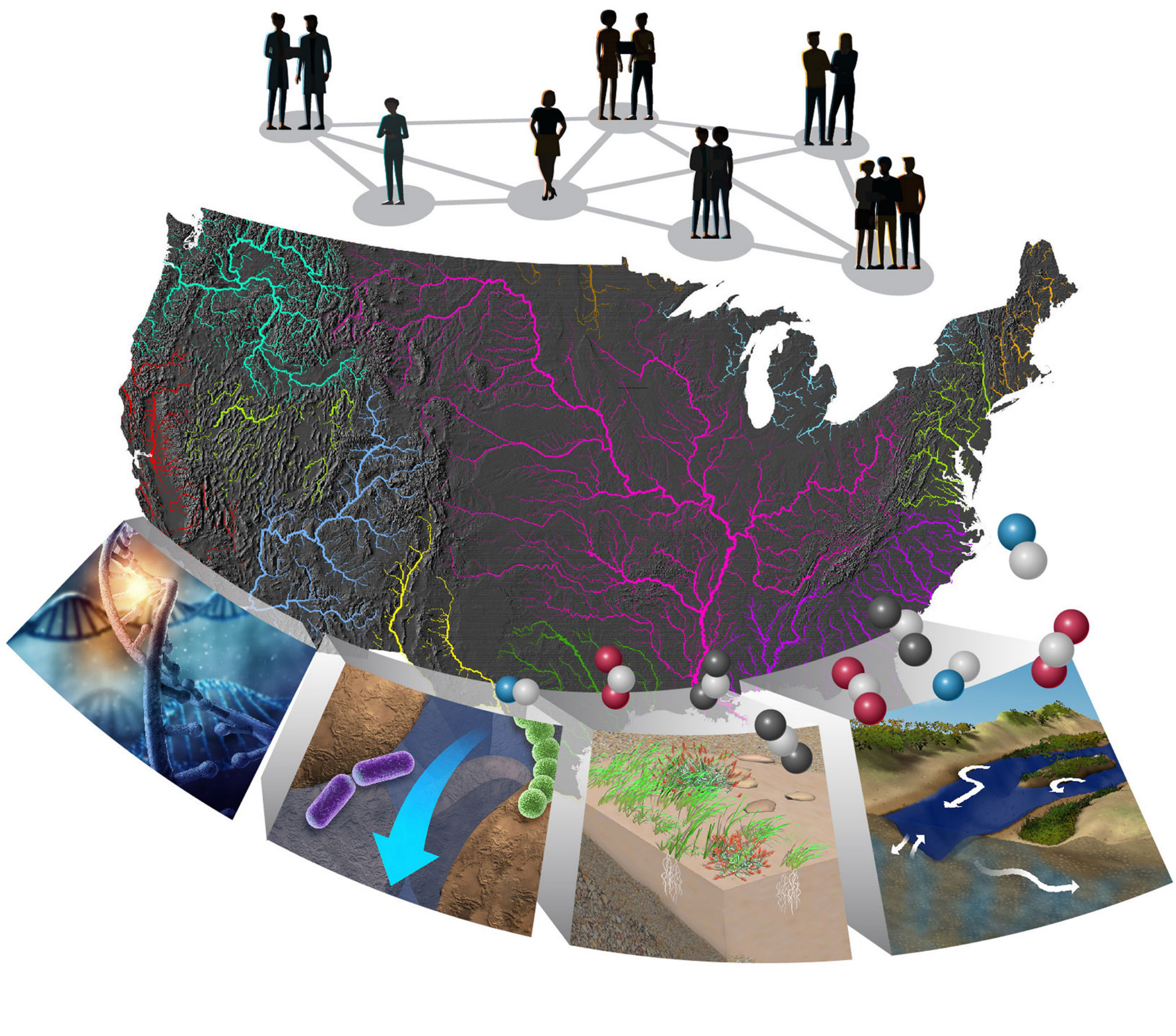
DOE/SC–0200

Open Watershed Science by Design

Leveraging Distributed Research Networks to Understand Watershed Systems

Workshop Report



U.S. DEPARTMENT OF ENERGY | Office of Science

Office of Biological and Environmental Research

Open Watershed Science by Design: Leveraging Distributed Research Networks to Understand Watershed Systems

January 28–30, 2019, Workshop
Rockville, Maryland

Convened by

U.S. Department of Energy
Office of Science
Office of Biological and Environmental Research (BER)

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About BER

The Biological and Environmental Research program (BER) advances fundamental research and scientific user facilities to support U.S. Department of Energy missions in scientific discovery and innovation and energy and infrastructure security. BER seeks to understand biological, biogeochemical, and physical principles needed to predict a continuum of processes occurring across scales, from molecular and genomics-controlled mechanisms to environmental and Earth system change. BER advances understanding of how Earth's dynamic, physical, and biogeochemical systems (atmosphere, land, oceans, sea ice, and subsurface) interact and affect future Earth system and environmental change. This research improves Earth system model predictions and provides valuable information for energy and resource planning.

About the cover: Watersheds and their associated basins organize terrestrial landscapes (map of continental United States with different colors indicating different basins) and integrate physical, chemical, and biological processes across scales (lower boxes showing molecular to river corridor scales). The vision of open watershed science by design is for the community to pursue integrated watershed science as a collective network (indicated by connected people in the graphic) that does together what would be impossible to do alone. [Pacific Northwest National Laboratory]

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Preface and Acknowledgements

The workshop upon which this report is based was convened in response to a community-recognized need for greater openness and coordination of multiwatershed distributed research efforts that integrate across capabilities within the U.S. Department of Energy's (DOE) Office of Biological and Environmental Research (BER) and link to those of other agencies. The science enabled by such an approach targets challenges and strategic directions articulated in the Biological and Environmental Research Advisory Committee's (BERAC) 2017 grand challenges report (BERAC 2017) and the 2018 Climate and Environmental Sciences Division (CESD) strategic plan (U.S. DOE 2018). The BERAC report and CESD strategic plan both focus heavily on the need for integrative research to connect environmental microbes, multiomics, plant system dynamics, biogeochemical interactions, and hydrological processes to understand ecosystem function. The need to develop such connections across scales of space, time, and biological complexity is framed in the context of improving predictions of the Earth system in response to disturbance, including extreme events. This report summarizes the discussions and ideas that came from the watershed systems research community on how to use integrated, coordinated, open, and community-networked watershed science to advance BER's efforts to link fundamental processes to emergent properties of watershed structure, function, and evolution. The ultimate goal is to enhance predictive capacity across scales up to the integrated Earth system.

The objectives of the workshop were as follows:

- Identify specific BER CESD science challenges associated with hydro-biogeochemical uncertainties that require an integrative, distributed watershed system science approach.
- Define capability gaps and solutions for sensing; data transmission, storage, and integration; and data analytics for integrating data streams across biological, physical, and chemical domains.
- Develop implementation plans, including model-informed and practical recommendations for leveraging existing infrastructure and the optimal spatial and temporal deployment of distributed hydro-biogeochemical sensing systems and direct sampling.
- Synthesize strategies to maximize community engagement and identify tractable strategies for sustaining institutional and community support for distributed watershed system science.
- Frame an approach to simultaneously engage the use of capabilities at DOE's Joint Genome Institute, Environmental Molecular Sciences Laboratory, Systems Biology Knowledgebase (KBase), and Environmental Systems Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE) to enable a Subsurface Biogeochemical Research (SBR)–supported science strategy.
- Outline plans to tie current SBR watershed test beds into other networks such as the U.S. Geological Survey's super gauges and National Science Foundation's National Ecological Observatory Network, among others, as well as a constellation of other sites run by researchers not funded by DOE.

BER appreciates the tireless efforts of the workshop organizers, co-writers, and contributors who energetically participated in workshop discussions and generously gave their time and ideas to this important activity. The workshop would not have been possible without the scientific vision and leadership of its organizing committee. BER extends special thanks to the speakers who gave thought-provoking presentations: Eoin Brodie, Ethan Coon, Jesus Gomez-Velez, Maoyi Huang, Praveen Kumar, Kate Maher, Bill McDowell, David Mellor, David Moulton, Carly Robinson, Audrey Sawyer, James Stegen, Charuleka Varadharajan, and Kelly Wrighton. In addition, session rapporteurs deserve acknowledgement for capturing the ideas discussed in breakout sessions for use in the creation of this report: Eoin Brodie, Sujata Emani, Jesus Gomez-Velez, David Mellor, Jessica Moerman, David Moulton, Carly Robinson, Audrey Sawyer, James Stegen, Charuleka Varadharajan, and Kelly Wrighton. Lastly, BER lauds the efforts of the workshop writing team who created this document: Martin Briggs, Eoin Brodie, Amy Goldman, Jesus Gomez-Velez, Kate Maher, David Moulton, Carly Robinson, James Stegen, Charuleka Varadharajan, Roelof Versteeg, Andrew Wickert, Mike Wilkins, and Kelly Wrighton.

Also acknowledged are the outstanding efforts of the staff from Oak Ridge National Laboratory's Biological and Environmental Research Information System, who helped create the workshop visuals and edited and prepared this report for publication.

Executive Summary

The Climate and Environmental Sciences Division (CESD) within the U.S. Department of Energy's (DOE) Office of Biological and Environmental Research (BER) funds basic research that addresses key uncertainties in the understanding of Earth system components, such as watersheds and the subsurface, and spans a wide range of spatial and temporal scales, from molecular to global and from nanoseconds to decades.

Within CESD, the Subsurface Biogeochemical Research program (SBR) is focused on advancing a robust, predictive understanding of how watersheds function as integrated hydro-biogeochemical systems and how these systems respond to disturbances such as changes in water recharge, availability, and quality; contaminant release and transport; nutrient loading; land use; and vegetative cover. SBR investments in watershed system science directly support CESD's mission to enhance the predictability of the Earth system by supporting process research and long-term field studies, making use of BER and other DOE user facilities, undertaking data analytics, and enhancing advanced codes and using best-in-class computing resources. SBR research contributes specifically to CESD's integrated water cycle, biogeochemistry, and data-model integration grand challenges (U.S. DOE 2018).

In addition to addressing CESD's mission and grand challenges, the SBR program is integrating research activities funded by both CESD and BER's Biological Systems Science Division (BSSD), by continuing to support a wide range of spatial and temporal scales of research. For example, the SBR program supports research activities spanning molecular-scale studies of geochemical stability, speciation, and biogeochemical reaction kinetics to field-scale processes involving flows of groundwater and surface water, nutrient loading and cycling, contaminant transformation and transport, and other key hydro-biogeochemical processes. Collectively, SBR research activities directly address the Microbial to Earth System Pathways grand challenges identified by the Biological and Environmental Research Advisory Committee (BERAC) in its 2017 grand challenges report (BERAC 2017), as well as some aspects of the Earth and Environmental Systems Sciences grand challenges.

Over the last decade, SBR has pioneered a complex system science approach to advance a predictive understanding of the hydro-biogeochemical structure, functioning, and dynamics of integrated watershed systems, from subsurface aquifers to surface waters. This approach has led to significant advances in understanding watershed function and dynamics. It was shaped by previous SBR workshops on complex system science (U.S. DOE 2010) and building virtual ecosystems (U.S. DOE 2015a) and designed around a strategic collection of watershed test-bed field sites in the continental United States (CONUS) coupled with a software ecosystem of interoperable codes at scales from molecular to basin.

SBR scientists use test-bed field sites to conduct integrated, process-based research to understand the influences of hydrology (and other physical processes) over fine-scale biogeochemical and microbiological processes and to link those processes to larger-scale phenomena spanning watershed structure, function, and evolution. There are six primary test beds distributed across CONUS that span watershed settings from headwaters to wetlands and ponded systems to main-stem rivers. Data from research within these test beds are incorporated into models that explain hydro-biogeochemical system behavior at multiple spatial and temporal scales. In parallel with this approach, model and code developments are advanced for these test beds to guide additional measurement and experimentation, leading to an iterative cycle of modeling and experimentation.

Despite the significant integration of process research with data analytics and modeling at each test-bed site, there has been relatively little exchange or coordination among the test beds or with other observational networks such as the National Science Foundation's (NSF) Critical Zone Observatories (CZOs). Enhanced coordination is an unexploited opportunity that would amplify SBR science by enabling the transfer of data and process knowledge across watershed systems. Moreover, data sharing is critical for the development of generalizable principles and models that can be used to nimbly deploy predictive capabilities across watersheds as disturbances and other challenges arise. Connecting data and process knowledge across multiple watershed systems would enable comprehensive understanding of the structure, function, and evolution of watershed systems and enable DOE to address a variety of environmental and energy challenges.

To explore innovative methods and approaches for enabling enhanced research coordination across watersheds and advance new strategic partnerships, BER convened the Leveraging Distributed Research Networks to Understand Watershed Systems workshop on January 28–30, 2019, in Rockville, Maryland (see Appendices 1–3, p. 57). This workshop brought together for on-site discussions a number of physical, chemical, and microbial scientists from DOE national laboratories, DOE user facilities, universities, and independent organizations, as well as representatives from other agencies. In addition to the on-site participants, many of whom are funded by SBR and other CESD and BSSD research programs, a number of scientists not funded by or affiliated with DOE received invitations and provided input in the form of premeeting virtual sessions and white papers (see Appendix 4, p. 66).

On-site workshop participants were guided through exercises based on design thinking to identify community needs, challenges, and opportunities in the areas of multiscale integration, measurement, computation, and cyberinfrastructure to enhance coordination among watershed field sites. Four overarching principles, defined together as ICON (see below and Chapter 2, p. 11, for more detailed explanations), were identified as necessary for advancing watershed system science by linking fragmented research networks:

- **I**ntegration of biological, chemical, and physical processes across scales.
- **C**oordinated use of consistent protocols across systems to generate specific data types needed to inform, develop, and improve models for application across systems.
- **O**pen exchange of ideas and consistently structured and usable data that are findable, accessible, interoperable, and reusable (FAIR) such that all are enabled to contribute and leverage resources.
- **N**etworked efforts, whereby data generation and sample collection are done by the broader scientific community in a way that provides resources (e.g., data and sensors) to contributors that otherwise would be difficult or impossible for them to access.

To build greater research capacity through integration of existing investments within SBR, across BER, and with other agencies, use cases incorporating these ICON-FAIR principles and spanning a broad range of scales were proposed and developed. Use case development employed iterative design-thinking processes to incorporate from the project's inception the necessary forethought, planning, and governance required to integrate watershed processes across scales and coordinate scientific activities across research networks and federal agencies.

Three of the use cases focus on a particular scale (including reaction, watershed, and basin scales), while two others operate across scales. Linking across these use cases provides transformative opportunities to address integrated hydro-biogeochemistry across watersheds. Brief summaries of the use cases follow.

The Worldwide Hydrobiogeochemistry Observation Network for Dynamic River Systems (WHONDRS) use case serves as an example of an existing BER research program that embodies ICON-FAIR principles. WHONDRS operates across scales, linking detailed biological and chemical processes to physical features and dynamics within sites, throughout watersheds, and across the planet. More specifically, WHONDRS is a global research consortium working to understand connections among dynamic hydrology, biogeochemistry, and microbiology in river corridors, from local to global scales. It designs studies with the science community, provides free access to sampling materials and analyses, and is enabled by the science community, which volunteers to sample at globally distributed study sites. WHONDRS generates model-relevant data products across watersheds as open resources for the community, enabling access to detailed molecular data (via BER user facilities), unique field instrumentation, and more standard data types (e.g., ion concentrations and sediment texture). Because all data are generated using consistent methods, there is an opportunity to set up models across all sampled locations and use these models to extract fundamental principles that are transferable across watersheds, while also discovering features that are system specific.

Because reaction-scale challenges span both biological and environmental sciences, the Reaction-Scale use case would likewise integrate capabilities across BER divisions. The aim is to develop seamless coordination among BER capabilities through enhanced cyberinfrastructure associated with data and code exchange and paired with consistent methods, from field to laboratory to analysis across watersheds. Key BER capabilities associated with the Reaction-Scale use case include DOE's Environmental Molecular Sciences Laboratory (EMSL) and Joint Genome Institute user facilities, cyberinfrastructure investments such as the Environmental Systems Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE) data archiving and Systems Biology Knowledgebase (KBase) software ecosystem, and the interoperable modeling software ecosystem being developed by the SBR-funded Interoperable Design of Extreme-scale Application Software (IDEAS)–Watersheds project. In addition to these more established capabilities, the emerging capabilities planned under DOE's National Microbiome Data Collaborative provide additional opportunities to integrate microbial data with other molecular data (i.e., at EMSL), as well as with chemical and physical data that are the purview of ESS-DIVE. The integration of BER capabilities coupled with consistency in methods and protocols can be used to address outstanding challenges associated with interactions between fundamental biological and chemical processes. A primary outcome of implementing this forward-looking use case would be a transformation in understanding how chemical-biological interactions vary across physical settings distributed within and across watersheds. This outcome will enable transfer of reaction-scale knowledge, data, and predictive models across watersheds, thereby enhancing understanding and predictive capacity of reaction-scale processes and, ultimately, their influence over larger-scale phenomena.

The Watershed-Scale use case is designed to address challenges that arise due to significant spatial heterogeneity within watersheds. Current approaches to understanding local spatial domains are often but not always conducted using methods that vary across sites. Greater consistency in methods provides opportunities to integrate outcomes across local sites to improve synthetic understanding of governing processes and dynamics throughout a given watershed. Enhanced synthetic understanding will improve the ability to predict how disturbances influence functions relevant to downstream municipalities, ecosystems, and the Earth system. The Watershed-Scale use case envisions coordinated field campaigns distributed within watersheds in which local results are placed in the context of watershed-scale remote-sensing data products. Archived data (e.g., via ESS-DIVE) that are FAIR are to be linked and integrated through the IDEAS-Watersheds project software ecosystem. By providing integrated process understanding throughout the watershed, outcomes should increase the capacity of models to predict impacts of disturbances on watershed hydro-biogeochemical function.

The Basin-Scale use case addresses challenges surrounding the coupling and co-evolution of natural and human systems over a domain encompassing several watersheds. Specifically, a river basin integrates the hydro-biogeochemical function of its watersheds with a variety of human systems (e.g., dams, reservoirs, and diversions), and it supports a variety of natural and human needs, from fish stocks to drinking water, agriculture, and power generation. To meet the needs of this broad range of stakeholders, water-management practices cause disturbances to the natural system that are comparable to those anticipated to be caused by climate change, including changes in peak flows, low flows, and contaminant concentrations. Thus, this use case explores the ways in which ICON-FAIR practices, as well as advances in mechanistic modeling and model-data integration, can be used to enhance collaborations across agencies and more effectively support the challenge of water management under climate change. For example, the increasing use of FAIR principles is supporting the growing integration of new and historical data in national databases and providing the opportunity for more unified and flexible cyberinfrastructure that can serve data analysis, data-driven models, and data integration in mechanistic models. Similarly, the inclusion of effective representations of human systems (e.g., diversions and irrigation) in mechanistic models that can respond to management actions is a relatively new, important area for interagency collaboration and coordination. The outcome of these collaborations and advances will be an increase in the predictive understanding and capacity for supporting the river basin-scale challenges in water management.

The Multiscale use case is designed to address challenges resulting from feedbacks and interactions across scales that influence the resilience of energy sustainability strategies to disturbance. This use case will be based on key multiagency partnerships needed to study watersheds across CONUS in a coordinated and systematic way. In particular, U.S. Geological Survey monitoring data on stream discharge and solute concentrations and NSF field capabilities (e.g., CZOs) will be essential. The concept is based on an iterative "zoom in–zoom out" approach from CONUS to basin to watershed to reaction scales and back again. The use of consistent data products and experimental designs throughout inherently link finer-scale data and knowledge to larger-scale phenomena and vice versa. Deploying this approach across watersheds binned into functional categories (e.g., based on concentration-discharge relationships) will allow data, knowledge, and models to be passed across scales and watersheds. Outcomes should promote multiwatershed understanding and hydro-biogeochemical predictive capacity that can be used as a scientific foundation to help inform decision making associated with energy sustainability strategies.

In addition to developing tangible use cases that embody ICON-FAIR principles, a major emphasis of the workshop was to enable progress through open science. In this spirit, prior to the in-person open watershed science workshop, a series of four public webinars were held to solicit input from the scientific community at large about current perspectives on challenges, solutions, and needs for advancing watershed system science. White papers were solicited from the community on topics related to the role of distributed research networks in watershed science. Attendance across the webinar series topped 150, and 23 white papers were submitted, a large fraction of which came from researchers not attending the in-person workshop. Moreover, following the workshop, the community continued to be engaged through discussions, webinars, conference sessions, and a number of activities at the BER 2019 Environmental System Science Principal Investigator meeting.

Emergent from activities before, during, and after the workshop is a vision for SBR termed "open watershed science by design." This vision combines open-science principles with design-thinking techniques to generate outcomes within the watershed context that are highly relevant to human society, including improved water quality and availability. This novel approach is designed to leverage individual agency research programs to reduce fragmentation across studies, creating an interoperable ecosystem of scientific capabilities, knowledge, data, and models that advance the understanding of watershed system structure, function, and evolution across the United States.

Chapter 1. Introduction

Watersheds fundamentally organize terrestrial landscapes (see Fig. 1.1, this page) and connect fine-scale processes (e.g., microbial metabolism) to Earth system function (e.g., global biogeochemical cycles). Processes occurring throughout watersheds also generate outcomes that are immediately relevant to human society, such as influencing water quality and the timing and magnitude of water delivery to downstream regions. Changes in water quality and hydrological regimes have significant implications for sustainable energy, agriculture, environmental health, and human society. For example, elevated water temperatures have shut down water-cooled nuclear power operations (McCall and Macknick 2016) and negatively affected endangered fish populations (Richter and Kolmes 2006). Given that mountain snowpacks are effectively natural water towers (Viviroli et al. 2007), changes in snowpack dynamics challenge operation of hydroelectric dam operations and can lead to altered thermal and biogeochemical dynamics within river corridors. Furthermore, the key role of watersheds within the Earth system was emphasized in the most recent report from the Biological and Environmental Research Advisory Committee (BERAC), calling out the need to understand fundamental processes in watersheds to achieve BERAC's 20-year vision for resilient energy systems (BERAC 2017). More generally, watersheds offer physically definable, yet complex, systems that can be understood only by integrating expertise and capabilities across disciplines.

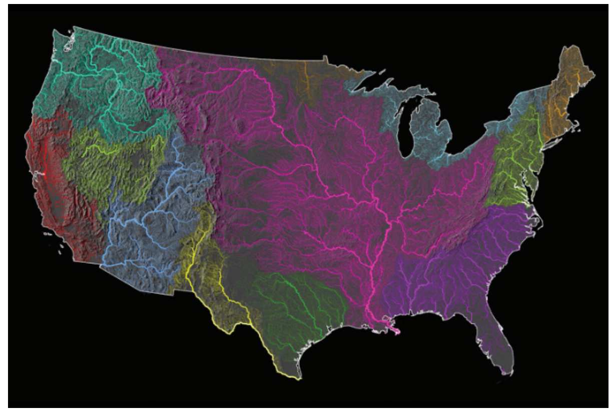


Fig. 1.1. U.S. Drainage Basins. Watersheds and their associated basins fundamentally organize terrestrial landscapes, connecting terrestrial and aquatic processes through space and time. Outcomes of these processes affect Earth system function and locally relevant ecosystem services. Different basins across the United States are shown as different colors. [Pacific Northwest National Laboratory. Adapted from Visualcapitalist.com.]

Watersheds operate through integration and feedbacks among physical, chemical, and biological processes (see Fig. 1.2, p. 2). These processes occur throughout the watershed continuum, from headwaters to the coast and from bedrock to the top of the vegetative canopy. These processes also influence watershed structure (e.g., topography and subsurface geology) through erosion and chemical weathering that are themselves influenced by biological processes such as vegetation establishment and succession. Integrated physical, chemical, and biological processes also underlie watershed function. In the context of the U.S. Department of Energy's (DOE) Office of Biological and Environmental Research (BER), watershed function is most commonly conceptualized as integrated hydro-biogeochemistry, which focuses on how coupled processes influence the movement of material and energy through watersheds. Due in part to a changing climate and direct impacts to land use, watershed structure and function are increasingly affected by disturbances that alter the movement of material and energy. Watershed "evolution" is conceptualized as subsequent changes in how watersheds are physically structured (see Fig. 1.3, p. 3) or function. The concept of watershed evolution is meant to emphasize that watersheds are not static entities—they are continually changing due to a variety of influences, some of which are natural (e.g., seasonal flooding that changes streambed structure) and some of which are directly or indirectly anthropogenic (e.g., pollutant releases).

BER efforts within watershed system science are currently centered within the Subsurface Biogeochemical Research program (SBR), with strong contributions from and connections to other BER programs in both the Climate and Environmental Sciences Division (CESD) and Biological Systems Science Division (BSSD). A major goal of the SBR program is to understand and predict the influences of disturbances (e.g., floods, droughts, and changes in snowpack) on

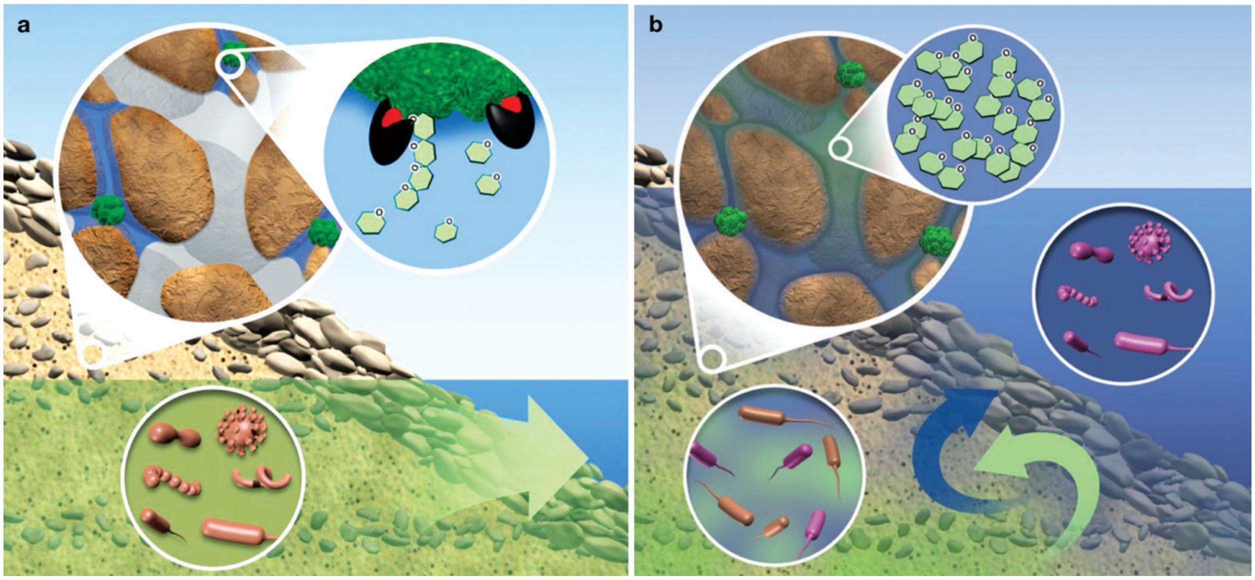


Fig. 1.2. Processes Are Coupled Across the Watershed Continuum. Physical, chemical, and biological processes feed back on each other to influence watershed structure, function, and evolution. Shown is a rise in river elevation that changes groundwater and surface-water mixing, which in turn influences connections between microbial communities and organic matter degradation. These tight couplings among physical, chemical, and biological processes occur throughout the watershed continuum, lead to complex hydro-biogeochemical behavior, and require understanding and representation in predictive models. Green and blue arrows represent groundwater and surface water, respectively. Also shown are groundwater and surface water microbes (brown and purple, respectively), particulate organic matter (POM; green particles), extracellular enzymes (black and red in panel a) degrading the POM into monomeric organic carbon that can be used to fuel microbial metabolism. See Stegen et al. (2018) for additional details. [From Stegen, J. C., et al. 2016. "Groundwater-Surface Water Mixing Shifts Ecological Assembly Processes and Stimulates Organic Carbon Turnover," *Nature Communications* **7**, 11237. Available via a Creative Commons license, CC-BY-NC-ND-4.0.]

emergent watershed structure, function, and evolution. As indicated by BERAC, robust watershed predictions require knowledge of governing processes (e.g., vegetation controls on evapotranspiration) and spatially and temporally varying nonlinear dynamics. Current models are, however, unable to provide robust predictions of integrated watershed structure, function, and evolution. Enhanced predictive capacity is needed to address pressing energy and environmental challenges.

There is a need, as well as an opportunity, to build new predictive capacity through enhanced mechanistic representation of hydrological, biogeochemical, microbial, and plant-rhizosphere processes and their interactions and feedbacks throughout the watershed continuum. Some of the capabilities required to build the associated mechanistic knowledge and mathematical representation are within BER, but not all, highlighting a need to leverage resources across DOE programs and other federal agencies. For example, the U.S. Geological Survey (USGS) undertakes significant monitoring of surface water quantity and quality across the United States. These data are used extensively by the watershed science community, and emerging opportunities can be further leveraged to enhance understanding and predictive capacity. In particular, USGS is developing a Next Generation Water Observing System that will use "super gauges" to monitor additional watershed components and processes, such as near-stream groundwater dynamics. Other opportunities could enable the use of these super gauges as platforms for extended and deeper investigation through additional sensing and measurements that complement USGS efforts. As another example, the National Science Foundation (NSF) has significant investments focused on environmental monitoring and experimentation distributed across the National Ecological Observatory Network (NEON), Critical Zone Observatories (CZOs), and Long-Term Ecological Research (LTER) network. These efforts vary in their focus on watershed processes, but, similar to USGS, there are significant opportunities to use NSF infrastructure as a platform for enabling science directed at enhancing understanding and predictive

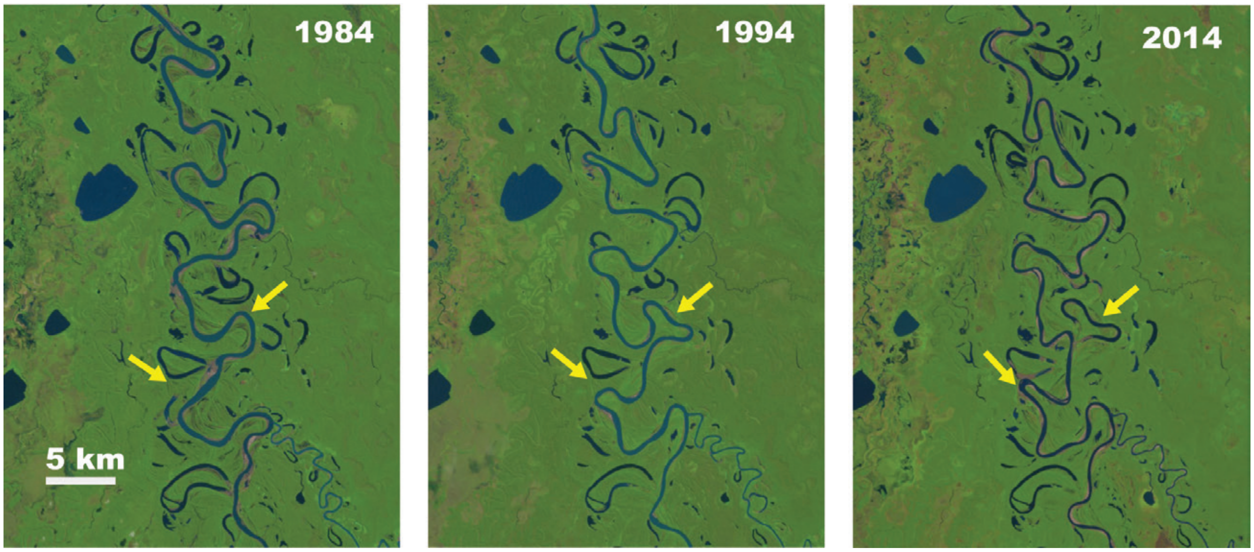


Fig. 1.3. Watersheds Are Dynamic. Watersheds are continually evolving, and watershed system science aims to understand the integrated processes leading to and resulting from these dynamics. Shown here are temporal dynamics in stream morphology in the Mamore River, Bolivia, from 1984 to 2014. [U.S. Geological Survey images: 1984 and 1994 from Landsat 5; 2014 from Landsat 8.]

capacity. For example, the SBR-funded consortium known as the Worldwide Hydrobiogeochemistry Observation Network for Dynamic River Systems (WHONDRS), detailed in subsequent sections, is working with the NEON, CZO, and LTER networks to generate data across most of their associated field systems to inform hydro-biogeochemical models and elucidate transferable principles. Numerous other opportunities to address watershed-relevant gaps in knowledge and data include leveraging existing and emerging resources across agencies such as the National Aeronautics and Space Agency's (NASA) remote-sensing products and the Long-Term Agroecosystem Research (LTAR) initiative within the U.S. Department of Agriculture's (USDA) Agricultural Research Service. The watershed science community can use these opportunities to tackle scientific challenges that would be impossible to address within a single field site or with resources from a single agency.

Within BER too, resources and expertise can be leveraged and linked across CESD and BSSD (see Fig. 1.4, this page). For example, understanding fundamental processes linking water quality to the movement of surface water through the rooting zone is most powerfully pursued by linking detailed molecular measurements across capabilities at DOE's Joint Genome Institute (JGI) and Environmental Molecular Sciences

Fig. 1.4. Resources and Capabilities Need to be Connected. There is significant need, as well as opportunities, to build formal, robust connections among capabilities supported by the U.S. Department of Energy's Office of Biological and Environmental Research (BER) that include data generation, data archiving, and analytics and modeling. Watershed system science would advance more rapidly with a deeper mechanistic foundation if connections were built across BER capabilities, in addition to other agencies. Doing so will require sustained focus, particularly in terms of new cyberinfrastructure. [Pacific Northwest National Laboratory]

Laboratory (EMSL) and tying those facilities to mechanistic models developed in part using the DOE Systems Biology Knowledgebase (KBase) and implemented using reactive transport codes funded by SBR. Currently, there are few formal and robust connections among these BER capabilities, but this situation is improving. The Facilities Integrating Collaborations for User Science (FICUS) program linking EMSL and JGI is one example of synergy among BER user facilities. Although other related efforts are under way (e.g., linking KBase to EMSL data through an application programming interface), much more attention needs to be focused on linking BER capabilities through enhanced cyberinfrastructure to enable seamless connectivity across data, models, and analytics. Essential to such efforts are robust connectivity among data-generating entities (e.g., EMSL and JGI) and data archives such as the Environmental Systems Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE) and the National Microbiome Data Collaborative (NMDC), as illustrated in Fig. 1.4.

1.1 BER Watershed Studies: Encompassing Interdisciplinary System Science

Watershed science within BER uses a complex system science approach to advance a predictive understanding of watershed system structure, function, and evolution. This approach is enabled by close collaboration, integration, and iteration among observational, experimental, and modeling efforts. Several past SBR-sponsored workshops have guided this current approach to watershed system science. For example, a 2009 workshop on complex system science (U.S. DOE 2010) was a key element in turning from a strong reliance on reductionist methods to a systems approach. This pivot was a result of recognizing that important elements of watershed structure, function, and evolution are not merely the sum of smaller-scale processes. Instead, watersheds are now conceptualized, studied, and modeled as complex systems with nonlinear feedback loops and adaptive mechanisms, which lead to emergent behavior that differs from predictions based on "summing up" underlying processes. In turn, BER watershed system science now combines "top-down" and "bottom-up" approaches to identify macroscopic features of system behavior and interactions among underlying processes that govern that behavior, analogous to systems biology.

Follow-on workshops have built upon the foundation laid by the complex system science workshop, such as the 2015 virtual ecosystems workshop (U.S. DOE 2015a). That effort further shifted the SBR approach to watershed system science through an emphasis on developing a new generation of multiscale models that couple physical, chemical, and biological processes. These models are meant to adapt to and facilitate the emergence of complex system behavior through feedbacks and nonlinearities occurring through linkages among key system features (e.g., vegetation, soils, aquifers, and surface waters). A particular focus is placed on developing multiscale models spanning microbial to watershed scales based on coupling surface-subsurface hydro-biogeochemical processes with above- and belowground elements of vegetation and microbial systems.

The virtual ecosystems workshop also influenced the approach to developing models and associated software for watershed system science. Based on the workshop's recommendations, a new community approach was established within SBR. This community approach was first implemented within an SBR-funded project called the Interoperable Design of Extreme-scale Application Software (IDEAS; U.S. DOE 2019), which focused on the development of an open and interoperable software ecosystem (see Fig. 1.5, p. 5). This approach allows flexible and seamless linkages among models that differ in (1) scale (e.g., microbial-scale metabolism coupled to reach-scale hydro-biogeochemistry), (2) capability (e.g., biogeochemical reactions coupled with subsurface flow), and (3) watershed component (e.g., rhizosphere coupled to surface water). For example, the software ecosystem developed by IDEAS was key to developing an intermediate-scale model of thermal hydrology in polygonal tundra for the Next-Generation Ecosystem Experiments (NGEE)–Arctic project (Jan et al. 2017, 2018) funded by CESD's Terrestrial Ecosystem Science (TES) program. This modeling capability has since been extended to reactive transport in fully coupled surface-subsurface systems, such as those associated with hyporheic exchange within river corridors. More broadly, SBR's systems approach to both data-generating and modeling efforts within watershed science is the cornerstone of achieving robust, predictive capacity of watershed structure, function, and evolution in response to disturbance.

