CI-WATER: Cyberinfrastructure to Advance High Performance Water Resource Modeling

Norman L. Jones[1], Jim Nelson[2], Gus Williams[3], Fred Ogden[4], David Tarboton[5], and Steve Burian[6]

[1]Civil and Environmental Engineering, 242L Clyde Building, Brigham Young University, Provo, UT 84604; PH (801) 422-7569; e-mail: njones@byu.edu
[2]Civil and Environmental Engineering, 242K Clyde Building, Brigham Young University, Provo, UT 84604; PH (801) 422-7632; e-mail: jimn@byu.edu
[3]Civil and Environmental Engineering, 242F Clyde Building, Brigham Young University, Provo, UT 84604; PH (801) 422-7810; e-mail: williagp@byu.edu
[4]Civil Engineering, Dept 3295, 1000 E University Avenue, University of Wyoming, Laramie, Wyoming 82071 (307) 766-6171, E-Mail: fogden@uwyo.edu
[5]Utah Water Research Laboratory, Civil and Environmental Engineering, 8200 Old Main Hill, Utah State University Dept 3295, 1000 E University Avenue, Utah State University, Logan Utah 84322-4110 (435) 797-3172, E-Mail: david.tarboton@usu.edu
[6]Civil and Environmental Engineering, 110 Central Campus Drive, Suite 2000, University of Utah, Salt Lake City, Utah 84112-0561 (801) 585-5721, E-Mail: burian@eng.utah.edu

ABSTRACT

We present a collaborative research project called CI-WATER which involves a consortium of Utah and Wyoming researchers. The objective of the project is to acquire and develop hardware and software cyberinfrastructure (CI) to support the development and use of large-scale, high-resolution computational water resources models to enable comprehensive examination of integrated system behavior through physically-based, data-driven simulation. The scientific problem that this project addresses is: How are the quality and availability of water resources sensitive to climate variability, watershed alterations, and management activities? The CI challenge that we are addressing is: How can we best structure data and computer models to address this scientific problem through the use of high-performance and data-intensive computing by discipline scientists coming to this problem without extensive computational and algorithmic knowledge and experience? The project thus aims to broaden the application of CI and HPC techniques into the domain of integrated water resources modeling.

INTRODUCTION

Population growth, shifting land uses, and climate variability are altering the magnitude and timing of water fluxes, stores, and availability in the arid intermountain U.S. These alterations are driven by coupled human-natural system interactions at spatial scales ranging from farm plots and buildings to entire river basins and temporal scales from seconds to centuries. The pressures produce interconnected responses in atmospheric, surface, and subsurface processes threatening the sustainability of natural water systems supporting fragile ecosystems and the resiliency of constructed water systems serving tens of millions of people

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who depend on them. Numerous researchers have investigated the individual atmospheric, hydrological, geological, environmental, economic, and sociological components of this complex human-natural water system. However, components are only infrequently integrated to characterize the overall system sustainability. Furthermore, it is rare for comprehensive evaluation of integrated system behavior to inform or guide land use or water system planning or management by individual users, cities, water conservancy districts, or states. And yet, integration is needed to understand system sustainability and to support planning and management within these water systems. Successful integration requires vision, data, software and simulation models, hardware, and tools to visualize and disseminate results, and outreach to engage stakeholders and impart science into policy, management, and decisions. Computational requirements increase by one or more orders of magnitude when we use stochastic Monte-Carlo methods to consider uncertainties, finer spatial or temporal resolutions to improve accuracy, and dynamic processes to include feedbacks among system components. An integrated software, hardware, and visualization system that meets these needs does not exist for water resources and explains why water system planning and management has largely proceeded without an integrated perspective.

CI-WATER is a cooperative research grant funded by the National Science Foundation involving researchers from two states and four universities: Brigham Young University, the University of Utah, Utah State University, and the University of Wyoming. CI-WATER is being used to establish a robust and distributed cyberinfrastructure (CI) consisting of data services, visualization tools, and a comprehensive education and outreach program that will support this integration and revolutionize how computer models are used to support long-term planning and water resource management in the Intermountain West.

