A Cyber-Infrastructure for a Virtual Observatory and Ecological Informatics System -VOEIS

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*Abstract***— The Virtual Observatory and Ecological Informatics System (VOEIS) provides a framework for data acquisition, analysis, model integration, and display of data products from completed workflows including geospatially explicit models, graphs from statistical analyses, and GIS displays of classified ecological attributes on the landscape. VOEIS is intended to complement the capabilities of the Consortium of Universities for the Advancement of Hydrologic Science (CUAHSI) Hydrologic Information System (HIS) by providing sound data and metadata management capabilities for field observations and analytical lab actions. Functionality provided by VOEIS is supported by a Field Data Model (FDM) that enhances the limited geospatial capabilities of CUAHSI's Observations Data Model (ODM). Access to VOEIS data and metadata is also made accessible via programmatic APIs which facilitates integration with other service oriented "*e-Science*" architectures and distributed frameworks.**

Keywords—framework; cyber infrastructure; data and meta-data management

I. INTRODUCTION

CUAHSI's Hydrological Information System (HIS) is an internet-based system that supports the distribution of hydrologic data. CUAHSI's HIS "is comprised of hydrologic databases and servers connected through web services as well as software for data publication, discovery and access." [1,23] Though HIS provides exceptional server side support, data entry and quality control client tools, HIS presumes that individual research labs posses sound internal data management practices, doesn't provide tools for managing metadata about field and analytical lab actions, and has a limited data model for geospatial reference. CUAHSI's Observations Data Model (ODM) [6] is founded upon an information model for observations at stationary points. This model is insufficient to characterize complex spatio-temporal relationships that arise under circumstances where hierarchical and dynamic sampling locations occur. VOEIS is an integrated sensor and ecological informatics system that complements CUAHSI's HIS capabilities by supporting all-encompassing workflows; from the collection of streaming senor data to the application of those data in simulation models and visualizations. VOEIS facilitates the management of data and science metadata within individual research labs, solves the problem of the static geospatial data model, and interfaces with HIS to allow labs to share some or all data via the HIS protocols.

The VOEIS infrastructure is designed to extend the functionality and knowledge representation capabilities of CUAHSI HIS by providing necessary interfaces, software components, and a complementary Field Data Model (FDM) schema [18] that captures data processed in the lab or collected by scientists in the field.

VOEIS has three basic research elements: 1) the development and deployment of sensor networks which requires the cyber-infrastructure enhancement of hardware at two field hubs (FLBS and HBS described in section III B); 2) the development and deployment of an informatics system to manage and serve hydrological and meteorological data and metadata, and to interface with CUAHSI's HIS and ODM; and 3) the development and usage of protocols and APIs to interface with partnering technologies (i.e., WaterML [27]).

II. BACKGROUND

The challenges of managing scientific data are significant, and over the years they have typically fallen in the hands of investigators. There exist significant obstacles in workflows supported by cyber-infrastructures; from operation and field deployment of sensors – to data streams – to data management – to data analysis – to the use of integration tools. These multifaceted obstacles involve hardware, middleware and software. However, significant work and progress has been made to tackle the challenges of managing these workflows, discovering data, storing data, and publishing scientific data in architectures that are conducive to ease-of-use, dissemination, documentation and research for scientists. PIs, researchers, managers, and scientists alike need the ability to easily access (and possibly integrate) information that is housed in distinct geographical and distributed sites. Additionally, such information is very likely to be stored in different formats and disseminated using a diverse range of communication protocols. The Tupelo middleware [4] developed at the National Center for Supercomputing (NCSA) and the

