

## Challenges in using scientific workflow tools in the hydrology domain

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**Abstract:** Scientific workflow tools are used to perform complex analysis on scientific data. The strength of scientific workflow tools lies in their ability to capture a complex analysis as a sequence of steps using simple components. The components may run on different computers or clusters located at different geographical locations and access data from heterogeneous sources. Scientific workflow tools are popular in specific scientific domains (e.g., ecology, genomics, and astrophysics) for the integration of simulation models. However, this kind of software framework has not been widely embraced by the hydrology domain.

Typically hydrologists use a combination of off-the-shelf software systems such as The Invisible Modelling Environment (TIME) or Matlab along with other ad-hoc software to perform integration and to implement the workflow as their environment for hydrology simulations. In a large scale hydrology study, such as the Murray Darling Sustainable Yields undertaken by CSIRO, a substantial fraction of the overall cost is devoted to developing a collection of software tools to implement the processing flow required for the project. Scientific workflow tools offer significant potential to allow this software to be modularised, reused and shared. The process composition can be semi-automated. For an organisation such as the Bureau of Meteorology Water Division, which is responsible for the routine production of data products like a national water account, these tools can provide greatly improved transparency into the method and auditability of the result.

There are several challenges to the application of scientific workflow in hydrology domain. This paper explores some of these challenges: managing and processing large volumes of data, integration of heterogeneous data and model integration.

Grid computing could be used as an interoperability platform to manage compute and data resources. Considerable work has been carried out in the grid computing community to develop methods to discover and efficiently access data by enabling services such as Fast Data Transfer, GridFTP and RapidFTP. We recommend the compute and data resources to be stored in a same grid infrastructure to provide effective execution. We also describe some applications that use grid computing to improve the execution speed of the hydrology models.

Finally, we report on the adaptation of Kepler for hydrology domain. Kepler is a service-based workflow tool used extensively in some scientific domain (e.g. Ecology). We report on some preliminary work through modifications of existing actors to suit our needs and development of new actors that allow access to the Open Geospatial Consortium- Sensor Web Enablement web services.

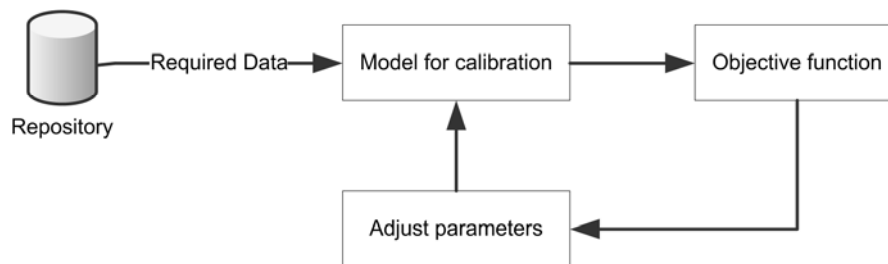
**Keywords:** *Scientific workflow, Hydrology Domain, Kepler.*

## INTRODUCTION

Hydrology is a complex science of understanding the water cycle of the Earth. Traditionally, hydrologists use domain knowledge and mathematical models to solve water-related problems. The problems could be water availability, quantity, quality, usage and distribution. Often these problems focus on a catchment scale but, with the understanding of the earth atmosphere and land surface, the problems can be scaled to larger areas (e.g., river basin and continental scale). This is called macroscale hydrology (Lettenmaier, 2001). In recent times, new observation systems (e.g., satellites, in-situ sensors) are used to capture phenomenon, which leads to an increase in the volume of available data. This poses a challenge of effective use of these data to improve the modelling capability of a hydrology phenomenon. Other challenges are managing the data, developing a suitable model to use the data and discovering new knowledge. Scientific workflows provide an opportunity to address these challenges. Workflows are defined as a tool to access scientific data and run complex analysis on the retrieved data (Gil *et al.* 2007). This paper argues the need of a scientific workflow in the hydrology domain and investigates the challenges to adapt scientific workflow in this domain.

### 1. HYDROLOGY MODELLING CHALLENGES

Let us consider a simple scenario of modelling a river flow. Hydrologists need to identify the rainfall-runoff model suitable for the catchment, gather required data, calibrate and validate the model. The complexity of the model can vary considerably but the outputs of most models are surface runoff. However, most models attempt to replicate the signal in runoff of surface and groundwater processes. The data sets required for model calibration could be catchment characteristics, rainfall, evapotranspiration and river flow. The data sets need to be checked for gaps in time-series and should be filled with necessary gap filling techniques. The model will be calibrated against the observed river flow and the model parameters are tuned to get the best result. For gridded models, the calibration process will be performed for each grid cells and the parameters are also tuned for every grid. Figure 1. shows different processes involved in the calibration process. This is a computationally intensive task and is similar to the training phase of neural network algorithms.