The scientific problem being addressed by CI-WATER is *how the quality and availability of water resources are sensitive to climate variability, watershed alterations and management activities*, while the cyberinfrastructure challenge that we are addressing is *how to best structure data and computer models to support addressing this scientific problem through the use of high performance and data intensive computing by discipline scientists coming to this problem without extensive computational and algorithmic knowledge and experience*. The project thus aims to broaden the application of CI and specifically HPC techniques into the domain of integrated water resources modeling. This project provides cyberinfrastructure that improves access to data and sophisticated models, combines models and model components from different sources, enables scientists to populate models with readily accessible data, harnesses high-performance computing resources to perform multi-decadal simulations over large spatial areas with high space-time resolution, and transforms the way hydrologic knowledge is created and used in water resource planning. Our CI developments leverage and extend our expertise and ongoing and previous research investments from NSF in informatics and cyberinfrastructure. They also build on research investments from other government agencies and private corporations in modeling and informatics. To meet these goals, our project consists of four primary objectives:

1. Enhance cyberinfrastructure facilities.
2. Enhance access to data and computationally intensive modeling.
3. Advance high-resolution multi-physics watershed modeling.
4. Promote STEM learning and water science engagement.

CYBERINFRASTRUCTURE FACILITIES

In addition to their proximity in the mostly high deserts of the Intermountain West, Utah and Wyoming share a number of similarities in their CI opportunities and challenges. For large-scale data center development, both states offer relatively inexpensive electric power. Their cool, dry climates promote the use of ambient air most of the year for data center cooling, thus greatly reducing the operational costs of these facilities. The State of Wyoming is a major investor in the new National Center for Atmospheric Research (NCAR)/Wyoming Data Center (NWSC) outside Cheyenne and has committed $40M in state funds to the facility. Concurrently, the University of Utah is making an investment in excess of $25M to convert a former industrial building in downtown Salt Lake City into a campus and statewide HPC and Data Center; half the facility is initially devoted to HPC, including 1.25 MW of power and space for 100 racks of HPC and storage hardware.

At each university, we have identified new CI facilities required to supplement these resources and to address the scientific needs posed by Components 2 and 3 of this project. Accordingly, are acquiring and deploying appropriate development and staging environments that is enabling the project teams to develop and prototype the needed software and modeling components of this project. In addition, we are purchasing and deploying production web servers and enhanced storage resources within the UU data center to host project websites, data services, and datasets developed by this project. The enhanced storage resources in the UU's data center will serve as a staging area for assembling large data packages to be sent to HPC resources at the time of model execution.

With NSF support, both States have also made or are currently implementing major investments in optical networks to connect the four research university campuses and the two new data centers to proximate national research and education network nodes in Salt Lake City and Denver. Networking investments have provided the University of Wyoming (UWYO) with excellent connectivity via redundant 10-Gbps connections along the Bi-State Optical Network (BiSON) to the Front Range GigaPOP.

Currently, the largest scientific computers at UWYO are a 512 CPU cluster and a 64 GPU compute cluster. Through this project, UWYO has acquired a 100+ TFLOPs hybrid multi-processor computer system and associated storage resources dedicated to supporting the combined HPC modeling needs of our consortium. The UWYO computer system is lighter on disk storage than normal since we intend to use the proposed data facilities at UU to house large data sets that will be read at the beginning of simulations and saved after the simulations are completed. A significant portion of the disk storage at UWYO will act as a large disk cache where all consortium members can stage large datasets and model packages for timely execution on the large machine. The NWSC machine also will have a GPU component so we easily can migrate code developed on the proposed UWYO machine to NWSC.

At the UU's new data center, we are deploying a Utah/Wyoming atmospheric and hydrologic data repository (CI-WATER STORE) with 180 Terabytes (TB) of usable storage initially and at least one 96 TB couplet added annually thereafter (roughly 0.4 Petabyte overall). This will provide the CI foundation to meet the data storage, sharing, analysis, and curation requirements of the high-resolution, data-intensive modeling proposed. We plan to utilize the capabilities of the UU's new data center, including reliable power, engineering and operational support, and an existing HPC-based storage array that can accommodate the proposed growth with minimal impact on users and system administrator time. CI-WATER STORE will be managed centrally and deployed as dedicated or shared storage resources. File system allocation policies can be tuned at the name space, directory, and individual file levels to meet the mixed usage requirements. This system granularity also will enable snapshots, auto-tiering (usually used to move unused files to slower but more economical disks, drives, or tape), replication, and quotas. Additional storage resources and development server capability are being established at USU and BYU to support development work at those institutions.

