A COMMUNITY MODEL FOR WATER IN THE CONTINENTAL EARTH SYSTEM

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SUMMARY

The ability to simulate water in the continental Earth system is scattered among myriad disciplines and this lack of focus is impeding scientific progress. We suggest that EarthCube should develop a Community Water Model designed to bring the scientific community together to link data and computations that will provide the best available simulations of the hydrologic cycle and coupled water-related processes. It will be an open-source code managed by the scientific community and its capabilities will grow through contributions from the community. The Community Water Model can serve as the connection point for other disciplines that require prediction of water movement, including general atmospheric and ocean circulation, landform evolution, biogeochemical, vegetation, ecological, geodetic and economic models.

INTRODUCTION

Water permeates the geosciences. It is central to hydrology, ocean and atmospheric sciences and glaciology, but it plays important roles in many other geosciences, from geochemistry to geomorphology, tectonics, geophysics and sedimentary geology. It is the most essential earth resource and no discussion of sustainability can avoid it. It ties the geosphere to ecosystems, and is one of the primary factors affecting human health and quality of life worldwide.

Computer simulators are important tools to the diverse cadre of scientists working on water. The physics of water movement in the atmosphere are much different than for water flowing on the ground surface or through the pores of the subsurface, so separate models have traditionally been developed for each of these domains. Recent advances have enabled hydrologic models to couple water flow in the subsurface to flow on the ground surface, and some of them can also include coupling to water transport in the atmosphere.

These efforts, although promising, are currently fragmented across many research groups and across disciplines. This has resulted in redundancy and inefficiency, which have limited progress in water sciences. It has also hampered progress in other disciplines, such as atmospheric and ocean sciences, where simulators of weather, climate and ocean circulation are limited by their ability to make use of state-of-the-art simulations of continental water.

The problem is not limited to redundancy and inefficiency in code development. Many grand science challenges require fundamental understanding of water processes that cannot be met by the capabilities of current models. Some science questions require understanding at the scale of a pore or plot, which must then be tested in other hydrogeologic settings and applied over large watersheds or continents. Simulating this broad range of spatial and temporal scales, and readily accessing the requisite data remain unrealized goals. Other limitations are caused by coupling diverse processes across hydrologic domains that are dominated by different physics operating over a range of time scales.

Community Water Model

Scientific progress could be accelerated by a new generation of simulator that integrates the community-wide breadth of knowledge and skills into an extensible *Community Water Model*. Such a model would serve as a benchmark against which to measure progress as new models are developed, and as a standard reference model for water movement that can be extended for use by all other disciplines where water plays a role.

The objective of the Community Water Model (CWM) would be to provide the best available simulations of water-related processes anywhere in the U.S. and beyond. Considerable progress has been made on this type of simulation, yet the best numerical solvers for specific problems and the appropriate process representation at any given scale remain open research questions. As a result, the Community Water Model needs to be built on computational infrastructure designed with the versatility to explore these questions. Precedent exists for this type of computational diversity with the development of multiphysics codes (e.g. Comsol, CFD ACE+, Adina, Simulia, Ansys, Elmer, Algor).

Despite their considerable strengths, current multiphysics codes are designed for general analyses and can perform relatively poorly on some problems of particular importance to water science. Moreover, they lack the facility to create the specialized geometries required to represent subsurface conditions. What is needed is a simulation platform with the versatility of current multiphysics codes, but with specialized, open-source capabilities developed to solve problems within the water science domain.

An important aspect of this approach would be the ability to record workflow describing how a particular analysis was conducted. Different workflow configurations describing water movement and its interaction with the earth system would be constructed to meet different objectives (such as flash flood prediction, nutrient cycling, or vegetation response to climate scenarios). Sharing these different workflow configurations will enable the community to explore alternate representations of processes, parameterizations, and model geometries to understand how these factors interact.

Ultimately, the Community Water Model would consist of the best workflows developed by the community to simulate water-related processes. This mechanism will allow the capabilities of the CWM to evolve and continuously improve as innovations are recognized.

