execution. Finally, the *provschema* collection contains a skeleton structure that is used to map the resulting *userscenario* into a provenance trace in order to assess the quality and reliability of input data and results generated from the model run (Villanueva-Rosales et al., 2017).

3.3 Backend

SWIM's design follows a Service Oriented Architecture (SOA) allowing the backend components to interface with other software modules through communication protocols based on standard Web technologies. The backend, also referred to as the Model Distributor, is a Java middleware application composed of a self-contained Web service wrapper. The Web service interface is leveraged by the Dropwizard Framework. The "uses view" representation of the Water Distributor Application is illustrated in Figure 2, showing usage dependencies with external software packages.

The current version of the Water Model Distributor entails functionality such as: i) input processing, ii) input validation, iii) model interaction, and iv) data persistence. The addition of new models will decouple model runner modules residing in the Water Distributor into standalone Web service components. The separation of these modules will enable registered models in SWIM to potentially be independently invoked from third-party integration platforms. More importantly, a single runner module and its paring offline modelling software, coexist on the same operating system environment. SWIM will provide automated orchestration between the Model Distributor and standalone model runner modules. The envisioned orchestration is informed by our previous work with Semantic Web Service orchestration in the ELSEWeb project (Del Rio et al., 2013) and leverages SWIM's SOA architecture and use of JSON-LD.