DATA AND COMPUTATIONALLY INTENSIVE MODELING

Currently, there exists a digital divide among most hydrologic researchers (experimentalists and modelers who have process-based modeling expertise) and HPC experts who have technical hardware and programming knowledge to efficiently use HPC resources and the resource managers who need to translate the outcomes to practical planning. This divide limits comprehensive modeling and the greater understanding of integrated hydrologic-human processes that we believe it would provide. Additionally, modelers spend much of their time finding and organizing required model input data, rather than engaging in analyses that lead to scientific discoveries. Thus, the significant CI challenges tackled by the work proposed under this component are to: (1) provide hydrologic researchers, modelers, water managers, and users access to HPC resources without requiring they become HPC and CI experts and (2) to reduce the amount of time and effort spent in finding and organizing the data required to execute the models. This challenge is really the CI to elevate water resources modeling to fully exploit the "fourth paradigm" use of computational simulation and data-intensive modeling to gain understanding from massive datasets that have emerged as avenues for scientific discovery [Hey, Et al, 2009].

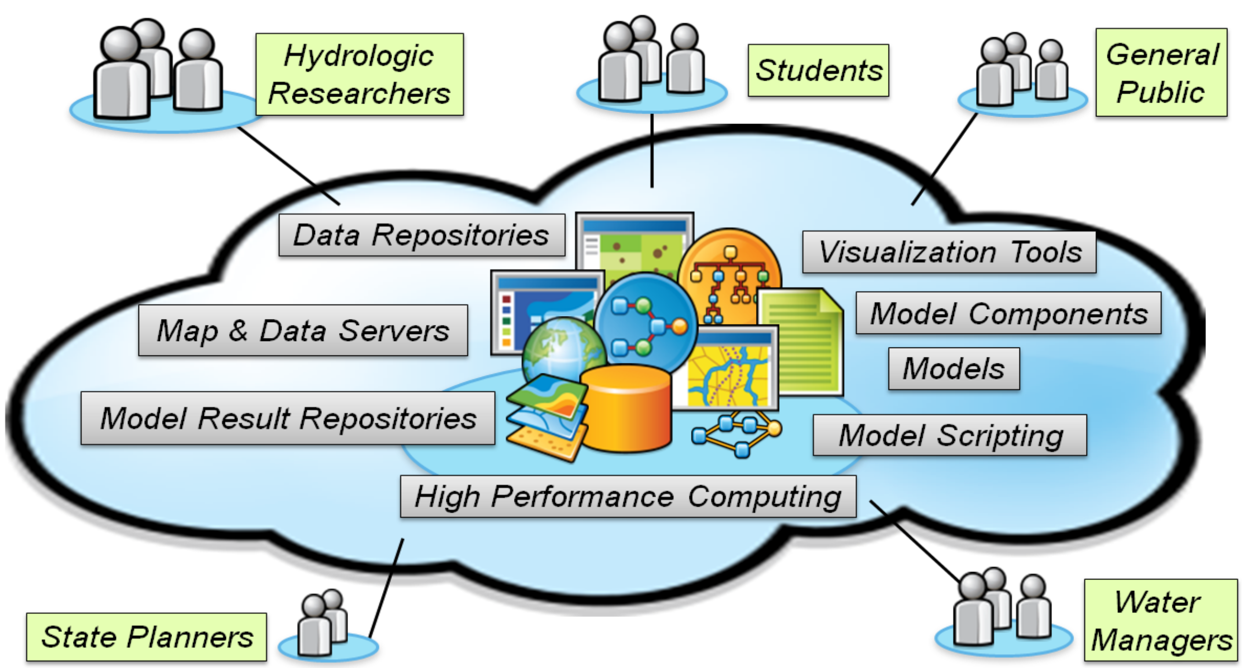

Figure 1. Data- and Computationally-Intensive Modeling Collaboratory.