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University of Illinois is an open source semantic content management framework (middleware technology stack) designed to manage e-Science projects. This is an all-purpose solution whose goal is to manage information from a broad range of sources and to provide functionality that supports data management, provenance, workflows, people, and temporal and geospatial relationships. Similarly, the NSF sponsored Data Observation Network for Earth (DataOne) [2] project has undertaken the task of developing a distributed framework and cyber-infrastructure to support the needs of the e-Science community. DataOne tackles the data integration problem by developing standards based technology to support all encompassing biological sciences domains, i.e., hydrology, ecology, atmospherical, oceanographic, etc. DataOne uses a service oriented architecture centered on collaborating nodes that maintain registries of available data and their addresses. To participate in DataOne, a researcher may choose to create a member node and implement its associated interfaces. Additionally, participating member nodes may choose to implement a full set of APIs that allows the member node to also accept data from other participating nodes. This allows clients to access and share information, which reduces the possibility of data loss and allows researchers to aggregate and analyze data from many sources. Clients interact with member nodes by using anyone of many services available through an investigator toolkit.

VOEIS, in contrast, is focused on hydrological and meteorological data only. VOEIS enhances and expands the information made available by CUAHSI's ODM through its associated HIS server. A VOEIS server can be integrated into any service oriented framework. For example, you can turn a VOEIS server into a DataOne member node by implementing the desired interfaces, registering it with a coordinating node, and mapping content schemas. VOEIS provides a programmatic RESTful API that can easily interface (via a façade for example) with other APIs, and our underling evolvable schema technology design [8] allows for the flexibility to represent content in other formats and provides a mechanism that supports dynamic changes to schemas. Participation in the greater e-Science community is a VOEIS goal, and the technical aspects of interfacing in the DataOne network and the Tupleo technology stack are currently being assessed. In the next section we describe the VOEIS architecture and all services made available to potential client nodes.

III. ARCHITECTURE AND FUNCTIONALITY

This section contains abridged structural and behavioral details of VOEIS. A high level description of the software architecture, related data collection functions and user interface provide an overview of VOEIS functionality.

A. Architecture – High Level Overview

The VOEIS Data Hub is an open source data management and publication software stack designed to store and organize hydrological, water quality, water chemistry, and meteorological data. Investigators can organize data into projects and create geospatial sites that are associated with temporal-tagged observations, sample readings, and sensor measurement data. VOEIS is designed to support research lab style data management, data collaboration and data publication through its own web presence and through the CUAHSI HIS services.

VOEIS (see Figure 1) is implemented using the Yogo Framework [9] with Ruby on Rails [20] to take advantage of the data management tools providing flexible schema management, RQL API, Role Based Access Controls (RBAC), versioning and support of multiple database back-ends making it platform independent. Currently the system uses PostgreSQL [19] as the backend storage system. Data processing has been optimized for PostgreSQL; however generic implementations can make use of any DataMapper ORM supported backend such as MySQL [13], SQLite3 [22], Persevere [17], MongoDB [12], etc. Yogo is open source software and is available for download [26].