1.2 BER Watershed System Science: Major Strengths and Opportunities

Watershed system science within BER is pursued via three primary efforts associated with SBR: (1) Science

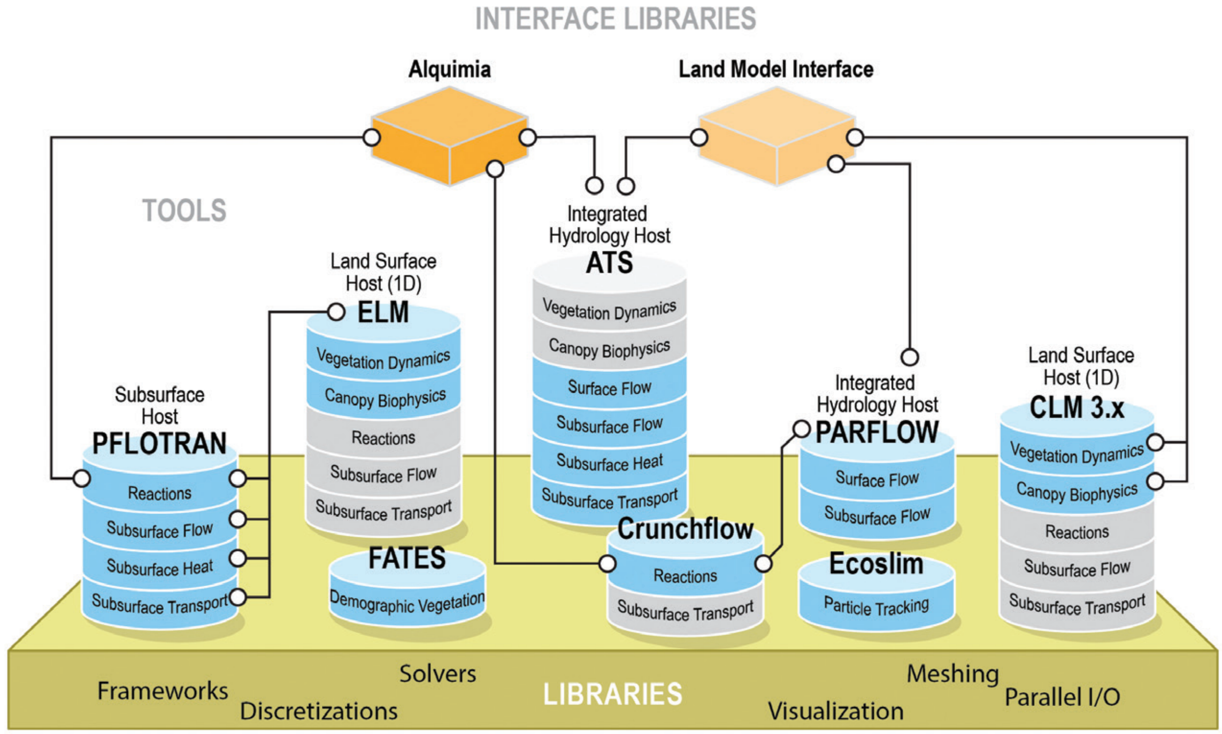


Fig. 1.5. Software Ecosystems: Enabling Connectivity Among Computational Codes. Central to the realization of the "open watershed science by design" vision is the development of coordinated, open efforts in both modeling and software and in data generation. The Interoperable Design of Extreme-scale Application Software (IDEAS)-Watersheds project, funded by the Subsurface Biogeochemical Research program, is developing the necessary, interoperable software ecosystem. Shown is an overview of the connectivity among computational codes enabled by this software ecosystem. Within the U.S. Department of Energy's Office of Biological and Environmental Research, there is currently less formal organization with respect to coordinated, open-data generation relevant to watershed system science. A key element of the open watershed vision is enhancing coordination for data generation, processing, archiving, and integration with models to improve predictive capacity. [Pacific Northwest National Laboratory]

Focus Area (SFA) projects associated with DOE national laboratories; (2) university-led projects, most of which are associated with SFAs; and (3) the IDEAS-Watersheds project, which spans multiple national laboratories and includes university partners. These three efforts are connected to a variety of other investments and capabilities across and beyond BER. A major aspect of the SBR program that ties these three efforts together is a collection of watershed test beds. These test beds are associated with national laboratory SFAs and have enabled integrated, sustained, and team-oriented systems-based research of watershed structure, function, and evolution.

The SBR test beds are distributed across the continental United States and span much of the watershed continuum (see Fig. 1.6, p. 6) from low-order headwater streams in the East River Watershed in Colorado (Lawrence Berkeley National Laboratory), to mid-order streams associated with East Fork Poplar Creek in Tennessee (Oak Ridge National Laboratory), to the high-order Columbia River in Washington State (Pacific Northwest National Laboratory). In addition, there are smaller-scale and emerging capabilities in other watershed systems, such as the Riverton site in Wyoming (SLAC National Accelerator Laboratory), the Tims Branch watershed near the border of Georgia and South Carolina (Argonne National Laboratory), and a freshwater pond system at the Savannah River Site in South Carolina (Lawrence Livermore National Laboratory). Within each test bed, SBR researchers carry out detailed, process-based investigations from molecular to watershed scales with strong coupling and iteration between data and models. This is a powerful approach, and the network of test beds is an essential BER capability needed to inform phenomena and processes relevant to the functioning of the

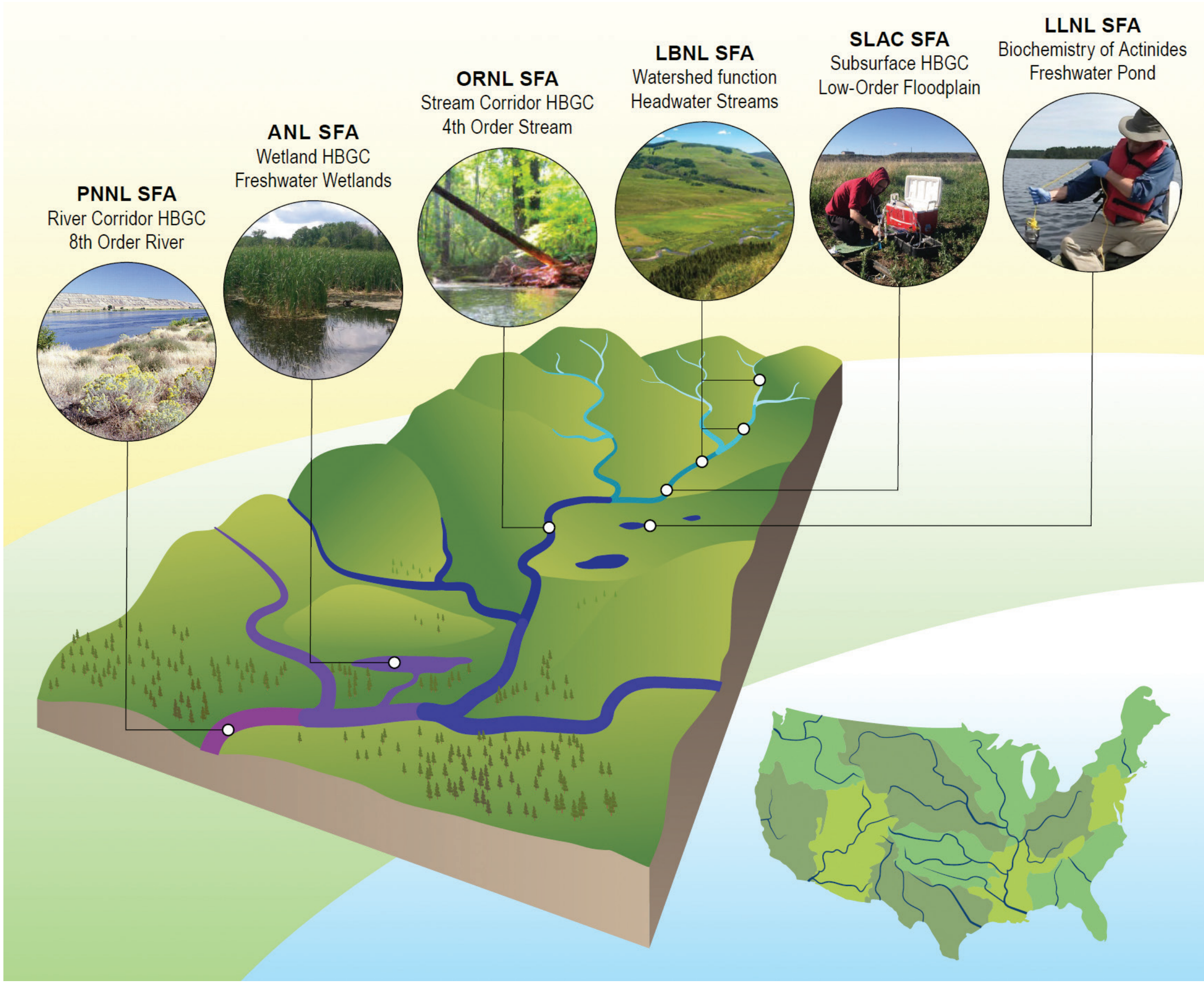


Fig. 1.6. Subsurface Biogeochemical Research Program (SBR) Test Beds. SBR test beds span the watershed continuum, from small headwater systems to a high-order main-stem river. Major field infrastructure in the test beds is complemented with fine-scale mechanistic efforts. [Pacific Northwest National Laboratory]

broader Earth system (e.g., water and biogeochemical cycles) and direct impacts of water quality and supply on resilient energy systems.

While powerful and essential, the scientific contributions of the SBR test beds could be elevated significantly through enhanced coordination. At present, integrative multiscale science is done primarily within test beds, with relatively little exchange of information, coordination of research activities, or focus on data interoperability among test beds. There is a concerted effort associated with the IDEAS-Watersheds project to enhance software and model interoperability, but relatively little has been done to have similar impact on the data collected. Increasing recognition is surfacing within BER, however, of the need for interoperable data that are formatted, annotated, and archived following community standards. In response, emerging BER efforts are focused on this challenge, primarily related to the ESS-DIVE archive, WHONDRS consortium, and NMDC. Although challenges are associated with enhancing coordination and interoperability of both the software/model and data sides, meeting these challenges is critical for developing data, knowledge, and models that are transferable across watersheds. Data, knowledge, and model transferability represent a lynchpin for the development of robust, predictive capacity that can be applied across watersheds.

Individual watershed system studies are crucial for understanding and modeling watershed processes and necessary for creating opportunities to evaluate the transferability of derived data, knowledge, and models, but they are inherently limited. Much of the intrinsic value from these studies cannot be realized without cross-site comparison enabled by uniform protocols and standardized data and metadata structures. Cross-system analysis is a powerful tool to evaluate transferability and relevance of processes across sites, as well as inform hypotheses and study design. However, if cross-system comparison is not anticipated as part of the study design, it can be slow, expensive, and ultimately intractable. Much of the motivation for the open watershed science workshop was predicated on this insight. Likewise, much of the "open watershed science by design" vision—developed from the workshop and described in more detail in subsequent sections—targets challenges, solutions, and opportunities associated with enhanced coordination.

Of importance is recognizing the need for enhanced coordination beyond the SBR watershed test beds, toward a "network of networks" that provide multiplicative benefits to each other through coordination. BER watershed system science depends heavily on connections with numerous capabilities and expertise domains across both CESD and BSSD, as well as across other parts of DOE and other federal agencies. SBR researchers make heavy use of the following examples:

- EMSL (CESD funded) and synchrotrons (funded by DOE's Office of Basic Energy Sciences) for molecular characterization (e.g., environmental metabolites).
- JGI (BSSD funded) for microbial analysis (e.g., metagenomics).
- KBase (BSSD funded) for analysis and modeling (e.g., flux balance modeling).
- AmeriFlux Network (TES funded) data (e.g., ecosystem fluxes of carbon dioxide).
- USGS and U.S. Environmental Protection Agency (EPA) water resources data (e.g., stream discharge and water quality).
- USDA (e.g., agroecosystem function and data).
- EMSL (CESD funded) and the National Energy Research Scientific Computing Center (NERSC; funded by DOE's Office of Advanced Scientific Computing Research) for high-performance computing.
- ESS-DIVE (CESD funded) for data archival and publication.

In addition, SBR researchers are currently interacting with the NMDC microbiome data archive (BSSD funded) as it is being developed, and they collaborate with projects outside SBR, such as those funded through BSSD's Genomic Science program, the TES NGEE–Arctic project, DOE Small Business Innovation Research/Small Business Technology Transfer program, NSF Rules of Life program, and USGS Next Generation Water Observing System. Other opportunities and capabilities could be better leveraged to advance BER watershed system science. For example, NSF has significant field infrastructure and personnel distributed across watersheds spanning all major U.S. biomes through its NEON, CZO, and LTER programs (see Fig. 1.7, p. 8).

While SBR scientists have some connection to these programs (e.g., via NEON drone flights), they represent mostly untapped potential partnerships that could be used for mutual benefit across agencies. This situation is beginning to change, however, as the SBR-funded WHONDRS consortium expands across all these NSF capabilities. One challenge to developing coordinated collaborations among SBR test beds and the NSF programs is that, much like the SBR test beds, there is relatively little coordination across the CZO and LTER programs. NEON represents a unique situation in which there is coordination among all sites. While NEON is not designed to inform integrated watershed structure, function, and evolution, it does encompass a robust set of field capabilities that BER watershed system science could build upon through close collaboration with NSF. In addition, NSF recently initiated an effort for greater coordination among its CZOs, which will facilitate connections between BER and NSF watershed science and lead to new research opportunities that bring together BER and NSF capabilities. In addition, the U.S. Forest Service has numerous experimental forests containing large-scale, long-term, watershed-scale manipulations. Furthermore, to determine watershed-scale outcomes of implementing conservation practices, the USDA Conservation Effects Assessment Project (CEAP) develops tools and provides data online through

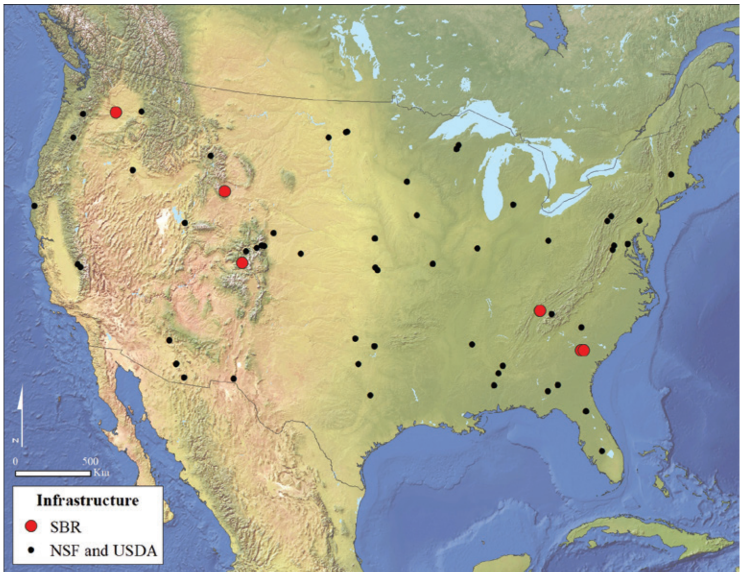


Fig. 1.7. Subset of Federal Field Infrastructure Across the Continental United States. A broad range of field infrastructure exists among federal agencies distributed across U.S. watersheds. There are opportunities to enhance knowledge of and predictive capacity for watershed systems through the development of stronger connections among these capabilities. Shown is the spatial distribution of the Subsurface Biogeochemical Research (SBR) program's watershed test beds and a subset of field infrastructure associated with other agencies, such as the National Science Foundation (NSF) and U.S. Department of Agriculture (USDA). There are numerous relevant field capabilities not shown for simplicity (e.g., U.S. Geological Survey stream gauging network and U.S. Forest Service experimental forests). [Pacific Northwest National Laboratory]

the Sustaining the Earth's Watersheds-Agricultural Research Data System (STEWARDS; see Fig. 1.8, p. 9). In addition, USDA's LTAR initiative addresses the sustainable intensification of agriculture within watersheds. These and other untapped opportunities could connect BER watershed system science to experimental and monitoring efforts across agencies, such as through evaluation of watershed-scale hydro-biogeochemical impacts of land-use change. This integration is central to the vision of open watershed science by design.

1.3 Open Watershed Science by Design: Advancing Understanding and Predictive Capacity

While BER watershed system science has made tremendous progress over the decade since the complex system science workshop, the next phase of advancement could make significant improvements in coordination among capabilities spanning measurements, models, and cyberinfrastructure. To meet this challenge, a vision of open watershed science by design has been developed and is articulated through the remainder of this workshop report. The essence of this vision is to combine highly coordinated, multiwatershed distributed research networks with the principles of open science by design. The key concepts of open science by design were recently summarized in a report from the National Academies of Science, Engineering, and Medicine (NASEM 2018) and are discussed in the following paragraph.

The open watershed science by design vision is based on the philosophy that the watershed science community must and can do together what would be impossible to do alone. It also recognizes that significant investments have been made across multiple agencies to improve the understanding of watersheds and the terrestrial and aquatic ecosystems they comprise. This vision takes advantage of opportunities to enhance coordination among individual researchers and agencies to accelerate the rate of information exchange through mechanisms that complement traditional publishing models. The goal is to transform the capacity of the watershed science community to generate data, knowledge, and models that are transferable and generalizable across watersheds. Achieving this goal is critical to meeting DOE and BER missions because transferable data and knowledge are cornerstones of mechanism-based predictive models and are essential to properly steward the public investment in watershed science.

Importantly, the vision of open watershed science by design recognizes that not all watershed science should be highly coordinated across watershed systems, though there are clear benefits to making all watershed science open. A continued need exists for single-site, more individualistic research that can more nimbly explore new concepts. In addition, smaller team efforts

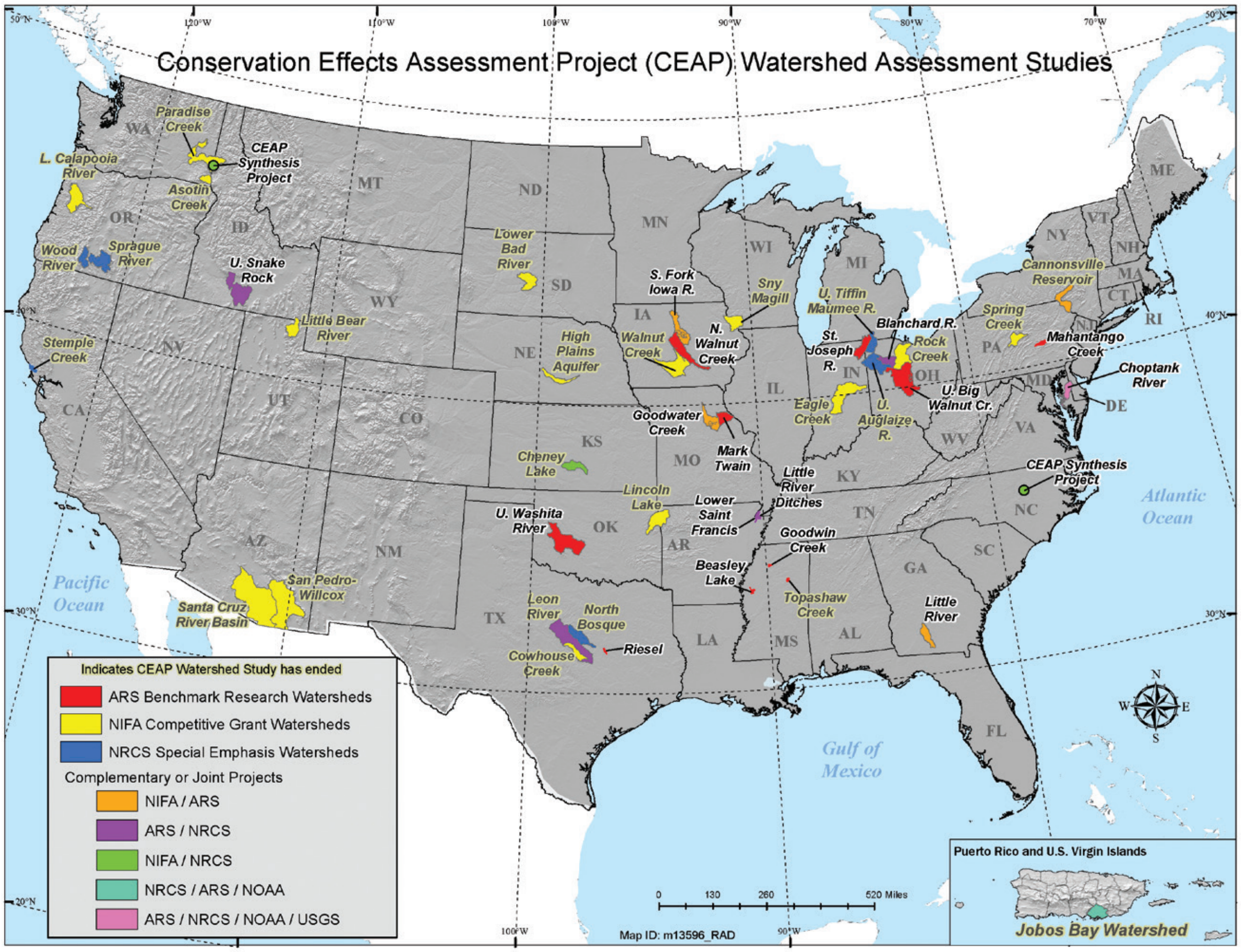


Fig. 1.8. Conservation Effects Assessment Project (CEAP). The CEAP watershed initiative is managed by the U.S. Department of Agriculture's Agricultural Research Service (ARS) and collaborators. Shown here are current and past CEAP watershed research sites and their corresponding watersheds. [U.S. Department of Agriculture]

can be more efficient and lead to key breakthroughs (Danchev et al. 2019; Fortin and Currie 2013). Also critical is emphasizing that highly coordinated, multisite watershed science—often comprising large interdisciplinary teams—must be mutualistic with more traditional single-site, small-team efforts. In fact, coordinated watershed science relies on the existence and persistence of scientific knowledge and research infrastructure across individual field sites. Similarly, research within individual systems can be amplified when placed in the context of data, knowledge, and models enabled by coordinated multisite efforts.

DOE is in a particularly strong position to lead the development of open, coordinated, multisite watershed system science and to do so with the watershed science community to ensure mutually beneficial outcomes between large coordinated efforts and more individualistic efforts. This effort requires being deliberate in the design of coordinated, open watershed science aimed at building transferable understanding and models of watershed structure, function, and evolution, which is the essence of the open watershed science by design vision.

Current BER-funded efforts have already begun responding to the need for watershed system science that integrates across physical, chemical, and biological processes in the context of coordinated, open networks of research distributed across watersheds. A primary example of this approach—and a microcosm of the broader vision—is the SBR-funded WHONDRS project (see Fig. 1.9, p. 10; whondrs.pnnl.gov; Stegen and Goldman 2018). WHONDRS is a consortium of researchers and other interested parties that aims to understand coupled hydrological, biogeochemical, and microbial function within river corridors. The WHONDRS business model is designed to be mutualistic with the community, whereby the community collects samples in their local watersheds following standardized protocols, and WHONDRS provides data and resources that are difficult or impossible for most researchers to access.

The vision of open watershed science by design builds upon the foundation provided by WHONDRS, expanding on the scientific scope while formalizing and improving the approach. A significant amount of community engagement has been leveraged in the development of the broader vision. These community activities included a series of open webinars from November 2018 to April 2019; an open call for white papers (see Appendix 4, p. 66); the in-person workshop in January 2019 (see Appendix 1, p. 57); numerous post-workshop discussions; and a collection of presentations, town hall discussions, and breakout sessions at the 2019 Environmental System Science Principal Investigator meeting. Information gathered across this spectrum of community activities has been used to develop the open watershed science by design vision. Key elements of this vision are summarized throughout the following chapters, including why more open science is needed, how to achieve it through design-based methodologies and guiding principles, what it looks like in the context of watershed systems, and the cross-cutting capabilities that must be integrated to realize open watershed science by design.

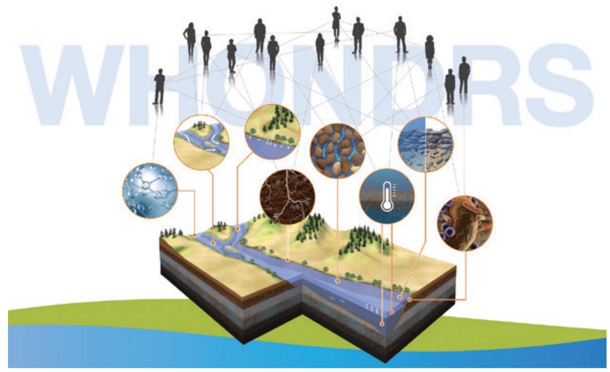


Fig. 1.9. Worldwide Hydrobiogeochemistry Observation Network for Dynamic River Systems (WHONDRS). WHONDRS is a microcosm of the open watershed science by design vision. This Subsurface Biogeochemical Research–funded effort aims to galvanize a global community around understanding river corridors, from local to global scales, and ultimately to provide the scientific basis for enhanced representation of river corridors in reactive transport, regional, and Earth system models, as well as improved management of river corridors throughout the world. WHONDRS targets specific data types that are needed to inform and develop mechanistic river corridor models and provides resources to the scientific community to generate these data across watersheds using consistent methods and data structures. Key to this effort is making data immediately open and unrestricted, while also developing open-access tools to enable analyses of these data by the community. [Pacific Northwest National Laboratory]

Chapter 2. Open Watershed Science: Vision and Approach

In the digital age, open science is critical for strengthening the efficiency and reliability of research and enhancing the public's access to knowledge generated from publicly supported research. Open science allows researchers to address new questions, including those that cross disciplinary, institutional, and national boundaries, and enables broader groups of researchers to collaborate on a global basis (NASEM 2018). In the wake of studies highlighting nonreproducible results across several scientific fields (The Economist 2013), the ability to easily address reproducibility issues and enable new science through availability of data and code is crucial (Harris et al. 2018). This same data and code availability—coupled with new informatic tools—allows researchers to quickly collaborate and identify complex phenomena that would be impossible to discover otherwise. These efforts have quantifiable benefits (Nosek et al. 2015); open-science strategies have been shown to have a positive impact on innovation (Jong and Slavova 2014), encourage entry by new researchers (Aghion et al. 2010), and increase the diversity of research topics (Williams 2010; see Fig. 2.1, this page). These opportunities have been recognized by both governmental funding agencies and private foundations. For example, NSF's National Ecological Observatory Network (NEON) generates open data to quantify complex, rapidly changing ecological and ecosystem processes. Such an endeavor would not be feasible through investigations at discrete sites by individual researchers. Similarly, a diverse group of private funders including the Ford Foundation, Alfred P. Sloan Foundation, Bill and Melinda Gates Foundation, and the MacArthur Foundation also have developed robust, open-access policies for their funded research.

Fig. 2.1. Benefits from Open Data. Making data open provides numerous benefits to researchers (as displayed above), but making data public is not the same as making data open. To be truly open (and thus useful), data need to be findable, accessible, interoperable, and reusable (FAIR). Making data open should be prioritized and built into the research workflow and priorities. [Australian National Data Service. Adapted from Danny Kingsley and Sarah Brown via a Creative Commons license, CC-BY-2.0.]

2.1 Open Science

The concept of open science—the practice of science in ways that allow for others to participate, collaborate, and contribute (e.g., open laboratory notebooks, data, software, and publications)—incorporates both principles (e.g., participation, reuse, and transparency) and practices (e.g., data sharing, citizen science, and open publications) that are tightly linked with traditional scientific values and norms. Indeed, as noted by the Royal Society in 2012: "open communication and deliberation sit at the heart of scientific practice."

More recently, the U.S. National Academies of Sciences, Engineering, and Medicine released a report in 2018 providing guidance to research enterprises and stakeholders about how to achieve open science (NASEM 2018). The report identifies the following benefits of open science:

- Scientific rigor and reliability enhanced by allowing researchers to reproduce and replicate reported work more easily.
- New areas of inquiry and opportunities for interdisciplinary collaboration enhanced by

bringing together data and perspectives from multiple fields.

- Faster and more inclusive dissemination of knowledge occurring when scientific articles are openly available.
- Increased opportunities for broader participation in research, including those for citizen scientists.
- Data and resources more effectively used by researchers in other fields who can aggregate multiple studies and test new hypotheses.
- Improved performance of research tasks by more accurate recording of research workstreams and automation of data curation.
- Recognition that publicly funded research should be available to the public.

In addition to outlining these benefits, the report reviews the National Academies' broad scope of open-science activities, and it identifies barriers and recommends solutions to overcoming those barriers by encouraging research communities to think about open science throughout the entire scientific lifecycle.

Figure 2.2, this page, illustrates a modified version of the scientific lifecycle identified in the National Academies report. In this figure, the inner circle identifies the steps involved in the lifecycle, from initial inspiration to final publication of the research. The outer overlapping terms depict a set of principles by which the scientific lifecycle is purposely designed to be open and transparent. These principles include:

- **Provocation:** Exploring or mining open-research resources and using open tools to network with colleagues.
- **Ideation:** Developing and revising research plans and sharing research results and tools so that they are findable, accessible, interoperable, and reusable (FAIR).
- **Knowledge generation:** Collecting data and conducting research using tools compatible with open sharing and using automated workflow tools to ensure accessibility of research outputs.
- **Validation:** Preparing data and tools for reproducibility and reuse and participating in replication studies.

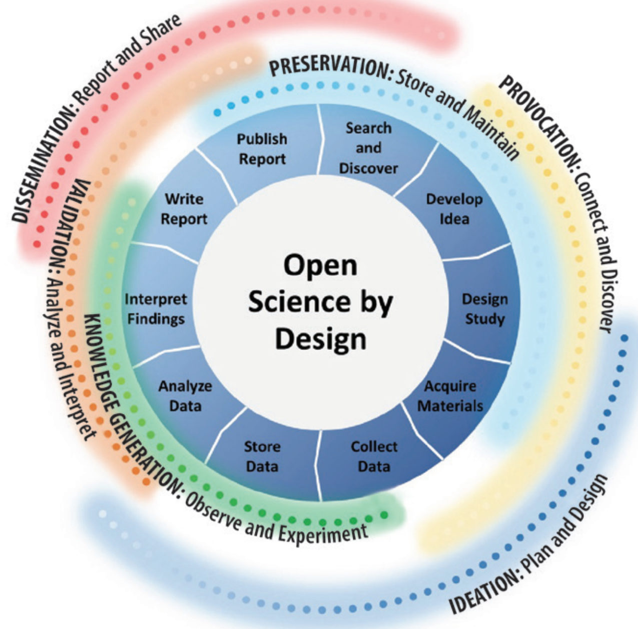


Fig. 2.2. Open-Science Principles Throughout the Research Lifecycle. As articulated by the National Academies of Sciences, Engineering, and Medicine (NASEM), open-science principles must be purposefully implemented across all phases of the research lifecycle, from provocation to preservation. Research lifecycle phases contain numerous elements, all of which can be enhanced by either leveraging the open efforts of others or making one's own efforts open. One key element is making data FAIR (i.e., findable, accessible, interoperable, and reusable), but there are numerous other elements of open science that go beyond data (e.g., code, protocols, ideas, and publications). [Inner ring, Center for Open Science. Outer ring adapted with permission of NASEM from *Open Science by Design: Realizing a Vision for 21st Century Research* (2018); permission conveyed through Copyright Clearance Center, Inc.]

- **Dissemination:** Using appropriate licenses for sharing research outputs and reporting all results and supporting information (e.g., data, code, and articles).
- **Preservation:** Depositing research outputs in FAIR archives and ensuring long-term access to research results.

2.2 Open Data

In 2013, the White House Office of Science and Technology Policy (OSTP) instructed all federal agencies that spend more than $100 million per year on research and development to "develop a plan to support increased public access to the results of research funded by the Federal Government." This OSTP mandate has resulted in (1) the requirement for more defined data-management plans associated with federal funding opportunities, describing how resulting data will be made publicly available; and (2) the development of data repositories (e.g., ESS-DIVE; https://ess-dive.lbl.gov) as a mechanism to, in the case of ESS-DIVE, "preserve, expand access to, and improve usability of critical data generated through DOE-sponsored research of terrestrial and subsurface ecosystems." A more recent effort underlying open data is the concept of FAIR data. FAIR is now starting to be quantified using the following guidelines (Jones and Slaughter 2019):

- **Findable** refers to the ability to discover data and metadata through manual and automated searches [e.g., through use of persistent identifiers such as digital object identifiers (DOIs) and well-defined keywords in the metadata].
- **Accessible** refers to the ability for users to access the data (e.g., through storage in a well-curated repository) with the appropriate license that allows them to use the data.
- **Interoperable** refers to the ability to integrate data across providers and scientific workflows and applications (e.g., through use of community data standards and controlled vocabularies).
- **Reusable** refers to how well the metadata (e.g., sampling protocols, analysis methods, and data processing) are described and how well the data are standardized (e.g., units and file structures) to enable easy and efficient reuse of the data beyond the purpose for which they were originally collected.

Generating such data requires purposeful design that accounts for increased planning, data curation, use of persistent identifiers, long-term hosting, and data discovery.

Within BER, the Subsurface Biogeochemical Research program's (SBR) portfolio is poised to especially benefit from the increased use of open-science principles. While the program previously had a more reductionist focus, it now "seeks to advance a robust, predictive understanding of how watersheds function as integrated hydro-biogeochemical systems," and thus BER requires approaches that enable the interrogation of inherently complex systems that often are beyond the scope of single–principal investigator (PI) studies. Instead, the integration of disparate spatiotemporal data streams is essential for achieving this aim. Although the use of multi-PI Science Focus Area projects has already successfully catalyzed this effort, these investigations primarily focus on individual watersheds. Moving forward, the increasing availability of code, data, and publications will enable collaboration with other researchers and agencies—such as USGS and the National Oceanic and Atmospheric Administration (NOAA)—that collect and host complementary data, enabling new insights into watershed structure, function, and evolution across scales.

2.3 Design Thinking for Watershed System Science

Just as scientists conceptualize physical processes unfolding in watersheds as complex dynamic structures with nonlinear feedbacks and adaptive mechanisms, the actual approach used to study them is often equally complex. Open watershed science by design emphasizes the benefit of an intentional and purposeful approach to constructing research focused on complex systems and the inherent cross-system transferability with enhanced connectivity and coordination that such research often requires. Ultimately, "by design" refers to the development of insights that lead to a novel idea for a product, system, or theory that is transferable and reproducible. In applying the concept to watershed science, the objective is to construct research systems designed to enable innovation and that leverage resources across BER and other agencies. The outcome of such "innovation systems" is transformative knowledge and predictive capacity of watershed structure, function, and evolution with the goal of advancing BER research missions. Key to the development of innovation systems is embedding intentionality, flexibility, and purpose into the architecture of research infrastructure, a process that is analogous to applying the lens of the scientific method to the systems used to conduct research.

How might new research architectures focused on innovation to enable open watershed science be defined? Design thinking is one framework that focuses on creative transformation of cross-domain knowledge, including integration of different expert domains in a creative problem definition and solution process. Design thinking is framed as a stepwise process focused on a flexible problem finding and solving framework, with a structure analogous to the scientific method (see Fig. 2.3, this page). Layered into the framework are mindsets and abilities designed to evoke innate creativity, foster collaboration, and focus attention on key elements of the systems being studied. An experienced research scientist moves flexibly through the phases of a research project toward knowledge generation by employing skills such as synthesis and iteration. Similarly, design thinking emphasizes a set of synergistic abilities that promote flexible navigation through a project toward the end goal of a novel idea or approach. Thus, at the core, design thinking can be viewed as a purposeful approach to scientific endeavors, one that aims not only to design key research questions, but also to design the systems needed to meaningfully address them.

As a concrete example, numerical models for watershed function must strive to continuously update their library of scientific knowledge with the most recent insights from the scientific community and, in so doing, continuously test the transferability of those insights. Achieving these aims requires a three-way interaction among the developers of models, the users of models, and the larger scientific community that can evaluate the models. Because the application of models across an array of watersheds may predict an important systemic response that has not been previously measured, it is unknown whether the response is an emergent property of watersheds or an artifact of incomplete knowledge or process representation. Conversely, models may fail to capture key observations across systems. Both cases present opportunities to advance the understanding of watershed systems. From a design-thinking standpoint, a scientist can take advantage of unexpected model (or experimental) outcomes and failures. This is done by intentionally putting aside biases to approach a design challenge with an open mind (i.e., allowing oneself to *learn from others* by embracing a beginner's mindset). Combining an open mind with *synthesis* and *flexible prototyping* often leads to innovative ideas and approaches. Through this process, three often disparate communities (i.e., model developers, users, and testers) can connect to more rapidly advance understanding and predictive capacity of watersheds as integrated hydro-biogeochemical systems.

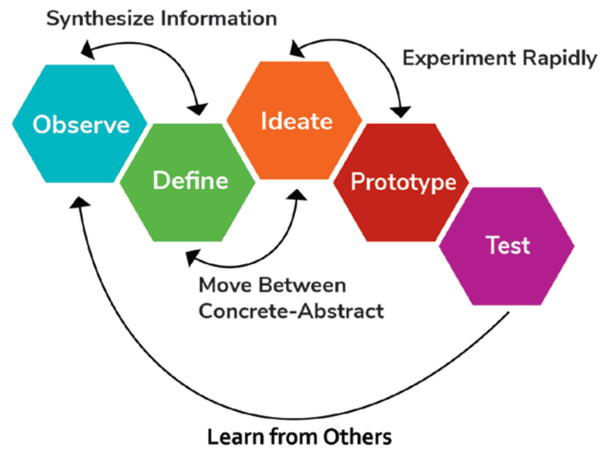


Fig. 2.3. Using Design Thinking to Advance the Research Process. The hexagons illustrate a traditional linear approach to design or research. In reality, as shown by the arrows, research can follow multiple interconnected loops and may not progress in a linear fashion. The various design abilities, shown here with arrows indicating how they may connect among various stages of research, are illustrated as an example of how abilities support fluid movement through the research process. The value of articulating the process and acknowledging the related abilities is that this process enables intentional advancement of research by focusing on the mindsets and approaches that are relevant to the particular challenge. [Stanford University]

The utility of design thinking is highlighted through the recognition that project structures and approaches that were previously successful are unlikely to meet research needs in the next 5 years due to the breakneck pace of data generation, knowledge acquisition, and tool development. Purposeful design of innovative research is, therefore, critical in advancing complex system science. Innovations in work practices and thinking are central to achieving the scientific advances needed to assess and predict watershed structure, function, and evolution in a changing world.