To address these challenges, we are developing easy-to-use model and data interfaces that link integrated system models running within an HPC environment to multiple data sources, allow users to efficiently and effectively explore alternative physical representations of study systems, and describe the sensitivity to and consequences of alternative representations on the integrated system represented by the models. Additionally, we are developing user interfaces hosted on the Cloud that summarize and visualize data and model outputs to support research, hypothesis testing and inform water management decisions. This combination of data, modeling, analysis, and visualization capability will result in a collaboratory in support of data- and computationally-intensive water resources modeling (Figure 1). In this context, collaboratory refers to a community-specific computational environment for research and education that provides HPC services, data and information services, knowledge management services, human interface and visualization services, and collaboration services, all of which are essential to facilitating high scientific productivity [Tech Working Group, 2005].

The focus of this component is the CI framework that enhances access to data- and computationally-intensive modeling. It is complementary to Component 3 below, which focuses on enhancing multi-physics modeling capability. Teams working on Components 2 and 3 will be closely coordinated and have considerable overlap in membership.

HIGH-RESOLUTION MULTI-PHYSICS WATERSHED MODELING

The Upper Colorado River Basin provides a natural setting for a collaboration between Utah and Wyoming since continued trends towards increases in temperature will likely result in reduced runoff from upper basin States [NRC, 2007; Milly, Et al, 2007; Christensen & Lettenmaier, 2007; Gleick, 2000]. Effective water management requires watershed-scale integration of data and simulation models within a socio-economic and prior-appropriations water rights framework that seeks to minimize the negative impacts of management decisions upon stakeholders and the environment [NRC, 2007]. In the western U.S., watershed management is most often performed at the scale of river basins, with key points where water must be delivered on demand according to in-state water rights or interstate compacts. These points consist of irrigation, industrial, or municipal diversions, are identified at the boundaries between States and other points defined by interstate compacts. Current models use grids of >1 km^2 and run overnight on a single CPU, whereas important processes such as snowmelt occur at scales of 100 m^2. Furthermore, existing models do not represent the built environment and water rights with sufficient detail to evaluate infrastructure and land-use changes at scales where they predominantly occur. Effective management with uncertain forcing and inputs requires consideration of large numbers of scenarios. The CI associated with this project will allow results to be obtained in a timely fashion so as to be useful to government agencies, water managers and planners and the community in general.

Hydrological modeling of large river basins in the western United States has been possible for decades. However, detailed, high-resolution research hydrologic models [Downer & Ogden, 2004; Qu & Duffy, 2007; Maxwell & Miller, 2005] either do not run on HPC systems or simulate the complexity of the built environment or prior-appropriation water rights. Two models that have been used with significant success in the Colorado River Basin are the Variable Infiltration Capacity (VIC) model [Gao, Et al, 2010], and Riverware [Zagona, Et al, 1998]. These models have been successfully applied at large scales, and rely on empirical relations or statistics to account for subgrid features that cannot be resolved within the model spatial discretization.

Neither of these models contains fully-coupled hydrodynamic processes necessary to simulate all feedbacks associated with land-use and climate changes that make management of over-allocated rivers in the western U.S. challenging.

There is a need for high space-time resolution models that can simulate the effects of changes at the scale of pine stands and agricultural fields on the response of the Colorado River basin. This model will have broad applications for hydrological studies, watershed management, economic analysis, as well as evaluation of changes in environmental policy and law. To be useful, the results must be available in minutes and we must be able to perform "what if" inquiries using Monte-Carlo techniques [Liu, 2008; Vrugt, Et al, 2003] and ensemble Kalman filtering methodologies [Evensen, 2009; Slater & Clark 2006] for data assimilation without re-running the entire simulation.

We are creating a new model to fill this important need that is specifically developed for HPC environments, not single PCs. Our goal is to include all hydrologically important processes and anthropogenic influences at scales of relevance using a physics-based approach wherein parameter values are measurable and identifiable and provide useful results for non-researchers. The CI-WATER HPC model will operate at grid sizes as small as 10 m, and ingest data from remote sensing sources, atmospheric models and geophysical techniques. The model uses an unstructured grid with adaptive grid capabilities [Thompson, Et al, 1985; Thompson, Et al, 1998].