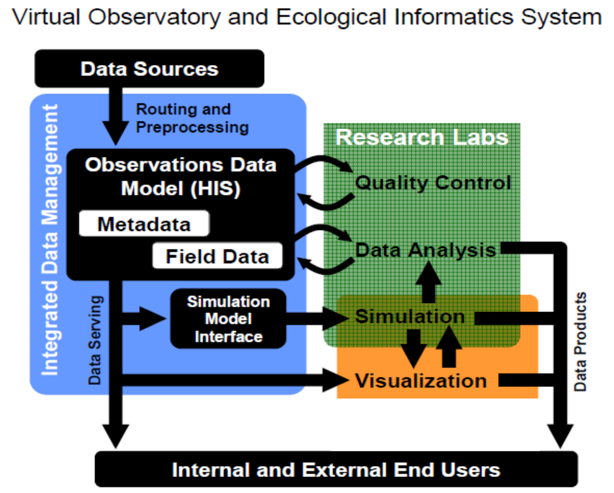


Figure 1. High level architectural view of VOEIS

B. Sensor Data Collection

The means of collecting ecological data include deployed lake, river and meteorological sensor systems. Moving vast quantities of real-time data from deployed sensor systems requires innovative wireless, satellite, cell, and/or combinations of these systems. The VOEIS Data Hub currently collects streaming data from three different sources. The Big Sky sensor array consists of four stations deployed in distinct stream localities and one weather station used to collect raw data transmitted from each station via high radio frequencies. All stations are equipped with Campbell Scientific CR1000 data loggers that store hydrological and meteorological data. The other two data sources are deployments in lakes. Both Flathead Lake Biological Station (FLBS) located in Montana and Hancock Biological Station (HBS) located in Kentucky import meteorological data and lake buoy hydrology and water quality measurements into the system. VOEIS currently supports parsing CSV files from data loggers and text based data from samples organized as time-series. Both biological stations are constantly inundated with requests for data from researchers and also the public. The data managers of both stations are busy handling operations for importing and curating data as well as creating reports and archives, and are thus challenged and confronted with meeting the expanding demands for data from their internal clients and from a public that has become aware of the usefulness of the data for fishing and boating purposes. VOEIS aims to alleviate some of the demand on these individuals by allowing that both internal and external clients have appropriate access to the data and are able to search and acquire it in their own time with little intervention.

C. Data and Meta Data Management

VOEIS is designed to manage information, and the science and administrative metadata required to make the data useful to other data consumers. VOEIS is able to capture the current data and metadata that CUAHSI HIS ODM 1.1 is designed to capture plus additional data types and additional metadata significant to the research and lab data management processes.

VOEIS uses an evolvable schema technology and data paradigm in order to easily support the ability of scientists to modify data models quickly [8]. Unlike relational technologies that require significant design work *a-priori*, an evolvable schema supports schema alterations *during runtime* that are necessary to support new functionality.

D. Field Data Model (FDM)

The goal of FDM is to provide a complementary schema that characterizes complex spatio-temporal relationships that cannot be realized by ODM. FDM captures the structural relationships necessary to augment ODM. It is not the intention of FDM to accommodate for the modeling of information fluxing through an environment. A simulation modeling interface, depicted in Figure 1 will be provided to support the ability to interface with VOEIS in order to generate said simulations. Significant work to develop simulation, hydrological modeling frameworks has been done by [5,7,25].

FDM is a significant contribution (developed over two decades) to evolving a data schema that allows functional integration of data from field observations, analytical labs, and data loggers whose format can be efficiently queried regardless of data source. The FDM can be broken into five basic components (shown in Figure 2), and a resulting unified database of results.

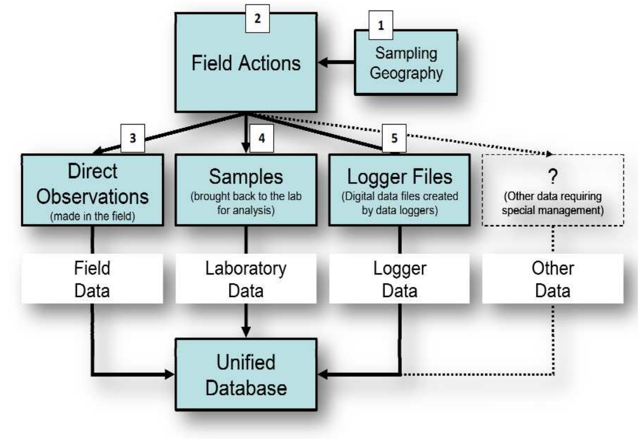


Figure 2. Schematic of general data flow for integrating data from field observations, lab analysis of samples, and results from data loggers

The components address the management of 1) geographic (meta)data describing the locations of study sites and sampling locations; 2) (meta)data describing actions that occur in the field (direct observations, sample collection, and logger deployment/retrieval) at study sites and sampling locations; 3) (meta)data about direct field observations; 4) (meta)data describing and tracking laboratory analyses that generate lab data; and 5) (meta)data describing logger deployments, retrievals, and resulting raw data files.