2.4 Challenges and Solutions for Open Watershed Science by Design

There is a clear opportunity for greater coordination and openness within watershed system science, and design thinking is one method for developing innovative approaches to achieve these goals. Making watershed system science more coordinated and open from the inception of research projects will increase research visibility, data and model reuse, transparency, and the pace of scientific discovery. While smaller, decentralized teams can be more efficient in terms of producing publications than centralized efforts

(Danchev et al. 2019; Fortin and Currie 2013), the coordination of data collection, integration, and archiving across multiple independent groups can be extremely challenging. Although coordinated, open science is a priority for the community, a series of cultural, economic, and institutional norms and realities currently pose particular challenges to the full embrace of open science. This is true across many scientific fields and is not unique to watershed system science. Perhaps most significant is the strong emphasis placed on *individual* production and accomplishments when assessing research effectiveness (e.g., by hiring and promotion committees). This is directly tied to the traditional approach of using scientific articles for dissemination of new research. Publication in "high-impact" journals (as inferred from the frequently problematic journal impact factor) has been seen as essential for career progress in many fields and is a metric commonly used by administrators and funding agencies to assess the quality of science. The fear of getting "scooped" by other researchers following release of scientific data ties into the publication-based research evaluation mindset, likely precluding some individuals from engaging in open science. Another barrier to engagement in open-science practices may be the discomfort felt when engaging in complex interdisciplinary studies, where a researcher's own specific discipline may play a relatively minor role in solving the scientific issue at hand. In addition, the generation of well-curated, FAIR datasets for public access is time consuming and can be expensive. This is especially true for projects with smaller budgets as the cost of making data FAIR is greater per bit of data for smaller datasets. If considered at the beginning of the research process, however, the time and costs associated with making data FAIR can be significantly reduced. Critically, the challenges of engaging with open science are greater for early-career researchers relative to their more senior colleagues, although early-career scientists may often, but not always, be better equipped with the technical skills (e.g., reproducible programming) needed for open science. However, due to many of the issues previously mentioned, it likely will be critical for senior scientists to lead the adoption of open-science principles across a range of scientific disciplines.

What are potential solutions or incentives? Many of these issues are linked to the systems by which researchers are evaluated by their institutions and funding agencies. Education—of both individuals and agencies—on the benefits of making science open, such as increased visibility and citations and the tools that can assist with these goals, must be a cornerstone of a framework for enhancing adoption of open-science principles. While there are many conflicting studies detailing the impact of open-access articles on citation counts (NASEM 2018), a series of recent studies concluded that open publication increased citations to the highest-quality articles and decreased citations to the least-cited articles (McCabe and Snyder 2014, 2015). Open-science efforts should be incentivized to ensure that those who create valuable research outputs (e.g., data and software) are recognized and rewarded. Recognizing the increasing acceptance of preprints as valuable scientific output and providing recognition for data dissemination via DOIs assigned to data publications (e.g., as in ESS-DIVE) are critical first steps. Also critical is that DOE-supported infrastructure components such as ESS-DIVE continue to actively enhance the ability of researchers to obtain DOIs for datasets that can be subsequently cited, shared, and accounted for when evaluating scientific contributions.

Similarly, new efforts to track the extent to which researchers follow open-science practices are also being established. The Center for Open Science (COS), in partnership with several journals, has led an initiative where "badges" are associated with published papers that include shared data or materials. In addition, *alternative metrics* (alt-metrics) such as file downloads are increasingly being used to assess the impact of a publication or dataset. Some of these efforts are reliant on modification of researcher evaluations, rewarding open-science practices. Both the 2013 San Francisco Declaration on Research Assessment and the 2015 Leiden Manifesto for Research Metrics have gained signatories among institutions, funding agencies, and journals in an effort to emphasize the importance of expert judgement in the evaluation process. Related to this, the Peer Reviewers' Openness Initiative proposes that data and materials must be openly available before peer reviewers provide critical feedback on submissions. Additionally, a new concept is development of an "openness index" for individual researchers that could be akin to the author citation h-index, but would be influenced by other factors such as quantitative evaluation of how FAIR their data are and how often their data are reused or cited. Many other potential solutions and incentives can be imagined and eventually developed, such as invitations to data-synthesis activities for those providing FAIR data and temporary co-authorship embargos to protect junior researchers but that allow public use of data. Additional innovative solutions are likely to emerge, especially if design thinking is used. These efforts, coupled with top-down controls from funding agencies and other stakeholders that require, value, and reward FAIRness of data, code, and publications, are essential to maximize the acceptance and beneficial impacts of open science.

Other challenges associated with rapid data release not previously detailed include concerns of participants about the exposure of errors in experimental design or data collection. The preregistration of studies represents one opportunity to correct any such issues prior to beginning work, and it is a practice rewarded through the COS badge system. Finally, open-science principles require infrastructure—tools and metadata—to organize and curate data, effectively link disparate datasets, and also provide long-term stewardship of data. These resources may be provided by funding agencies (e.g., data repositories) or by individual institutions. Given the costs associated with generating FAIR data, funding agencies might in the future require a separate budget line item for performing these activities, as well as increased levels of detail in data-management plans.

2.5 Attributes to Guide the Design of Open Watershed Science

To achieve the vision of open watershed science by design, research programs need to be purposefully built—using design thinking and methodology—to embody a set of fundamental attributes. During workshop planning and discussions, organizers and participants identified and implemented a set of these attributes that they referred to as ICON (i.e., integrated, coordinated, open, and networked), defined as follows.

Integrated refers to designing models, experiments, and observational campaigns to intentionally target the coupling among biological, chemical, and physical processes within and across scales. Such a target avoids the stove piping of disciplines in which studies focus, for example, primarily on hydrology, microbiology, or carbon chemistry without explicitly connecting the associated processes or considering how they influence larger- or smaller-scale phenomena. Attempting to integrate across process domains *post hoc* is fraught with challenges if models and data were not developed or generated with the goal of integration. If integration is the *a priori* goal, this changes how models are built and data are generated. Greater, more purposeful integration is essential as watershed structure, function, and evolution are phenomena that emerge via feedbacks among these process domains that operate across scales. For example, understanding and predicting watershed hydrology are made more robust when considering influences of groundwater flow on transpiration (Maxwell and Condon 2016). In addition, linking hydrological, chemical, and microbiological data can reveal attributes of system function that could not be inferred with data from any one of those data types (Stegen et al. 2018).

Coordinated refers to the purposeful use of consistent protocols across systems to generate specific data types needed to inform, develop, and improve models for application across watersheds. To enhance the ability to understand and predict the structure, function, and evolution of watershed systems, scientists need knowledge, data, and models that are transferable across watersheds. Developing transferability is most rigorous and efficient when starting with data that are generated using consistent methods and are archived using consistent standards for the data and metadata. When using different methods across systems, synthesizing data across studies and watersheds is very difficult, and often impossible. However, with an understanding of biases and differences across methods, the data generated using different methods can be reconciled and made to be interoperable, though this requires concerted effort. Cross-watershed, synthetic analyses are required to evaluate the transferability of fundamental principles that, in turn, underlie mechanistic predictive models that can be used within and across watersheds. This is the fundamental reason that networks such as NEON use standardized sensors and field and laboratory protocols to generate data across their sites (see Fig. 2.4, p. 17). Using consistent methods across watersheds is very different, however, and requires significant planning, governance, and coordination among researchers. There are examples of successful coordination of consistent methodologies

Fig. 2.4. National Ecological Observatory Network (NEON) Field Sites. Funded by the National Science Foundation, NEON is a coordinated network of field monitoring capabilities that uses highly standardized protocols across all sites, spanning both terrestrial and aquatic watershed components. This high degree of coordination and consistency is an essential element of the open watershed science by design vision. There is significant need to use the same level of consistency across other efforts focused on watershed system science, including those supported by the U.S. Department of Energy's Office of Biological and Environmental Research. In addition to challenges associated with coordination and standardization, also important are leveraging and developing mechanisms for reconciling data from nonstandardized methods to maximize data interoperability across all sources. Shown is a screenshot displaying the distribution and type of field sites monitored by NEON. [NEON]

[e.g., NEON, USGS stream gauges, and the Worldwide Hydrobiogeochemistry Observation Network for Dynamic River Systems (WHONDRS)], but these efforts are more the exception than the rule.

Open refers to the free and easy exchange and accessibility of data, software, and models, and this concept should be designed into all phases of the research lifecycle (NASEM 2018). Openness is essential for advancing knowledge of watershed systems because scientific progress is fundamentally based on the exchange of knowledge. When data, software, or models are private or proprietary, researchers are pushed to focus on their individual research site or model and limited in their ability to draw out transferable principles through synthetic analyses. Making data, software, and models open is, therefore, essential, and it can confer many benefits to providers (see Fig. 2.1, p. 11). Importantly, making data, software, and models public is not sufficient for making them open. For example, many public datasets do not ascribe to community standards that define the data structure, formats, and metadata content, all of which are essential to reusing the data for other purposes. However, community data and metadata standards are often lacking for many watershed data types or can be difficult to use outside the informatics community. To be open, data need to be provided in a way that makes them FAIR (Wilkinson et al. 2016; Boeckhout et al. 2018; FORCE 11 2018). The degree of FAIRness is now being quantified in terms of how close the data are to the FAIR ideals summarized in Section 2.2, p. 12 (Jones and Slaughter 2019). This concept originated from the data-management field, but it can be broadly applied to other key components of a research program that include data, software, and even testable hypotheses and ideas.

Similar concepts have been developed over several years in the software arena, including scientific computing, around open-source and reusable code. Critical elements here include availability through code-sharing platforms (e.g., github, gitlab, and bitbucket), good documentation, adoption of software standards for modular design and interfaces, continuous integration, and version control (Adorf et al. 2019). A particular challenge for models is making them interoperable. Efforts like the Interoperable Design of Extreme-scale Application Software (IDEAS)–Watersheds SBR-funded project are focused on solving that challenge through the development of an interoperable software ecosystem (U.S. DOE 2019).

Networked refers to a research approach, whereby sample collection and data generation are conducted with and for the broader scientific community. Studying watershed systems, often involving field sampling and instrumentation, is costly in terms of both time and money spent to send researchers into the field. An individual research group working across a large number of field sites is often intractable for many reasons, including costs and limited working knowledge of each site. This cost intractability poses a challenge because (as discussed earlier) developing transferable data, knowledge, and models requires integrated, coordinated, and open information across watershed systems. One solution is to develop research programs that are purposefully designed to be conducted with and for the science community. Essential to such efforts is the inclusion of elements that are mutualistic between a given research project and the broader science community. BER is well positioned to develop such watershed research programs as a result of its unique capabilities spanning (1) molecular characterization including, for example, the Environmental Molecular Sciences Laboratory (EMSL) and Joint Genome Institute (JGI); (2) cyberinfrastructure such as ESS-DIVE and the National Microbiome Data Collaborative; and (3) modeling tools available through resources such as the DOE Systems Biology Knowledgebase (KBase) and IDEAS. WHONDRS is an example of an SBR-funded effort developed in this mold, with the science community providing local field site expertise and the person hours to conduct field sampling (see Section 3.1, p. 23, for more information about WHONDRS). In return, WHONDRS provides data and analysis tools to the community via BER capabilities that would be difficult or impossible for much of the science community to access. In addition, the AmeriFlux Network (see Fig. 2.5, p. 19) is another BER project that is networked in the sense that data collection is distributed across a broad range of individual researchers, though those researchers provide all equipment. Another key aspect of networked research programs is scalability, whereby resources can be deployed and used across a large number of watershed field systems. Such systems include sensors and physical sample collection followed by laboratory analysis, pointing to particular needs in the development of less expensive sensing systems and high-throughput analyses.

2.6 Incorporating ICON-FAIR into Open Watershed Science by Design

Developing research programs using ICON-FAIR principles has benefits to current and future scientific discovery and enhanced predictive capacity. The individual researcher also receives benefits, but they are not always immediate and there are costs that present obstacles to participation. In particular, there are unique costs associated with the governance and implementation of ICON-based research programs. For example, research teams must build consensus, distribute resources across sites, design data and metadata acquisition and formatting to conform with standards that might exceed the needs of the immediate project, upload data to a FAIR archive, and support users who seek to employ these data. To enable researchers to engage in ICON-FAIR research, funding agencies need to provide concrete and substantial support both to smaller, more individualistic teams and to larger, more coordinated teams. This support

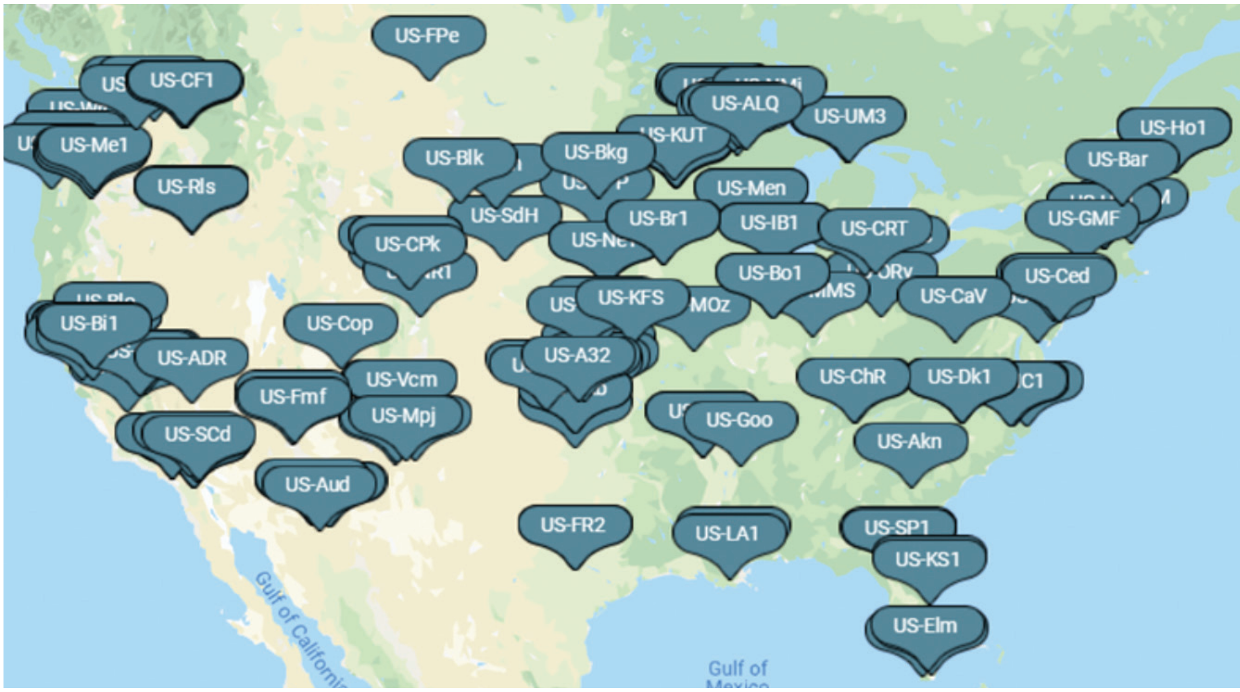


Fig. 2.5. AmeriFlux Network Across the Continental United States. With support from the U.S. Department of Energy Office of Biological and Environmental Research, AmeriFlux is a network to which individual investigators contribute data from their eddy covariance flux towers to a centralized database using consistent data formats and instrument settings. Developing transferable understanding, which requires generating data and knowledge across a broad range of systems, can be achieved through distributed efforts to which numerous participants contribute. Enhancing predictive capacity requires purposefully networked efforts within watershed system science. Shown is the distribution of AmeriFlux sites across the continental United States. [AmeriFlux Network]

could be accomplished through funding that covers governance costs and the sustained development of physical and cyberinfrastructure needed to streamline both ICON research programs and FAIR data. Key is the development of funding agency–based incentives such as supplemental grants to pursue coordinated research across independent teams or the provision of access to pools of funding based on FAIRness of previously produced data. In addition, further investments are needed both in cyberinfrastructure to reduce the costs of making data FAIR and in the physical infrastructure required for ICON research programs.

Important to recognize is that much of the scientific enterprise runs on discrete, 3-year research grants that support relatively small teams. This individualization enables diverse perspectives and novel insights but makes coordination difficult. In addition, the cost of making data FAIR is higher per bit of data for smaller datasets. If smaller, more individualized teams running on short-term grants can lean on ICON-FAIR infrastructure built and maintained by larger, more coordinated, and longer-term teams, the ICON-FAIR approach will be significantly more accessible to the entire watershed science community.

The two primary elements needed are (1) incentives that provide immediate, tangible benefits to individual researchers and (2) tools that decrease the costs of ICON governance and making data FAIR. Incentives will come from funding agencies and a change in culture (e.g., in hiring and promotion practices). Within DOE, the national laboratory system is ideally suited to provide long-term investment in the development and maintenance of the tools and infrastructure needed to enable ICON-FAIR watershed science. Support also could come by way of providing greater rewards for participation, such as by having data publications peer reviewed with assignment of titles and DOIs (as can be done via ESS-DIVE), so that scientists can be recognized more easily for their contributions (e.g., via citations of data products). More generally, building support for ICON-FAIR research programs into the structures that underpin scientific advancement (e.g., funding agencies, journals, and promotion opportunities) is critical to the realization of the open watershed science by design vision. Numerous other elements are also needed to enable ICON-FAIR watershed science, however, as summarized in the following subsections.

2.6.1 Integrated

Integrated research programs require that the entire research lifecycle is designed by an interdisciplinary team that spans physical, chemical, and biological domains. They must define robust *a priori* plans for how to carry out data analyses and modeling that will link physical, chemical, and biological data types to address identified science challenges. The research design must account for the early lifecycle phase of data collection from samples and sensors, including new and existing datasets, as well as the later phase of data analysis and modeling. Without the forethought and planning needed to make use of the data, collecting high-quality data may be a wasted effort. Thus, integrated research programs inherently require a team that knows the strengths and limitations of all data types, analysis methods, and simulation models and that understands or is able to hypothesize how different kinds of processes can influence each other (e.g., how hydrology can influence the supply of resources that can influence microbial metabolism and growth that can feed back to influence subsurface hydrology through the development of biofilms that can clog pore channels).

2.6.2 Coordinated

Using design thinking to develop integrated research programs will identify the types of data to be generated. The subsequent data generation from samples and sensors must then be coordinated through the use of consistent protocols across systems. Although individual researchers are often hesitant to transition away from their personally developed protocols, coordination ensures interoperable data that can increase the impact of individual studies and enable multi-system studies that are needed to inform, develop, and improve models for application within and across watersheds. Coordinated research programs require input from an interdisciplinary team that understands cross-system variability to create standardized protocols that can be applied in diverse settings. Existing protocols and widely accepted methods or standards should be leveraged during development. Protocols should be made publicly available to increase standardization, reduce resources required to create new studies, and allow for feedback from the community. Although stable protocols are most likely to be interoperable through time, there must be a way to engage with improved methods and new data types. Updating protocols requires significant input from the community of users and should be done in a way that is not disruptive to data collection. In some cases, generating data using both the original and updated protocols may be possible. If this can be done across a broad range of watershed systems, the data could be made interoperable through the development of data-driven algorithms that effectively translate data from one protocol to another.

2.6.3 Open

As detailed by the National Academies report on open science by design (NASEM 2018), research should be open at every stage of the research lifecycle. For example, during initial idea generation and planning, research programs can invite the scientific community to contribute to study design either informally using tools such as social media or more formally using distributed proposals or webinars. This early engagement encourages innovation, identifies roadblocks to data sharing or usability, and offers solutions to bridge those gaps. One of the most critical elements of open science is making data FAIR. The FAIR data principles must be built into research programs from their inception. Much work remains to be done, however, to enable increased adoption of FAIR data principles, including the development of community data and metadata standards. The scientific research community is increasingly aware of the need to make data public as funding agencies have imposed requirements and the number of public data repositories accepting environmental data has increased. However, despite the data-management tools being made available, relatively few researchers make their data FAIR, potentially causing these data to be unusable and effectively lost. This practice may occur because doing so is not yet the cultural norm within watershed system science, or researchers may feel it is too much of a burden, especially for individual researchers generating small datasets. Important, however, is enabling all projects and researchers to access the resources (e.g., funding and personnel) needed to prepare and publish FAIR data. This access is currently difficult because, although funding agencies require project data to be made public, they do not necessarily require data to be FAIR, highlighting the need to modify the current value system for researchers and funding agencies by placing greater value on robust data dissemination. Greater recognition of FAIR data practices by funding agencies, peers, and promotion or hiring committees could help to incentivize a shift to these practices, which may ultimately make them more viable for smaller project teams.

Hence, innovative solutions are still needed to guide researchers and streamline the process of submitting FAIR data to established repositories. These solutions require the involvement of domain scientists, who are in the best position to judge how well suited the various metadata and data standards are for different data types. Most importantly, scientific workflows and culture need to undergo a shift, whereby the incorporation of FAIR principles into the research data lifecycle is the norm (Stall et al. 2019). Research programs should be designed to be FAIR compliant at their inception (i.e., during the proposal planning phase) because many project features are difficult to change once the project has begun.

Choices to be made upfront and described in data- or software-management plans include:

- Selection of appropriate repositories and software-sharing platforms that (a) support FAIR principles to archive and publish the program's data and codes and (b) provide the means for easy discovery of archived data products by the science community.
- Choice of open-data and software-management policies with a defined time to publication and licensing terms that enable reuse with minimal restrictions. Examples include the Creative Commons licenses CC0 (public domain) and CCby4 (attribution, for data) and open-source policies such as the BSD-3-Clause and MIT licenses for software.
- Identification of the community data and metadata standards that will be adopted by the research program. Some of these standards may be determined by the choice of repository, but there may be domain-specific standards that are more suitable for the program's data (e.g., netCDF formats for climate datasets). Similarly, software must be developed using best practices and accompanied with sufficient documentation and examples to encourage reuse. Resources developed by the Better Scientific Software community provides guidance on best practices for curating, creating, and disseminating software (https://bssw.io).
- Selection of the scientific workflow tools (e.g., Jupyter notebooks) that the program will adopt to make data preparation and analysis as well as modeling more transparent and reproducible.

Importantly, the concept of FAIRness must be prioritized by program leadership (e.g., PIs and program managers), and sufficient time and resources must be allocated to ensure that a program's data and software are FAIR.

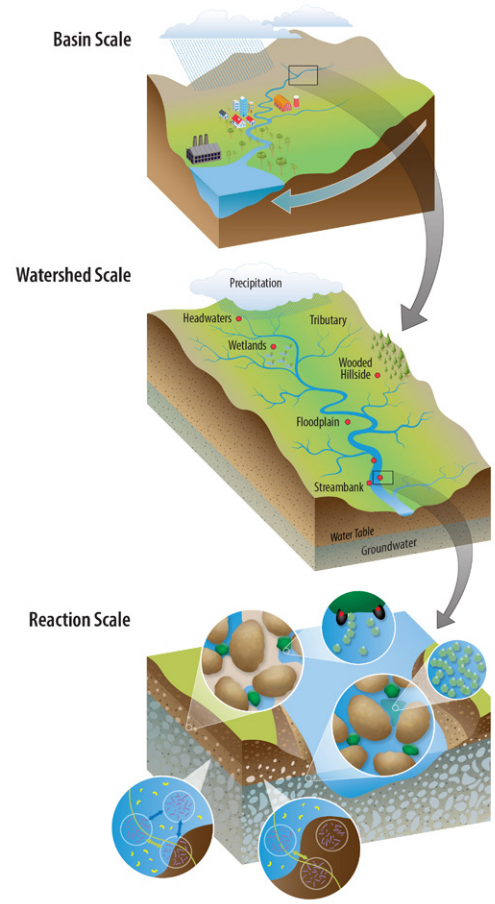
2.6.4 Networked

Networked research programs depend on engagement with the scientific community, and should occur early in the design process and continue throughout a project's lifecycle. During the early design process, the study can be configured so that the supply of resources (e.g., sampling equipment, sensors, data, and infrastructure) comes entirely from the research program, the network of collaborators, or a blend of the two. Research programs (e.g., WHONDRS) may send free sampling supplies or sensor technology to a network of collaborators. This can be done on a temporary basis so that tools can be loaned to other researchers. Sending out supplies is an additional cost to research programs that must be integrated with the design from the outset. Programs (e.g., AmeriFlux Network) may choose instead to have the community (1) use their own materials while following standardized protocols or (2) purchase standardized materials that are used or installed in their systems. A critical need is that networked research programs designed with and for the community can be leveraged by individual research projects. Networked research must be mutually beneficial across all engaged parties, which can be achieved through multiple mechanisms, but all require *a priori* thought and design. For example, unique BER resources (e.g., EMSL and JGI) can be used to generate high-value data that are difficult for many individual researchers to access. Providing these data to individual researchers in exchange for being part of a large, networked research campaign provides an incentive to join the larger effort and thus gain mutual benefit.

This scenario points to a new model for the BER user facilities in which they could actively engage the research community to jointly design networked research campaigns. Some portion of the facility resources could be allocated to supporting such efforts. In turn, individual researchers would effectively gain access to user facilities by being part of the networked effort. This model represents a complementary approach to the traditional user facility proposal process and would significantly increase the number of users while generating standardized datasets across watershed systems. Such datasets are enormously valuable for developing transferable understanding. In addition, samples collected using standardized methods from across a broad range of physical, chemical, and biological settings could be used to develop new laboratory methods needed to optimize the use of advanced user facility instruments. Such sample sets also could be used to develop long-term archives of physical samples for future interrogation. User facility–initiated, networked research campaigns would, therefore, have numerous mutual benefits spanning the facilities themselves, individual investigator efforts in localized systems, and synthetic multiwatershed research programs. User facility–based sample archives also would be highly beneficial to future efforts focused on long–time series analysis, potentially through the use of future advancements in analytical technologies.

Chapter 3. Open Watershed Science by Design: Use Case Examples

Five different use cases are described in this chapter to offer examples of how science challenges can be addressed across a range of scales using open watershed science by design. These use case examples include overviews of technical limitations and knowledge gaps inhibiting understanding of and the ability to predict watershed structure, function, and evolution. They also discuss what information and tools are needed to overcome current limitations and gaps and describe approaches for resolving these challenges using ICON-FAIR research programs that leverage and integrate existing capabilities, such as those provided by the DOE Systems Biology Knowledgebase (KBase), ESS-DIVE, DOE Joint Genome Institute (JGI), DOE Environmental Molecular Sciences Laboratory (EMSL), USGS, and NASA. All five use cases provide tangible ideas of research efforts embodying ICON-FAIR principles that, if implemented, would turn the vision of open watershed science by design into reality. The use cases begin with the Worldwide Hydrobiogeochemistry Observation Network for Dynamic River Systems (WHONDRS) project, an existing example that uses a nimble approach to target a variety of scales using different study designs. The next three use cases represent a given scale—reaction, watershed, and basin (see Fig. 3.1, this page)—and are more forward looking, though they build from existing efforts and capabilities. The final use case is also forward looking and emphasizes how at-scale ICON-FAIR research can be integrated to understand emergent functional attributes of watershed systems across scales. These use cases are not intended to be comprehensive and do not attempt to address all challenges or relevant scales in watershed science. Instead, they offer a subset of potential examples to help clarify how to turn the vision of open watershed science by design into reality. The research community is encouraged to build upon the foundation the use cases provide.



3.1. Use Cases Represent a Broad Range of Scales. The use cases span reaction, watershed, and basin scales while also integrating across these scales. The **reaction scale** is focused on the integration of fundamental biological (e.g., interactions among bacteria, fungi, and viruses) and chemical (e.g., enzymatic degradation of organic matter) processes within the context of physical settings throughout the watershed continuum. The **watershed scale** focuses on the integration of physical, chemical, and biological processes from ridge lines to receiving waters in coupled surface and subsurface domains that are relatively unimpacted by direct human modifications. The **basin scale** incorporates multiple watersheds and spans both pristine and human-modified systems (e.g., reservoirs, agricultural landscapes, and urban environments). In addition to the use cases developed at these three scales, the WHONDRS and Multiscale use cases span and integrate across scales. [**Watershed-scale** panel adapted from Allegheny County Conservation District. **Reaction-scale** panel adapted from (1) Stegen, J. C., et al. 2016. "Groundwater-Surface Water Mixing Shifts Ecological Assembly Processes and Stimulates Organic Carbon Turnover," *Nature Communications* **7**, 11237, and (2) Jansson, J. K., and K. S. Hofmockel. 2018. "The Soil Microbiome—from Metagenomics to Metaphenomics," *Current Opinion in Microbiology* **43**, 162–68. CC-BY-4.0.]

3.1 WHONDRS: An Existing BER Use Case

The WHONDRS project aims to galvanize a global community around understanding the coupled

Fig. 3.2. WHONDRS Is Designed to be Mutualistic with the Watershed Science Community. WHONDRS field campaigns are conducted with the community to generate resources for the community, enabling an iterative cycle of enhanced understanding and predictive capacity that feeds back to influence subsequent efforts. [Pacific Northwest National Laboratory]

hydro-biogeochemical function of dynamic river corridors from local to global scales (Stegen and Goldman 2018). The purpose is to provide a scientific basis for enhanced predictions of integrated watershed function under contemporary conditions and in response to disturbance (e.g., hydrological disturbance). Such predictive capacity is essential for using watersheds as a framework to connect processes from microbial to Earth system scales and to improve watershed management aimed at sustainable and resilient ecosystem services (e.g., providing high-quality water). Of particular interest is understanding how dynamic hydrology couples with other macroscopic features (e.g., vegetation composition, stream order, and geological properties) to influence organic carbon chemistry, microbial community composition, and biogeochemical activity in surface water and in groundwater–surface water mixing zones within river corridors. Community-enabled sampling campaigns are designed to advance this understanding.

WHONDRS is part of the Pacific Northwest National Laboratory (PNNL) Subsurface Biogeochemical Research program (SBR) Science Focus Area (SFA) and fills a unique role within the SBR program, and within watershed science more broadly. This consortium is enabled by the science community and generates model-relevant data products across watersheds as open resources for the community (see Fig. 3.2, this page). An essential element of the WHONDRS philosophy is that resources, knowledge, and data belong to the community, not to individual researchers, and that this approach leads to more rapid and robust scientific advancement. In turn, WHONDRS provides free access to detailed molecular data (via BER user facilities), unique field instrumentation, and more standard data types (e.g., ion concentrations and sediment texture). Collectively, WHONDRS-generated data include what is needed to set up one-dimensional (1D), genome-informed numerical models of hyporheic zone hydro-biogeochemistry. Because all data are generated using consistent methods, models can be set up across sampled locations and used to extract fundamental principles that are transferable across watersheds, while also discovering features that are system specific.

Purposefully designed to embody ICON-FAIR principles, WHONDRS represents a microcosm of the broader open watershed science by design vision and serves as an example for how to develop and implement additional, expanded watershed science research programs that collectively embody open watersheds by design.

WHONDRS is *integrated* by emphasizing connections among microbial community composition and

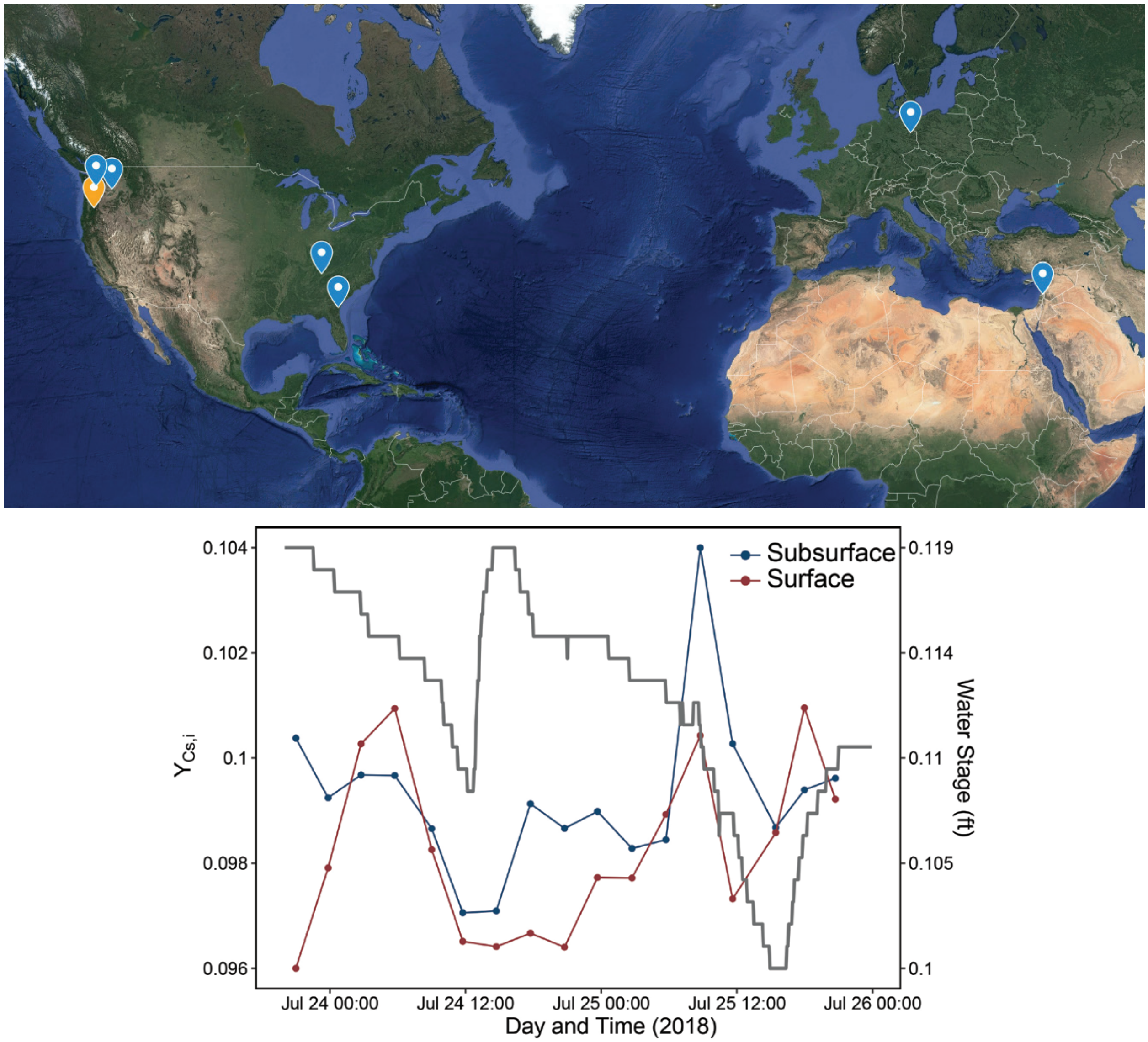


Fig. 3.3. WHONDRS Field Campaigns Generate Fundamental Knowledge Generalizable Across Systems. Data are generated using consistent methods across field systems to enable transferable understanding. **(Top)** Spatial distribution of time-series sampling campaigns carried out in 2018. **(Bottom)** Stream-depth dynamics (grey line) and associated dynamics of an organic carbon thermodynamic property ($Y_{Cs,i}$) relevant to hydro-biogeochemical function and models. $Y_{Cs,i}$ is the stoichiometric coefficient of the *i*th organic carbon source in a metabolic reaction. The value of $Y_{Cs,i}$ is a quantitative estimate for how many moles of organic carbon need to be consumed to provide the energy required for the synthesis of one mole of microbial biomass (Song et al., in prep). These data are from the H. J. Andrews Experimental Forest (orange symbol in the top panel). [Pacific Northwest National Laboratory. Map based on WHONDRS data publication in ESS-DIVE (Stegen et al. 2019), Google Map data © 2018 INEGI, Imagery © 2018 NASA, TerraMetrics.]

function (biology), major ions and detailed properties of organic carbon (chemistry), and surface and subsurface hydrology (physical). For example, in 2018, WHONDRS collaborators conducted surface and subsurface time-series sampling in seven globally distributed river corridors that were all characterized by subdaily river stage/discharge fluctuations (see Fig. 3.3, this page). A goal of subsequent analyses is to evaluate cross-system variation in the relationships among dynamic hydrology (measured via *in situ* sensors), carbon chemistry (measured via EMSL), and microbial functional gene profiles (measured via JGI). Outcomes of these analyses will help to guide multiwatershed, hydro-biogeochemical modeling efforts that couple microbial metabolic models to carbon chemistry and dynamic hydrological fluxes.

WHONDRS is *coordinated*, whereby field sampling and laboratory handling and analysis protocols have been standardized. Many different people collect the field samples associated with WHONDRS. Oftentimes though, one-off sampling is conducted for a given system, so there is no opportunity for collaborators to become familiar with WHONDRS sampling methods through repeated experiences. These instances pose a challenge to achieving consistency in field-sampling methodology. The project uses multiple approaches to resolve this challenge and achieve maximum consistency. First, WHONDRS provides materials to conduct sampling, yielding consistency in the type of vessels (e.g., glass or plastic) and preservation methods (e.g., filtration and acidification) that are used. Second, WHONDRS provides sampling kits that are simple to use, require minimal time in the field, and have built-in features to minimize potential contamination (see Fig. 3.4, this page). Third, WHONDRS provides comprehensive, easy-to-follow written and video protocols (see the WHONDRS YouTube channel at https://tinyurl.com/y5mqfzmd/). In developing the protocols, team members emphasized discovering, highlighting, and solving potential pitfalls that could lead to inconsistency in sample collection. Fourth, samples are sent to PNNL for analysis so that sample handling and laboratory analysis are as consistent as possible. For example, WHONDRS worked closely with EMSL to develop standardized procedures for preparing and analyzing water samples via high-resolution mass spectrometry. These procedures span the sample lifecycle, including storage, preparation, instrument settings, and data processing. Collectively, this multipronged approach enables WHONDRS coordination through purposeful application of consistent methods across all sampled watershed systems.