The new model includes the following features: three-dimensional groundwater simulation capabilities for predicting mountain-front infiltration and the effects of groundwater pumping on stream flows. The vadose zone is simulated using a one- and two-dimensional multi-physics algorithm [Talbot & Ogden, 2008] that can simulate variably-saturated matrix, macropore, crack, and film flow. Surface flow algorithms include two-dimensional overland flow routing, and one-dimensional full-dynamic channel flow routing on a dendritic (vector) channel network. The channel network interacts with lakes, reservoirs, detention basins, irrigation diversions, and trans-basin transfers.

The accumulation, re-distribution, sublimation, and melt of snow above 2400 m (8000 ft) elevation provide the dominant source of water in the western U.S. [Bales, Et al, 2006]. The CI-WATER HPC model will include published snowmelt routines and facilitate testing of advanced routines to simulate these processes. High spatial resolutions employed will allow simulation of snow redistribution in mountainous terrain [Liston & Elder, 2006; Liston, Et al, 2007], while above-ground LiDAR returns that quantify the location and distribution of above-ground canopy will allow explicit simulation of stand-level effects of vegetation on snow accumulation and melt [Stork, Et al, 2002]. Large eddy simulations will allow explicit simulation of snow/topography/vegetation interactions [Lehning, Et al, 2000], which is very important given the pine bark beetle epidemic underway in the region [Bentz, Et al, 2010].

The model design will include development of application programming interface (API) standards to allow easy substitution of alternative process-level simulation routines [Kumar, Et al, 2006]. Existing widely-used and successful codes will be employed to avoid "re-inventing the wheel". The modeling system will include ensemble Kalman filtering [Vrugt & Robinson, 2007] to improve forecast prediction accuracy while quantifying the effect of model formulation errors on predictions. Monte-Carlo techniques [Liu, 2008] will allow evaluation of the effects of parameter, data, and model uncertainties when used in a predictive mode. We will use finite volume and finite element discretizations on various grid types. Explicit numerical solvers will provide highly scalable parallelism to take advantage of the UWYO CI. Fluxes are needed on multiple processors and we will employ an efficient, highly scalable database approach providing a virtual shared memory using either commercial or freeware versions of a similar system [52-54].

As smaller discretizations are employed and/or larger watersheds are studied, the parallelism will grow. At the 10 m land-surface resolution, the memory requirement for each ensemble member for a demonstration scale problem (Green River basin in Wyoming) is about 200 GB. For the Upper Colorado River basin above Lake Powell, it is about 5200 GB. While sensors and mapping databases would have to be improved significantly, in the future a 1 m LiDAR-derived land-surface resolution will require 100 times the memory. For a single ensemble member, at some land-surface resolution and number of state variables we will have to move to the NWSC facilities since we will be running simulations too large for the UWYO CI. Further, we need 20-100 ensemble members so the memory requirements might outstrip the capacity of the first computer at NWSC by the end of our three-year project and might be a candidate for the NWSC in the 2015-2016 timeframe.

STEM LEARNING AND WATER SCIENCE ENGAGEMENT

An update to the report *Rising Above the Gathering Storm* [55] indicates an immediate, high priority to increase America's talent pool, research, and incentives for innovation to assure U.S. security and competitiveness. The most pervasive concern is the state of U.S. K-12 education, which on average lags behind other industrial economies - while costing more per student than any other developed country. Utah and Wyoming educators face similar obstacles to engaging learners in environmental science. This project comes during a period when educators report a severe lack of timely science content for their formal and informal learning environments. According to a recent assessment by the Utah Society for Environmental Education, only 31% of Utah teachers received any pre-service training in environmental education, and the majority of elementary school teachers say they are not comfortable teaching environmental and natural history or environmental science issues [56]. Wyoming teachers report similar needs for environmental science content. Further, only 23% of Wyoming's adult population holds a college degree, pointing to the need to educate at all levels of the population.