In VOEIS, we extend ODM with the FDM to provide investigators with the most flexible and robust solution that supports the ability to store, manage and publish data. Figure 3 is a simplified version of the structural UML [24] class diagram that represents the schema of FDM. There are four types of objects: 1) administrative objects represent the set of classes necessary to identify projects, their members, permissions (not shown) and a TupleID used to associate a project with a campaign and visit tuple; 2) action objects represent various field actions, each of which can be associated with data collected for said activity; 3) temporal objects which represent the time characteristics associated with actions; and 4) spatial objects, which represent the geospatial information associated with the actions.

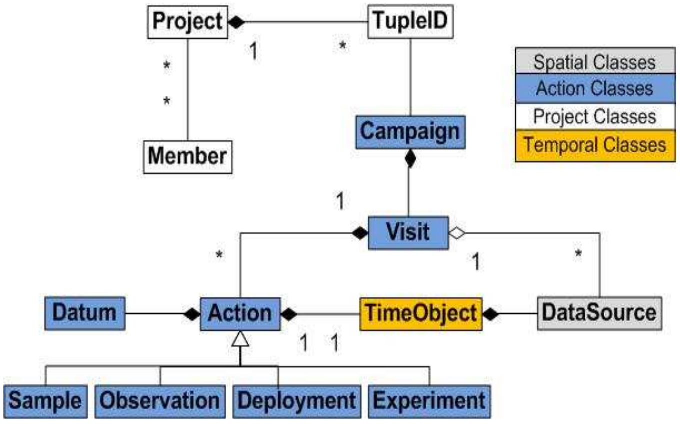
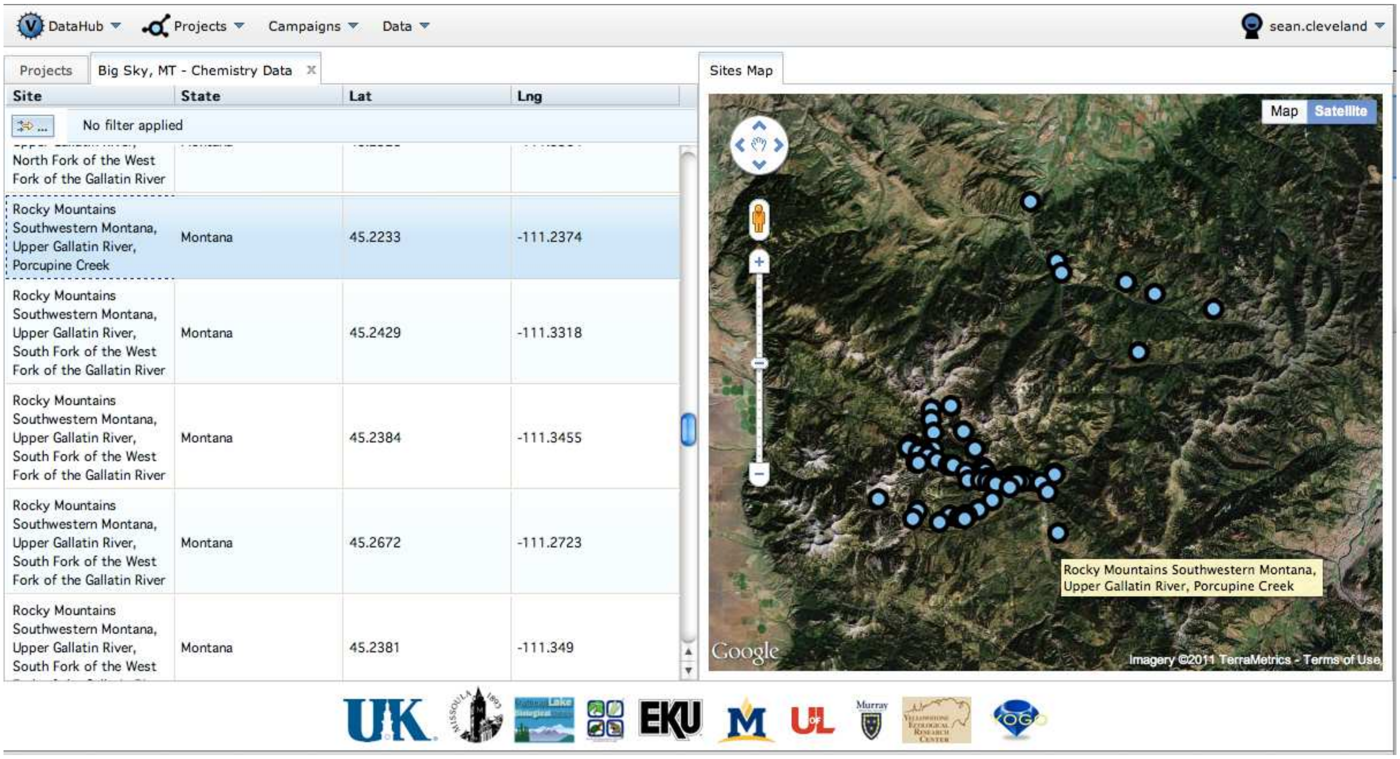