WHONDRS is *open* in that all data are made freely available following quality evaluation; there is no time-delayed embargo on when data become available. Data from WHONDRS are hosted on ESS-DIVE, and future sequencing data generated through JGI will likely be hosted via the National Microbiome Data Collaborative (NMDC). Importantly, WHONDRS data are not just public, they are truly open by ascribing to FAIR data principles. The data are *findable* through a built-in search function within ESS-DIVE that is paired with a digital object identifier (DOI) for each dataset.

Fig. 3.4. WHONDRS Sampling Kits and Detailed Protocols Enable Coordination and Consistency in Sampling Methodology. Shown is a stream water sampling kit that can be sent to anyone in the world interested in being involved with the project. The kit was designed to be simple and quick to use (sampling takes ~10 minutes), and it minimizes contamination by introducing the sample through a septum instead of opening the collection vials. These features make the kit amenable for use by both scientists and the public via citizen science efforts. [Pacific Northwest National Laboratory]

The ESS-DIVE search allows discovery of the full datasets, and the underlying data are *accessible* through an open-access license (CC0) and via a WHONDRS-developed graphical user interface (GUI) that enables searching within WHONDRS data (see Fig. 3.5, p. 27). The GUI has a variety of search criteria (e.g., spatial bounding box and data types of interest) and, following sample selection, provides consistently formatted, machine-readable output that includes all data types in one ready-for-analysis package. WHONDRS data have been made *interoperable* through the use of community data standards. In particular, the solute concentration data follow standards developed by USGS, such that the data can be merged with USGS or any other data generator that follows the same standards. For example, envisioned is that researchers will be able to merge WHONDRS water quality data with EPA data by pulling from ESS-DIVE and EPA's Water Quality Portal (www.waterqualitydata.us). Other data types such as mass spectrometry currently lack community standards, but WHONDRS is using a consistent format and engaging with the community to develop standards. WHONDRS data are *reusable* through the inclusion of detailed metadata spanning the entire sample lifecycle. These metadata include field, laboratory preservation, instrument, and data-processing methods. In addition, data are standardized in terms of units and file structures that are machine readable.

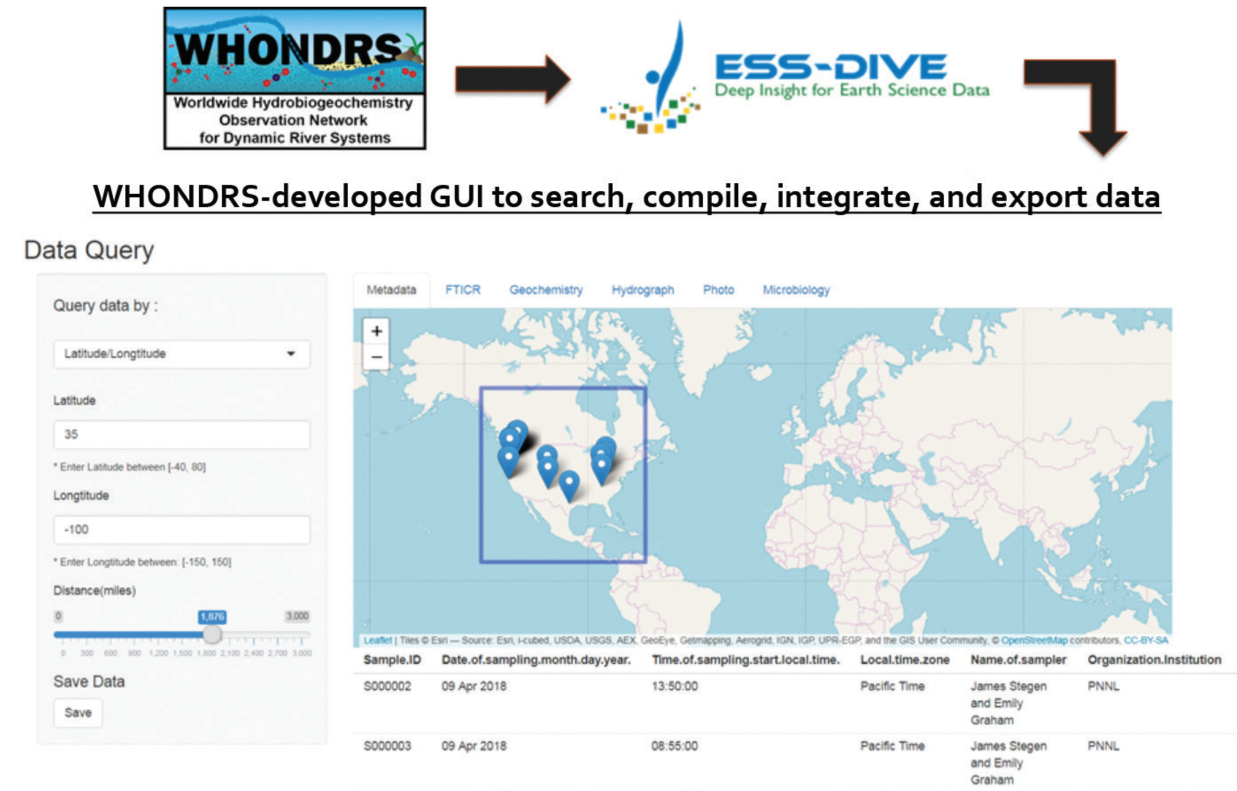


Fig. 3.5. All WHONDRS Data Are Published via an Open-Access License. Shown is a screenshot of the WHONDRS graphical user interface (GUI) on ESS-DIVE. Once selected, data are output using a standard, machine-readable format that allows integration across diverse data types. [Pacific Northwest National Laboratory]

Importantly, there was and continues to be significant emphasis on making WHONDRS data open by design. Doing the work *a priori* to build open watershed research programs is intrinsic to the vision of open watershed science by design.

WHONDRS is *networked* such that sample collection and data generation are conducted with and for the scientific community, whereby the community provides input on data targets and performs field sampling (see Fig. 3.6, p. 28). This networked approach is designed to be mutualistic between the science needs of the PNNL SBR SFA and the broader science community (see Fig. 3.2, p. 24). For example, the PNNL SBR SFA is developing methods to represent detailed properties of organic carbon in numerical hydro-biogeochemical models. A key data type needed to inform such models is provided by Fourier-transform ion cyclotron resonance mass spectrometry (FTICR-MS). FTICR-MS is a major EMSL capability, but this instrument is relatively uncommon, making this data type difficult for most researchers to generate. This provides an ideal situation to build a mutualistic research program with the community, whereby the community provides field samples (using WHONDRS sampling methods), and WHONDRS collaborates with EMSL to generate and provide FTICR-MS data from those samples. Resulting data are freely available for use by the community and for PNNL SBR SFA modeling needs. Similarly, the PNNL SBR SFA has developed new sensor technology for estimating the flux of water through subsurface sediments under both dynamic and steady-state conditions. This unique capability, which is otherwise not available, is provided to the community for free via WHONDRS. As with FTICR-MS, the resulting data are needed to inform models being developed by the PNNL SBR SFA (across watersheds and coupled to FTICR-MS data), but the broader community also needs these data to understand the hydrology of local field sites. In this mutualistic relationship,

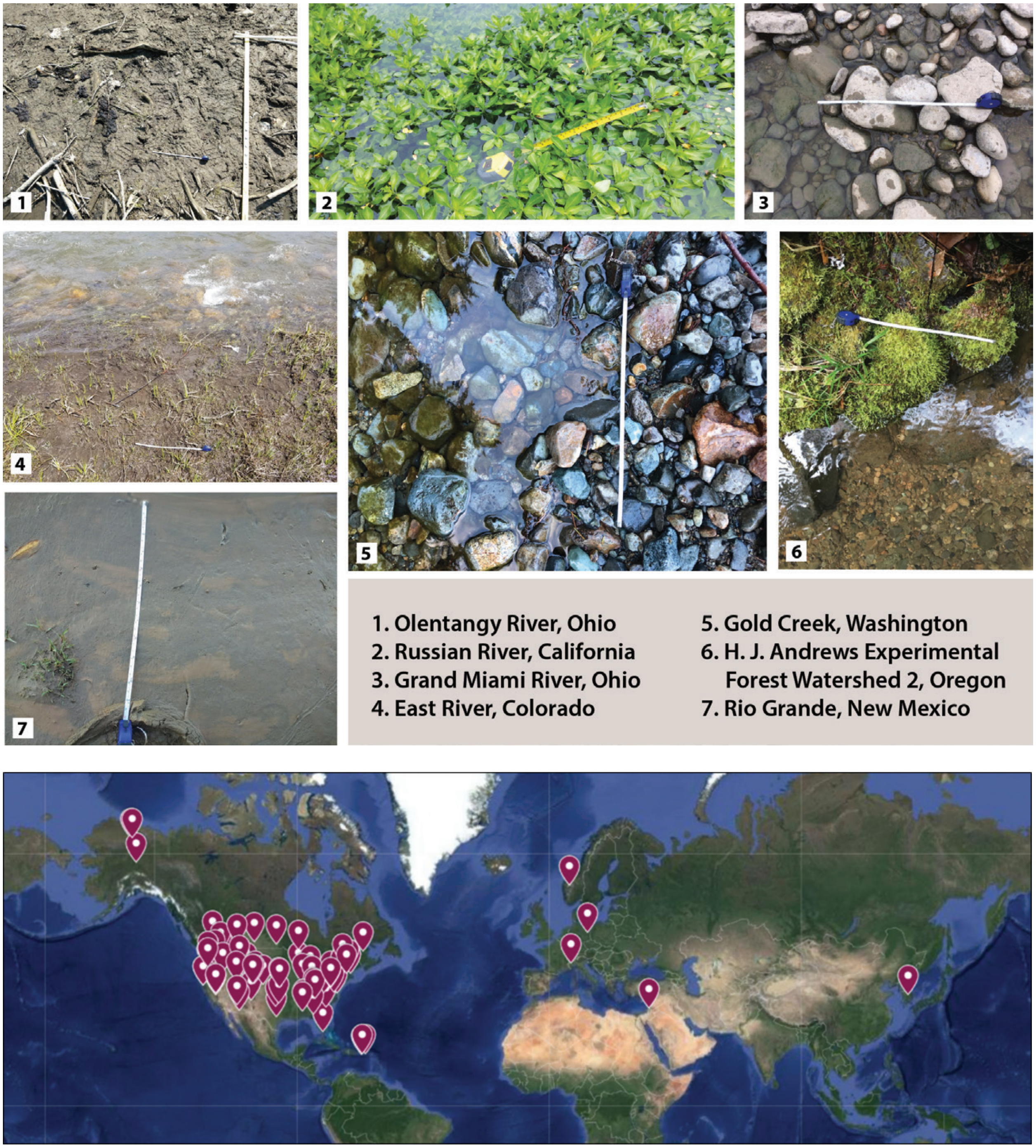


Fig. 3.6. WHONDRS' Success Hinges on Engagement of a Large, Globally Distributed Network of Collaborators. These collaborators collect samples across river corridors that differ significantly in their physical, chemical, and biological attributes. Generating consistent data across divergent systems is essential to the development of transferable principles. **(Top)** Examples of river corridor systems sampled by WHONDRS collaborators. **(Bottom)** Spatial distribution of a WHONDRS sampling campaign of roughly 100 globally distributed river corridors during August 2019. [Photos: **(1)** Olentangy River, Garrett Smith, The Ohio State University. **(2)** Russian River, Michelle Newcomer, Lawrence Berkeley National Laboratory (LBNL). **(3)** Grand Miami River, Mohamadreza Soltanian, University of Cincinnati. **(4)** East River, Nicholas Bouskill, LBNL. **(5)** Gold Creek, Jackie Wells, Pacific Northwest National Laboratory (PNNL). **(6)** H. J. Andrews Experimental Forest Watershed 2, James Stegen, PNNL. **(7)** Rio Grande, Vanessa Garayburu-Caruso, PNNL. Map: Google Map data © 2018 INEGI, Imagery © 2018 NASA, TerraMetrics.]

WHONDRS provides instrumentation, the community provides people power to deploy it, and everyone benefits from the resulting data.

Using discrete studies within the network allows WHONDRS the flexibility to investigate different scales of watershed science. An example is a globally distributed sampling campaign that was carried out in the summer of 2019. For this campaign, the WHONDRS team first identified research questions including:

- At the global scale, is there a core metabolome in river corridors, and what combination of ecosystem features explain variation in the transient metabolome?
- Across U.S. biomes, what are the relative contributions of ecosystem metabolomes and microbial communities in explaining variation in respiration rates of surface water and riverbed sediments?
- Across U.S. biomes, what is the relationship among ecological assembly processes influencing metabolomes, communities, and metatranscriptomes in river corridors, and can assembly processes be predictive of respiration rates?

The team then outlined a study design that was feasible, provided the needed data, and would be useful to other research teams. The study was further designed to provide the data necessary to develop genome-informed reactive transport models within each sampled field site, enabling an extension of WHONDRS that couples distributed observations to distributed modeling. A distributed modeling approach based on the same model setup across watersheds and informed by consistently generated data can be used to run numerical experiments across watersheds to elucidate general principles of physical, chemical, and biological interactions and feedbacks. The WHONDRS study design also included an iterative process with input from experts on specific data types, modelers planning to use the resulting data, and a watershed science community of over 100 researchers who agreed to collect samples across the world. The same general approach to study design can be used at any scale, such as within a given watershed (e.g., sampling intensively across stream orders) or basin scale (e.g., sampling across land-use types, within and outside reservoirs, and in pristine and contaminated sub-basins).

These iterative, design-based approaches focus heavily on molecular and hydrological measurements within river corridors, which are important to the understanding of and ability to predict watershed function. WHONDRS is finite, however, and a much broader scope is needed to span other watershed components (e.g., hill slopes, deep subsurface, and vegetation) and include additional methods (e.g., geophysics and remote sensing). There are exciting opportunities to use the WHONDRS approach to build additional ICON-FAIR watershed research programs. Doing so is at the heart of realizing the open watershed science by design vision. The following sections summarize a series of such opportunities spanning reaction, watershed, and basin scales, as well as an ICON-FAIR approach to link across these scales.

3.2 Reaction-Scale Use Case

3.2.1 Challenge: Identifying Model-Relevant, Reaction-Scale Data

Microorganisms govern critical watershed functions ranging from nutrient processing to the remediation of waste streams, but genome-enabled knowledge from these microbial catalysts is rarely incorporated into contemporary hydro-biogeochemical models. An open question is whether genome-resolved strain abundances or encoded functions can act as explanatory variables that improve predictions of watershed hydro-biogeochemical function. Across ecosystems, emerging evidence shows that molecular data (e.g., genomes and other omics) can uncover transient biotic and abiotic aspects of biogeochemical processes (Hansel 2016). For example, metagenome-enabled community proteomics was used to identify active bacterial sulfate reduction despite the presence of unfavorable redox conditions at the Rifle, Colorado, Integrated Field Research Challenge (IFRC) site (Wrighton et al. 2014). New knowledge of simultaneously active metal- and sulfate-reducing bacteria was incorporated into reactive transport models, revealing increased biogenic sources of iron [Fe(II)] and improving predictions during an *in situ* uranium bioremediation field experiment (Yabusaki et al. 2011). Additionally, multiomics data can reveal new geochemical signatures that are currently latent or undefined in watersheds. Gene expression data coupled to metabolite data, for example, uncovered new reactive components of dissolved organic matter that represent a previously unidentified and likely sizable portion of marine organic carbon and sulfur cycling (Durham et al. 2014). Based on these and other examples, multiomic datasets from across watersheds will likely uncover an intricate web of chemical-biological interactions that can be used to improve predictions of hydro-biogeochemical function in response to disturbance. Resulting enhancements to predictive capacity will be important for accurately forecasting the ecological consequences of ongoing global environmental change.

To improve the incorporation of fundamental chemical-biological interactions (i.e., reaction-scale processes) in predictive hydro-biogeochemical models, there is a growing need to (1) enhance the spatiotemporal distribution of samples and associated data to elucidate the spatiotemporal organization of interacting chemical (e.g., organic carbon species) and biological (e.g., combinations of complementary genomes) features, (2) illuminate the mechanistic linkages between chemical and biological processes, and (3) improve the incorporation of these processes into numerical models.

In response, a forward-looking ICON-FAIR Reaction-Scale use case is presented that would address these three challenges by significantly enhancing integration among BER capabilities through the development of new cyberinfrastructure spanning data processing to model integration. These cyberinfrastructure modifications could enable the seamless linkage of genome-enabled information to reactive transport models. Another key element is leveraging distributed scientific efforts, such as WHONDRS, to pursue coordinated sample collection across watersheds. These efforts will generate coupled, high-resolution chemical and biological data to identify variables that are predictive of fundamental biotic-abiotic interactions across a broad range of conditions. An envisioned outcome of implementing this use case is a transformation in understanding of how chemical-biological interactions vary across physical settings distributed within and across watersheds. This advance will enable the transfer of reaction-scale knowledge, data, and predictive models across watersheds, thereby enhancing understanding and predictive capacity of reaction-scale processes and (ultimately) their influence over larger-scale phenomena. For example, such knowledge and models could be used to explain concentration-discharge (C-Q) patterns of solutes at watershed to basin scales. Beyond improved models, this use case also addresses fundamental scientific grand challenges articulated in a report by the Biological and Environmental Research Advisory Committee (BERAC; BERAC 2017) including (1) understanding biological complexity from molecules to ecosystems (BERAC grand challenge 2.1), (2) optimizing large datasets to reveal biological paradigms (BERAC grand challenge 2.3), and (3) defining the influence of microbial communities on ecosystem and Earth system phenomena (BERAC grand challenge 4.3).

3.2.2 Current Needs

ICON-FAIR Research Efforts Leveraging High-Resolution Molecular Data to Reveal Patterns of Conserved Reaction-Scale Processes

Beyond easy-to-measure water quality variables (e.g., pH, conductivity, and temperature), few research campaigns to date have shared data collection methods. As a result, cross-watershed comparative analyses are hindered, or limited to biogeochemical features that do not adequately capture processes at the reaction scale. However, increasing accessibility to mass spectroscopy and genomic technologies, provided by BER user facilities such as EMSL and JGI, respectively, offer new opportunities for collecting standardized, high-resolution measurements of reaction-scale chemistry and biology. Tools such as metabolomics enable the characterization of microbial substrates and other nutrients at environmentally relevant concentrations, while genome-enabled tools (genomes, proteomes, and transcriptomes) survey the enzymes catalyzing the transformation of such compounds. Computational methods currently being developed (e.g., within the KBase platform) will be able to integrate these chemical and biological data into genome-resolved flux balance analyses (FBA), resulting in reaction-based descriptions of the overall stoichiometry of chemical reactions performed by each genome under observed environmental conditions. Also possible is the ability to produce approximate rate predictions and biomass yield predictions from these FBA models. Such predictions are, however, currently limited to a relatively small number of well-curated genomes, highlighting the need for further development of genomic tools for modeling *in situ* microbial

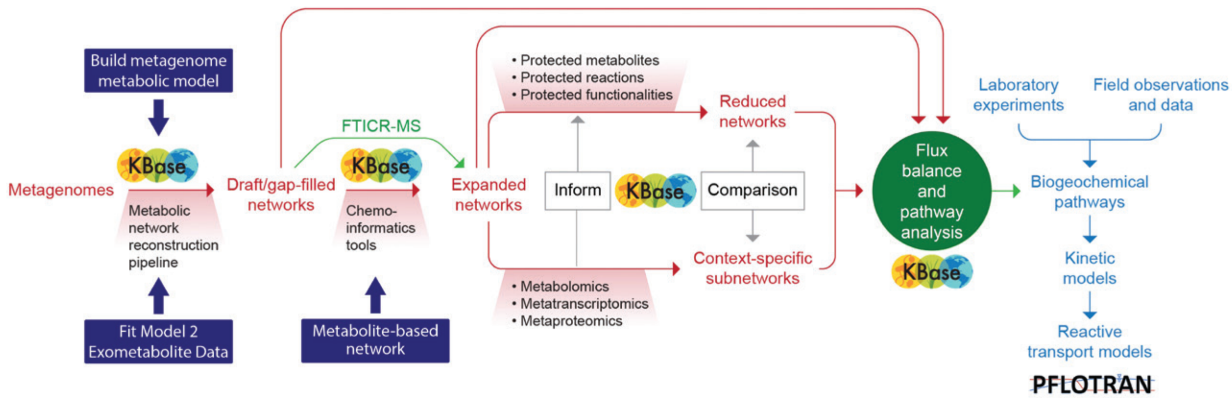


Fig. 3.7. Overview of How Genomic and Metabolomic Data Can be Coupled Within KBase to Generate Flux Balance Analysis Models, Which Are, in Turn, Integrated with Reactive Transport Models (e.g., PFLOTRAN). This approach can uncover coupled pathways, help refine kinetics, and lead to more informed reactive transport models. [Hyun-Seob Song and Pacific Northwest National Laboratory]

communities. Nonetheless, FBA predictions can, in principle, be seamlessly integrated into dynamic biogeochemical reactive transport models to define the metabolic pathways and transformations that govern biogeochemical processes and rates within and across watersheds (see Fig. 3.7, this page).

How can this new information advance knowledge of reaction-scale processes? The integration of high-resolution chemical and biological data could elucidate how microbial function is organized with respect to physically defined watershed features or properties (e.g., stream order), as well as how this organization is influenced by environmental disturbances (e.g., changing carbon inputs and fluctuating redox conditions). Furthermore, common patterns shared across similar watershed components or conditions could enable the development of new predictive indices, potentially through data-driven (e.g., machine-learning) approaches. Alternatively, detailed chemical and biological data can feed into FBA models that are applied across watersheds. Linking these FBA models to reactive transport models would enable distributed reactive transport modeling using a consistent model architecture (e.g., 1D-PFLOTRAN) informed by consistently generated, high-resolution data. Coordinated numerical experiments (e.g., across a hydrological disturbance regime) can then be run across watersheds to help elucidate conserved linkages between fine-scale processes and emergent hydro-biogeochemical phenomena. Outcomes of the numerical experiments could be used to guide additional field or laboratory experimental campaigns aimed at testing model predictions and improving mechanistic understanding of reaction-scale processes across environmental regimes. Such advances have the potential to leverage—and extend beyond—WHONDRS efforts, ultimately strengthening both efforts.

Refined Cyberinfrastructure Enabling Translation of New, Mechanistic Insights into Reactive Transport Models

Current distributed efforts could enable the collection of more and new types of data from a larger number of points in space and time, but current cyberinfrastructure hinders the feasibility, scalability, and use of these distributed efforts at the reaction scale. Therefore, a key challenge is the development of cyberinfrastructure that enables more seamless data retrieval, integration, and analysis. Fortunately, the individual components enabling data collection (e.g., JGI, EMSL, and SLAC National Accelerator Laboratory), data processing and database creation (NMDC and KBase), storage and archiving (NMDC and ESS-DIVE), and analyses and linkages to models (KBase and PFLOTRAN) already exist as active BER capabilities (see Fig. 3.8, p. 32). However, to translate high-resolution chemical and biological data into models, improved cyberinfrastructure for ingesting, archiving, and processing these data is needed.

Connecting any kind of data is challenging, but making connections across divergent kinds of data associated

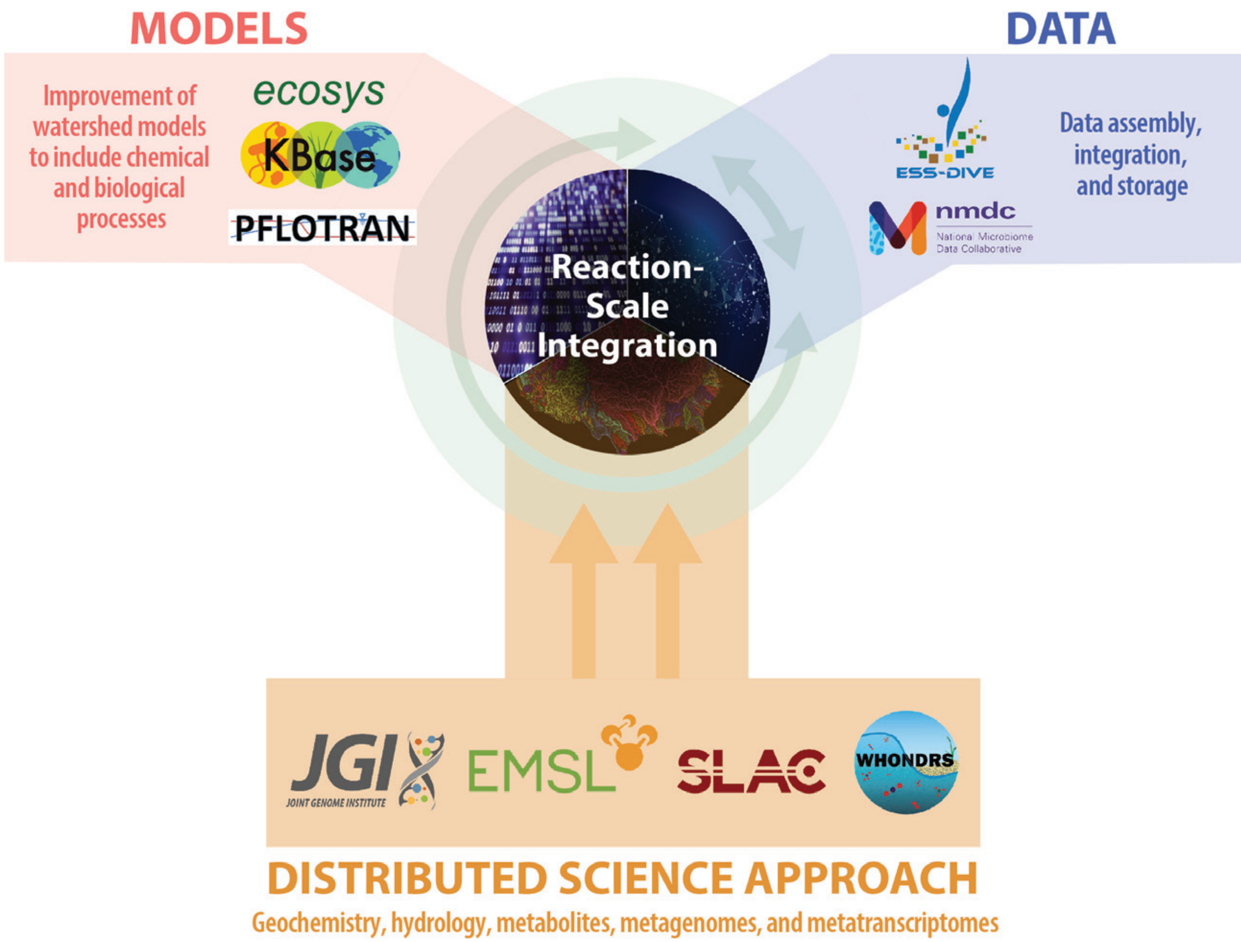


Fig. 3.8. Overview Schematic Combining ICON-FAIR Approaches with Existing DOE Capabilities. Some of the key DOE capabilities include the Joint Genome Institute (JGI), Environmental Molecular Sciences Laboratory (EMSL), SLAC National Accelerator Laboratory (SLAC), and WHONDRS. Reaction-scale data are archived and processed within BER resources such as ESS-DIVE and the DOE Systems Biology Knowledgebase (KBase) to generate flux balance analysis models that can, in turn, be coupled to reactive transport models. Coordinated, multiwatershed data collection, processing, and analyses will provide fundamental knowledge of reaction-scale processes that are conserved across watershed components or conditions. [Mikayla Borton, Colorado State University]

with environmental microbiomes (e.g., genomics and metabolomics) is particularly difficult. (1) These data are voluminous and, especially for genomics, can require vast storage requirements; cloud computing and storage offers one solution. (2) These data require substantial post processing, which is highly variable and often not well documented, pointing to a need for standard reporting requirements potentially through the use of reproducibility tools like Jupyter notebooks. In addition, ongoing development and standards by the newly formed NMDC will likely regulate and control the processing and analyses of these data in future applications. (3) Omics data (as compared to data like water temperature) require interpretation in the context of the original sample's overall physical and chemical environment, which can be facilitated through data-analysis environments (e.g., KBase) capable of integrating molecular (e.g., genomes) and nonmolecular (e.g., sediment texture) data. (4) Data-management tools that have been developed for omics data, and specifically the DOE-funded KBase software, enable data upload, curation, and analysis tools, but often require substantial domain knowledge and computational power that pose challenges to the distributed approaches (with high sample numbers) envisioned here. Significant progress can be made toward tackling these challenges through a combination of additional researcher training, interdisciplinary collaboration with domain experts, and purposeful development of informatics and modeling tools to be compatible with high-performance computing, which represents a large DOE investment.

Resolving these four computational challenges will require focused and sustained efforts from multiple research and infrastructure groups. As noted previously, some solutions are readily apparent—and are currently being pursued—while others will require more iteration around innovative solutions. Seamless integration among BER capabilities also poses some very specific challenges. For example, EMSL-generated data need to be connected to KBase. This link can be accomplished with the development of an application programming interface (API) through which KBase can pull EMSL data into its informatics ecosystem; such a capability is actively being developed and will be a powerful step forward as a central element of the envisioned Reaction-Scale use case, in part because JGI and KBase are already connected. Such a capability also would make leveraging data generated through BER's Facilities Integrating Collaborations for User Science (FICUS) program significantly easier. FICUS is designed to link EMSL and JGI resources. Similar solutions will likely be effective for connecting KBase to ESS-DIVE and NMDC, so that all relevant data can be brought together within a single-analysis environment. Another key element is connecting KBase outputs (e.g., FBA models), as well as ESS-DIVE data (e.g., water quality and hydrological data), to the Interoperable Design of Extreme-scale Application Software (IDEAS) ecosystem, which potentially can also be achieved through APIs. Ultimately, overcoming these existing computational challenges will enable new, more efficient capacities to link high-resolution, reaction-scale data to reactive transport models, making these data accessible to multidisciplinary teams and enabling answers to fundamental questions on watershed function and evolution.

3.2.3 Expected Outcomes

Reaction-scale, genome-enabled studies will uncover currently cryptic linkages between biological and chemical processes, advancing understanding of the degree of conservation across space, time, and environmental gradients. Refined cyberinfrastructure for DOE capability integration will enable this scaling across watersheds, as well as seamless incorporation of these data into predictive models. The combination of multiomic data collection and enhanced cyberinfrastructure will result in unprecedented advances in the understanding of coupled processes and predictive capacity. For example, machine learning–based analyses could reveal chemical-biological linkages that influence emergent phenomena such as C-Q relationships and their responses to disturbance (e.g., nutrient loading). Chemical-biological linkages that are conserved across watersheds may also point to the need for new, *in situ* sensor technology offering real-time and affordable monitoring of key variables. This coupling between mechanistic insights and sensor development will provide an informed approach, enabling a move away from time- and cost-intensive methods (e.g., laboratory-based mass spectrometry and nucleic acid sequencing) toward scalable, open-source *in situ* sensing. Beyond watershed science, the envisioned ICON-FAIR approach to develop transferable reaction-scale data, knowledge, and models can serve as a general approach for studying coupled chemical-biological processes and associated emergent phenomena in other environmental settings.

3.3 Watershed-Scale Use Case

3.3.1 Challenge: Developing Next-Generation Models Capable of Characterizing and Predicting Watershed Structure, Function, and Evolution

Characterizing and predicting watershed structure, function, and evolution require a holistic perspective that encompasses physical, chemical, and biological processes. An integrated approach can lead to deeper understanding and quantification of disturbance impacts, as well as play a central role in management, decision making, and policy from local to regional scales. Decades of federally funded watershed research emphasizing the stream reach and hillslope scales has substantially advanced understanding and state-of-the-art modeling and data acquisition. In particular, myriad complex models have emerged to simulate watershed dynamics in response to the wide availability of new and diverse data sources. Though these models are able to match past and current observations, they often fail to accurately predict new baselines and impacts of episodic disturbances. Such fundamental limitations indicate a latent need to fully integrate observations into the next generation of models capable of predicting emergent phenomena that arise via nonlinear feedbacks and other complex system dynamics.

Current modeling tool limitations can be partially explained by the uncertainty of model conceptualization (i.e., model structure and primary processes and feedbacks) and the lack of appropriate field data to estimate parameters and validate predictions. Current watershed research efforts often focus on specific component processes, with complementary efforts only loosely coordinated among field, laboratory, and modeling teams. This approach results in weak strategies to test alternative model structures, highlighting the reality that modeling and observational efforts tend to develop in parallel and with minimal interaction. Further, research outcomes are often difficult to integrate across studies into a synthetic body of transferable knowledge due to differences in methods, data types, and scale mismatch between data and model needs. Finally, the coupling among the critical zone and deeper subsurface systems, which offer high-level control on coupled water flow and reaction, are rarely characterized in sufficient detail to place short-term, process-focused research efforts (e.g., typical 3-year research grant) into temporal and system-scale context. Resources dedicated to multiscale, remote-sensing data collection (land and air based) comprehensively across watersheds can address some of these challenges, but they could be better coordinated and shared among individual projects and integrated at multiple stages into the modeling process.

Purposeful design of watershed-scale research programs ascribing to ICON-FAIR principles can be used to address challenges associated with model evaluation through the development of integrative, model-relevant datasets and process knowledge. The East River Watershed, a highly studied cluster of nested watersheds in western Colorado, demonstrates this approach. Research at this site is led by the Lawrence Berkeley National Laboratory (LBNL) SFA and has adopted key principles of the open watershed science by design vision since its inception. Importantly, while this use case is developed around a single watershed, this is for demonstration purposes. The open watershed science by design vision is ultimately focused on deploying ICON-FAIR research programs across watersheds to develop transferable data, knowledge, and models.

This Watershed-Scale[1] use case serves as an evolving example of coordinated, integrated watershed research, and by following the ICON-FAIR principles will lead to transferable, mechanistic understanding that can be applied to any watershed. Although there is progress yet to be made, the East River Watershed demonstrates the budding potential of adopting ICON-FAIR principles in the context of deriving and predicting critical watershed functions. Furthermore, this Watershed-Scale use case directly addresses several BERAC grand challenges (BERAC 2017), including (1) new technologies to understand (watershed) processes and inform models with novel analyses (BERAC grand challenge 3.2); (2) understand and model water-cycle processes to predict water availability and response to extremes (BERAC grand challenge 3.5); and (3) characterize the biogeochemical exchanges driven by food-web and plant-microbe interactions and evaluate their process-level impacts, sensitivity to disturbances, and shifting resource availability under changing environmental regimes (BERAC grand challenge 4.1).

The East River Watershed is a nested system of experimental watersheds specifically designed to address spatiotemporal heterogeneity in coupled surface-subsurface systems within (and between) watersheds. These heterogeneities challenge the ability to predict how disturbances impact functions relevant to downstream municipalities, ecosystems, and the Earth system. This Watershed-Scale use case builds from growing efforts to holistically integrate watershed-scale, remotely sensed data with process-focused research efforts. Multiscale remote sensing from a range of platforms (e.g., satellite, manned aircraft, drone, and surface geophysics) can act as the "glue" to tie together various process- and place-based watershed research efforts and coordinate synoptic sampling efforts.

The LBNL SFA was established to quantify nested processes impacting the ability of mountainous systems to retain and release water, nutrients, carbon, and metals. The East River sub-watersheds have varied legacies of mining activity and differing vulnerability to numerous future disturbances. The East River is managed as a scientific "community watershed" and

[1] Here, watershed-scale refers to the integration of physical, chemical, and biological processes from ridgelines to receiving waters in coupled surface and subsurface domains.

hosts ongoing research spanning a wide range of spatial scales and physical, chemical, and biological processes. Activities of a multidisciplinary, multi-institutional team of investigators supported by DOE, USGS, NSF, and the Rocky Mountain Biological Laboratory are coordinated in a manner that emphasizes integration, openness, engagement, and communication.

Upland areas of the Colorado River Basin (including the East River Watershed) are critical in controlling downstream water quantity and quality, but they are experiencing some of the fastest rates of ecosystem change due to global warming and land-use dynamics. At a regional scale, the East River is one of two major tributaries that form the Gunnison River, which, in turn, accounts for just under half of the Colorado River's discharge at the Colorado-Utah border. The Colorado River provides public municipal water supplies to 30 million people, both within and outside the basin, including numerous Native American tribes. Colorado River water is also used to irrigate nearly 4 million acres of agricultural lands. At a local scale, stakeholders include the Crested Butte Ski Resort, ranchers, recreational users of public lands, and trout anglers. This diverse group of local and regional stakeholders underscores the necessity of coordinated watershed research to improve the prediction of watershed function.

3.3.2 Design Vision

This use case is designed to integrate watershed-scale remote-sensing data to help bin the watershed into refined functional units that can be used to guide detailed process investigations. Watershed functional zones are spatial domains within watersheds that have a defined suite of features, such as particular types of vegetation, soil, and hydrology. The data used to define functional zones can be conceptualized as watershed functional traits derived from readily available data (e.g., climate, geology, geomorphology, and vegetation). A given functional zone is likely to occur in multiple discrete spatial domains such that the spatial distribution of any given functional zone can be mapped throughout a given watershed. In the Watershed-Scale use case, representative spatial domains of each functional type, such as high alpine hillslopes, wet meadows, and alluvial floodplains, will be interrogated with ICON-FAIR process-based investigations. These studies could address a variety of processes such as those influencing fine-scale patterns of groundwater discharge along the river corridor and the associated influences on subsurface microbial metabolism. This approach would provide a natural connection point between the watershed functional zones defined in this Watershed-Scale use case and the high-resolution chemical and biological data and associated cyberinfrastructure of the Reaction-Scale use case. Regardless of which processes are studied, the associated research campaigns will need high-level coordination and integration, as well as a template of remotely sensed FAIR data to define the physical and reactive controls on watershed function.