**Figure 1.** Model Calibration process

Calibration and flow forecasting processes look simple for a single catchment. However, to study the river basin, several catchments need to be considered to understand the water balance of individual hydrological response units through the interaction of climate, vegetation and soils (Mulligan, 2005). For example, the Murray Darling Sustainable Yields Project (MDBSY) (CSIRO, 2009) modelled all of the catchments within the Murray Darling River basin. Each catchment is modelled as grid cell of  $5 \times 5$  km and the entire basin consists of 4000 grid cells (Fitch *et al.* 2008). A rainfall-runoff model will run for each grid cell and the output of a catchment is the sum of the output of all the grid cells considered in the catchment. Overall, the model is calibrated for 240 gauged catchments. This is a complex process which involves managing large volumes of data (in terabytes) and requires substantial computational resources.

### 2. MOTIVATION FOR WORKFLOW SYSTEM IN HYDROLOGY

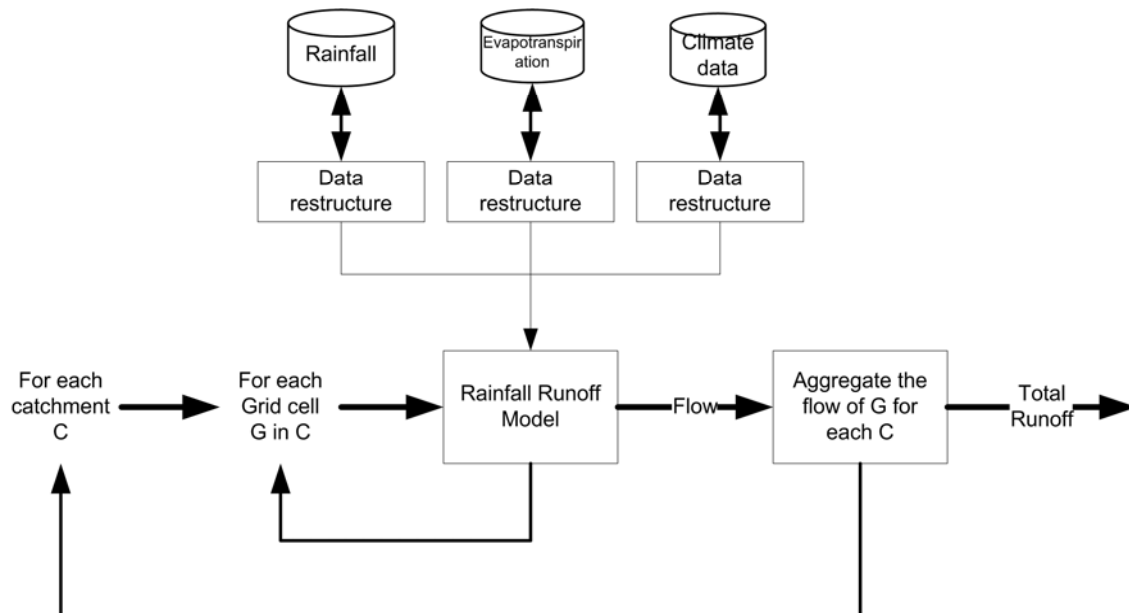
The MDBSY project uses different file formats and structures to store data. The initial data includes a mapping from a grid cell to a catchment, historical time series of observed rainfall and climate data. Hydrologists need to pre-process the data before calibrating a model, check calibration results and tune the parameters if required, verify the parameter set mapping for each grid cell and submit for simulation. Each step of the process is performed as a separate task and there is no direct interaction between the processes. This methodology requires constant intervention from hydrologists, lacks flexibility and is time consuming.

There are very few systems that systematically construct and simulate hydrology systems. To achieve this goal, the first step should be to develop a workbench for hydrologists based on scientific workflow. This should enable them to address the challenges of data management, integration of data with models that

represent hydrology phenomenon and process integration. Scientific workflows will be used to develop new tools based on the existing ones that would enable the integration of heterogeneous data resources with state-of-the-art hydrology models and visualisation tools. It helps scientists to share data and computation resources by using underlying “cyberinfrastructure”. Cyberinfrastructure is a term coined by the United States National Science Foundation (NSF): “*it consists of computing systems, data storage systems, advanced instruments and data repositories, visualisation environments, and people, all linked by high speed networks to make possible scholarly innovation and discoveries not otherwise possible*”. This helps scientists to concentrate more on discovering new scientific knowledge instead of worrying about accessing data, finding resources to run the experiments and transformation of different formats of data.