Figure 3. Simplified UML class diagram of the Field Data Model (FDM)

The modular design of VOEIS is intended to allow integration of other components and data types that originate as a function of field work, but require different data management pathways. To illustrate why an FDM is necessary, consider that observations are made, samples are taken, and sensors are deployed at specific points in three dimensional spaces. In order to catalog and track the location of field “actions” (e.g., observations, samples, or deployments) in a database, the action occurs at a “place” (e.g., monitoring water quality at a conceptual location such as the “mouth of a river”), but that the geographic location of virtually any conceptual “place” may change over time (e.g., lateral erosion of a river bank during high flow can cause the location of the “river’s mouth” to migrate to a new geographic location). FDM allows field actions to occurs at “places” (DataSource in Figure 3), while “places” can be associated with multiple spatial locations for different periods of time (TimeObject in Figure3).



Site	State	Lat	Lng
North Fork of the West Fork of the Gallatin River			
Rocky Mountains Southwestern Montana, Upper Gallatin River, Porcupine Creek	Montana	45.2233	-111.2374
Rocky Mountains Southwestern Montana, Upper Gallatin River, South Fork of the West Fork of the Gallatin River	Montana	45.2429	-111.3318
Rocky Mountains Southwestern Montana, Upper Gallatin River, South Fork of the West Fork of the Gallatin River	Montana	45.2384	-111.3455
Rocky Mountains Southwestern Montana, Upper Gallatin River, South Fork of the West Fork of the Gallatin River	Montana	45.2672	-111.2723
Rocky Mountains Southwestern Montana, Upper Gallatin River, South Fork of the West	Montana	45.2381	-111.349

Figure 4. VOEIS UI interface for project browsing

E. *Graphical User Interface*

The VOEIS UI is served through basic html and Dojo Toolkit JavaScript widgets [3] to support multiple browsers. The VOEIS UI is specifically designed for investigators. A contextual inquiry process along with numerous requirement validation meetings were carried out before settling on a project centric UI. VOEIS allows investigators to display managed projects with options to upload, browse, search and download data. The current UI supports simple upload of workflows for logger and sample/chemistry data within a project with options that allow saving the resulting parsing instructions for re-use. Simple data graphs are supported for displaying time-series data. The VOEIS UI provides simple views of project data that support the end-to-end public drill down of data products. In Figure 4 we display a simple representative example of the UI.

F. *Programming Interface and Data Sharing*

The VOEIS Data Hub is designed to offer developers programmatic access to data via RESTful APIs. The APIs provide significant flexibility for users to create personalized tools and views to interact with the data stored in VOEIS. Access to API methods is role based and is implemented using API keys that are linked to user accounts. Thus, API access is managed in the same manner that regular user access is handled. Further, the implementation of a Resource Query Language (RQL) REST interface allows dynamic data querying API functionality resembling SQL database queries without the security risks and complication inherent in exposing an SQL interface for a complex database schema.