Community-driven, multiscale remote-sensing efforts at the East River Watershed demonstrate a novel approach to the adoption of ICON-FAIR principles at true watershed scales, augmenting coordinated direct measurement and synoptic sampling-based field data collection. As mentioned previously, watershed research efforts typically lack high-level coordination and representative spatial distribution. Moreover, they tend to be spatially focused on hot beds of reach-scale research on specific processes, as shown conceptually by the patchy distribution of process-based study sites in Fig. 3.9a, p. 36. Complementary, multiscale remote-sensing methods assess various watershed compartments or functional zones providing context and common supporting data types to guide consistently implemented, place-based, process-specific studies (see Fig. 3.9b, p. 36). Two general spatial scales of remote sensing are currently collected at the East River Watershed: (1) Point-in-time remote sensing at watershed scales that is comprehensive across space, but often with reduced spatial and temporal resolution (e.g., satellite and manned aircraft). (2) Transect, grid, and reach-/hillslope-scale remote sensing with higher spatial resolution and often repeated over time to document change (e.g., manned aircraft, drone, and surface geophysics). Specific examples of recent large-scale datasets include light detection and ranging (LIDAR)–derived estimates of snow depth and microtopography; hyperspectral estimates of foliar properties obtained using the National Ecological Observatory Network's (NEON) Airborne Observation Platform; and subsurface geological structure using airborne, time-domain electromagnetics (see Fig. 3.9c, p. 36). Finer-scale remote-sensing data include drone-based infrared, multispectral,

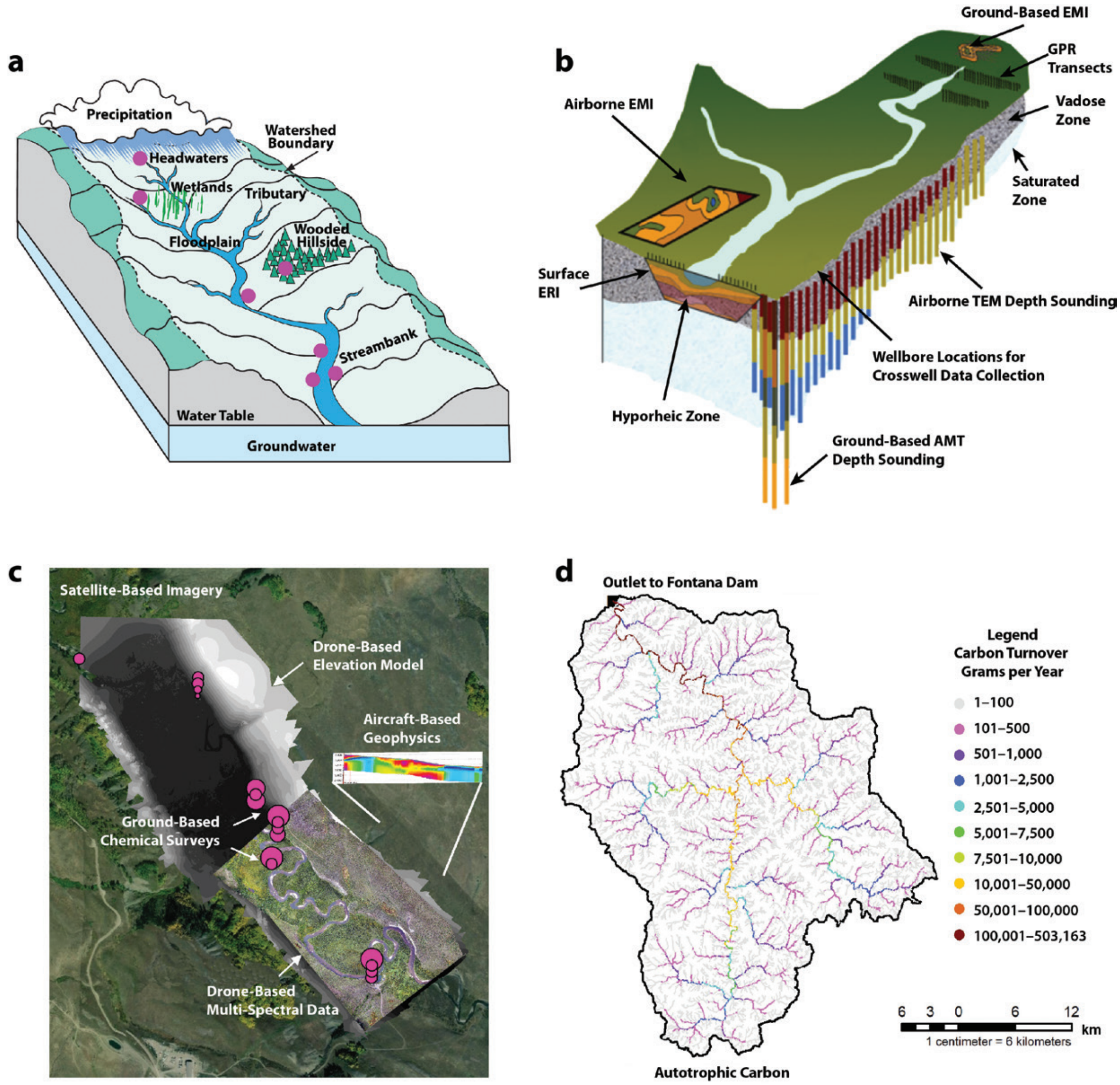


Fig. 3.9. Opportunities to Develop Transferable Data, Knowledge, and Models via Enhanced Coordination Within Large Projects, Across Multiple Smaller Projects, and Through More Rapid and Purposeful Data Sharing. Individual process-focused watershed research efforts are inherently constrained by funding and other logistics that lead to intensive data collection efforts at a small number of locations, which can identify deep insights about particular sites. While powerful, this approach can result in relatively sparse spatial coverage at the watershed scale (as shown conceptually with pink circles in **panel a**). In addition, access to comprehensive, remotely sensed data collected by other studies in the same watershed can be *ad hoc*, which highlights the opportunity to enhance the utility of spatially distributed field campaigns through tighter coordination with remote-sensing efforts and data. Recent advances in multiscale and objective remote-sensing technology and data products could enable better integration of disparate research studies to elucidate the controls on watershed function (**panel b**). The application of multiscale, remote-sensing data collection from satellite, aircraft, drone, and on-foot techniques, with input and contributions from diverse research teams, is being demonstrated at the East River Watershed through the SBR-funded LBNL Science Focus Area (**panel c**). Specific data types include aircraft-based electromagnetic induction to map watershed-scale geological structure to hundreds of meters of depth, paired with high-resolution surface vegetation, structure, and thermal mapping conducted via drone. The desired outcome of these integrated efforts is transferable, predictive understanding of function across watershed functional zones, particularly regarding the reactive transport process (e.g., dissolved carbon export) in response to baseline change and disturbances (example model output, **panel d**). [**Panel a**: Adapted from Allegheny County Conservation District. **Panel b**: Reprinted from Robinson, D. A., et al. 2008. "Advancing Process-Based Watershed Hydrological Research Using Near-Surface Geophysics: A Vision for, and Review of, Electrical and Magnetic Geophysical Methods," *Hydrological Processes* **22**, 3604–35. DOI:10.1002/hyp.6963. © 2008 John Wiley & Sons, Ltd. **Panel c**: U.S. Geological Survey. **Panel d**: Danielle K. Hare, University of Connecticut.]

Fig. 3.10. Watershed-Scale Use Case Links Cross-Project FAIR Data to Machine Learning. This linkage identifies fundamental properties and enhances predictive capacity. [U.S. Geological Survey]

and visible-light imagery, along with direct contact, near-surface geophysics (see Fig. 3.9c, p. 36).

When the drivers of watershed function are understood, predictive capability at the watershed scale is possible, as shown conceptually with a river network model of distributed organic carbon turnover rates in Fig. 3.9d, p. 36. Efforts are under way at the East River Watershed to incorporate process-based study findings into process-based predictive models such as ParFlow, but the coordination among field data, process understanding, and model calibration and validation remains challenging.

If multiscale remote-sensing efforts, and the ground-based efforts they support, are going to substantially advance watershed function predictive capability (see Fig. 3.9d), data need to be highly accessible and searchable, requiring efficient mechanisms to distill processes and patterns from large, multiparameter datasets. The LBNL SFA's data-management framework enables data management and distribution according to DOE's digital data requirements and ensures that data collected at the East River Watershed are broadly available, open, and useful. In particular, the framework provides infrastructure and services to (1) manage, archive, and publicly release data collected by the SFA as per the LBNL SFA's data policy; (2) enable the SFA team and the broader community to discover and access relevant datasets; (3) perform quality assurance and quality control (QA/QC) of datasets; and (4) enable efficient data collection, data integration, and product generation. Notably, the SFA has developed a number of tools for data management and preservation, QA/QC, data discovery, advanced search, and visualization (Hubbard et al. 2018).

3.3.3 Expected Outcomes

Understanding and predicting watershed functions involve a suite of compartments and properties from bedrock to the top of the vegetative canopy, including bedrock structure; soil characteristics; and plant functional types, structure, and dynamics. Characterizing each of these properties is a major challenge and has even been considered intractable, given their high degree of heterogeneity influenced by complex terrains, geology, and other factors. Advances in computing power and the availability of "wide" multiparameter datasets have enabled the application of machine-learning techniques, which could shed light on some of these complex relationships and improve predictability. Machine-learning methods are typically used to make continuous (i.e., regression) or categorical predictions (e.g., through classification or clustering) and are easily implemented for a variety of data types (e.g., continuous, binary, and categorical). Moreover, machine-learning methods can be used as exploratory tools to understand the potentially complex relationship between a wide array of datasets and environmental processes of interest, making them a powerful tool to predict and understand watershed functioning. ICON-FAIR principles could further maximize the potential of these approaches (see Fig. 3.10, this page).

Significant advances in understanding watershed organization and the interactions among different compartments have been made over the last decade, particularly through NSF's Critical Zone Observatories network (Brantley et al. 2018). For example, Pelletier et al. (2018) highlighted the control of topography (slope aspects) on ecosystem and critical-zone systems, including soil moisture, deeper weathering, and larger nutrient retention in soil. Machine-learning approaches could further advance such understanding of watershed organization and functions, taking advantage of airborne and satellite remote-sensing datasets (including hyperspectral and airborne geophysics) to capture spatiotemporal patterns of plants, topography, and subsurface. In particular, the subsurface-surface co-variability— among geology, geomorphology, and vegetation—can be identified and exploited to reduce the dimensionality of parameters that are relevant for complex hydro-biogeochemical processes (Falco et al. 2019). Unsupervised learning or clustering algorithms can help identify such co-variability and delineate the zones with unique distributions of bedrock-through-canopy properties relative to neighboring parcels. In addition, these patterns can be linked to the watershed "functions" of interest, such as water quality and disturbance sensitivity, through supervised learning or regression algorithms. LBNL has been developing the watershed functional zonation approach to use both unsupervised and supervised algorithms for delineating the zones that capture watershed heterogeneity relevant to key watershed functions, and for tractably describing watershed organization and functions.

Such examples highlight the positive feedbacks and substantial return dividends that can accompany the design and operation of experimental watersheds as open, community-accessible, integrated research programs from their inception. Coordinated East River Watershed SFA research efforts across biological, chemical, and physical compartments have put a premium on conducting watershed-scale remote-sensing campaigns for surface and subsurface properties with input from SFA research groups on the front end. Recent example efforts include NASA's Jet Propulsion Laboratory Airborne Snow Observatory airborne mapping, NEON Airborne Observation Platform airborne mapping, airborne time-domain electromagnetic imaging of underlying SFA geology, and reach- to hillslope-scale drone-based imaging with various sensors across seasons (see Fig. 3.9c, p. 36). A recently published example by Briggs et al. (2019) demonstrates how drone-based infrared and visible imaging, combined with near-surface geophysics and flow path–oriented biogeochemical synoptics, was used to identify beaver dams as an important control on floodplain-to-river metals mobility. There is an emphasis on understanding and predicting C-Q relationships throughout the East River sub-watersheds, and multiscale remote sensing is helping to define the component processes that drive temporal water quality dynamics. Integrated hydrological models are concurrently being developed to explore how streamflow may be impacted by disturbances such as changing vegetation and baseline warming throughout the East River Watershed (Pribulick et al. 2016).

The remote-sensing datasets provide common data coverage for essentially the whole watershed, guiding on-the-ground spatially distributed research efforts that are using consistent protocols to generate common data types across point locations. Remote-sensing data can be used to characterize large-scale physical controls (e.g., bedrock structure, snow distribution, and surface topography) and fine-scale landscape patterns in attributes such as soil moisture, vegetation type and health, and river corridor groundwater and biogeochemical function. These characterizations tie together the patchwork of watershed functional zones in a watershed function framework that can be augmented by process-focused field work in a directed way. As field data collection efforts are better designed and coordinated with the support of, and integrated with, multiscale remote-sensing campaigns, and large datasets are analyzed more efficiently and intelligently, codesign of field efforts and models can be optimized. Recent advances in remote sensing can be coupled with newly refined watershed-scale hydrological field methodology such as parsing young from older groundwater discharge with stable isotopes, geolocating exchange zones using dissolved radon, and high–spatial resolution mass balancing of stream water using various tracers. Models of watershed function are likely to both grow and shrink in complexity due to iterative comparison to evolving field data streams and analysis as the coupling of fundamental watershed processes across time and space is better understood. In this way, the watershed community will gain real traction on transferable characterizations of complex watershed systems, which would not be possible with piecemeal watershed research studies. Large, multiparameter remote-sensing datasets have great potential for advancing watershed research, but they also present unique challenges, particularly in distilling controlling processes using more traditional (e.g., piecemeal regressions and bivariate plots) analysis techniques.

Multiscale remote-sensing data can be integrated to provide fundamental knowledge of each local field site, and, by ascribing to FAIR data principles and using consistent methods, these data can also be integrated across local sites by placing all outcomes in the broader watershed context. This context is what provides the connective tissue among the individual sites, and the ICON-FAIR principles enable integration. Purposeful design of research programs to include these features offers more holistic knowledge of watershed function than could be achieved with information from any single field site or through *post hoc* attempts to link inconsistently generated and structured data. Instead of being less than the sum of the parts, the whole becomes greater than the sum of the parts. As a result, the significant heterogeneity that exists within watersheds becomes addressable, advancing the ability to predict disturbance outcomes on watershed function, which is critical to meeting local- to regional-scale stakeholder needs.

3.4 Basin-Scale Use Case

3.4.1 Challenge: Developing Predictive Understanding of Basin-Scale Responses to Disturbances and Extremes to Inform Water-Management Strategies

An important and perhaps defining characteristic of river basins is that they span a spatial extent that is sufficient for collecting and storing a significant amount of water, ideally enough to support the broad range of services required by large human populations. At the river basin scale, humans begin to view themselves as critical stakeholders in both the water and surrounding natural resources, and, hence, this is the scale at which the co-evolution of natural and engineered systems comes into view. The engineered systems that humans couple to the complex natural ecosystem include features such as irrigation for agriculture, energy storage and production through dams and reservoirs, and diversion and distribution to local and distant urban populations. The scale and complexity of this integrated river basin system have focused data collection and models toward simplified representations suitable for decision making, but they have not adequately addressed the increasing uncertainty in water quantity and quality due to climatic trends in precipitation and snowpack; disturbances such as fire, insects, and drought; and impacts on consumptive use such as crop selection and human population dynamics. These human elements of the integrated, complex river basin system are generally outside SBR's fundamental, process-oriented research portfolio, but their coupling and feedbacks with the natural system can play a critical role in water management. Thus, ICON-FAIR principles could be leveraged in the open watershed science by design vision to both improve predictive understanding of river basins and support the development of more resilient and effective water-management strategies.

From this river basin-scale perspective, a high-level scientific challenge is developing a predictive understanding of river basin-scale response to disturbances and extremes, in terms of both water quantity and quality, to inform holistic water-management strategies.

Specifically, the objective of this use case is to identify questions, resources, and approaches that facilitate a phased approach to the exploration of integrated, natural-human basin-scale systems. This use case seeks to identify physical, chemical, and biological processes and features across finer scales (e.g., reaction and watershed scales) that have a significant impact on basin-scale predictions and, hence, on management practices. For example, understanding the larger-scale influences of finer-scale processes may motivate development of multiscale or surrogate models that are significantly more efficient, yet still capture important couplings and feedbacks (Painter 2018). In addition, key processes or model features may be identified and added to models to improve understanding and prediction accuracy. Testing of these models critically depends on available data. SBR has significant data at SFA test-bed sites, but data across larger scales require coordination and collaboration with a wide range of agencies. Similarly, as data from multiple agencies and across larger scales are integrated and viewed, patterns and connections may emerge. Even more powerful is the iterative development of understanding and improvement of conceptual models both within and across river basins as multiscale, mechanistic models are better integrated with and become consistent with the available data and inform future data collection objectives.

A critical factor in making this river Basin-Scale use case ideal for open watershed science by design is the growing recognition of the importance and uncertainty of water resources across local, regional, and state governments. This realization has led most state governments across the United States to develop a "water plan" and begin the challenging task of integrating and coordinating water management within and across all the river basins within state boundaries. Widespread water plan development provides an

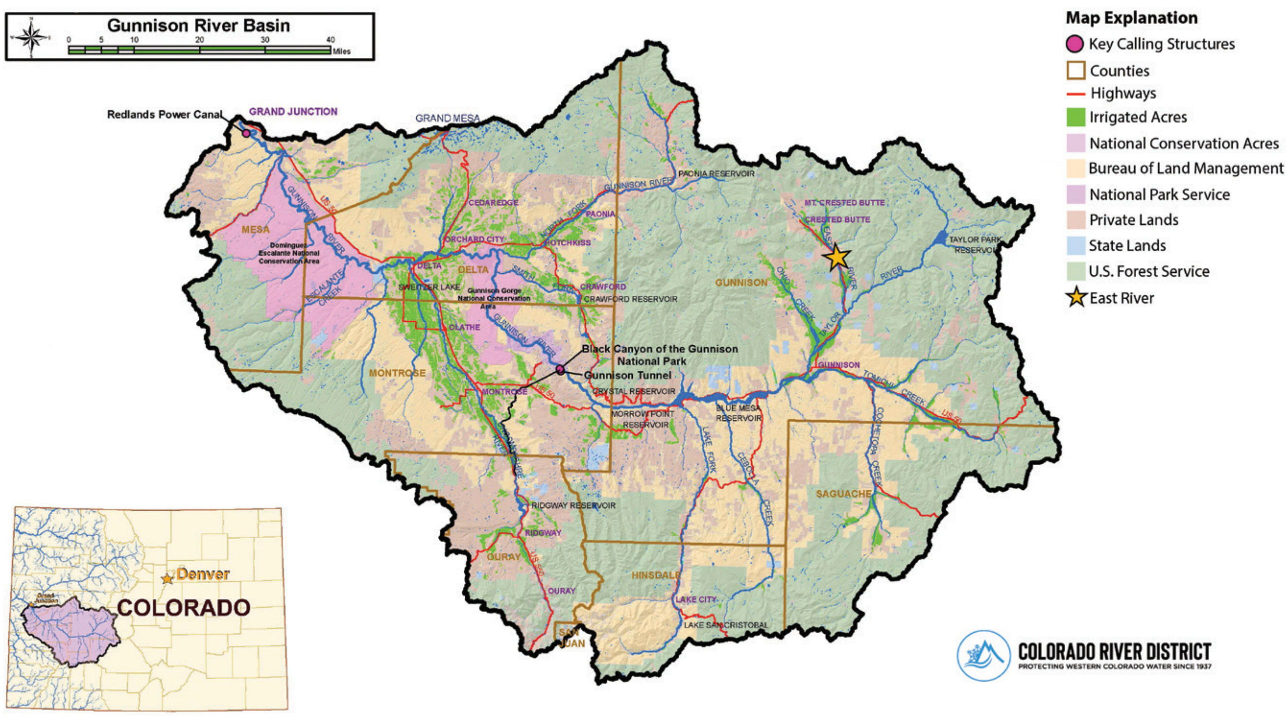


Fig. 3.11. Gunnison River Basin, Colorado. This river basin encompasses a diverse mixture of land uses (shown as different colors), including pristine watersheds and human-impacted landscapes. The basin provides an ideal setting for understanding basin-scale processes and how they are influenced by human infrastructure and other impacts. [Colorado River Water Conservation District]

incredibly valuable resource for the scientific community and underpins the transferability of the approach developed in this use case to other river basins.

This use case focuses on the Gunnison River Basin (see Fig. 3.11, this page) in Colorado. From several perspectives, this river basin is ideal as an example use case. First, it is a significant size (~8,000 mi^2) and includes pristine headwaters, managed tributaries with diversions and reservoirs, and intensely irrigated lower valleys, as well as the spatial domains of the Watershed-Scale use case. Second, the Gunnison River Basin is one of the eight basins within Colorado, each of which formed a roundtable for the collection and coordination of information gathering and planning and community outreach. These community-driven entities played a critical role in the development of the state's water plan, working with the Metro roundtable (defined by metropolitan Denver) and the Interbasin Compact Committee. These entities and their infrastructure provide valuable resources for technical work as well as the use of ICON-FAIR principles within the community. Finally, the Colorado Water Plan seeks to reduce the water gaps across its watersheds to zero by 2050. This interest in long-term goals in the face of potential impacts from climate change and disturbances can benefit significantly from mechanistic, multiscale models and data integration, which are flagship areas of SBR research.

3.4.2 Current Needs

Advances in Cyberinfrastructure

Data collection and synthesis at the river basin scale represent an immense task. Fortunately, many data sources have been identified, the majority are open and readily available, and some of these data have already been collected to support the Colorado Water Plan. In addition, the shared vision of state-level water plans is to increase the coordination and commitment of a broad range of stakeholders to publish their data in national databases. This trend in the use of FAIR principles is greatly expanding the types of data available to include digital elevation maps, hydrogeology of the subsurface, meteorological data (e.g., precipitation and radiation), land-use maps, and several chemical components of interest to water quality. Moreover, accessibility and use of these data are improving through the development of interfaces and RESTful APIs that enable scientists' access both interactively through a web browser and noninteractively through scripting and low-level computer languages. This noninteractive access provides a range of significant research opportunities, from data-driven, machine-learning techniques for classifications and analysis to significant automation of mechanistic model setup and model-data integration. For example, scripting capabilities enable various assessments of data coverage, and strategies could be developed to fill data gaps for future disturbance scenarios with suitably processed historical data.

Advances in Modeling

A wide range of models have been developed and used to simulate water quantity and quality at river basin scales. From the perspective of water management, coarse-grained, nonmechanistic models have dominated because of limited data and the need for computational efficiency. The strength of these models is that they can be calibrated to predict sufficiently integrated quantities (e.g., water availability) over larger spatial domains, given that the current state and forcing of the system is within bounds of previously observed states. However, under climate change, future system states are likely to be driven far from current states, with disturbances and extreme forcing being much more common. Thus, new approaches based on ICON principles are needed to leverage the growing expertise and strength in finer-scale, mechanistic models at the basin scale. Previously, integration of computational and domain scientists led to the development of parallel, open-source integrated hydrology codes. These codes significantly expanded the domain size over which high-resolution integrated hydrology simulations can be performed and used to improve fundamental understanding of processes and their feedbacks. For example, using integrated hydrology simulations of the continental United States (CONUS) with ParFlow studies highlighted the importance of lateral groundwater flow, the impact of groundwater pumping on streamflow losses, and evapotranspiration (Condon and Maxwell, 2019). Furthermore, groundwater pumping that depletes storage can actually increase future irrigation demand and overall system sensitivity to stress (Condon and Maxwell 2014). These connections highlight the potential for conjunctive management tradeoffs and the need for integrated groundwater–surface water models that can simulate managed systems. They also pinpoint the need for expanded integration to include stakeholders and water managers, as well as additional coordination across agencies to access existing expertise and models. Recent work in this direction used a collaborative modeling approach to integrate beyond traditional disciplines and include stakeholders and water managers by using an integrated hydrology model (GSFLOW) within a decision-support system to explore management decisions that boost recovery of a terminus lake basin (Niswonger, Allander, and Jeton 2014). The model was modified to include management of reservoir releases, river diversions, and irrigation and, hence, offers a starting point for a coordinated effort to develop models of engineered features that can be shared broadly across the scientific community.

3.4.3 Design Vision

The Gunnison River is heavily managed, with several dams, power plants, and a major water diversion for agriculture in the Uncompahgre Valley. These human systems have enabled incredible economic growth in Colorado but have had devastating impacts on natural systems. For example, the flow provided by the diversion tunnel along with the region's hydrogeology led to significant salt and selenium releases through subsequent irrigation (Mills et al. 2016). These contaminants had a negative impact on both agriculture as well as downstream fish populations (USDOI-BR 2011). In addition, the reduction of the low-flow regime and alteration of peak and shoulder flow behavior have caused significant problems for the fish populations, as has the decrease in dissolved oxygen in the water caused by hydropower generation (USDOI-BR 2012).

In all these cases, mitigation strategies have been implemented and water quality improvements have been realized (USDOI-BR 2011; Henneberg 2018). However, further improvements are still needed, particularly amid a growing gap between water supply and demand. From recent collaborations between USGS and EPA based on FAIR principles, in conjunction with outreach to engage the Gunnison River Basin community, a wealth of current and historical data is available. In addition, various soil-type, vegetation, and crop data are available from USDA, and meteorological forcing data (e.g., precipitation and snowpack) are available from NOAA. These data will be used to guide the development of both climate and management scenarios that stress the river basin in ways that challenge both the mechanistic models as well as management practices. To support these scenarios, ICON principles will be used to enhance capabilities in both cyberinfrastructure and mechanistic modeling. For example, cyberinfrastructure will focus on enabling the merging of integrated, consistently structured FAIR data into predictive, open-source models that enable modeling advancements through community-wide efforts.

In cyberinfrastructure, this use case is focused on workflows and tools that enable more effective use of data in models with a range of mechanistic complexity. Specifically, ongoing work at the watershed scale would be leveraged and extended to develop interfaces and tools that can access and aggregate data from various national databases (e.g., Water Quality Portal) and project-specific databases (e.g., ESS-DIVE) to prepare it for flexible model application. Flexibility in model application is critical to building confidence in both process conceptualization and representation in the model, parameter estimation and model calibration, and the ability to explore a wide range of climate forcing and management scenarios. These enhanced tools will preprocess available data to develop model inputs, for example, creating a mesh from available digital elevation models, mapping hydrogeological information to the mesh, and generating boundary conditions (e.g., precipitation) and sources (e.g., well locations and historical withdrawals). Automating this mapping between the original data, which have specific time and spatial scales associated with them, and the time and spatial scales of the model input is critical to realizing the desired flexibility and efficiency. This important combination of automating access to data sources and mapping the data to the model representation is what is needed and will be developed.

Building on this efficient and flexible development of models and model inputs, mechanistic models need to represent human-engineered components and management manipulations. First, by integrating with water managers and coordinating across agencies (e.g., USGS), requirements for the representations of engineered features will be developed and existing models will be assessed. After a subset of models is selected for this use case, implementations of these components with well-documented interfaces will be developed, tested, and released as open source. Most of these engineered components have suitable representations at the scales of interest, and the important advances are collaboration and coordination across agencies and stakeholders to promote the sharing of common interfaces, tests, and practices. Second, a scenario-based approach will be used to develop requirements for model interaction with decision-support systems, assess existing approaches and interfaces, and develop design recommendations for the support of various management scenarios through effective simulation restarts and backtracking controls of mechanistic models. For example, management tool interfaces would support both the straightforward modification of pumping rates at a given time, as well as be able to backtrack to an earlier time to adjust diversions and extractions to meet demands. In this latter case, the nonlinear feedbacks in the system, coupled with additional constraints (e.g., water rights and service decrees), require support for iteration in conjunction with backtracking scenarios. This design requirement is often overlooked but will be effectively addressed through collaboration with other agencies and stakeholders. An additional advantage of these mechanistic modeling approaches is that they are transferable and thus networked with the broader scientific community.

These advances in cyberinfrastructure and model development will be further focused to explore scenarios that highlight the factors at play in the projected 25% water shortfall for the Gunnison River Basin by 2050. Drought and anticipated population growth are key factors in this projection, and this use case will focus on drought. The recent prolonged drought led to a significant depletion of groundwater to mitigate the loss of storage in reservoirs (Castle et al. 2014), while the use of groundwater for irrigation affects levels of selenium and other trace elements in the system. In addition, low flows in rivers during drought are more susceptible to contaminant loads that may impact fish populations. These components and their nonlinear coupling and feedbacks are well represented in the Uncompahgre Valley, Colorado, which is a shallow aquifer system that relies on both groundwater and diversion-controlled surface water to meet the demands of a range of stakeholders, including the second largest agricultural region in the state. The hydrogeology leads to complex interactions of the groundwater system with the weathering Mancos Shale to create challenges for water quality. For example, the mobility of selenium from the weathering process is impacted by the leaching of nitrate from irrigation, while surface water from the diversion also contains selenium. Scenarios will be used to explore representations and controls of these coupled processes in mechanistic models to support management decisions over the whole basin.

3.4.4 Expected Outcomes

Cyberinfrastructure enhancements at the river basin scale will streamline the integration of data from a wide range of stakeholders and agencies for use in analyses and models that can inform water-management practices. In this use case, these enhancements leverage the community's support for the sustainability of the Gunnison River Basin, which has ensured data are being shared with new national databases as well as DOE SFA scientists who are sharing their data through ESS-DIVE. Since most communities and states are developing water plans and following FAIR principles, these enhancements will provide uniform access to data and enable transferable workflows for analyses and models across basins. Similarly, interagency collaboration and coordination on modeling both the human system components (e.g., dams and reservoirs) and management controls of the natural system (e.g., flow rate from a dam or diversion) in mechanistic models will offer several benefits for water management. Specifically, this work will enable the development of interoperable and extensible capabilities to enable the use of mechanistic models either directly in decision-support systems, or indirectly through the development of suitable surrogate or metamodels that can be used when additional efficiency is needed. As with the enhancements to cyberinfrastructure, modeling work will use open-development practices and distribute open-source software. In addition, given the anticipation that similar data are available across basins, these mechanistic models are readily transferable. This transferability highlights an important point, in that this use case is developed around a single basin for demonstration purposes, but the open watershed science by design vision is ultimately focused on deploying ICON-FAIR research programs across watersheds distributed among multiple basins (e.g., Delaware, Columbia, and Mississippi). Thus, the outcome of this use case will be an increase in the predictive understanding and capacity for supporting the river basin-scale challenges in water management arising from the co-evolution of natural and human systems.

3.5 Multiscale Use Case

3.5.1 Challenge: Integrated, Coordinated, Open-Research Networks Operating Across Scales

Fresh water is an increasingly scarce and precious resource. Pressures related to climate, land use, manufacturing, and energy production interact across local to continental scales to influence the quantity and quality of water available to humans and ecosystems. Consequently, there is a growing need to understand the impacts on this resource from extreme events such as floods and droughts.

Uncertainties in predicting future water quantity and quality manifest across multiple scales. At basin scales, the factors that influence water quantity and quality include climate, vegetation, and land use; at watershed scales, they include geology, geomorphology, and weather; and at reaction scales, highly localized microbial and geochemical processes (see Fig. 3.1, p. 23). These factors and their interactions make accurate predictions of water quality and quantity an indivisible problem that no one person, discipline, or organization can solve alone. Consequently, the entire scientific enterprise must be engaged and leveraged across disciplines, agencies, and scales to inform sustainable energy strategies that do not compete with ecosystem function or the availability of fresh water.

The way current watershed research is conducted, however, is suboptimal for predicting the hydrobiogeochemical outputs of watersheds due to the complexity and coupling of processes that occur at reaction to basin scales. Although the same biogeochemical processes may be studied in similar and disparate systems across the globe, barriers to sharing, communicating, assimilating, and integrating the resultant findings have effectively hampered the discovery of generalizable mechanisms describing the organization of biological and geochemical processes from reaction to basin scales.

How can generalizable principles for watershed functioning be derived in this context? A perspective by McDonnell et al. (2007) highlights the remaining challenges in watershed science and the need for a change in philosophical approach: moving from the view that "if enough hillslopes and watersheds around the world are characterized through detailed experimentation, some new understanding is bound to emerge eventually" toward testing "hypotheses governing general behavior (across places and scales)." Although the complexity and sophistication of physically based watershed models continue to increase, they remain primarily based on theories derived from scales smaller than their application. Factors such as spatial heterogeneity of landscapes and nonlinear process interactions result in highly unconstrained outcomes across scales with great sensitivity to parameterization. McDonnell et al. (2017) also proposed the adoption of an ecological approach for defining the key attributes of watershed function as sets of "functional traits" that represent the complex co-evolution of watershed landscape and process patterns. Connecting watershed function (i.e., the composite of its traits, called the phenotype) to functional traits that are increasingly observable across scales within and across watersheds has great potential for improving understanding of the relative importance of landscape heterogeneity and for leading to the observation of reproducible and diagnosable patterns.

More than a decade following McDonnell et al. (2007), some technological barriers have been reduced, but many social hurdles remain. The community requires a shift in philosophy to approach disparate systems using common hypothesis testing with consistency in approach and data. Adopting the ICON-FAIR principles proposed in this report would be a major step toward generalizable principles describing the origins of watershed heterogeneity and a move to watershed classification based on functional traits.

The Multiscale use case integrates outcomes from the previously described Reaction-, Watershed- and river Basin-Scale use cases to determine the scale-relevant attributes that influence watershed functional traits from the perspective of hydro-biogeochemical functioning. In particular, this use case aims to diagnose the origins of aggregated concentrations and fluxes of compounds observed in stream chemistry. Reaction- to hillslope-scale processes can culminate in reproducible and characteristic patterns (i.e., a phenotype) of changes in stream chemistry. The C-Q relationships represent a commonly used method to understand how the water quality in watersheds changes due to hydrological perturbations and other drivers (see Fig. 3.12, p. 45; Kim et al. 2017; Maher 2011). Yet basin-scale traits such as land-use and water-management practices also impact C-Q patterns, sometimes leading to a state of low biogeochemical variability (i.e., chemostasis), wherein concentrations of specific chemicals remain stable despite large variations in flow (Chanat and Yang 2018; Bieroza et al. 2018). Such simple phenotypes describing the relationship between water movement and its physical properties or chemical composition are powerful aggregators of the complex reaction-scale processes that underpin watershed function and are a consequence of a collection of watershed functional traits. In the future, extending C-Q relationships to more complex analytes like dissolved organic constituents detectable by high-resolution mass spectrometry (see WHONDRS and Reaction-Scale use cases, p. 23 and p. 29, respectively) may be a powerful approach for illuminating the microbial metabolic pathways active within hillslopes or reaches and contributing to the typically observed inorganic elemental fluxes.

Across the United States, watershed phenotypes such as stream C-Q relationships are widely available for a number of biogeochemical parameters (e.g., major cations, nutrients, and trace elements), which could enable a matrix of C-Q data to be employed to classify streams, rivers, watersheds, and basins using C-Q relationships as watershed functional traits (see whitepaper, "Using Machine Learning to Leverage the Value of Big Data and High-Frequency Monitoring in Characterizing Watershed Sediment Dynamics," Appendix 4, p. 122). A further analogy to the ecological term "guilds" is appropriate; watersheds may be grouped together into guilds based on a suite of common functional traits such as their C-Q response to disturbance. This approach provides a framework for compressing complexity and enabling diagnosis.

Such an approach would require collecting C-Q data in a *coordinated* (e.g., common sensor platforms), *networked* manner with the watershed science community so that representative watersheds of representative basins are targeted, resulting in data that are *open* and *FAIR*. These data could be *integrated* to classify catchments into functional guilds and, through comparative analyses, derive the causal mechanisms driving changes in water quality, as reflected in dynamic C-Q relationships. Once derived, watershed functional

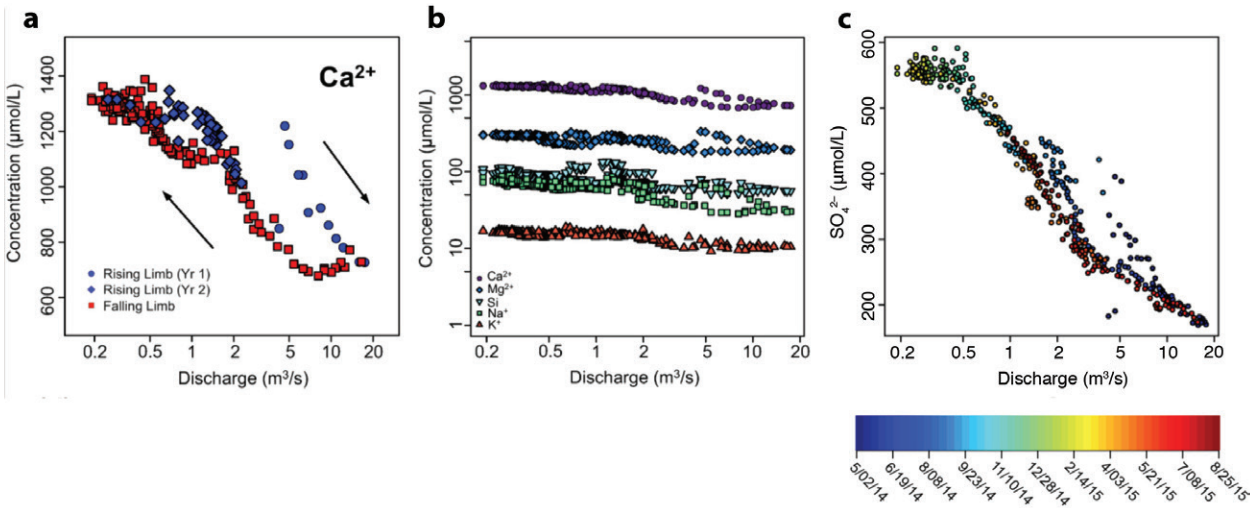


Fig. 3.12. Examples of Concentration-Discharge (C-Q) Relationships at the East River Pumphouse Site in Colorado. **(a)** Semi-log calcium ions (Ca^{2+}) show an annual hysteresis pattern, **(b)** log-log C-Q for all base cations indicating chemostatic behavior, and **(c)** sulfate (SO_4^{2-}) C-Q. Blue points represent the rising limb of the hydrograph, red points represent the falling limb, and first-year and second-year rising limbs are denoted by shape. [Adapted from Winnick, M. J., et al. 2017. "Snowmelt Controls on Concentration-Discharge Relationships and the Balance of Oxidative and Acid-Base Weathering Fluxes in an Alpine Catchment, East River, Colorado," *Water Resources Research* **53**(3), 2507–23.]

traits can provide an extensible approach for predicting watershed and basin responses to disturbance, through the use of process-rich numerical models strengthened by reaction-scale knowledge, or through the use of data-driven/hybrid models.