### 3. SCIENTIFIC WORKFLOWS FOR HYDROLOGY DOMAIN

Scientific workflows in hydrology should support a distributed infrastructure to enable hydrology research. It should enable the integration of data resources, processes and computation. Scientific workflows could leverage the services of grid infrastructure for data storage, computation, data discovery and processing. For a large part of hydrology forecasting, hydrologists perform the same processes repetitively. For example, to forecast the streamflow from a catchment for a gridded model, hydrologists gather the required time-series data sets; restructure the data sets to the targeted rainfall-runoff model. Since each catchment is divided into grid cells, the rainfall-runoff model is simulated for each grid cell. The aggregated runoff of the grid cells is the total runoff of a catchment. Figure 2. shows the conceptual level workflow of this process.



**Figure 2.** Conceptual level workflow to simulate runoff from a catchment.

There are number of workflow tools and frameworks available. Most were initially developed for a particular domain but have since been extended to work in other domains. Workflow systems can be classified as task-based and service-based (Montagnat *et al.* 2006). In task-based systems, users specify the computing task to be executed. The task is specified with a location of the executable code, input data, dependencies and a location of the output data that needs to be stored. The focus of task-based workflow is to map and execute the workflow. Pegasus (Pegasus 2008), which uses DAGMan (Dagman 2008) as a workflow engine uses this approach to execute the workflow. In service-based environments, the application is wrapped around an interface. The workflow knows about the interface and accesses the application through it. The focus here is more towards the composition of a workflow. Taverna (Taverna 2008), Triana (Triana 2008), Kepler (Kepler 2008) are examples of service-based workflow systems.

In the following sections we discuss some of the challenges and opportunities in the application of scientific workflows to the hydrology domain. Similar to any other domains, hydrological science involve: large volumes of data, different models to represent physical phenomenon, and high performance computation capabilities to simulate the model and discover knowledge from data. Some of the issues we will discuss in this section are data integration, data management and model integration.

### 3.1. Data Integration

In Australia, it is estimated that 260 organisations gather hydrological data and transfer it to Bureau of Meteorology (BOM, 2008). Each organisation uses different methods to gather information and several organisations gather same data leading to duplication. Data are also stored in different formats (spreadsheets, database, text file etc.) and most organisations provide none or very little metadata. Therefore, data are heterogeneous from syntactical, structural and semantic perspectives. Apart from data, there will also be differences from system operations. Different technologies are used for data transfer (e.g., FTP, HTTP), remote invocation and platform representation.

Grid computing architectures could be used as a system interoperability platform. Grid computing consists of a number of loosely coupled computers working together to solve a large task (Foster, 2004). The computing infrastructure can be heterogeneous and geographically dispersed. Grid software running on a computer allows the use of unused resources by the other computers in a network. Computers that are part of grid computing perform different tasks and may be running different applications independently. However, in a cluster computing, a group of identical computers are inter-connected to perform the same task. The computers that are used as clusters cannot be used as individual resources.

A Data grid, a part of grid computing, provides services that help users discover, transfer and manipulate large datasets stored in distributed repositories. Data grids provide high performance and reliable data transfer mechanism, and a scalable replica discovery and management mechanism (Chervenak *et al.* 2001). There are several hydrology domain cyberinfrastructure projects that uses grid computing infrastructure. The Cyberinfrastructure for End-to-End Environmental Exploration (C4E4) aims to integrate heterogeneous data and modelling tools in an integrated environment across different spatial and temporal scale (Govindaraju *et al.* 2009). The C4E4 framework uses TeraGrid ([www.teragrid.org](http://www.teragrid.org)) to store, manipulate and query large data sets for environmental research. The Soil and Water Assessment tool (SWAT) model was used over the St. Joseph watershed in Indiana, USA as a case study to realise C4E4 (Chang *et al.* 2008). SWAT is a process-based distributed-parameter river basin scale model to quantify the impact of land management practices in a watershed. It is a conceptual model and that needs calibration of parameters to reproduce observed streamflow. The amount of time required to calibrate a model depends on the number of parameters, the number of subwatersheds and the volume of data used for calibration. The simulation consists of 28 configurations, which includes six watersheds, each involving two resolutions of soil data, and one sub-watershed has 16 configurations, to calibrate four parameters with 7 years daily streamflow data. On a desktop machine, the estimated computation time is about one year based on each configuration taking 2 weeks to complete the computation. However, it is reported that using C4E4 framework, the entire computation was completed in 3 weeks. This was accomplished using TeraGrid facility to run multiple calibrations in parallel thus reducing the execution time. Other authors (Theiner and Wieczorek, 2006) report speed of upto 5x increase in calibrating the WaSiM-ETH model using grid computing.