Once data are in common formats, the system will store data locally as well as have the capacity for rapid sharing regionally (e.g., to campus-based HPC centers and collaborators throughout the VOEIS community) and globally (e.g., international colleagues, TeraGrid) via UIs or programmatic APIs. This sharing will be the basis for bi-directional flows of data between storage and analysis, simulation, and eventually visualization components. This interoperability among storage and science user components of the VOEIS Data Hub will allow for rapid iterative exchange among different types of data, models, and user components. At this time we plan to implement WaterML communications for VOEIS by implementing a WaterML gateway (see section III G) to the VOEIS server. The design specifies a gateway similar to the HIS-gateway (described below) implemented through a custom DataMapper REST adapter. The WaterML gateway will respond to RESTful WaterML formatted queries within the context of a VOEIS project and will use the existing API security protocols to ensure data integrity. WaterML is currently a candidate standard in the Open Geospatial Consortium (OGC) [14] for the representation of in-situ hydrological data. WaterML 2.0 makes use of the OGC Observations and Measurement (O&M) standard [15]. The success of ecological informatics is highly dependent on the usage of common standards and the goals of VOEIS include continued support of these standards.

G. *HIS Gateway*

A specific goal of the VOEIS project is to integrate with the CUAHSI HIS through HydroServer. In order for VOEIS to leverage the power of the CUAHSI HydroServer and its corresponding suite of tools, a fully functional REST interface that allows for the pulling and pushing of data objects was needed. We have constructed a HIS gateway using Ruby, Sinatra [21] and the DataMapper ORM to provide the necessary REST functionality. Associated requirements for the HIS gateway include a simple authorization system to prevent malicious access, and the ability to serve up JSON [10] and XML results from simple URL style queries that can behave like full APIs to the ODM data-store. The initial implementation of the VOEIS HIS gateway is currently available for use as a standalone JRuby [11] server application that can be deployed on any platform and configured to connect to any ODM database.

H. Workflows and Data Provenance

Preprocessing of data involves development of data paths through a standardized workflow framework. During quality control, errors are corrected, missing data are annotated, and metadata are created. This provides robust validation and tracking of original data which is required for comprehensive, reliable analysis later in the data workflow. More advanced workflow support with features offered by tools such as NCSA's CybeIntegrator is also currently being investigated. Research groups have well-developed data management systems and protocols. However, as typical throughout the sciences, these protocols have been largely developed to fit the specific needs of the research group. VOEIS will integrate these separate systems into a single, interactive management platform and implement data provenance (processing history) tracking. VOEIS (through its underlying implementation Yogo Framework technology) maintains data provenance by natively versioning all data stored in the system. As a result, for each VOEIS project, the data that is stored is never revised or erased. When raw data is modified (through the QA/QC process, or by some other means) the prior values are stored for provenance. Any time a change is made to any record in VOEIS a copy-on-write is performed of the pre-modified record (with the addition of a user-defined comment on the change) and is stored in a version table associated with the model. These version records are time-stamped with creation dates allowing the system to identify when any record was versioned and what version of the other records it was associated with. Therefore, as any piece of information is modified it is possible for VOEIS to ensure that for a given time the entire system could be reconstructed. Since the previous versions are read-only, the interface only allows for them to be viewed; they cannot be edited. The most recent versions of the data are the values that are used for data mining and exposed via the data retrieval APIs.

IV. CASE STUDIES

A number of projects are currently exercising VOEIS functionality and the numbers are expected to grow. This section provides a brief description of the types of projects that are or will be using VOEIS data management capabilities.

A. The Spanish Creek Case Study

The Spanish Creek site on the Flying D Ranch, Montana, is instrumented in support of undergraduate education at Montana State University. We are using VOEIS to instrument the site with four real-time nodes. The physical and chemical characteristics of the stream are monitored to provide data for use in Poole's class "Stream Restoration Ecology." Parameters include river stage, temperature, conductivity, dissolved oxygen, precipitation, wind speed, and incoming solar radiation. In past years, students in the class have conducted individual research projects on the creek, which have provided the foundation for each year's class to compile an integrated set of stream restoration recommendations and present them to ranch staff. Data for the VOEIS network nodes on Spanish Creek will help next year's students determine how land management and any restoration actions may be affecting the physical and biological aspects of water quality in the creek.