3.5.2 Current Needs

Several field, cyberinfrastructure, and modeling challenges must be addressed to achieve the vision presented in this Multiscale use case.

Field Measurements

Despite the wide prevalence of sensor networks used to routinely conduct water monitoring at unprecedented resolutions in the nation's rivers and streams, high-frequency, spatially dense biogeochemical measurements remain sparse. Long-term datasets of discharge and corresponding water quality variables do not have uniform spatial or temporal coverage. Emerging lower-cost methods to sense dissolved organic matter and nutrients (Pellerin et al. 2016) have not yet been implemented at scale across the nation. Many other parameters such as carbon, metals, microbial biomass, and community composition are not directly sensed due to the lack of affordable and reliable sensors to measure these variables. Enabling this Multiscale use case would require data collection of these variables at higher temporal and spatial resolutions across monitoring networks sponsored by different organizations and, in particular, expansion of scope to unrepresented, ungauged basins.

Expanded Cyberinfrastructure

The cyberinfrastructure to streamline data exchange and integration among providers is currently limited. Such exchange and integration are critical for enabling multiscale research, which needs to combine data generated by federal, state, and local agencies and organizations across scales of interest. This requires data to be provided with open-usage policies that enable creation and distribution of products without restrictions. Currently, years of effort are needed to obtain, perform QA/QC, and integrate data from different providers, resulting in several one-off products that are not updated on a regular basis. Adoption of community data and metadata standards would ease efforts to continually integrate the data from different providers. Also needed are innovative tools to integrate diverse data types (e.g., geology, hydrology, water quality, remote sensing, and genomics) that are of different structures (e.g., time series, image, gridded, and hierarchical) and scales (reaction, reach, watershed, and basin) into unified views for data analysis and modeling.

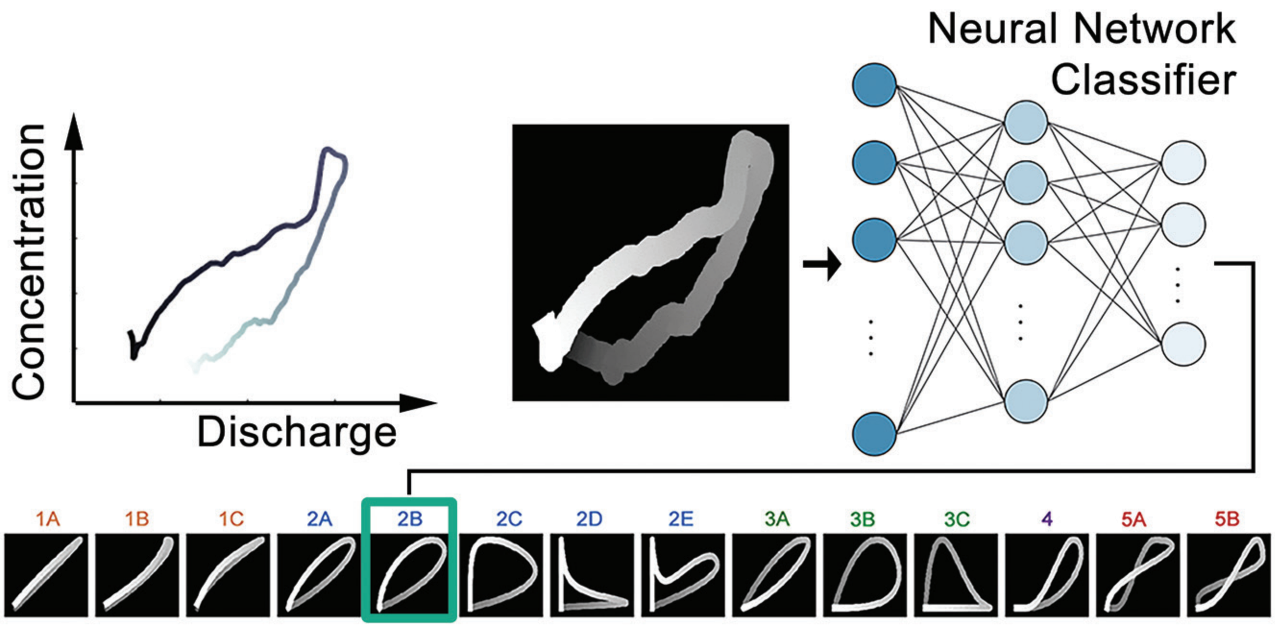


Fig. 3.13. Application of Machine Learning to Analyze Concentration-Discharge (C-Q) Relationships of Individual Hydrological Events and Categorize Those Events Using Visual Patterns. This approach takes advantage of machine-learning methods termed deep belief neural networks that are based on the restricted Boltzmann machine (RBM) for feature extraction, pattern recognition, and classification. Shown is the automated classification of C-Q event hysteresis directly from the C-Q images. [University of Vermont, Burlington. See also whitepaper, "Using Machine Learning to Leverage the Value of Big Data and High-Frequency Monitoring in Characterizing Watershed Sediment Dynamics," Appendix 4, p. 122.]

Improved Modeling Tools

Additionally, significant improvements to modeling tools are required. Current mechanistic approaches represent physical, chemical, and biological processes in the models, thus being limited by an incomplete process understanding that propagates to model structural deficiencies. These mechanistic models cannot be scaled, especially while attempting to represent highly resolved, complex processes across spatial scales that span several orders of magnitude. A multipronged effort can help with improving prediction accuracies and efficiencies. (1) Reactive transport models—spanning the Reaction-, Watershed-, and Basin-Scale use cases—can be placed into a multiscale modeling framework capable of more accurately representing fluxes at the larger scales, while considering smaller-scale heterogeneities (U.S. DOE 2015b). (2) Model structures can be improved based on the new process understanding from investigations at reaction to basin scales. (3) Use of exascale computing resources can enable hyper-resolution mechanistic modeling at multiple scales (Wood et al. 2011).

The application and development of machine-learning techniques for data mining and prediction (see Fig. 3.13, this page), including the use of data-driven and hybrid (physics-informed, machine-learning) models, can provide a complementary modeling approach that uses the vast amount of data available from the enhanced networks, with some level of process understanding built into the predictions.

3.5.3 Proposed Conceptual Framework for Integrated Multiscale Studies

A research approach for using data and models across scales can be viewed as two converging lenses (see Fig. 3.14, p. 47). This involves a co-design approach, wherein integrated studies that collect model-guided observations for near-term predictions are conducted at the relevant scale and informed by the other scales. Information gained at the various scales is then synthesized and used to inform the design of long-term data collection efforts for benchmarking model projections. Application of this approach to the C-Q Multiscale use case starts from the top down. The C-Q observations

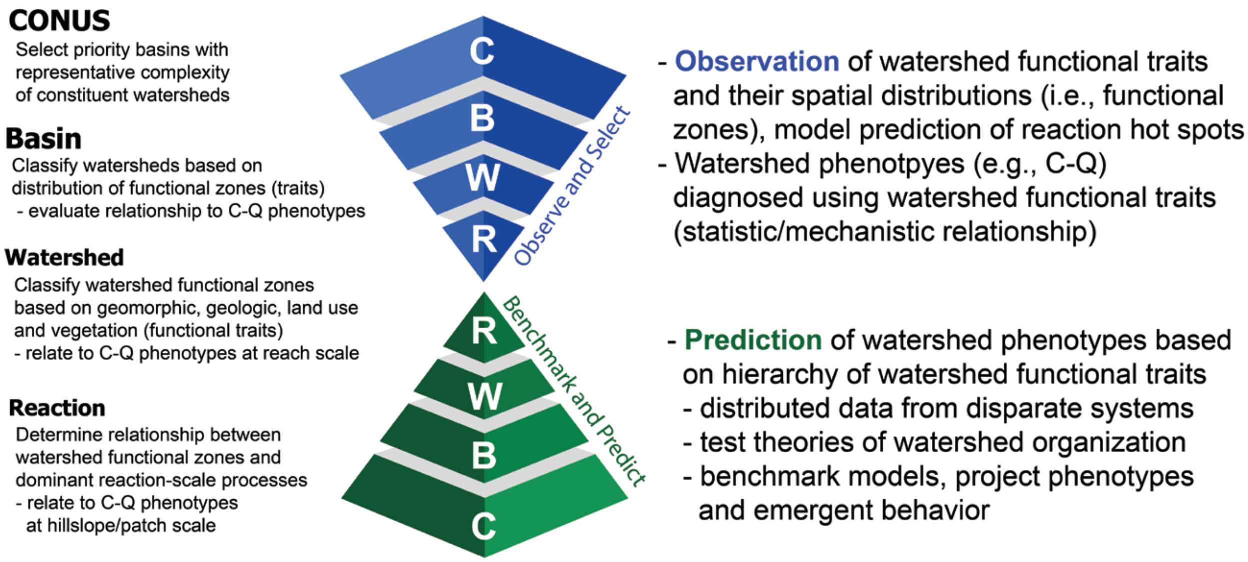


Fig. 3.14. Multiscale Concept of Addressing Watershed Complexity Through Watershed Classification Based on Functional Traits. Beginning at the continental United States (CONUS) scale, basins are selected based on the features of (e.g., topography and elevation) or influences on (e.g., managed, unmanaged, and urban) their constituent watersheds. At the watershed scale, watershed functional zones are identified from landscape analysis by quantifying the distribution of watershed functional traits derived from readily available data (e.g., climate, geology, geomorphology, and vegetation). Landscape locations with similar trait distributions are classified into watershed functional zones. Watersheds with similar distributions of watershed functional zones are predicted to display similar phenotypes such as concentration-discharge (C-Q) responses to disturbance. To evaluate these predictions and reveal underlying processes, representative functional zones and appropriate sub-zone heterogeneity (e.g., microtopography or interfaces between larger functional zones) that are expected to contribute significantly to reaction-scale processes underlying C-Q relationships are prioritized for local observation and experimentation. New discoveries, improved mechanistic understanding, and updated parameters at the reaction scale directly contribute to improved process representation in models that are then evaluated for quantitative improvement in prediction of C-Q relationships across scales. [Lawrence Berkeley National Laboratory]

at CONUS to basin scales are clustered, and machine-learning approaches are used to identify explanatory variables according to scale (e.g., climate, vegetation, and land use at basin scales; geology, geomorphology, and weather at watershed scales). This approach would help to identify commonalities in watershed response to disturbance at the basin or CONUS scales. To derive the causal mechanisms, representative watersheds could be prioritized for intensive community campaigns to study reaction- to watershed-scale processes and their contribution to C-Q properties using approaches summarized in the associated at-scale use cases. Resulting process understanding would then be used to improve mechanistic models with the ability to project watershed and cumulative basin-scale response to disturbance. Alternatively, the explanatory variables can be used as predictors in data-driven/hybrid models that use the data collected in representative watersheds as training datasets and data collected from the larger CONUS-wide monitoring networks for validation.

As part of a research plan to execute this Multiscale use case, a network of energy sustainability testbeds (NEST) is envisioned, as proposed in the BERAC 2017 grand challenges report (BERAC 2017). The NEST testbeds are strategically chosen to quantify the coupling between energy strategies and scale-relevant air-water-land processes. Field observations, data processing and synthesis, and modeling are conducted across a network of sites with different air-water-land forcings or vulnerabilities and are designed to investigate processes at different scales of interest relevant to water quality and quantity (see Fig. 3.15, p. 48). The interactions within and among scales will largely define the resiliency of different watersheds. Thus, predictions of C-Q relationships in response to disturbances require a multiscale understanding of the interconnectedness of these systems.

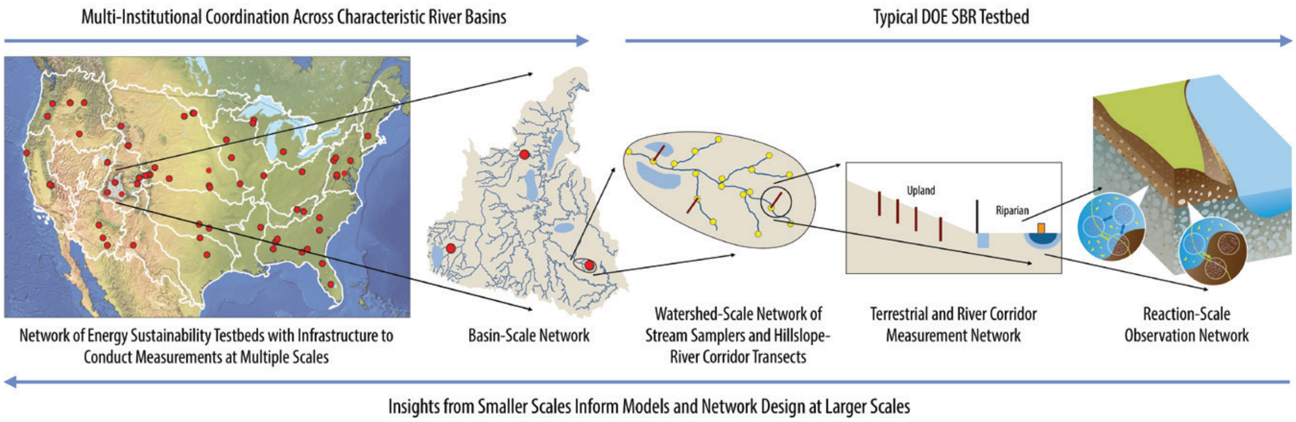


Fig. 3.15. A Multiscale Network of Energy Sustainability Testbeds (NEST) Spans a Range of Scales Necessary to Understand and Predict the Interconnectedness Between Land- and Water-Management Practices and Air-Water-Land Forcings on Water Quantity and Quality. NEST testbeds are networks of observations and model predictions that iterate across basin, to watershed, to reaction scales to predict water availability and quality across different types of energy and land-use strategies. The testbeds can include current or future Subsurface Biogeochemical Research investments that are strategically selected across the continental United States in coordination with other institutions and stakeholders and operated using ICON-FAIR principles. The colored circles represent real and hypothetical testbeds, many of which are already being led by different organizations. [**NEST map**, Pacific Northwest National Laboratory. **Basin-scale network**, **watershed-scale network**, and **terrestrial and river corridor network** modified and reprinted with permission from Springer from McClain, M. E., et al. 2003. "Biogeochemical Hot Spots and Hot Moments at the Interface of Terrestrial and Aquatic Ecosystems," *Ecosystems* **6**(4), 301–12. © 2003 Springer-Verlag New York, Inc. **Reaction-scale network** from Jansson, J. K., and K. S. Hofmockel. 2018. "The Soil Microbiome—from Metagenomics to Metaphenomics," *Current Opinion in Microbiology* **43**, 162–68. DOI:10.1016/j.mib.2018.01.013. CC-BY-4.0.]

This plan would use data from multiple agencies and employ rapid advances in remote sensing to describe watershed functional traits (see functional zone concept in Watershed use case, Section 3.3.2, p. 35) and in *in situ* environmental sensor networks (Rode et al. 2016; Blaen et al. 2016). Notably, USGS is now developing its Next Generation Water Observing System, initially deployed in the Delaware River Basin, with a second site being considered in the western United States. These high-resolution datasets are complemented by routine water quality monitoring conducted by many local and state agencies in coordination with EPA. Corresponding remote sensing and climate and meteorological data are available from NASA and NOAA. BER's ESS-DIVE can provide data for local- to watershed-scale research generated by the SBR SFAs. Some DOE data will be available through other suitable repositories; for example, microbial data may be available through NMDC and the National Institutes of Health's National Center for Biotechnology Information (NCBI). Remote-sensing data will be obtained through public portals from relevant agencies (e.g., NASA, National Snow and Ice Data Center, and NEON). Data at watershed to basin and CONUS scales will be pulled from the National Water Information System, and other interagency (USGS, EPA, and USDA) manual measurements of water quality available through the Water Quality Portal.

Thus, the Multiscale use case will reap the benefits of efforts at the federal and state levels to broaden public access to water data, such as the national Open Water Data Initiative (Blodgett et al. 2016) and California's AB1755 Open and Transparent Water Data Act (water.ca.gov/Programs/All-Programs/AB-1755/).

3.5.4 Expected Outcomes

As Pellerin et al. (2016) point out, there are multiple opportunities for coordinating efforts and investments from federal and state agencies, and scientific research institutions will "accelerate sensor development, build and leverage sites within a national network, and develop open-data standards and data-management protocols that are key to realizing the benefits of a large-scale, integrated monitoring network." The development of new conceptual frameworks and capabilities for synthesizing and distilling information in a consistent manner across reaction to basin scales will help to dramatically improve understanding and prediction of watershed structure, function, and evolution.

Chapter 4. Building Cross-Cutting Capabilities

4.1 Data Wrangling, Archives, and Distribution

Watershed science has now reached a point where a typical research project must iteratively obtain and integrate diverse data types from multiple sources to glean insights (see Fig. 4.1, p. 50). Several advances in data management for watershed research efforts are needed to enable easier scientific discovery, access, integration, processing, and reuse of data (U.S. DOE 2015b).

First are community data repositories that comply with findable, accessible, interoperable, and reusable (FAIR) principles and provide long-term archival with the ability to search and download data with appropriate citation information. Data compliant with the first two of these principles, findable and accessible, are becoming more common because of increasing repository options that accept programmatic (e.g., ESS-DIVE) or thematic (e.g., Hydroshare and National Microbiome Data Collaborative) data packages, which are bundles of data files with metadata. Still lacking, however, are physical sample (i.e., sediment and water) archives, which would support FAIR data and future research. Physical archives preserve irreplaceable samples, provide an opportunity for new research queries without the cost of sample collection, and open the possibility of using yet-to-be discovered technologies or methods from which to derive new information (Cary and Fierer 2014). Tools to archive streaming data from sensor networks and time-series data from repeat sampling represent another area that requires further thought and cyberinfrastructure investments. Time-series data (i.e., from sensors or samples) are constantly evolving, either with new data additions or with data processing, thus requiring storage and versioning models different from the ones supported in current repositories and digital library options [e.g., digital object identifiers (DOIs)]. In the "big data" realm, large sensor networks will produce massive volumes of data in various forms, from raw to processed, that have undergone quality assurance and quality control (QA/QC). Consequently, alternative storage architectures (e.g., edge- or fog-computing or data compression) will be needed to enable efficient data retrieval.

Much more work remains to make data compliant with the last two principles, interoperable and reusable. Community-accepted standards for data and metadata need to be identified, developed, and adopted to enable data exchange and reuse, including metadata reporting templates that describe aspects of sampling such as sensor and acquisition system models, sensor location and placement, calibration procedures, sample collection metadata, reporting units, time zone, owner, and use restrictions. Many of these metadata are typically missing but are necessary for data interpretation or integration. Examples of metadata templates in use by the DOE Environmental System Science community include BADM (Biological, Ancillary, Disturbance, and Metadata) for flux measurements (ameriflux.lbl.gov/data/badm-data-templates/) and FRAMES for ecohydrological observations (Christianson et al. 2017). Furthermore, if the research community adopted standards to produce machine-readable files in common formats, the repositories could then build capabilities for advanced searches, subsampling, visualizations, and analytical tools with data extracted from the files using parsers. Efforts to research existing standards and define community data standards for DOE's Subsurface Biogeochemical Research and Terrestrial Ecosystem Science programs are under way through ESS-DIVE. These efforts are important, because several existing standards for environmental data (e.g., Open Geospatial Consortium and International Organization for Standardization spatial standards and EPA's Water Quality Exchange) have not been broadly adopted by the scientific research community.

Also needed are queryable databases and tools to store and integrate heterogeneous data types. The diversity and multiscale nature of watershed data pose considerable challenges for data synthesis and typically require elaborate efforts to harmonize data across sources from individual resources. Current solutions to automate and simplify data integration across providers are focused largely on time-series data. These providers include the Consortium of Universities for the

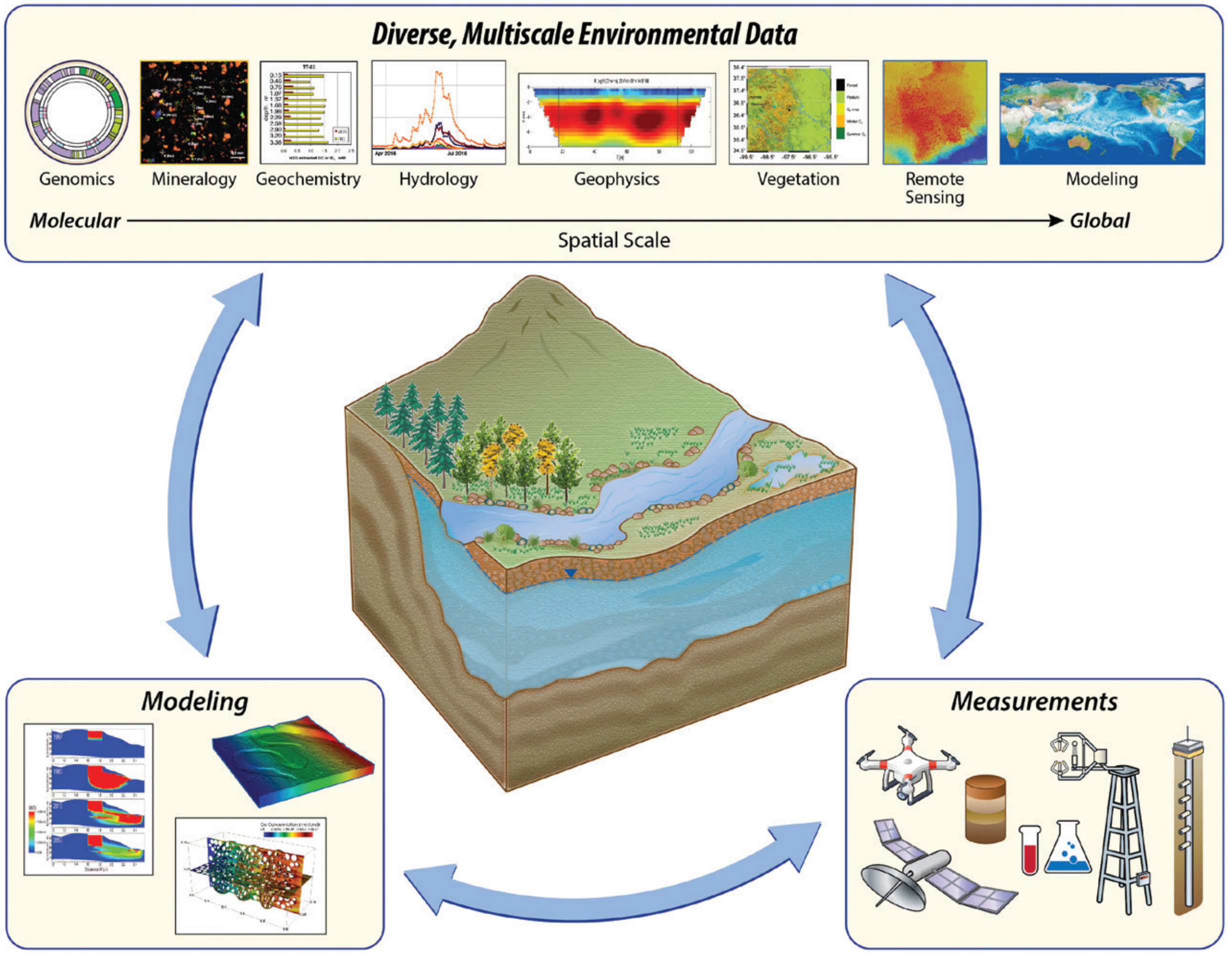


Fig. 4.1. Watershed Science: Generating Diverse Data from Multidisciplinary Earth Sciences. Data sources, including hydrology, ecology, climate, geology, geophysics, geochemistry, and microbiology, produce data in different formats and structures (e.g., time-series, gridded, and imagery data). An iterative model-experimentation approach requires not only the use of data in models, but also the ability to use model output and other datasets to inform measurements. [Lawrence Berkeley National Laboratory, from Varadharajan, C., et al. 2019. "Launching an Accessible Archive of Environmental Data," *Eos* **100**. DOI:10.1029/2019eo111263.]

Advancement of Hydrologic Science, Inc.'s (CUAHSI) Hydrologic Information System (HIS), which maintains a metadata catalog of about 100 data providers and from which data can be retrieved via web services. HIS contains a mixture of data hosted by CUAHSI and others, whereby CUAHSI regularly harvests information for the metadata catalog from the data providers to ensure that the catalog is kept up to date. Although there is an effort to use the Observations Data Model 2 (Horsburgh et al. 2016), not all data within HIS conform to this data model. Nonetheless, HIS is an important tool that can be combined with other brokering solutions that collectively unify data into an integrated view, such as the BASIN-3D software used to synthesize data for the East River (Hubbard et al. 2018). In the future, tools will be needed to integrate additional data types such as remote sensing, genomics, and model output.

Technologies for QA/QC and preprocessing of data are urgently needed. QA/QC involves the detection and correction of suspicious or bad data such as gaps, spikes, drift, level shifts, and outliers. Most QA/QC methods are time consuming and semiautomated, requiring expert evaluation and subjective decisions. Automated methods for detecting issues, such as machine learning for anomaly detection, can save significant resources and improve detection accuracy. In addition, coordination of data-quality efforts among agencies, particularly to specify uniform definitions of the extent to which data QA/QC has been performed (e.g., raw, provisional, and approved status), will provide clarity to users regarding data quality.

The integration of data with models also presents unique challenges, particularly when observations and measurements vary in resolution and spatial scale. Preparation of datasets for use in modeling is onerous and burdensome. Besides being derived from multiple sources for model parameterization or training, data for input into models typically need to be checked for quality and have gaps filled before they can be fed into the model. In many cases, the variables need to be translated into formats that can be read by the model. Data may need to be up- or downscaled, leading to errors or uncertainties in model predictions. Urgently needed are data-to-model pipelines that acquire and integrate diverse, multiscale datasets (e.g., meteorological data for climate drivers, geophysical and subsurface characterization for model parameterization, discharge- and groundwater-level data for model initialization, and water quality data for validation) into models.

4.2 Model Development and Analysis

Achieving major leaps in understanding and predictability of watershed response requires integrated observational and modeling frameworks that combine "bottom-up" and "top-down" approaches to assess models, observations, and uncertainties. These frameworks should be iterative in nature, allowing for the design of observational networks aimed at the *formulation* and *testing* of model conceptualizations and the implementation of models aimed at the *assessment* and *refinement* of observational networks and prediction. This iterative approach is critical for gaining deeper mechanistic understanding and enhancing capacity to overcome the limits of predictability for new baselines and impacts of episodic disturbances.

From the bottom-up perspective, multiscale observations play a critical role. For example, at the "bottom," detailed local observations (i.e., smaller than the size of the modeling grid resolution) and first principles are used to propose model conceptualizations for predictions at the watershed scale. Then, these predictions can be tested by their ability to reproduce integrated metrics (e.g., concentration-discharge relationships at the watershed outlet) and the emergence of complex behavior (e.g., soil moisture patchiness or power-law scaling) captured by synoptic networks of small-scale sensors (e.g., discharge gauging stations) and large-scale observations (e.g., soil moisture estimates from remote sensing). These are strong tests for model structure that require a targeted, multiscale observational effort. From the top-down perspective, the use of large-scale patterns, obtained from observations or models at the "top," becomes a fundamental guide to propose locations for targeted experimental and numerical efforts. Finally, and critical to this integrated observational and modeling framework, is the need to understand observational uncertainty and how it propagates through models and into predictions.

Reactive watershed models currently have a wide range of complexity and capability, existing on a spectrum from process-based models to empirically based representations of underlying physics. When calibrating model output to past observations, particularly using complex models with many degrees of freedom, parameter equifinality, where various parameter combinations yield the same simulated result, is often encountered. This means that getting the "right" answer for the "wrong" underlying reasons is quite common when matching field data with model simulations. In these situations of falsely calibrated models, watershed response to change cannot be reasonably predicted. To better avoid equifinality and achieve true model calibrations, a diverse array of model-relevant data streams is needed, including traditional synoptic-type measurements that are coordinated and better distributed in space and time and emerging multiscale remote-sensing techniques.

Data-driven approaches present a complementary approach that uses the vast amounts of available data for pattern classification, feature extraction, and prediction. Advances in artificial intelligence (AI) and particularly deep learning over the past decade are spurring new research paradigms in the Earth sciences (Bergen et al. 2019; Reichstein et al. 2019). Several challenges and opportunities for large-scale use of AI and machine learning (AI/ML) in watershed science include the (1) availability of training data, particularly for predicting outcomes under conditions that have never been observed previously; (2) appropriate model choice from a variety of options and development of new algorithms; (3) hyperparameter optimization to improve model performance and reduce prediction uncertainties; (4) incorporation of physics into model training to create hybrid models (also known as physics-informed ML); and (5) development of appropriate compute and high-performance computing architectures (e.g., central processing unit or graphics processing unit) for compute-intensive processes. Coordination of efforts among Earth scientists, computer scientists, and industry is needed to make more progress in this area.

4.3 Sensing Technologies: Structure, Function, and Evolution

Open and distributed watershed science requires access to high-quality data that is derived across a broad suite of watershed systems. These data cross-cut multiple categories and include the following nonexhaustive list.

Examples of Data Categories

- Remotely sensed
  - Optical
  - Multispectral
  - Hyperspectral
- Thermal
- Electromagnetic
- Microwave
- Gravity
- Stream-gauging and groundwater hydrology
- Weather
  - Basic "point" weather station
  - High-end atmospheric, including gas composition, temperature gradient, and flux tower
- Belowground temperature, mineralogy, structure, moisture, electrical properties, and organic matter content
- Geophysical surveys such as seismic, electrical resistivity, and ground-penetrating radar
- Organic and inorganic aqueous chemistry (e.g., metabolomics) of groundwater and surface water
- Potential and expressed microbial metabolisms associated with soils and sediments, plants, and groundwater and surface water
- Above- and belowground plant functional traits
- Snowpack dynamics

Applying these data to projects requires a variable amount of effort. Some data are publicly available, including many remotely sensed data products and stream gauges maintained by USGS. In other cases, individual projects must manage their own data collection, infrastructure, and curation. Many of these project-related, data-collection efforts require long-term *in situ* sensors that can provide continuous data. However, not all data types are currently amenable to *in situ* sensing. New sensors are needed to monitor important features of watershed systems that cannot currently be monitored *in situ* (e.g., microbial communities). In addition, a significant gap remains between the ability to characterize aboveground systems through remote sensing and the ability to characterize belowground systems. Belowground physical, chemical, and biological properties have major influences over watershed structure, function, and evolution. Although aboveground and belowground watershed properties and processes have co-evolved to some extent, developing a capability for evaluating the extent of this co-evolution and using it to predict hard-to-observe subsurface properties is a promising path forward (e.g., Falco et al. 2019). This highlights a critical need to develop sensing methods that can provide high-resolution characterization (e.g., decimeter scale) of subsurface properties across broad spatial domains (e.g., whole watersheds). Current sensing efforts are, nonetheless, powerful and are broadly used to monitor at both the reaction scale (i.e., points and profiles) and the watershed or basin scale (e.g., in networks). Appropriate use of these technologies alongside remotely sensed data can help scientists to explore the impacts of scale on the key physical and biogeochemical processes that control near-surface environmental change.

In situ sensors present both financial and data-standardization challenges. First, installing and maintaining these sensors require both direct (purchase) costs for the sensor—as well as the data logger, power system, and any telemetry—and indirect (staff time, travel, and training) expenses. This total-lifecycle cost of sensor ownership is not considered as often as the price of the sensor, but it is the variable to optimize when funding ICON-FAIR monitoring networks. Second, effective data integration requires standardization of a suite of well-characterized and comparable sensors to ensure that spatial variability in measurements is rooted in environmental differences rather than sensor properties. Analogous to the broad range of available numerical models is that there will always be different sensors that measure similar parameters (i.e., either sensors from different vendors or sensors from the same vendor but with improved performance). Scientists must be able to relate data from different sensors by characterizing and calibrating their responses, just as they need to be able to compare models.

The need to reduce the total cost of ownership and improve measurement standards is driving the development of novel, cost-effective, and scalable instrumentation solutions as part of the open watershed science by design vision—a so-called "sensing grand challenge." There is a fundamental appeal to address this challenge through an open-source *hardware* approach that would parallel open-source *software* approaches. However, despite the ready comparison with open-source software, it should be recognized that (1) many more open-source software projects succeed and thrive within academic environments than open-source hardware projects and (2) there are fundamental differences between hardware and software.

Computer code can be developed in parallel by multiple groups with minimal cost; testing and development cycles are very rapid (e.g., installing and testing PFLOTRAN takes about an hour), and the associated coding skills are present in multiple groups. On the other hand, while basic hardware breadboard prototyping using, for example, Arduino or Raspberry Pi with low-cost sensors is cheap, easy, and rapid, and within the skillset of most geoscientists, moving from such prototypes to a field-robust, stable, and scalable Internet of Things sensor package is challenging and time consuming. This limitation is due to the development cycles (e.g., delivery times of prototype printed circuit boards are typically 1 to 2 weeks), skillsets, and resources available in geoscience research groups, as well as the challenges associated with coordinating open-source hardware. These challenges are demonstrated by two examples of successful open-source data loggers, including the Mayfly (github.com/EnviroDIY/EnviroDIY_Mayfly_Logger/) and ALog (github.com/NorthernWidget/ALog/). The loggers took 4 to 8 years to mature during the slow and iterative process of single-group small-scale design, testing, and development. A final difference between open-source hardware and open-source software is that open-source software is free to the end user. Although the design of open-source hardware is free, the actual hardware will not be and will still require mass production, distribution, and support. Notwithstanding these differences, there is substantial value in community-developed, open-source, and transparent sensing solutions.

This sensing grand challenge could be addressed by coordinating community-driven, open-source sensor development solutions, spreading labor and effort while ensuring co-development of a standardized approach. Hardware development efforts should be purposefully designed to ascribe to ICON-FAIR principles in ways that are analogous to "by design" ICON-FAIR research programs. Such efforts will ideally bring together national laboratories, academic researchers, and commercial entities, with the latter being structured to mass produce, sell, and support these sensors. Multi-institution ICON-FAIR hardware development would ensure community acceptance and allow multiple parties to review the designs while reducing costs and replacing some of the current "black-box" commercial sensing systems with those whose measurement characteristics and errors can be systematically traced through the sensors and circuitry. This process could enable distributed sensing efforts similar to the AmeriFlux Network, but with a focus on watershed processes and with a much greater number of sensors for more spatially intensive monitoring. For example, highly scalable thermal methods for monitoring hydrological exchange within groundwater–surface water mixing zones could be used to develop a multiwatershed "hydrological flux" network with standardized hardware, software, calibrations, and data format as well as centralized real-time data hosting. Direct outcomes of such efforts will be data that are more robust, transparent, and interoperable and hardware systems that are more scalable to enable monitoring of a broader range of watershed systems. Indirect outcomes will include significant acceleration toward data, knowledge, and models that are transferable across watershed systems to enable enhanced predictive capacity.

A final point to consider is the value of new discoveries and retrospective analyses. Once key variables have been identified, sensor platforms provide a new dimension of understanding through increased spatiotemporal observations. However, watershed understanding is in continuous evolution, meaning new discoveries and changing paradigms. Thought should be given to augmenting sensing networks with automated sampling networks and community environmental sample archives for water, sediments, and soils. Sample repositories are notoriously costly to maintain and represent a long-term commitment for the organization or agency that commits to the task. While a centralized watershed sample archive—potentially enabled through user facilities—represents the ideal, an interim step that embraces community interactions and collaborative goals is the use of a common sample registration system [e.g., International GeoSample Number (IGSN), www.geosamples.org]. Systems like IGSN allow global access to a registry of sample information. Combining this registration approach with community-accepted approaches for sample collection, preservation, and sharing would significantly improve the potential for both retrospective analyses and new collaborative discoveries.

Chapter 5. Conclusions and Path Forward

The vision of open watershed science by design will transform watershed system science through the purposeful development and implementation of research programs based on ICON attributes and FAIR principles. Despite technical and cultural challenges, the watershed science community is poised to turn this vision into reality.

As far as the technical challenges, many of the necessary elements exist but are not yet coupled. Focused effort is needed to link current BER capabilities such as the Environmental Molecular Sciences Laboratory, Joint Genome Institute, Systems Biology Knowledgebase, ESS-DIVE, and National Microbiome Data Collaborative. Further coupling an integrated set of BER capabilities with investments from other agencies such as NSF, USGS, and NASA is also essential so that the community can do together what would be impossible to do alone.