In recent times, there are initiatives from Consortium of Universities for the Advancement of Hydrologic Science Inc (CUAHSI) to develop infrastructure and services to improve access to hydrology data (Maidment, 2008). The project is CUAHSI-HIS (Hydrologic Information System) and the goal of the project is to *“Provide better access to a large volume of high quality hydrologic data, storing and synthesizing hydrologic data for a region, supporting science by providing a stronger hydrologic information infrastructure and bringing more hydrologic data into the classroom”*(Indiana, 2007). The project architecture is service oriented and has a capability to access 3<sup>rd</sup> party web services. WaterML is used as a standard water data transfer language. Data structure problems can be solved by adopting Open Geospatial Consortium (OGC) Observation and Measurement (O&M) standards to represent data. This enables the use of OGC- Sensor Web Enablement (SWE) standards to publish data. This will be an initial step towards creating a Hydrological Sensor Web (Guru *et al.* 2008).

Currently, standards are not mature enough to represent a hydrology data. The standards are not consistent and interoperability remains a major issue. This is a hindrance to share data in a hydrology community. The data should be represented semantically to enable automatic processing and identification. There is an initiative to develop domain ontology for hydrology metadata (Bermudez and Piasecki, 2004) but, still more work is needed to capture entire hydrology concepts.

### 3.2. Data Management

The fundamental aim of scientific workflow is to analyse large volumes of data. In a large project, data sets are often stored in different geographical locations. Management of these data sets in a distributed grid environment is a major challenge. Data undergoes different transformations in a workflow lifecycle. During

the workflow creation phase data needs to be identified for a given task and could be discovered by querying catalog services that store metadata (Deelman and Chervenak, 2008). These services are used to map metadata to one or more physical locations where data sets are stored. It is a common practice to store mapping information in relational databases for easy and effective access. The workflow task should select desired data from replicas based on different criteria (e.g., latency and bandwidth of a network).

The grid enabled databases are relatively new. Oracle 11 supports database grid to deliver database services for grid computing (Olofson, 2008). If centralised database is used for data storage, it can be exposed as a web service. Open Grid Service Architecture - Data Access Integration (OGSA-DAI) is a middleware which allows access to remote data sources (e.g., relational, XML, file databases) through web services. The request to OGSA-DAI web service is independent to the data source.

Efficient placement of data during the workflow execution improves the performance of data-intensive workflow. Data transfer relies on services like GridFTP, Fast Data Transfer (FDT), FTP, HTTP and RapidFTP. Data replicators are used to manage data in large data volume experiments. For example, the Laser Interferometer Gravitational Wave Observatory (LIGO) project which, was conceived to detect gravitational waves produced by violent events in the universe gathers large volume of data (Brown et al. 2007). During the experimental phase 1 terabyte of data is collected per day for analysis. Data is managed by LIGO Data Replicator (LDR) and make copies of data sets to distribute and replicate. Data is stored with metadata for easy discovery. This helps to implement a fall-back mechanism when one of the data source do not respond for data access. In certain applications, storage available at the execution site may not be sufficient to successfully execute a workflow. Workflow scheduling algorithm should estimate the storage availability while submitting a task. It also should remove unwanted data set to reduce workflow footprint.

Intermediate data may be useful for different workflows. For example, some of the hydrology data collected from a field may have several deficiencies such as large gap, unusual spikes. Data cleaning step will always be performed before it is used for analysis. The cleaned data set can be reused as long as it is tagged with metadata and complete provenance information is available. It is a challenging task for workflow system to determine what data to store when the storage space is a constraint. Provenance management is an important issue to efficiently reuse data, processes and workflows.

Provenance by definition is a record of the history of ownership. From scientific workflow perspective, provenance is classified into data and process (Simhan et al, 2005). Data provenance shows an evolution of created data. It consists of data, processes used, date of creation and intermediate steps of creation. Process provenance provides the origin of derived processes. Provenance helps to make a judgement about the derived data quality, validity and also to reuse the data and processes with confidence. Provenance framework is supported both by Kepler (Altintas, 2006) and Pegasus (Kim, 2007).