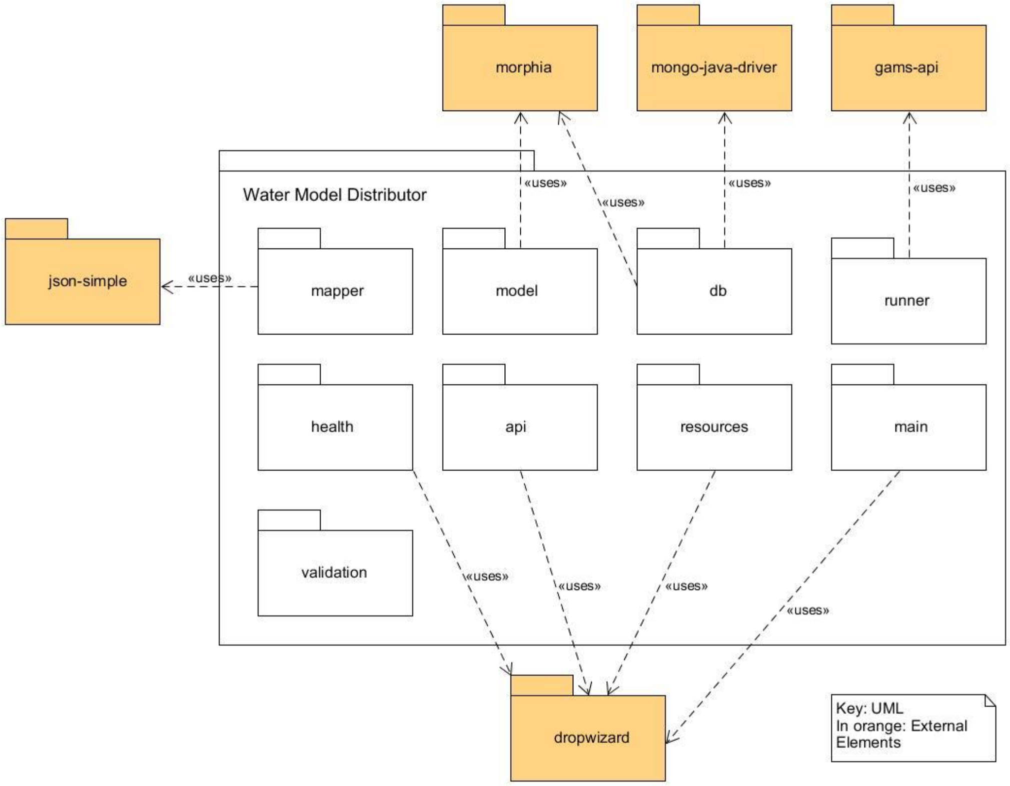

Figure 2. Water Model Distributor UML Uses View

4 RELATED WORK

The SWIM framework is one of many approaches that are underway, attempting to solve the data and model integration challenge (Belete et al., 2017; Laniak et al., 2013a; Nativi et al., 2013). This challenge has proven to be enormously difficult, yet critically important for understanding plausible future scenarios of socio-environmental systems (Filatova et al., 2016; Maier et al., 2016; Polhill et al., 2016). Despite the difficulties, data and model interoperability must be achieved (Laniak et al., 2013b). We believe it is of great importance to provide mechanisms that allow for true engagement and inclusion of non-specialized stakeholders into the modelling environment. The creation of well-thought user interfaces and apps are a good strategy to engage a wide variety of stakeholders.

The CI-Water project, a Utah-Wyoming Cyberinfrastructure Water Modelling Collaboration, include among their work the Tethys Platform (Swain, 2015), an open source software platform that can be used for data and computational needs common to water resources web application development. The Web apps published by using this platform aim to facilitate the process of water-resource modelling and decision making. Tethys is an alternative platform to the SWIM frontend, however SWIM's model distributor can potentially be invoked from a Tethys Web app.

The private sector is also working on providing software solutions for data scientists and modelers - the Forio Team (Forio, 2001) released Forio Epicenter in 2014. Epicenter is a computational platform for hosting server-side models, interactive web applications, mobile applications and sharing insights, it integrates with modelling software and languages such as: Vensim, R and Python, which are complementary to SWIM's integration with GAMS.

Important progress has been made in robust platforms for the sharing of data and models. The HydroShARE platform is an online collaborative system for open sharing of hydrologic data and models (Tarboton et al., 2014). HydroShARE is currently supported by The Consortium of Universities for the Advancement of Hydrologic Science Inc. (CUAHSI) in the U.S. The Hydroshare platform has shown significant progress with the integration of modelling tools such as SWAT (Merwade et al., 2016).

SWIM was designed with interoperability in mind. Our platform will enable the integration of data and models with data and services provided by efforts which are relevant at the infrastructure and scientific level.

5 CONCLUSIONS AND FUTURE WORK

Our experience in developing SWIM provided us with a better understanding of fine-grained requirements from stakeholders interested in sustainable water resources. The main features and services provided by SWIM include: a generic module for manipulating mathematical models, which currently interfaces with GAMS; a robust document-based data model that is flexible enough to be extended or simplified on-the-go as required at the application level; and user-friendly interaction mechanisms for stakeholders who are neither trained nor have experience in modelling.

Our future work includes implementing higher levels of abstraction into the system by adding top layers that would allow: i) alignment with widely-accepted model and data integration standards, ii) interaction with community supported data and model sharing platforms such as HydroShARE, iii) decoupling of backend functionality for model reuse with other integration platforms, and iv) migration of the SWIM user interface into a generic, but highly customizable participatory modelling platform.

We have conducted a number of usability tests, primarily with students and members of our research team before using SWIM with external stakeholders in a workshop on April 25, 2018 (Pennington et al., 2018). Preliminary results from the workshop evaluation indicate that 83% agreed or strongly agreed that the interface was easy to learn, 100% that they could use it on their own, and 92% that the interface improved their understanding of different factors related to water sustainability. No stakeholder disagreed or strongly disagreed with any of the ten questions that were on the survey.

SOFTWARE AVAILABILITY

The frontend implementation of SWIM is part of our main project website. Detailed system documentation and open source code is available online through the portal links presented in Table 1.

Project Website	https://water.cybershare.utep.edu/
SWIM Frontend	https://water.cybershare.utep.edu/bucket_05/home
SWIM Documentation	https://water.cybershare.utep.edu/resources/docs/
Backend Source Code	https://github.com/cybershare/SWIM-IT/

Table 1. Software Availability Hyperlinks

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