In some ways, tackling the cultural challenges may be more difficult than the technical challenges. Throughout the scientific enterprise, there is a deep history of single-investigator research, as well as a need to protect the identity and contributions of individual investigators. This mindset is directly linked to the mechanisms used by institutions and funding agencies to evaluate individual researcher contributions. On the surface, this history and these needs would seem to run counter to the vision of open watershed science, but creative solutions will allow open community science and individual research programs to coexist and elevate each other. Many of these solutions are discussed throughout this workshop report (e.g., networked research purposefully designed to be mutually beneficial), and new creative solutions are constantly developing. Some solutions are grassroots and come from the community (e.g., ICON-FAIR principles), while others are top down (e.g., funding agency requirements to make data FAIR). Sustained support tailored to both small, individualistic and larger, coordinated teams to engage in ICON-FAIR watershed science is essential for overcoming challenges associated with technical, cultural, and governance considerations. The watershed science community can also learn from solutions pushed forward in other scientific domains, such as advanced governance schemes developed within the atmospheric sciences. In all cases, strong leadership is required, as well as a willingness to experiment with and iterate on potential solutions using design-based thinking and approaches.

No single investigator or funding agency can realize the vision of open watershed science by design. To succeed, all entities involved in watershed system science will need to embrace the vision's core elements: purposeful design of ICON-FAIR research and development to generate data, knowledge, and models that are transferable across watershed systems. This approach is not meant to replace single-investigator or single-site research but rather to complement it. Also imperative is that the identity and contributions of individual researchers are maintained as open watershed science is expanded. Through careful design, open watershed science can elevate individual researchers by enabling them to better leverage existing and future resources. Moreover, open watershed science cannot exist without a large number of individual researchers actively studying watershed systems that span a broad range of physical, chemical, and biological conditions. In ecological terms, open watershed science is an "obligate mutualist" with individual, localized research efforts. Optimizing this mutualistic relationship is fundamental to realizing the open watershed science by design vision and will transform the ability to predict the impacts of disturbance on watershed structure, function, and evolution with myriad direct and indirect benefits to society and the scientific enterprise.

Appendix 1. Workshop Agenda

Leveraging Distributed Research Networks to Understand Watershed Systems

U.S. Department of Energy
Office of Biological and Environmental Research

January 28–30, 2019
Bethesda North Marriott Hotel, Rockville, Maryland

Sunday, January 27

8:00 a.m. – 10:00 p.m.	*Mixer* (Bethesda North Marriott Hotel Bar)

Monday, January 28: Linden Oak Conference Room

7:30 a.m. – 8:30 a.m.	*Continental breakfast*
8:30 a.m. – 8:35 a.m.	Welcome (Jessica Moerman, U.S. Department of Energy)
8:35 a.m. – 9:05 a.m.	Overview of agenda, vision, goals, and outcomes (James Stegen, Workshop Co-Chair, Pacific Northwest National Laboratory)
9:05 a.m. – 9:15 a.m.	Participants write "I like, I wish, I hope" statements related to workshop vision and one sentence on what "open science" is. (Share with partner; post to big board during break)
9:15 a.m. – 9:30 a.m.	Open science overview (Carly Robinson, U.S. Department of Energy)
9:30 a.m. – 9:55 a.m.	Preworkshop feedback presentations (5 minutes each) • Key functions to predict, governing processes, and scales of understanding (Eoin Brodie, Workshop Co-Chair, Lawrence Berkeley National Laboratory) • Measurements (Audrey Sawyer, The Ohio State University, with Marty Briggs, U.S. Geological Survey) • Computation (Jesus Gomez-Velez, Vanderbilt University) • Cyberinfrastructure (Kelly Wrighton, Workshop Co-Chair, Colorado State University) • Data standards (Charu Varadharajan, Lawrence Berkeley National Laboratory)
9:55 a.m. – 10:05 a.m.	Group discussion on preworkshop outcomes (Panel style; Jessica Moerman, record in Google Doc file)
10:05 a.m. – 10:20 a.m.	*Break* (Post "I like, I wish, I hope" and open science sentences to big board; mingle, discuss, and/or draw a picture; <u>NO email</u>)
10:20 a.m. – 10:25 a.m.	Take 5 minutes to plan a birthday party using "yes, BUT" versus "yes, AND" (Kate Maher, Stanford University, and David Moulton, Los Alamos National Laboratory)
10:25 a.m. – 10:40 a.m.	Provocative ideas for national-scale distributed research (Eve Hinckley, University of Colorado; Audrey Sawyer; and Ethan Coon, Oak Ridge National Laboratory; 5 minutes each)
10:40 a.m. – 10:50 a.m.	Group "yes, AND" discussion exploring synergies among the three provocative ideas (Everyone; Jessica Moerman, record in Google Doc file)
10:50 a.m. – 11:15 a.m.	Exchange of big ideas around national-scale distributed research in a "yes, AND" exercise using the Solo, Share, Synergy (S^3) approach (3-minute description of S^3 by Kate Maher; 20 minutes to do S^3). Capture ideas on paper, capture the synergy between ideas with a drawing, and write a headline.

	Post to big board. (Everyone, partnered with neighbor)
11:15 a.m. – 11:30 a.m.	Describe how breakout will work, including its goals, and organize people into groups (Participants align breakout theme to their expertise; James Stegen)
11:30 a.m. – 1:30 p.m.	Working Lunch and Breakouts: Three concurrent groups, each focused on challenges and opportunities in measurements, cyberinfrastructure and standards, or computation (Audrey Sawyer and James Stegen: measurement; Kelly Wrighton and Charu Varadharajan: cyberinfrastructure; and Eoin Brodie and Jesus Gomez-Velez: computation)
1:30 p.m. – 2:00 p.m.	Report outs from breakouts and associated discussion (One lead from each)
2:00 p.m. – 2:15 p.m.	*Break* (Explore the big board, mingle, discuss, and/or draw a picture; NO email)
2:15 p.m. – 2:30 p.m.	Describe how breakout will work, including its goals, and organize people into groups (Mix people from across first breakout; James Stegen)
2:30 p.m. – 4:30 p.m.	Breakouts: Three concurrent groups, each focused on challenges and opportunities in linking measurements, cyberinfrastructure and standards, and computation (Audrey Sawyer and Eoin Brodie, Kelly Wrighton and James Stegen, and Charu Varadharajan and Jesus Gomez-Velez)
4:30 p.m. – 5:00 p.m.	Report outs from breakouts and associated discussion (One lead from each)
5:00 p.m. – 6:00 p.m.	*Break*
6:00 p.m.	*Dinner* (On your own in groups of four to five)

Tuesday, January 29: Linden Oak Conference Room

7:30 a.m. – 8:30 a.m.	*Continental breakfast*
8:30 a.m. – 8:50 a.m.	Overview of agenda, including Day One outcomes, themes, and major ideas (James Stegen)
8:50 a.m. – 9:10 a.m.	Hot Topics: Open to all who want to speak for 2 minutes on any topic, especially on ideas that emerged during informal evening discussions. (Use one slide or no slides; self-identify; Jessica Moerman, record in Google Doc file)
9:10 a.m. – 9:25 a.m.	Vision for how to use models to guide the design (spatial and temporal layout) of field sensor or sampling programs (Eoin Brodie; Praveen Kumar, University of Illinois at Urbana-Champaign; and Maoyi Huang, Pacific Northwest National Laboratory; 5 minutes each)
9:25 a.m. – 9:35 a.m.	Group "yes, AND" discussion, exploring synergies among the three visions (Everyone; Jessica Moerman, record in Google Doc file)
9:35 a.m. – 9:55 a.m.	Exchange of big, wild ideas around model-guided data collection in a "yes, AND" exercise, using the S^3 approach. Capture ideas on paper, capture the synergy between ideas with a drawing, and write a headline. Post to big board. (Everyone, partnered with neighbor).
9:55 a.m. – 10:10 a.m.	*Break* (Explore the big board, mingle, discuss, and/or draw a picture; NO email)
10:10 a.m. – 10:55 a.m.	Vision and opportunities for connecting (5 minutes each) • National Ecological Observatory Network (NEON) to coordinated open watershed networks (Bill McDowell, University of Vermont) • Long-Term Ecological Research Network (LTER) and Critical Zone Observatories (CZOs) to coordinated open watershed networks (Bill McDowell) • U.S. Geological Survey (USGS) to coordinated open watershed networks (James Stegen via Marty Briggs) • Consortium of Universities for the Advancement of Hydrologic Science, Inc. (CUASHI) to coordinated open watershed networks (Jesus Gomez-Velez) • Interoperable Design of Extreme-scale Application Software (IDEAS) to coordinated open watershed networks (David Moulton)
10:55 a.m. – 11:05 a.m.	Group "yes, AND" discussion, exploring ways to link existing infrastructure to national-scale distributed watershed science programs (Everyone; Jessica Moerman, record to Google Doc file)

11:05 a.m. – 11:25 a.m.	Exchange of big ideas around infrastructure synergy in a "yes, AND" exercise, using the S^3 approach. Capture ideas on paper, capture the synergy between ideas with a drawing, and write a headline. Post to big board (Everyone, partnered with neighbor)
11:25 a.m. – 11:40 a.m.	Describe how breakout will work, including its goals, and organize people into groups (Mix people again; James Stegen)
11:40 a.m. – 1:40 p.m.	Working lunch and breakouts: Three concurrent groups, each focused on challenges and opportunities in model-guided field deployments, leveraging existing infrastructure, or connecting efforts across agencies (Kelly Wrighton and Eoin Brodie, Charu Varadharajan and James Stegen, and Audrey Sawyer and Jesus Gomez-Velez)
1:40 p.m. – 2:00 p.m.	Report outs from breakouts (One lead from each)
2:00 p.m. – 2:15 p.m.	*Break* (Explore the big board, mingle, discuss, and/or draw a picture; NO email)
2:15 p.m. – 2:30 p.m.	Vision for changing science culture and incentive schemes toward broader adoption of open science (David Mellor, Center for Open Science)
2:30 p.m. – 2:45 p.m.	Describe how breakout will work, including its goals, and organize people into groups (Mix people again; James Stegen)
2:45 p.m. – 4:45 p.m.	Breakouts: Three concurrent groups, each focused on challenges and opportunities in changing science culture and incentive schemes toward broader adoption of open science (Carly Robinson and Kelly Wrighton, David Mellor and Audrey Sawyer, and James Stegen and Charu Varadharajan)
4:45 p.m. – 5:15 p.m.	Report outs from breakouts (One lead from each)
5:15 p.m. – 5:45 p.m.	Closing remarks and next steps (James Stegen)
5:45 p.m. – 6:45 p.m.	*Break*
7:00 p.m.	*Dinner* (Seasons 52)

Wednesday, January 30: Linden Oak Conference Room

7:30 a.m. – 8:30 a.m.	*Continental breakfast*
8:30 a.m. – 12:00 p.m.	Writing team reviews material generated before and during the workshop, uses it to update the report storyboard, identifies key graphics needs, and assigns writing tasks (Lead: James Stegen, Workshop Team)

Appendix 2. Workshop Participants

Workshop Leadership

Program Managers

Paul Bayer
U.S. Department of Energy

David Lesmes
U.S. Department of Energy (formerly)

Co-Chairs

James Stegen
Pacific Northwest National Laboratory

Eoin Brodie
Lawrence Berkeley National Laboratory

Kelly Wrighton
Colorado State University

Leadership Team

Martin Briggs
U.S. Geological Survey

Jesus Gomez-Velez
Vanderbilt University

Charuleka Varadharajan
Lawrence Berkeley National Laboratory

American Association for the Advancement of Science (AAAS) Science and Technology Policy Fellows

Sujata Emani
U.S. Department of Energy

Jessica Moerman
U.S. Department of Energy

Participants

***Denise Akob**
U.S. Geological Survey

George Allen
Texas A&M University

***Martha Anderson**
U.S. Department of Agriculture

***Holly Barnard**
National Science Foundation

Enriqueta Barrera
National Science Foundation

***Nate Booth**
U.S. Geological Survey

Kristin Boye
SLAC National Accelerator Laboratory

Scott Brooks
Oak Ridge National Laboratory

Dana Chadwick
Stanford University

Nathan Chaney
Duke University

Ethan Coon
Oak Ridge National Laboratory

Kjiersten Fagnan
Lawrence Berkeley National Laboratory

Dave Gochis
National Center for Atmospheric Research

Emily Graham
Pacific Northwest National Laboratory

Scott Hamshaw
University of Vermont

***Jud Harvey**
U.S. Geological Survey

Chris Henry
Argonne National Laboratory

Eve Hinckley
University of Colorado

Kirsten Hofmockel
Pacific Northwest National Laboratory

Maoyi Huang
Pacific Northwest National Laboratory

* Invited but unable to attend due to the government shutdown.

***Joe Hughes**
U.S. Geological Survey

Dan Kaplan
Savannah River National Laboratory

***Julie Kiang**
U.S. Geological Survey

Praveen Kumar
University of Illinois at Urbana-Champaign

Kate Maher
Stanford University

Bill McDowell
University of Vermont

David Mellor
Center for Open Science

David Moulton
Los Alamos National Laboratory

Don Nuzzio
Analytical Instrument Systems

Cynthia Parr
U.S. Department of Agriculture

***Brian Pellerin**
U.S. Geological Survey

Pete Raymond
Yale University

***J. T. Reager**
National Aeronautics and Space Administration
Jet Propulsion Laboratory

Carly Robinson
U.S. Department of Energy

Audrey Sawyer
The Ohio State University

***Denice Shaw**
U.S. Environmental Protection Agency

Katie Skalak
U.S. Geological Survey

***Craig Snyder**
U.S. Geological Survey

Hyun-Seob Song
Pacific Northwest National Laboratory

***Ted Stets**
U.S. Geological Survey

Roelof Versteeg
Subsurface Insights

Andy Wickert
University of Minnesota

Mike Wilkins
Colorado State University

Ken Williams
Lawrence Berkeley National Laboratory

Yuxin Wu
Lawrence Berkeley National Laboratory

Dantong Yu
New Jersey Institute of Technology
Brookhaven National Laboratory

Jay Zarnetske
Michigan State University

* Invited but unable to attend due to the government shutdown.

Appendix 3. Running an Innovative Workshop

The Leveraging Distributed Research Networks to Understand Watershed Systems workshop, organized by the Subsurface Biogeochemical Research program (SBR), was undertaken in response to the watershed science community recognizing a need for research programs that are purposefully designed—from their inception—to be distributed (e.g., multiwatershed), coordinated with the community, and open. This approach builds from the current structure of the SBR program and is critical for addressing major challenges articulated in the 2017 Biological and Environmental Research Advisory Committee (BERAC) grand challenges report (BERAC 2017) and the 2018 Climate and Environmental Sciences Division (CESD) strategic plan (U.S. DOE 2018). The vision of "open watershed science by design" that has emerged from the workshop activities aligns with needs identified in these reports for integrative research to connect environmental microbes, multiomics, plant system dynamics, biogeochemical interactions, and hydrological processes to understand and predict ecosystem and watershed function. The key scientific target of the U.S. Department of Energy (DOE) Office of Biological and Environmental Research (BER) is developing connections across scales of space, time, and biological complexity to enhance understanding of and the capacity to predict nonlinear changes to the Earth system and local ecosystems in response to disturbances (e.g, extreme weather).

In the Earth system, watersheds are the fundamental organizing unit that mediates the hydro-biogeochemical functioning of terrestrial environments. Mechanistic models informed by field and laboratory research synthesize knowledge of the processes governing watershed structure, function, and evolution. Governing processes span physical, chemical, and biological domains, and a key challenge is developing transferable understanding, data, and models that integrate across these process domains throughout the watershed continuum. Transferability can be achieved by using standardized methods to purposefully study a broad range of watershed systems that differ along major physical (e.g., hydrology), chemical (e.g., nutrient inputs), and biological (e.g., vegetation) axes. This method is analogous to an approach often taken in macroecology, in which patterns are studied across very large spatial domains to reveal fundamental organizing principles that cannot be elucidated by studying individual systems or sites (Brown 1995). The need for transferability motivated the organizers to focus the workshop on challenges and opportunities associated with the purposeful development of distributed (e.g., multiwatershed) research programs that use integrated, coordinated, open, and networked (ICON)–findable, accessible, interoperable, and reusable (FAIR) principles to advance watershed system science.

The long-term goal is to develop a scientific approach based on ICON-FAIR principles that will develop into a network of networks focused on watershed hydro-biogeochemistry to do together what would be impossible to do alone. To identify challenges and solutions associated with ICON-FAIR distributed watershed science, workshop organizers brought together federally funded researchers doing science relevant to watersheds, with a focus on researchers with expertise spanning key technical domains such as cyberinfrastructure, sensor development, design thinking, machine learning, and remote sensing, as well as those with deep understanding of physical, chemical, and biological processes relevant to watershed structure, function, and evolution. In addition, the organizers included federal agency program managers funding watershed research, within and outside BER.

Attendees included program managers from the National Science Foundation (NSF), U.S. Department of Agriculture, U.S. Geological Survey (USGS), U.S. Environmental Protection Agency; researchers and investigators from Colorado State University, University of Colorado, Duke University, University of Illinois at Urbana Champaign, Michigan State University, University of Minnesota, University of North Carolina, The Ohio State University, Stanford University, Texas A&M University, Vanderbilt University, University of Vermont, and Yale University; and researchers from DOE national laboratories (Pacific Northwest National Laboratory, Lawrence Berkeley National Laboratory, Argonne National Laboratory, Savannah River National Laboratory, SLAC National Accelerator Laboratory, Oak Ridge National

Laboratory, Brookhaven National Laboratory, and Los Alamos National Laboratory).

The workshop was structured to pursue the following objectives:

- Identify specific BER CESD science challenges associated with hydro-biogeochemical uncertainties that require an integrative, distributed watershed system science approach.
- Define capability gaps and solutions for sensing; data transmission, storage, and integration; and data analytics for integrating data streams across biological, physical, and chemical domains.
- Develop implementation plans, including model-informed and practical recommendations for leveraging existing infrastructure and the optimal spatial and temporal deployment of distributed hydro-biogeochemical sensing systems and direct sampling.
- Synthesize strategies to maximize community engagement and identify tractable strategies for sustaining institutional and community support for distributed watershed system science.
- Frame an approach to simultaneously engage the use of capabilities at DOE's Joint Genome Institute, Environmental Molecular Sciences Laboratory, Systems Biology Knowledgebase, and Environmental Systems Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE) to enable an SBR-supported science strategy.
- Outline plans to tie current SBR watershed test beds into other networks such as the USGS super gauges and NSF's National Ecological Observatory Network (NEON), among others, as well as a constellation of other sites run by researchers not funded by DOE.

The workshop organizers openly engaged a broad community of watershed scientists before, during, and after the workshop. For several months leading up to the workshop, four interactive webinars were organized to expand the breadth of community members that could engage with the workshop. The webinars focused on soliciting input from the scientific community at large about current perspectives on challenges, solutions, and needs for advancing watershed system science. A theme resonating through the webinar discussions was that scientists believed that the intention of sharing data widely and the infrastructure to simplify data sharing and access were critical to developing integrated watershed data for robust model development to understand ecosystem function through distributed watershed system science. Attendees converged on the concept of open watershed science by design.

The open watershed science by design concept drove the workshop organizers to use a dynamic and creative process to engage the vibrant meshwork of scientists who explore pressing scientific questions across divergent watershed research sites. The complexity of the challenge encouraged the organizers to seek out unconventional methods that would parallel the need for unconventional ideas.

The organizers introduced design-thinking principles to creatively approach the workshop objectives. These principles required participants to listen deeply to each other to find common ground, break down assumptions, and build synergies, as well as identify insights that could be developed into innovative ideas and solutions. Throughout the workshop, attendees were encouraged to arouse their creativity in forms of drawing and writing and to engage their whole selves in the day's activities. Workshop attendees were offered colorful sticky notes, white paper, crayons, markers, and building blocks on their desks to jot down thoughts, ideas, notes, and concerns; make drawings; and expand concepts along the way (see Fig. A3.1, p. 64).

To begin the workshop, Carly Robinson, assistant director at DOE's Office of Scientific and Technical Information, introduced attendees to open science and federal public access policies concerning federally funded science. Organizers then summarized the needs shared by the research community during the preworkshop webinars. Attendees added their thoughts to the conversation in a discussion activity following the summary of the preworkshop webinars. These presentations seeded the basic information needed for attendees to contribute to subsequent discussions and activities.

Having an open mindset (i.e., the "beginner's mindset") is foundational to the design-thinking

Fig. A3.1. Creative Outlets on "Big Boards" at the Workshop. Workshop attendees tracked and shared their rapid-fire ideas through writing assignments, drawings, and other creative outlets. They shared their unfiltered ideas throughout the workshop on big boards with sticky notes. These ideas and concepts were continuously discussed and expanded in breakout sessions during the workshop.

framework. To emphasize this, workshop attendees participated in an open-mindset activity that folded into directed brainstorming on "provocative ideas for national-scale distributed research" shared in lightning rounds of presentations from researchers. Staying open to new possibilities was continuously encouraged throughout the workshop activities.

Kate Maher of Stanford University presented and demonstrated an activity from her research into group dynamics to equip researchers with ways to increase the collaboration in conversations. The activity, called Solo, Share, Synergy (S^3), incorporates the value of generating ideas individually before working and sharing with a team. The goal of S^3 is to find new possibilities through convergence or divergence of the individual ideas, ultimately seeking opportunities that may lead to a solution that exceeds the capabilities of the individual solutions. The S^3 exercise maximized participation and interaction while respecting individual contributions to the process of problem framing. Workshop breakout sessions focused on building and expanding ideas, and attendees were encouraged to think about opportunities for transformative change.

The initial breakout discussion was focused on challenges and opportunities in three themes: (1) measurements, (2) cyberinfrastructure and standards, and (3) computation. These themes were selected based on previous SBR community meetings. Organizers divided participants based on the alignment of their expertise with the three breakout themes. During the discussion, lead organizers were assigned as facilitators and notetakers. Attendees shared personal experiences relevant to the themes, which became the highlights that guided later ideation. After each breakout, lead organizers reported out the synthesized notes, which were captured via Google Docs for all to read and provide input.

The subsequent breakout discussion focused on identifying needs, challenges, and opportunities in linking measurements, cyberinfrastructure and standards, and computation. The initial breakout groups were mixed, with new groups comprising attendees of different expertise in terms of cyberinfrastructure, modeling, and measurements. Discussion topics spanned data access, storage and archiving, computational processing requirements, data cleaning and wrangling, and working with heterogeneous datasets. Following each breakout and report out from lead organizers, attendees were given time to interact, expressing ideas and concerns on sticky notes to a "big board" of unstructured ideas on open science and open watershed research and descriptions of what the future of watershed science should look like (see Fig. A3.2, p. 65).

In addition to structured breakouts, in a session after breaks called "Hot Takes," organizers opened the floor to attendees to share ideas as they emerged.

Fig. A3.2. Open Watershed Science Expressions. A panel of word clouds generated from sticky-note comments (e.g., see Fig. A3.1, p. 64) written by participants. The size of a word indicates its frequency of usage. Workshop participants were encouraged to explain what open science meant to them (**left panel**), what they want watershed science to be (**middle panel**), and what watershed science meant to them (**right panel**). The resulting word clouds are revealing and inspiring. They point to a significant interest in openly sharing data and ideas to pursue understanding of physical, chemical, and biological processes within a watershed context, and to do so together as a community.

This free-form activity allowed the attendees to share quickly and have their ideas vetted by the community. It was a rapid-feedback exercise, providing critique and sharing of techniques and emergent ideas with the goal of exchange and refinement.

Implementation was strongly emphasized in the latter part of the workshop. To transition from ideas to implementation, organizers asked representatives from various agencies' projects to share information on their sponsored research sites and networks. These projects included NEON; Long-Term Ecological Research; Critical Zone Observatories; Consortium of Universities for the Advancement of Hydrologic Science, Inc.; Interoperable Design of Extreme-scale Application Software, and Next Generation Water Observing System—all of which collectively span NSF, DOE, and USGS. Project representatives shared their vision on connecting their projects to networks for open watershed science. The participants shared their reactions and hopes for strengthening connections among these efforts to improve the transferability of data, knowledge, and models and enhance predictive capacity. Participants shared their thoughts with partners in the S^3 format discussions, followed by posting ideas on sticky notes to the big boards. The topics for the S^3 groups were to share big ideas around infrastructure synergy, followed by a breakout session focusing on challenges and opportunities in model-guided field deployments, leveraging existing infrastructure, or connecting efforts across agencies.

Finally, to begin to share strategies for maximizing community engagement and scientific culture change, organizers invited a speaker from the Center for Open Science (COS); David Mellor presented the mission and vision of open science in the scholarly community. COS conducts research, provides training services in openness, provides preregistration for research and reports, and offers policy roadmaps to help institutions make their scientific process more open. Workshop participants were able to take this fundamental information and discuss in breakout groups the challenges and opportunities in the changing science culture and the incentive schemes toward broader adoption of open science. This community-led discussion was focused on transformation of the community norms to continuously support ICON-FAIR distributed watershed science.

The entire workshop was organized with the goal of introducing an unconventional scenario to participants in which their mettle would be tested. All the participants were willing and ready to adopt a different framework and experiment with the hope for a result that would transform the possibilities for understanding watershed structure, function, and evolution through distributed watershed system science. Workshop discussions and the role of design thinking were expanded in later webinars and meetings for the Environmental System Science community and are continually being adapted for workshops organized by the community. All discussions and notes from the workshop are stored in a Google Drive Folder established for the workshop and are freely available (drive.google.com/.open?id=1eL3pPweqJ6mRiMKAUp9hJopXdGTGFuCR/).

Appendix 4. Contributed White Papers

To further encourage community members to provide their vision and feedback to workshop organizers, an open call for white papers was issued. The call included a series of guiding questions (listed below). The white papers are the authors' own work and were not influenced or modified (except for formatting and minor style changes) by the workshop organizers or writing team.

Guiding Questions

- **What aspect of watershed function do you feel is most critical to understand and predict, in particular with respect to changes in that function due to ongoing and future disturbances?**
- **Why is that function so critical to predict?**
  - » If we had improved capacity to predict this function, what would the implications be to society and stewardship of the environment?
  - » Who/what are the stakeholders, decision makers, aspects of society, etc., that would be impacted by and interested in the associated fundamental knowledge and predictive capacity?
  - » What would they do with that knowledge and the associated predictions?
- **What are the essential processes that must be understood to enable prediction of the selected aspect of watershed function?**
  - » At what spatial and temporal scales must these processes be understood?
  - » Where within watersheds must we understand these processes (e.g., within hydrologic exchange zones, hill slopes, rooting zones, surface water)?
  - » When in time must we understand these processes (e.g., during disturbance events, under steady-state conditions, within a particular season)?
- **How will mechanistic and/or data-driven models benefit from new data, concepts, and/or mechanistic understanding of the processes you described above?**
  - » Are there existing computational codes that are well suited for modeling/predicting key processes/scales you identified above, and, if so, why (e.g., do they integrate the necessary mechanisms, run at the right scales, have existing parameterizations, HPC compatible, open source)?
  - » What new model developments are required, and why? What would their essential elements be (e.g., what would they predict, what disciplines would they be built from, what scales would they run at)?
  - » What would the data-model integration strategy be (e.g., formal data assimilation methods, direct parameterization)?
  - » Would the approach provide opportunities to repeatedly iterate between data acquisition and model refinement, and if so, how would that iterative (i.e., MODEX) approach be pursued?
- **Are there opportunities to use models *a priori* to guide data generation?**
  - » How would these modeling efforts guide the type and scales of data generated and where/when those data would be generated (i.e., how would an iterative MODEX approach be implemented)?
  - » What would be the approach to doing this (e.g., which models, what spatial and temporal domains, parameter and structural sensitivity analyses)?

White Papers

1. An Initial, Preworkshop Vision for Distributed Open Watershed Science

James Stegen (Pacific Northwest National Laboratory)

This white paper summarizes the initial vision and point of departure for the U.S. Department of Energy (DOE) workshop, Leveraging Distributed Research Networks to Understand Watershed Systems. Distributed research is enabled by working with a large number of individual scientists from the broad scientific community. It is based on a well-defined and consistently implemented approach designed to resolve a specific science vision. This approach is carried out consistently by many scientists distributed across a wide range of systems (field sites or laboratories) envisioned to be supported by many organizations and agencies, not just DOE's Office of Biological and Environmental Research (BER). Bringing the data together from these distributed scientists enables synthetic understanding and elucidation of generalizable and transferable principles. Two additional elements that make this approach feasible and scientifically attractive are (a) that the required materials, protocols, and software are freely provided to individual researchers and (b) that the implementation is easy, low cost, and fast. These two elements make this approach highly scalable for implementation in many systems to enable broad understanding.

Distributed research has four primary components:

1. There is a core group or institution that engages with communities funded by BER's Subsurface Biogeochemical Research (SBR) program and Climate and Environmental Sciences Division (CESD) and also with the broader science community to develop concepts around a specific scientific vision.
2. The core group also engages with the broader community to define an approach (e.g., the measurements, models, and manipulative experiments) that will resolve or achieve the vision and that can be implemented by many individual scientists who are distributed across a large number of relevant ecosystems. Initial considerations include the recognition that, to be successful, the approach must be highly scalable (i.e., implementation within each system must be easy and low cost, requiring relatively few person hours so that implementation can occur in many systems). For the SBR program, the focal ecosystems are watersheds, river corridors, hyporheic zones, streams and rivers, and related hydro-terrestrial systems, but, for other CESD, BER Biological Systems Science Division (BSSD), and non-DOE programs, the relevant ecosystems will be different but are likely to include cropping systems, permafrost-associated landscapes, or even laboratory systems.
3. The core group provides the protocols, software, supplies, analytics, instrumentation, and other resources that are needed for individual scientists to implement the defined approach in their ecosystem (or laboratory system). The approach is designed to address the science vision that is driven by the core group and, thus, is not a free-for-all or user facility. Resulting data and associated informatics tools can, however, be used in any manner that is relevant to the science community, opening up significant flexibility and opportunities.
4. Individual scientists provide the time and people power to implement the approach, thereby distributing the workload across many researchers and accessing many different systems. Resulting data from all systems are centralized and accessible to all via ESS-DIVE. As a result, a rigorously defined approach designed to resolve a specific science vision is therefore carried out in a consistent manner across a large number of systems. This enables synthetic understanding and elucidation of generalizable and transferable principles.

This vision of distributed research is sufficiently distinct from other BER-associated scientific networks, such as AmeriFlux. Whereas AmeriFlux is focused on carbon dioxide (CO_2), water, and energy fluxes and provides impressive data management tools, in large part the necessary instrumentation (e.g., the flux tower itself) is not provided. The scientific focus—biological, physical, and chemical processes underlying watershed hydrobiogeochemistry (HBGC)—is also distinct from AmeriFlux, as is the planned approach to distributed research. In this vision of distributed research, the physical materials (as well as the cyberinfrastructure) are provided to individual researchers and the associated methods are much more nimble and scalable. These attributes will enable

(1) a much broader swath of the scientific community to become engaged and (2) a much larger variety of systems to be interrogated for enhanced cross-system, synthetic understanding. For example, while AmeriFlux currently has 110 active sites, the vision here is for at least an order of magnitude increase in the number of interrogated field systems and associated investigators. This expanded level of engagement is required for holistic understanding of integrated, watershed HBGC function across scales, including responses to perturbation.

There are non-BER scientific networks that are similar in philosophy to this vision, although none that share the same scientific focus. For example, the nutrient network (www.nutnet.umn.edu) is a grassroots collection of researchers around the world that are all imposing the same manipulative experiment in grasslands. This approach has produced a number of key insights on the linkages between diversity and ecosystem function, including a number of very high profile publications (e.g., Harpole et al. 2016). Similar to this distributed research approach, the intermittent rivers network (https://1000_intermittent_rivers_project.irstea.fr) is managed by a core group of researchers that have developed a defined vision and associated field-sampling approach. Other scientists carry out the provided protocol to generate a consistently collected set of samples that are analyzed in one laboratory. The focus of this network is on particulate organic matter accumulation in intermittent rivers, which is related to this scientific vision but is only a small sliver of what this effort aims to achieve (e.g., there are no sensor systems, real-time data, machine learning, microbiology, or numerical models). There are more examples, such as Drought-Net (https://drought-net.colostate.edu) and StreamPULSE (pulseofstreams.weebly.com), but none of them provide the necessary level of scalability and integration among biological, chemical, and physical processes to understand and robustly model watershed HBGC across scales and in response to perturbation. The vision presented here to solve environmental grand challenges, from environmental genomes to watershed systems, using a distributed research approach will therefore fill a critical gap in understanding the integrated Earth system.

Reference

Harpole, W. S., et al. 2016. "Addition of Multiple Limiting Resources Reduces Grassland Diversity." *Nature* **537**, 93–96. DOI:10.1038/nature19324.

2. Networked Understanding of Watershed Systems: The Stakeholder Dimension

F. S. Colwell (Oregon State University)

The importance of science and technology in the development of knowledge of complex coupled human and natural systems is well established (Cash et al. 2003). Knowledge development is most effective when it is accomplished across both disciplinary and institutional boundaries such that information can be effectively communicated and translated between different elements of society (Liu et al. 2007). In cases where deeper understanding of systems and knowledge development is aimed at improved decision making, it is important to include many interested parties to find solutions (Cash et al. 2006). In the context of understanding watersheds, knowledge derived across a spectrum of interested parties will be richly used and appreciated.

Many scientists who are not normally associated with national laboratories, universities, or federal agencies but are interested parties can contribute richly to watershed science. This is likely the case for all coupled human-natural systems. Stakeholder groups such as Native American tribes, landowners, watershed councils, conservation organizations, irrigation districts, nongovernmental organizations, and citizen scientists often have long histories with watersheds, as well as deep personal levels of understanding and commitment to a hydrologic system.

There are several advantages inherent to working with stakeholders dedicated to preservation and care for water resources. These groups are concerned about what happens in a watershed and have a level of insight and local knowledge that complements—and can help guide—a scientific approach to studying watersheds. Many such groups or individuals are locally situated or visit the watershed frequently, and they are poised to become partners in sample and data collection. This may be required to obtain timely evidence from sampling sites distant to the science team or as ways to ground truth data collected by sensors. Sensor networks may require some effort for placement and maintenance of nodes, and trained stakeholders can help with data collection and sensor servicing. Efforts that include citizen scientists may increase the degree to which federal research is appreciated as being beneficial to the public. Multiple two-way teaching and learning opportunities occur as disparate groups interact with a single entity (e.g., a watershed) as the focus. Consideration of watersheds that already have well-coordinated stakeholder teams where crucial issues have been identified may assist the selection of candidate watersheds to include in the networked approach.

In the context of distributed research networks to understand watershed systems, the engagement of citizen science partners will ultimately enrich the outcome of the networks as these partners will help to guide data collection and become advocates and users of the data and computational models resulting from the research. Essentially, this concept is based on the premise that by including such stakeholders the distributed research philosophy will be valued beyond the community of scientists dedicated to understanding a system. This outcome should result in an effort that reaches deeply into the communities that have an enduring dependence upon specific watersheds and a growing appreciation for how scientific data can be collected and merged with conventional knowledge to sustain the value of a watershed research network.

Strategies to encourage nontraditional scientists include: (1) inviting stakeholder groups and researchers who study watershed conflict/resolution and nontraditional forms of knowledge acquisition to attend the networked watershed project workshop; (2) developing funding opportunity announcements (FOAs) that encourage the engagement of stakeholders and ways to evaluate the effectiveness of stakeholder contributions; and (3) conducting surveys of stakeholder groups to determine the type of data and modeling that would best meet their needs with respect to open watershed science.

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3. Transcending the Tyranny of Scales and Disciplines in Watershed Monitoring

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The development of field sites has long been a blend of the field scientist's eye, the practical aspects of access and proximity to resources, and systematic simplification. These lenses are further shaped by epistemological foundations that vary across subdisciplines engaged in critical zone science. Although this approach to field measurement has greatly advanced our understanding of key processes, it tends to compound the "tyranny of scales" by isolating processes from one another, arguably a "tyranny of disciplines." The treatment of soil is a simple yet illustrative example—geochemists and pedologists have preferred to study soil profiles in quasi one-dimensional conditions. They include those that might occur on ridgetops or different geomorphic units, resulting in interpretations that inform our understanding of soil development processes but are difficult to extrapolate spatially or incorporate into modeling structures. Similarly, ecological studies, when they consider soil conditions, often extend only to shallow soil depths (10 to 30 cm), whereas we know that the influence of root and microbial activity on water and solute distributions and/or regolith stability can extend over many meters. As a result of these compounding differences, it can be difficult to even agree on where the critical zone begins and ends, let alone to build a model of it.

In a nutshell, all data and all models are biased by their intent. How do we prevent these biases from stifling knowledge production? Although a great deal of work has focused on scale in models, including the development of multiscale approaches, we do not think a similar theory has emerged for the development of field measurements to drive these models. We propose that a new methodology should be developed to transcend the tyranny of scales and disciplines inherent in current approaches to watershed sampling and monitoring. Based on our experiences using and modeling field data, we envision that the following concepts could be fruitful for a dedicated working group to consider:

- **Process control as a design principle:** Field measurements often focus on a series of state variables that describe the system, whereas models represent those state variables via the balance of interconnected fluxes. As a result, state variables can be highly nonunique. For example, a measurement of foliar phosphorous levels could be reproduced in a nutrient model through multiple combinations of growth rate, foliar resorption, and uptake rates. In turn, uptake rates depend on both the solubilization rate of litter and the supply of phosphorous from regolith, requiring additional constraints. Although fluxes are increasingly measured, they are among the most difficult to constrain and may reflect multiple functions (e.g., partitioning soil respiration between heterotrophic and autotrophic respiration). *Process control* refers to the engineering principle that is used to optimize large systems, such as factories, which may contain thousands of interconnected functions. Process controls are usually hierarchical and often consider different inputs and outputs distinct from the material balance. For example, instead of tracking carbon through the critical zone, potentially ignoring key inputs/outputs for certain functions, the variables and parameters may be defined as relevant combinations, or entirely different functions all together. This is one idea that may highlight the hidden interconnections and the variable time and spatial scales that would be independent of model structure, thus potentially avoiding issues of bias. It is not a new model structure, but a way to optimize measurements. Alternatively, actually investing in the use of models in field site design could be another approach.