Fast access to data

Fast access to the data needed to calibrate and force simulations is as important to the success of the Community Water Model as access to advance numerical algorithms. Some data describing the continental environment are available in electronic datasets supported by federal agencies, but other critical data are available only in hard copy (hydrostratigraphy is an important example). Assembling these data is tedious because of varying file formats and accessibility, and making large amounts of data available during execution of a simulator requires even further effort. This is a clear bottleneck to the development of an effective CWM, and one that will require a targeted effort to overcome.

Community contributions

The Community Water Model would be a resource for the broad, Earth system science community, including researchers from across academia, government agencies, national labs, and the private sector. Initial design and construction would be done by a core development team of experts in domain modeling and software engineering. Subsequent developments that improve the modules or create new ones will evolve from contributions of code from across the water science community, other science disciplines, and software engineers.

In addition to code, the science community will also contribute workflow describing how the platform was used to solve a particular problem. Workflow records identifying how the platform was configured to solve a problem will allow a particular approach to be documented and communicated to others (i.e., the workflow could be published).

EarthCube: an Invitation to Collaborators

We suggest that EarthCube should embrace a Community Water Model and the data needed to use it. This cyberinfrastructure would be a major scientific resource that would both contribute to, and benefit from, many of the geosciences.

The need for a Community Water Model was identified during a series of community workshops organized by the Consortium of Universities for the Advancement of Hydrologic Sciences (CUAHSI) and described by *Famiglietti et al.* (2011). A plan for developing such a model is outlined in *CUAHSI* (2011).

The water science community feels strongly that a community model will advance their science, but this can only by accomplished through the collaboration of the broader science and engineering communities. Water flow and storage are strongly coupled to many processes, so accurately simulating water requires that those other processes are also represented. Correctly representing these couplings is a key challenge that can only be met through collaboration with other domain scientists. This collaboration will not be just a one-way street, however. Improving the CWM will enable better representation of water dynamics, which will benefit many of the domain collaborators.

Scientific Functionality

Creating the needed functionality will require input from domain scientists from a range of geosciences and from other areas. Some of the collaborations we would seek as part of EarthCube include:

Atmospheric Sciences The CWM will need rapid access to data describing precipitation, temperature, moisture flux and other aspects of the atmospheric boundary layer, and it will also need to link with codes describing weather and climate. In turn, the CWM will provide improved predictions of water storage in soil and aquifers, and flux across the land surface, which should feed back to improve simulations of weather and climate.

Ocean Sciences Data describing the base level of the ocean during tidal cycles and over longer periods, as well as the distribution of flow in the near shore environment will be needed, along with coupling to codes that predict these processes. The CWM can provide improved estimates of the magnitude and distribution of water flow, and transport of dissolved compounds and sediment influx to coastal areas. This could be particularly beneficial to the prediction of storm surges, coastal contamination, estuary ecosystems, and other processes.

Geochemistry Data describing the distribution of dissolved compounds, along with the equilibrium and kinetic data describing reaction rates will be an important contribution to the CWM. In return, the CWM will be capable of providing better predictions of mass fluxes during reactive transport through time at locations across the continent.

Geomorphology Data documenting the erosion and deposition of sediment over the land surface and in channels, as well as methods of predicting sediment transport will be needed for the CWM. The geomorphology community could benefit from improved predictions of water flow rates and distributions during ambient and extreme events, which could be used to develop independent models of landform evolution and transport of earth materials.

Geology A 3-D electronic representation of the distribution of rock units, along with estimates of the permeability and porosity, will be critical to developing a hydrostratigraphic model for the CWM. This is among the most critical pieces of missing data needed for the CWM. Advances in predicting water flow, transport and reactions in the subsurface will help the sedimentary geology community understand diagenesis.

Ecosystems Water transpiration by plants is a major component of the hydrologic cycle and advances in both data and methods for predicting transpiration rates will be important for the CWM. Species redistribution occurring as a result of changes in soil water content and temperature will be required data for correctly anticipating effects of climate change on water. The movement of water across the landscape facilitates carbon and nutrient exchange between terrestrial and aquatic ecosystems, and hence the porous media property and groundwater-surface water connectivity, at a range of scales, are essential data required to support the CWM. Advances in the CWM will improve predictions of water content and temperature in soil, as well as water depth, flow rate, temperature and water composition in streams and lakes, and these data will have important applications in ecosystem models.