### 3.3. Model Integration

Integrating different hydrology models in a scientific workflow is a major challenge. Hydrology models are written in different programming language and use different data sets. There are hydrology model suites like TIME ([www.toolkit.net.au](http://www.toolkit.net.au)) which is based on .Net framework and hence platform dependent. The goal should be to integrate these tools into workflow systems with minimum modification. These models could be used as web services for computation. The services should be semantically annotated to enable effective service discovery. Taverna has access to more than 3000 bioinformatics related services. The existing workflows can be defined as services and shared with others. Taverna shares workflow to wider research community through myExperiment ([www.myexperiment.org](http://www.myexperiment.org)). The effective resource discovery, planning and scheduling algorithms are needed to use grid infrastructure in computation. Since the volume of data used in hydrology modelling varies, it is sensible to use same resource for computation and data storage to avoid latency. CUAHSI-HIS uses OpenMI ([www.openmi.org](http://www.openmi.org)) to link hydrology models and expose them as web services.

## 4. KEPLER FOR HYDROLOGY DOMAIN

A Workflow in Kepler is a composition of different actors. Kepler uses a graphical editing interface based on Vergil from Ptolemy II to compose workflow. There are different actors to perform different tasks. Actors are initialised through parameters. Two or more actors can be combined to form a composite actor to perform complex operations. Ports in an actor are used to input and output data. An Actor can have single port or multiple ports. Relations are used to branch the data flow and send same data to multiple actors. Resource allocation is performed in Kepler by configuring the parameters of actors in a workflow. If the resources are web services, they are searched using a registry which will be updated regularly to include new services.

Kepler uses its own run-time engine to execute workflow. It supports grid and web service resources that are represented as actors in a workflow. Directors orchestrate the workflow and Kepler provides five different directors, each providing different models of computation (e.g., sequential, continues time, discrete etc.). A large workflow can have different sub-workflow and each of them can be operated by different directors.

Preliminary work has been conducted in the use of Kepler in the hydrology domain. Some of the reasons to use Kepler are: Kepler was developed initially to work in ecology domain thus; some of the actors can be directly used in hydrology domain. Kepler has large pool of reusable actors. Different models of computation give flexibility to compose workflow. For example, Process Network (PN) director which supports multi-threaded dataflow could be used to orchestrate workflow of Figure 2. This enables the grid cell computations to run in parallel. Distributed execution of a workflow could be accomplished using a Distributed Composite Actor (DCA). This actor follows Master-Slave architecture where master is a machine from where the execution starts and slaves are remote machines. Grid facilities can be used to register the slaves and authenticate them.

Kepler has actors to invoke web services, Matlab expressions, R scripts, statistical tools and Globus<sup>1</sup> enabled grid facilities. We have developed actors to invoke OGC-Sensor Observation Services (SOS) which, is used to publish raw historical sensor data on the web. This is the step towards enabling Kepler to compose OGC-SWE web services. We also have had initial success in invoking models from the TIME suite.

There are some performance issues in existing Kepler actors. For example, the database query actor available in the Kepler actor library initially could not handle more than 6000 records. We modified the actor to handle 3.2 million records. In Kepler, actors are programmed in Java and the throughput and efficiency of an actor can be improved through efficient programming practices.

## 5. CONCLUSIONS

This paper describes some of the challenges and opportunities to develop scientific workflow workbench for hydrology domain. The work was motivated by the complexity of the hydrological science and the belief that the scientific workflow would improve effectiveness of hydrological experiments. The aim is to provide an opportunity for hydrologist to concentrate on their science with less emphasis on computer science aspect. The advantages of scientific workflow are improved efficiency, reusability and most importantly capability to explicitly document the processes used in the analysis through provenance. This is also an opportunity to demonstrate the capabilities of cyberinfrastructure to conduct experiments and discover new scientific outcome. Scientific workflows do not replace hydrologists but certainly enhance the capability of them.

Use of cyberinfrastructure driven by workflow will significantly minimise the hardship of data management. The grid technology is scalable and management is also efficient. But configuring a grid system is still not very easy. With the popularisation of cloud computing this may not be an issue because third party can maintain the infrastructure and the scientific community can buy and use the resources only when it is necessary.

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<sup>1</sup> Globus is a open source software toolkit with set of services and software libraries that support grids and grid applications

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