B. The Tenderfoot Creek Experimental Forest Case Study

The Tenderfoot Creek Experimental Forest (TCEF) is located in central Montana within the Lewis and Clark National Forest. As a result of collaborative hydrological and meteorological research, efforts between the Watershed Hydrology Lab at Montana State University (MSU) and the USFS Rocky Mountain Research Station, several hydrologic and meteorological monitoring stations have been set up within the forest. These include eleven streamflow gauging stations (flumes and open channel) and two eddy-covariance towers (tower at 40 m height and tripod at 3 m height). The streamflow stations collect stage, temperature, and conductivity data for each major tributary in the forest. Several sensors installed on the eddy-covariance towers assist with discerning ecosystem trends by measuring concentrations of water vapor, concentrations of carbon dioxide, and three-dimensional wind speed every tenth of a second.

Data can only be physically stored within data loggers at each station for a maximum of two to three months and is manually downloaded by Forest Service employees and MSU researchers for analysis. Access to the stations is difficult particularly in the winter months when snowmobiles must be used for travel within the forest. A remote communication system will provide a method for direct data transmission between TCEF and the VOEIS system at MSU. This will greatly reduce the potential for lost data, eliminate costly man-hours spent in the field, and will provide real-time data streams to forest managers and researchers. Such a system will provide the ability to monitor sensor activity and system power supplies as well as make watershed process predictions based on the real-time data.

C. The Timberlake Case Study

The Timberlake Observatory for Wetland Restoration (TOWeR) is a 440 ha former agricultural field on the coastal plain of NC that was recently abandoned, purchased by investors, and restored to a forested wetland for use as a wetland mitigation bank. This case study is a collaborative effort between Duke University, Wright State University and

Montana State University. As a result of hydrologic reconnection coupled with severe hydrologic drought, seasonal saltwater intrusion (via surface water) was documented for the first time in this site in 2007. It is anticipated that over time, these seasonal shifts will increase in both duration and salinity until ultimately TOWeR transitions to an estuarine ecosystem. Throughout this transition biogeochemical cycling will shift dramatically, but the rate and shape of this change is uncertain. Indeed, salt water intrusion and sea level rise introduce key challenges to basic understanding of coastal wetland biogeochemistry worldwide. The VOEIS system at MSU will be used to catalog and store data and metadata collected at the site. Researchers have instrumented a total of 43 permanent sampling stations throughout the site. Sampling sites are arrayed to encompass the full gradient of elevation across the site in order to capture natural variations in water levels.

V. FUTURE WORK

A challenge in ecological analysis is projecting ecological processes through time (past-to-present-to future) and across space (from field sensor locations across large landscapes). Simulation modeling provides the means for such projection. Data from sensors are used to both parameterize and to validate these models. VOEIS will be specifically designed to allow data resources to be accessed by simulation models. Collaborations with the University of Kentucky's visualization labs are currently underway to develop APIs that will facilitate high performance visualizations of these simulations. In particular, the VOEIS team is investigating the use of the Open Modeling Interface (OpenMI) [16] as a means to exchange data between operational models, thus facilitating data interchange at run time. Further, we are investigating leveraging technologies from the e-Science community (e.g., NCSA, DataOne) to avoid replication of services or the proliferation of unnecessary technologies. For example, client APIs, workflow management and provenance components.

VI. CONCLUSIONS

VOEIS provides cyber-infrastructure capabilities for managing various workflows and providing a data model that are directly aligned with the goals of other efforts currently undertaken by research and investigative groups working to promote an integrated environment for the sharing of scientific knowledge. The informatics system developed through this project is designed to manage vast amounts of legacy data as well as new data generated by the sensor networks deployed at the biological stations.

The development of the VOEIS framework enables a unique capability for PIs to manage and analyze information quickly. The informatics framework aligns itself with existing and broader efforts currently under development by the greater e-Science community.

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