We are advancing NSF Core Priorities, particularly science and technology education in formal and informal learning environments. We are fostering scientific cyber-literacy and improving educational and research capacity within the CI-WATER consortium through education activities designed to reach three audiences across the STEM learning pipeline: 1) High School Students and Teachers; 2) Higher Education and Water Professionals; and 3) Adult Learners. STEM learning and community engagement partners include the Utah Museum of Natural History (UMNH), the UU's Genetics Science Learning Center (GSLC), Wyoming PBS, and The Science Zone in Wyoming, each of which has a strong track record in STEM learning with educators and citizens. See Figure 2 for details of the activities proposed.

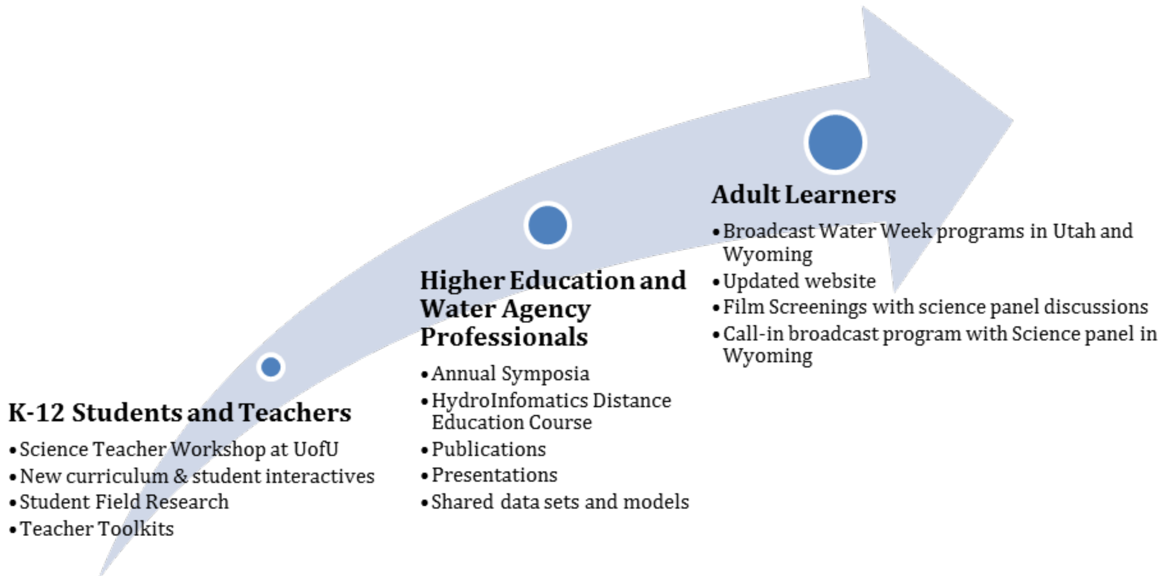

Figure 2. Audiences in the STEM learning pipeline.

Each participating organization is committed to building scientific literacy and strengthening the educational and research capacity throughout and beyond the Consortium. We specifically focus on cyber-literacy with a goal to improve an understanding of quantitative and computationally-intensive scientific methods, and water scarcity issues specific to the West. To accomplish this goal, the Utah Education Network (UEN) is serving as the lead education partner working with the WY EPSCoR office to create STEM learning opportunities designed to develop a diverse, well-prepared, globally engaged, and scientifically literate public for our specific target groups, as described below.

CONCLUSIONS

This project will result in unprecedented access to data for water resources modeling in the Western U.S. as well as unprecedented capability for non-HPC specialists to take advantage of these data and perform data- and computationally-intensive model simulations to evaluate hypothesis, quantify uncertainty and embrace computational thinking in their research. Implementing the data services, modeling tools, and model integration in a HPC environment will provide the ability to execute full-detail watershed models in long-term continuous simulation mode with incorporated uncertainty. The new data available on water resources infrastructure will facilitate previously impossible detailed simulations of water resources systems sensitivity properly accounting for the presence of human alterations in the system. This will enable a fundamentally deeper understanding of water resources in Utah and Wyoming. The CI-WATER HPC model being developed promises a significant advance that will revolutionize the way in which water is managed in the western U.S. The model also provides a bottom-up HPC modeling system for hypothesis testing and model rejection within a multi-university collaboration. The outreach activities will enable a new generation of scientists to utilize these tools to solve the water resource management challenges of tomorrow.

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