Neotectonics and Geodetics Deformation data collected during studies of recent tectonics and geodetics bear a signature of changes in water pressure, either due to changes in the level of lakes or ground water. Deformation data from InSAR or GPS arrays would be useful in the CWM. In turn, the CWM would provide improved predictions of changes in water pressures, which will help separate tectonic signals from poroelastic responses due to pumping.

Engineering and Water Management Movement of water on continents has been strongly affected by human actions, and both data and simulation techniques describing these effects will be needed. The location and characteristics of drains, sewers, canals, impoundments, impervious surfaces and other built structures affecting water flow will be required. Data describing pumping, dam releases, and other human controls on water will also be needed. In return, the CWM will be capable of providing improved estimates of water flow rates and levels during extreme events and in response to human actions, which will benefit decision-making by the engineering and water management communities.

Geophysics The seismic community would have important contributions to the subsurface structure defining hydrostratigraphy. Gravity data, both from satellites and land-based microgravity data would also be important contributions.

Other Community Modeling Approaches

Another strategy to develop a versatile model with community contributions is to use protocols like OpenMI or Common Component Architecture (CCA) used in Community Surface Dynamics Modeling System (CSDMS), where components can be extracted from different existing models and coupled together to create new capability. Coupling existing models or model components using CSDMS or OpenMI leverages the significant library of existing codes and is an important way to advance the science.

The Community Water Model proposed here would focus on solving multiple water-related physics problems that are fully coupled in the same matrix, which should be a more effective approach for representing strongly coupled processes than linking separate codes. Ultimately, we envision that the CWM would also be capable of coupling to other external codes to expand versatility, and we hope that CSDMS would be an important partner in accomplishing this capability.

Other national-scale water models have been developed and collaborations with these efforts would also be important. Many federal agencies (USGS, NOAA, NASA, USDA, DOE, etc.) have significant activities in this area, and they would be critical partners. A major modeling effort as part of the Australian Water Resources Assessment is an example of one of several international projects that would lead to productive collaborations.

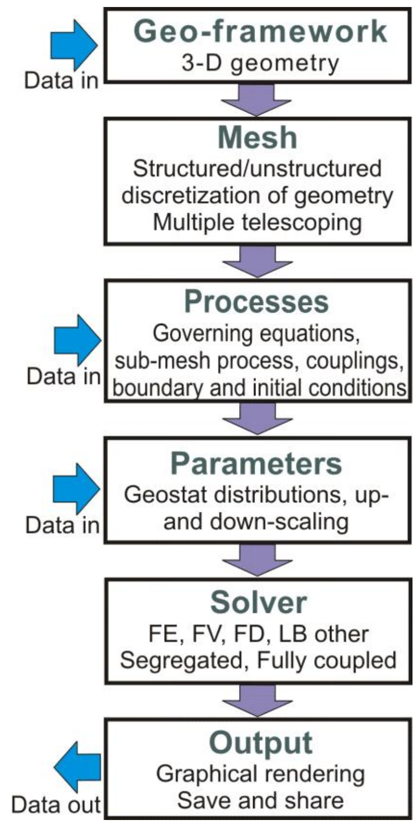

Figure 1. Major modules and basic workflow for developing an analysis using the Community Water Model.

Software Engineering

The development of a CWM will rely on close collaboration between domain scientists and software engineers. The conventional paradigm of domain scientists doing software development will be revised to include software specialists as major players in the development process. EarthCube will be an ideal forum for this type of development because of the breadth of skill sets that are involved. We recognize several major software components that will be required.

Interface

Graphical system for accessing functionality. It will be important that the interface is easy to use in order to facilitate access by scientists who are not necessarily expert modelers. Should save and retrieve workflows.

Numerics

Equation generators, element assembly and matrix solvers; data assimilation; up- and downscaling; parameter estimation; optimization.

Geospatial

Geosurfaces and volumes for topographic and geologic modeling; distributions of parameters and forcing terms; geostatistics; mesh generation and refinement;

Visualization

Geometries and distributions during model development; scalar and vector fields in 3-D; video.

Data Access

Fast exchange with data servers.

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