- **Toolsets for scale translation:** At a very basic level, most sites are designed with attention to upscaling via nested measurement schemes or representative properties. Despite this intent, seldom are large-scale correlations and emergent patterns interrogated in designing the point-based sampling approach. There are now long-term satellite datasets available that can shed light on the spatial organization and history of vegetation coverage, phenologic change, and community shifts—insights that could provide relevant information when selecting locations for intensive sampling.

On the other hand, when designing a site with the intention to scale from point measurements of watershed characteristics to spatially explicit predictions, it is necessary to consider the relationships that would underpin these extrapolations. Remote-sensing datasets can provide spatially explicit information on surface characteristics, including topographic characteristics and surface-reflectance properties. However, many site designs do not explicitly consider how it will be possible to link ground measurements in both time and space to remote-sensing datasets. Many attempts at this type of scaling are done *post hoc* and introduce question able linkages as a result. An example of a working group product could be a set of recommendations, linked to usable toolboxes, to explore scale in designing watershed networks.

- **Team character and leadership:** Watershed study sites can end up being less than the sum of their parts because, despite our best intentions, they are often set up as a geographic unit where each discipline conducts research traditional to its field, without an eye to integration across disciplines. Increased leveraging could be accomplished by bending, adaptation, and proactive integration across disciplines, rather than the current approach that often re-enforces disciplinary paradigms. How would a field site co-designed by an ecologist, hydrologist, and geochemist look different from one designed by a team of hydrologists? How would the questions differ? If we could use the boundaries where each of these fields presses up against the other and the assumptions being made by each discipline about the others as a starting point, is it possible to design field sites to answer questions that can reconcile divergent paradigms? Embracing transdisciplinary design of field measurements may also require new techniques for leading teams that acknowledge and explore the "tyranny" of disciplines.

Ideally, innovative approaches for field measurements and model structure could arise from leveraging our biases to redefine our approaches.

4. Leveraging Distributed Research Networks to Understand Watershed Systems

John Schalles (Creighton University, Nebraska), Aaron Thompson and Christof Meile (University of Georgia)

A central research area of watershed biogeochemistry is understanding how elements are introduced to subsurface and surface water, how they are processed in those waters, and how they are exported to the ocean via coastal zone hydrologic networks. The type and magnitude of elemental input are strongly influenced by the geological and climatic settings, and they are subject to anthropogenic influence. Controls on these inputs have been studied extensively in relation to the composition of the receiving waterbodies. However, the exchange between surface and subsurface water, as well as the extent and controls on biogeochemical transformations at these interfaces (how elements are internally processed), remains poorly quantified. This lack of knowledge includes biogeochemical transformations, as well as how elements are distributed between solid and aqueous phases of different mobility (i.e., dissolved, colloids, flocs, or suspended load).

Some key knowledge gaps regarding how elements are processed within the watershed include the effects of (1) temporally varying physiochemical conditions, (2) the presence and activity of vegetation, and (3) how interactions within coupled protist-plant-fungi-prokaryote systems influence chemical form and mobility. The relevant time scales for shifting conditions vary from the event scale [e.g., flushing associated with storm-driven torrential rainfalls and (semi-)diurnal and spring-neap tidal frequencies] to the seasonal scale, which influences patterns underlying ecological food-web structures. Closing these knowledge gaps is critical because they dictate how subsurface and surface waters interact to provide elemental filters between the terrestrial and marine systems and are themselves key waterbodies (e.g., rivers, lakes, and coastal zone) whose water quality—or, more broadly, ecosystem health—is of broad societal relevance for a wide range of industries and stakeholders (e.g., nursery habitats, fisheries, tourism, and algal blooms).

Experimental/Observational Efforts

Research networks like the WHONDRS characterization program shed light into the differences between the composition of surface and subsurface waters and also capture the dynamics of their interactions. We propose that such observations be paired with (1) biogeochemically relevant sensor measurements (e.g., field spectroradiometers) that allow for automated extension of these efforts over longer time scales and at high temporal resolution; (2) experimental efforts targeting processes and linkages between elemental cycles (e.g., complementing the carbon-focused measurements of WHONDRS with studies of iron cycling, which can exert a major control on elemental mobility); and (3) efforts that expand spatial coverage, such as drone georectified and repetitive satellite imagery to allow a high spatial resolution analysis of seasonal or event-driven (e.g., tidal, storm surge, and watershed flooding) perturbations.

Modeling

Data collected through such experimental efforts can and need to be incorporated into reactive transport models. Some sensor data may be suitable for data assimilation; however, in the short term, we consider iterative model-experiment approaches that establish robust process-driven formulations of key biogeochemical processes, validated through cross-site comparisons, to be an important step.

5. Revisiting the Role of Bio- and Photodegradation on the Global Distribution and Degradation of Dissolved Organic Matter in Watersheds

Malak Tfaily (University of Arizona; Pacific Northwest National Laboratory) and Rachel Wilson (Florida State University)

Dissolved organic matter (DOM) is an important component of watershed ecosystems' energy budgets (Yamashita et al. 2011). It affects many physicochemical and biological characteristics in freshwaters and is considered an important energy and nutrient source for microbes, thereby affecting whole-ecosystem metabolism (Adrian et al. 2016). DOM comprises the sum of energy input substrates, intermediate metabolites, and remnant biounavailable compounds. Biotic reactions driven by microbial communities and abiotic reactions, driven by physical factors such as sunlight and temperature, in combination control DOM production, transformations, and degradation (e.g., Doane 2017). Both biotic and abiotic processes strongly affect (1) DOM composition; (2) the physical, chemical, and biological template upon which watersheds operate and function; and (3) the rate at which ecosystem processes progress. For example, in-stream processes acting on DOM, such as biodegradation (biotic reactions) and photodegradation (abiotic reactions), can lead to DOM loss and thus increase carbon dioxide (CO_2) emissions to the atmosphere. Interactions between biotic and abiotic processes can also occur (Zhu-Barker et al. 2015), influencing the rates of DOM decomposition and, ultimately, CO_2 production. For example, (1) intermediates of biological nitrification/denitrification can, under some wetland conditions, undergo abiotic nitrosation reactions (Miyajima 2015) and (2) extracellular enzymes, amino acids, and sugars may participate in abiotic reactions, altering nitrogen bioavailability (Ikan et al. 1992; Barrett et al. 2002) and, in some cases, directly producing CO_2 as a byproduct (Thorn and Mikita 2000). The extent to which biotic and abiotic reactions influence the bulk DOM character and composition is likely influenced by the physicochemical nature of the system. For example, low pH may facilitate some reactions in peatlands, while warmer temperatures and higher sulfate content may stimulate other abiotic reactions in coastal and tropical wetlands. Additionally, both biotic and abiotic reactions are being affected by climatic factors and other environmental perturbations (such as increased temperature and rainfall). Changes in physiochemical factors can strongly influence some organisms, altering the rates of bacterial organic matter degradation and thus biotic reactions responsible for DOM degradation. Additionally, drought can lead to oxygen intrusion into previously anaerobic environments, an event which can have a detrimental effect on the methanogenic enzymes of microorganisms (Cedervall et al. 2010). Conversely, increased availability of nitrates resulting from water pollution could support a large population of algae, causing water blooms, thus increasing biotic degradation of DOM and reducing abiotic factors (light penetration into water column).

Current global changes (e.g., climate change, land-use change, and biological invasion) are shaking up the watershed environments by the global redistributions of DOM, as well as the emergence of new mechanisms of degradation and transformation through the modification of biotic and abiotic reactions. The analysis of interacting biotic and abiotic factors in DOM degradation within a watershed's boundaries is, therefore, critical to understanding controls on the rates of DOM degradation and thus CO_2 and methane (CH_4) fluxes between wetlands and the atmosphere. Understanding the role that DOM composition and abundance plays in regulating ecosystem function and structure remains a key question in watershed ecology. If we are to understand DOM lability and release to the atmosphere, then we need a way of understanding, and predicting, the rates of turnover. Therefore, we propose that we can understand rates of DOM turnover and, ultimately, CO_2 release into the atmosphere by investigating the role of biotic and abiotic reactions on DOM degradation, the interactions between biotic and abiotic reaction pathways, and how these factors could be affected by different hydroclimatic and landscape conditions. Even though biotic and abiotic reactions are increasingly acknowledged to change DOM composition and distribution, understanding the specific mechanisms by which these reactions affect DOM abundance, composition, and distributions has been an important challenge for biogeochemists and ecologists. In particular, the relative importance of biotic and abiotic reactions in DOM transformation remains unclear. Moreover, particular biotic and abiotic reactions and their coupling are underrepresented in modeling, but, if quantified, could improve

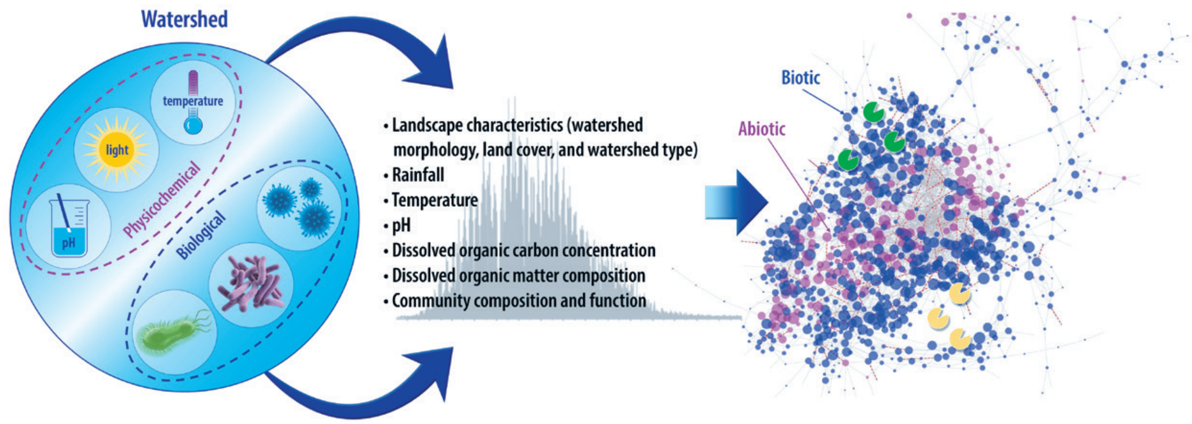

Fig. 1. Identifying "marker" transformations and reactions will require studying the coupling between the hydroclimatic, biological, and landscape conditions that influence dissolved organic matter degradation. [Tfaily Lab, University of Arizona]

model predictions. Improving our capacity to predict this function (i.e., quantify the contribution of biotic and abiotic reactions to DOM degradation and how it will be impacted by climate change) will be integral to proactively creating conservation/management plans to control future perturbations. Deciphering molecular principles and mining specific DOM molecular transformation mechanisms that govern DOM production and degradation represent one of the prerequisites to understanding how biotic and abiotic reactions shape watershed ecosystems and how these systems will be affected by future and ongoing perturbations.

Efforts to recognize the importance of both biotic and abiotic reactions in shaping DOM distributions across broad scales can be advanced by using new analytical tools that can be coupled via modeling to investigate and characterize "marker molecular transformations" that are key for each factor. These factors need to be addressed (1) in watersheds with different landscapes; (2) within hydrologic exchange zones, hillslopes, rooting zones, and surface waters because both abiotic and biotic factors could be different in these zones; and (3) during steady state, both during and after perturbations to be able to identify biomarker transformations responsible for DOM degradation by each factor. To accomplish this goal, we suggest using Fourier transform ion cyclotron resonance mass spectrometry (FTICR-MS) followed by Kendrick mass transform analysis (Kendrick 1963) to investigate molecular changes and transformation in DOM from different watershed systems. The Kendrick mass transform analysis identifies gain or loss of specific chemical moieties [e.g., methylene (CH_2), hydrogen gas (H_2), and formaldehyde (CH_2O)] via mass differences, and it will be used to infer and quantify potential microbial degradation and/or abiotic degradation pathways by which compounds were consumed/produced in these samples. In other words, we will characterize and quantify the exact reactions and transformations responsible for DOM degradation. When coupled with metagenomic analysis and hydroclimatic and landscape characteristics, and through multiple regressions and network analysis, we can then identify "marker" transformations/reactions carried out either by microbial communities (biotic reactions) or photodegradation (abiotic reactions) and how these reactions change with system perturbations and other physiochemical parameters (see Fig. 1). Because of the need to generate large datasets across many different watershed systems that include DOM composition, community composition, and other metadata (e.g., temperature, rainfall, and land morphology), some of the challenges include costs of sample processing and data analysis that could be overcome by leveraging user facilities and crowd resources. This experiment could highly benefit from existing investments in physical infrastructure [e.g., DOE Subsurface Biogeochemical Research (SBR) watershed test beds, NEON, and USGS], data archiving (e.g., ESS-DIVE and DataONE), and computational tools (e.g., KBase, CyVerse, Jupyter notebooks, and simulation codes). Datasets can be made publicly available to encourage people to analyze the data using different approaches. Datasets, for example, could be made available under ESS-DIVE where the public community could access the dataset and use it after appropriate recognition [i.e., dataset digital object identifiers (DOIs)].

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6. When and Where Are Hyporheic Zone Processes Important?

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The hyporheic zone (HZ) underlying and surrounding the stream channel is one component of transient storage in streams (other components include, for example, surface water eddies, back waters, and leaf packs). Water entering the HZ exhibits a range of travel times, giving that water characteristic residence times longer than those of the mean channel flow. In addition to the longer residence time, the HZ is characterized by higher surface area to volume ratios and different geochemical and microbiological environments than those of the surface water. Consequently, the HZ is an important location for nutrient and trace metal cycling and contaminant transformation, with important implications for water quality as supported by numerous experiments and modeling studies. Nevertheless, across multiple systems, the relationship between transient storage and nutrient cycling (e.g., uptake) is ambiguous. Some scientists report positive relationships between transient storage and nutrient cycling (Valett et al. 1996; Thomas et al. 2003; Ensign et al. 2005; Ryan et al. 2007), while others report weak or no relationship between these variables when comparing results across sites (Lautz and Siegel 2007; Bukaveckas 2007; Webster et al. 2003; Simon et al. 2005; Ensign et al. 2006). Additionally, some studies report different relationships for different nutrients (e.g., ammonium versus phosphate) within the same site (Hall et al. 2002).

One reason for the lack of agreement among studies may be the focus on identifying relationships between one or more physical characteristics [e.g., transient storage or the ratio of transient storage cross-sectional area to stream cross-sectional area (A_s/A)] and processes controlled by more complex interactions among hydrological, microbiological, and geochemical variables (Wondzell 2011; Helton et al. 2011; Zarnetski et al. 2011, 2012). In other words, previous assessments based on A_s/A were predicated on the assumption that the hydro-biogeochemistry within and between sites was either the same or the differences were inconsequential. It seems unlikely that such an assumption is valid. HZ flow and the biogeochemical gradients established in the HZ are intrinsically linked to surface-water flow (Kaufman et al. 2017; Li et al. 2017; Grant et al. 2018; Painter 2018), and the nature and implications of that linkage require further elucidation. New research efforts are needed to understand the temporal and spatial variability in the hydro-biogeochemistry of the transient storage zone and the drivers of that variability (Stegen et al. 2016, 2018; Harvey 2016). Subsequent incorporation of that understanding into a more comprehensive evaluation of unifying relationships within and among sites should yield more reliable prediction of watershed function (Ward and Packman 2019; Ward 2016).

Another contributing factor for the apparent lack of agreement may be related to the question of representativeness with respect to spatial scale, time, and location. Field experiments are typically conducted at the scale of meters to tens of meters. This leaves several questions unanswered. Do experiments at this scale yield parameter estimates that are representative of the stream (kilometers long) or watershed (greater than tens of km^2) under study? How do these parameter estimates vary with the scale of experiments? How do, or can, we best compare results among sites where experiments are conducted at different scales? Improved understanding of these and related questions will enhance our ability to scale understanding throughout a watershed and across different watersheds for better predictive capability of watershed function (Ward 2016).

The concept of "hot spots" (locations that exhibit disproportionately high reaction rates relative to surroundings) and "hot moments" (short periods of time that exhibit higher reaction rates than the longer intervening periods; McClain et al. 2003) has been around for decades. Our understanding of hot spots and hot moments continues to improve as has their representation in numerical models (Groffman et al. 2009; Wagena et al. 2017; Dwivedi et al. 2018). Nevertheless, significant challenges remain in our conceptual understanding, experiments and observations, and numerical models incorporating these phenomena in predictions of watershed function.

Site-specific hydrological and biogeochemical factors control the location and timing of hot spots and hot moments (Harvey 2016; Vidon et al. 2010). Some of these controls are well known. For example, flow transients and snow melt events generally increase solute flux from watersheds. These hydrological events can activate flow paths that are inactive during lower flow, transporting dissolved reactants to new locations and potentially relieving limiting factors (e.g., electron donor, acceptor, or nutrient limitations) that had been controlling reaction rates. For example, sulfate delivery into previously isolated anaerobic zones can accelerate methylmercury (MeHg) production. How do the intervening drier periods prime a system to develop hot spots at a later time? Desiccation of algae or macrophytes at stream margins can leave an inventory of labile organic matter that can fuel a hot spot at the stream-terrestrial interface when wetter conditions return. Fluctuating redox conditions that accompany changes in water level enhance the reactivity of manganese oxides [Mn(IV)]. Additionally, some fundamental concepts are poorly understood. For example, how large does a hot spot or an ensemble of hot spots in a river corridor or network need to be for these to be important at the watershed scale? How does the location or distribution of these hot spots affect our assessment? Are there times when hot moments are more important when considered in the context of intra-annual seasonal variability? Elucidation of the specific hydro-biogeochemical controls on hot spot and hot moment development, function, and importance in the HZ will greatly enhance watershed function predictive ability.

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7. Mixing Zones as Critical Components of Coastal Watershed Function

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"Mixing Zones" as a Watershed Function

Mixing zones are critical functional elements in watersheds for controlling the concentration, biogeochemical transformation, and release of water and, especially, solutes. A wide range of examples exist where mixing zones occur, such as in the hyporheic zone, wetlands, or between regions of vastly different physical or chemical properties (e.g., sea water intrusion in aquifers). Mixing zones also can occur at scales ranging from pores to reservoirs. Thus, given the great diversity of settings where mixing occurs, to give mixing zones meaning as a functional watershed element, we conceptualize them as interfaces across which a transition occurs (see Fig. 1); that is, they are the linkage between other functional elements within a watershed and, therefore, important nodes in defining connectivity of the overall system. Furthermore, processes may be reasonably well known and predictable on either side of the interface, but the connection between them that transfers mass and energy fluxes from one domain to another is poorly understood and makes modeling difficult and unpredictable.

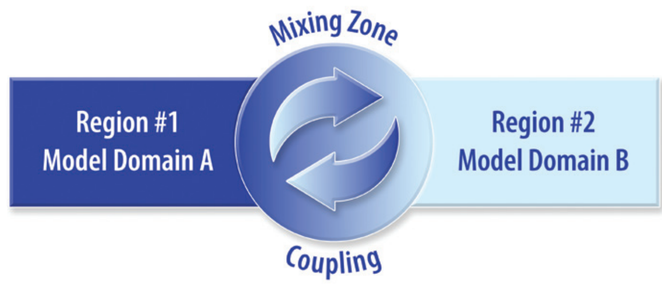

Fig. 1. Mixing zones as the coupling elements between relatively well known and predictable functional watershed components. [East Carolina University]

Mixing zones may also act as nonlinear elements or "control units" regulating mass and energy transport within a watershed. Changes in rainfall characteristics may, for example, produce differences in the functionality of the soil by shifting between slow flows through the soil matrix versus fast flows moving through macropores. Such shifts in behavior may influence runoff generation, but, perhaps more importantly, they lead to fundamental changes in the role that soils play as an interface for biogeochemical transformations at the boundary between the land surface and groundwater. As a consequence, mixing zones can provide overarching controls on mass transport in watersheds, such as the response time for carbon and nutrient cycles.

While mixing zones may be common in all watersheds, they are particularly distinct and important in coastal watersheds. Coastal watersheds are different from inland watersheds where topography is the major driver of flow systems. In contrast, bidirectional fluxes are common near the coast, driven by wind, tides, storm surge, water extraction, and other processes that shift the "typical" direction of water flow. It is, therefore, important to ensure that we investigate and understand the aspects of these watersheds that make them unique and different from the far more commonly studied inland watersheds.

Figure 2 illustrates a wide variety of areas in a coastal watershed where mixing zones between water sources are common. For example, low flows in coastal areas resulting from drought and/or high flow resulting from extreme weather events may contribute locally to the enhancement of saltwater intrusion along stream courses (Herbert et al. 2015). During recent droughts (e.g., in 2008), saltwater intrusion was documented as far inland as Greenville, N.C., along the Tar River (i.e., over 20 miles upstream from where the river discharges to the estuary). The factors influencing this inland migration of salt and the potential for transfer, storage, and release of salts from the hyporheic zone surrounding stream channels (or associated aquifers) have important implications for aquatic and riparian ecosystems. Since there is not always a consistent relationship between stream level, discharge, and salinity and there is limited monitoring of these variables in coastal regions, there is a poor understanding of flow-salinity relationships for many coastal rivers throughout North Carolina and the Southeast. Addressing this problem is, therefore, of high importance for maintaining ecosystems and the services they provide in riparian buffers, as well as for Coastal Plain utilities who need more information on the frequency, duration, and timing of saltwater intrusion to evaluate the resiliency of public water supplies.

Why Is That Function so Critical to Predict?

Coastal watersheds are facing a wide range of challenges, given the competing demands of population growth, economic productivity, and ecological diversity, especially with their high degree of vulnerability to sea level rise and extreme storm events (Bhattachan et al. 2018). Influxes of sea water and discharge of nutrients from the land create intermediate transition zones as boundaries between fresh and saline water, zones which are critical for maintaining ecological, agricultural, and water resource systems. Understanding these transition zones in different contexts (i.e., river systems, groundwater, and soils) is difficult because it requires investigation of linkages and feedbacks between processes coupling the atmosphere, soils, stream networks, groundwater, wetlands, and estuaries to each other and the ocean (see Fig. 2). While individual processes (e.g., groundwater flow or runoff generation) may be captured reasonably well with current models, we have a poor understanding of the behavior within different types of mixing zones (e.g., hyporheic zone or submarine aquifer discharge) and lack models of these interfaces that can act as linkages between coupled environmental regimes. As a result, it is difficult to predict how physical and chemical states, mass and energy fluxes, or the influence of geologic structures can be represented between domains to investigate fundamentally important processes such as salt and nutrient transition zones in coastal regions.

Populations in U.S. coastal counties have grown from approximately 47 million year-round residents in 1960 to over 87 million year-round residents in 2008 (Wilson and Fischetti 2010). This population growth has been accompanied by extensive land-use change, particularly evident in the southeastern United States (Exum et al. 2005). The southeastern United States has experienced rapid population growth since the 1950s, with a rate of population increase nearly 40% larger than that of the rest of the nation (Exum et al. 2005; O'Driscoll et al. 2010). This region accounted for more than half of the newly developed land in the contiguous United States during the period of 1982 to 2007 (USDA 2009). In the future, model simulations suggest that the extent of urbanization in the Southeast is projected to increase by 101% to 192% between 2010 and 2060 (Terando et al. 2014). These projected changes suggest that increased land-use change, water demands, and wastewater discharges will be expected for southeastern coastal communities in the future and lead to major shifts in mixing zones.

Coastal watersheds can be particularly vulnerable to water quality impacts associated with land-use change due to shallow water tables, sandy soils, dominance of groundwater inputs to streamflow, proximity to surface waters, and seasonal population fluctuations associated with coastal tourism (Lapointe et al. 2017; Humphrey Jr. et al. 2010;

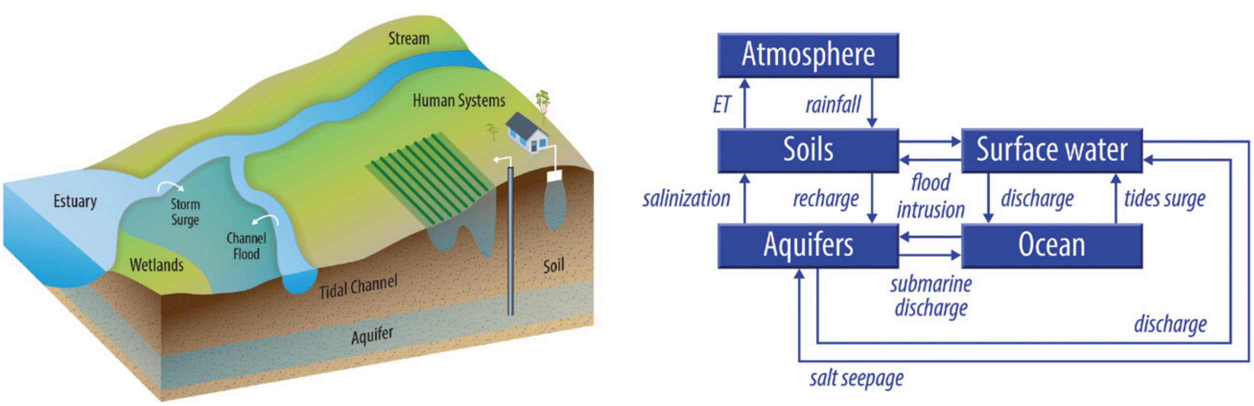

Fig. 2. Watershed Mixing Zones. (**Left**) Examples of the ubiquitous nature of mixing zones in coastal watersheds. (**Right**) Conceptual models linking different components of a watershed with different behaviors are common. Almost every arrow in the model, however, represents an opportunity for a different mixing process at the interface between domains. [East Carolina University]

Carlston 1963; Williams and Pinder III 1990). Coastal watersheds are typically located downstream of other land uses and as a result are at the receiving end of decisions made upstream, both locally and regionally. These systems are typically nutrient sensitive, and recent work has shown that the majority of U.S. estuaries assessed by the National Oceanic and Atmospheric Administration (NOAA) are impacted by nutrient enrichment, including impairments associated with elevated chlorophyll *a*, the presence of harmful algal blooms, low dissolved oxygen, fish kills, water clarity, and loss of submerged aquatic vegetation (Bricker et al. 2008). Additionally, coastal freshwater systems face threats from saltwater intrusion associated with sea level rise (Ezer and Atkinson 2015), storm surge, nuisance dry-weather flooding, and extreme tidal and wind events (Sweet et al. 2014; Michael et al. 2017). Recent work suggests that many coastal aquifers are facing a "coastal groundwater squeeze" (Michael et al. 2017), confronted with increasing contaminant inputs from the land surface and saltwater intrusion from the coast and below. Enhanced capabilities to quantify spatial and temporal variability in surface and groundwater stage, flow, and water quality to better understand the changing flow and solute behavior in dynamic coastal river and estuarine systems are needed, specifically in coastal North Carolina.

The Tar-Pamlico watershed, for example, is relatively water rich, receiving approximately 50 inches of precipitation a year. Evapotranspiration fluxes are also high, however, accounting for approximately 75% of these inputs (Sun et al. 2002), at times making availability of water for human and ecological demands an issue (Weaver 2016). Within eastern North Carolina, eight major rivers (i.e., Chowan, Pasquotank, Roanoke, Tar-Pamlico, Neuse, White Oak, Cape Fear, and Lumber) drain to the coast and discharge approximately 12 billion gallons a day. North Carolina has approximately 325 miles of ocean shoreline and 12,000 miles of estuarine shoreline. The Tar-Pamlico watershed is part of the larger Albemarle-Pamlico (A-P) Estuary System, which is the nation's second largest estuarine system containing over 3,000 square miles of open water and representing over half of the juvenile fish habitat between Maine and Florida (NC Department of Environmental Quality 2015). In 2016 the Coastal Plain, including the A-P Estuary System, was identified as the 36th global biodiversity "hot spot" (Myers et al. 2000) and one of only two hot spots located in North America. A recent study estimated the economic value of the A-P basin's natural resources at approximately \$6 to \$7 billion a year associated with select agricultural, forestry, fishery, ecosystem, and recreational benefits (Van Houtven et al. 2016).

In the contiguous United States, wetlands store ~12 petagrams of carbon (Pg C) and Coastal Plain wetlands store ~3.4 Pg C (Nahlik and Fennessy 2016). Despite federal protections, these wetland ecosystems are particularly vulnerable to human- and climate-induced environmental changes. Nutrient-limited systems are particularly sensitive to nutrient enrichment, resulting in changes to plant community composition and diversity (e.g., Harpole et al. 2016; Borer et al. 2017) and altering plant-microbe associations (Weese et al. 2015; Remigi et al. 2016). Saltwater intrusion has been shown to alter the carbon and nitrogen cycling of both natural and human-altered systems. This change includes increases in carbon dioxide (CO_2) gas fluxes from wetlands and increased nitrogen export from agricultural soils in the region (Craft et al. 2009; McLead et al. 2010; Ardon et al. 2013). Many coastal watersheds are nitrogen sensitive, and excess nitrogen can lead to eutrophication problems such as fish kills and harmful algal blooms.

From a practical perspective, understanding mixing zones will enable prediction of watershed response times, thereby aiding planners in understanding how to prepare for excess suspended sediment and nutrient runoff downstream throughout the watershed. These predictive capabilities are critical for downstream water resource utilities as well as agricultural communities. As sea level rises, lands that currently house forests, wetlands, communities, and agriculture will soon serve as the transition from terrestrial to aquatic and from fresh to brackish. As this transition zone moves, the vegetation and microbes will change due to changes in salinity and water levels. The movement of this transition zone has the potential to increase nutrient export to downstream systems. If we better understood the mixing zones, it would be possible for people with land in transition to adapt to sea level rise sustainably. It would allow policymakers to evaluate how land-use management practices might cause changes in fluxes that produce shifts in transition zones. It also would allow for better prediction of risk from future extreme events. Understanding mixing zones and their controls on downstream water quantity and quality also would help to drive more strategic approaches to the food-energy-water nexus, for example, via transitioning to less–water impactful energy-production options (e.g., growth of solar) and to promote solutions for dealing with energy risks (e.g., better assessing impacts of coal ash releases and optimizing investments to transform the most environmentally devastating hog waste lagoons in North Carolina to biogas-generation facilities).

Key processes that affect mixing zones are inward fluxes, state, and structure. As described earlier, for example, drought can cause shifts in the nature of mixing zones in streams due to shifting of the boundary between fresh- and saltwater. In the case of soils, antecedent water content plays an important role in defining how flow and biogeochemical processes will evolve. In groundwater systems, submarine discharge is dependent on the geologic structure of the subsurface. Thus, depending on the specific case of the mixing zone and why it exists, the knowledge needs will be different. In all cases, however, conceptualizing the mixing zone as a control node in the system implies that we may be able to make advances by abstractly considering the inputs, dynamic state, and fixed structures that define the operation of the node. Depending on the scenario, this may mean a range of approaches to defining and characterizing the mixing zone that span bottom-up integration of physically based models to top-down data-driven models obtained from machine learning. Soft methods of computation and indirect data sources may then become powerful tools for understanding what the appropriate inputs, dynamic states, and fixed structures are that need to be characterized in detail and how these are linked to other functional components of the watershed. The identification and characterization of mixing zones as control nodes of connectivity then further open opportunities to integrate a wide variety of data sources, from satellite imaging to genomics, as indirect or proxy data for understanding and simplifying the complexity of watersheds.

A focus on mixing zones as points of connection between functional units in watersheds is important for facilitating innovative new data streams or combining data from multiple spatial and temporal scales. In traditional environmental monitoring, water quality samples are collected at frequencies between weekly and monthly for laboratory analysis. This is analogous to watching a movie but only being able to see 12 clips that are each half a second long. It would be difficult to determine or discuss what occurred in the movie with only 6 seconds available. Similarly, it is difficult to calibrate and validate a model with nutrient dynamics as an output with monthly samples. Having high-frequency measurements will allow us to examine processes interacting at the storm event scale and calibrate models to the true dynamics during these events. Combining such data with less frequent, but spatially distributed measurements (e.g., using autonomous vehicles or remote sensing) would help to define the boundaries between functional units in the watershed and key elements needed for inclusion in the process controller (i.e., mixing zone) connecting them.

In general, there are many codes available that can describe processes within distinct compartments of a watershed (i.e., in both surface- and groundwater systems). In a few cases (e.g., the dynamics of macropore flow in soils), we do not yet have models (upscaled or otherwise) that can accurately represent the physical processes occurring at field scales. In most cases, however, existing models are sufficient for describing physical and, in many cases, biogeochemical processes. Our key challenge has always been in parameterizing these models given the complexity of the real world. As we move toward functional descriptions of watersheds, we are aiming to simplify our conceptualization of the system and, therefore, identify the key parameters and data that allow us to reduce this complexity. Consequently, identifying how to parse out functional units within a watershed is a key problem, but modular approaches to modeling will enable us to capture the behavior of these functional units. In contrast, an area of modeling where we need major advances is in understanding how to couple these functional units (i.e., how to describe the complexity and heterogeneity of mixing zones in a simplified way). Beyond the need for data-driven methods to identify functional units within a watershed, understanding how to model the complexity, heterogeneity, and dynamics of mixing zones to allow for coupling of other functional units in a watershed in a simplified way is the most important modeling challenge that we face. This challenge will benefit greatly from the data that can be obtained from intercomparison studies in vastly different watershed settings, from coastal to alpine environments.

The Way Forward

DOE and other federal agencies can facilitate intercomparison studies and community-based science by providing the logistics for the formation of national science networks. Many times there are investments in specific sites, such as DOE watershed test beds, NEON, and NSF Critical Zone Observatories. While such investments are critical, they are of limited scope and overlook the need for the infrastructure that connects and promotes inclusion of a diverse (i.e., technically, culturally, and spatially) community of researchers. There is a need for developing the standards, data and modeling tools, and educational and communication opportunities that would allow more breadth of experience, understanding, and environments within the scope of watershed science. There are currently no national observatories located in areas that directly parallel the unique natural environments, complex hydrologic conditions, or coastal threats (i.e., sea level rise and hurricanes) found in eastern North Carolina. Building networks that support science at risk environments like this are therefore needed.

Developing national frameworks and infrastructure to support a broader community of users, including decision makers and the public, should be a priority. In this way, premiere research sites can continue to provide a focal point for specific issues in watershed science and can be used as a key basis for comparison studies and watershed education. An inclusive infrastructure also would, however, enable a pathway for exploring and growing alternative sites and enabling critical understanding of watershed processes that may otherwise be overlooked by the narrow focus of existing sites. By facilitating the development of data standards, best practices, and accessible infrastructure to promote community engagement, interoperability, and knowledge dissemination, federal agencies can act as a critical enabling power to build a broad and dynamic water science community. Cloud-based solutions are key to achieving this by supporting models-as-a-service and data-as-a-service to the community. Cloud-based approaches will also engage industry and lower the barriers between those who have access to resources and those who do not. We live in an age where anyone should be able to log in and utilize massive datasets and modeling capabilities through a web browser. Working with the community to develop standards, promote interoperability, and ensure accessibility is the key to enabling the future of watershed science.

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8. A Proposal to Monitor and Archive Data of Standardized Porewater Signatures in Response to Hydrology to Transform Understanding of Groundwater Quality

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Motivation

Capturing the processes that dictate groundwater quality and its response to perturbations is an increasingly acute challenge around the world, as it is necessary for preserving groundwater resources. In many watersheds in the western United States (and elsewhere), shallow groundwater flow is a major contributor to surface water, in addition to being important drinking and irrigation water sources themselves. Unconfined or semiconfined shallow groundwater aquifers that actively interact with overlying soil and sediments are especially sensitive to seasonal and episodic hydrological variability. In these aquifers, changing water table elevations together with surface-driven (e.g., precipitation/snowmelt, flooding, and evapotranspiration) hydrological events will drastically change the exchange dynamics between the solid and aqueous phases, as well as the active biogeochemical processes. Thus, groundwater quality in these aquifers is heavily controlled by surface and near-surface hydrology that triggers both the biogeochemical processes that regulate nutrient and contaminant solubility as well as the transport processes and solute exchange that ultimately delimit what ends up in the groundwater and surface water.

To predict groundwater quality in response to projected future perturbations, it is critical to develop a robust understanding of the coupling between hydrology and biogeochemical processes from soil surface through the vadose zone, capillary fringe, and into the saturated zone. Current groundwater monitoring is normally limited to permanently saturated aquifers and ignores the important contribution of variable or unsaturated zones. Further, even for saturated zones, the spatial heterogeneity of sediment composition that may contribute to variability in water quality is largely unknown. Thus, there is a major need for expanding, both spatially and temporally, our examination of the biogeochemical reactions in soils and sediments that interact with groundwater sources, and to determine the extent to which they contribute to groundwater quality through episodic or seasonal hydrological cycles.

Watershed Science Community Capability Gaps and Open Science Opportunities

We know in general that transitions in soil biogeochemical processes are triggered by changes in water saturation and moderated by sediment properties that regulate water transport, oxygen supply, and biological oxygen demand. The corresponding switches in microbial metabolic activity; geochemical reactions; and redox transformations of carbon, nutrients, mineral constituents, and contaminants profoundly alter their susceptibility to transport and resulting impact on groundwater quality. Crucially, however, we lack a robust predictive understanding of when thresholds invoking a change in operative biogeochemical processes are reached in relation to soil moisture changes, metabolic responses, and rates and connection nodes of different reactions. These gaps reflect a lack of detailed conceptual knowledge about the biogeochemical reaction networks that govern redox transitions in the capillary fringe and transiently saturated zones. The resulting uncertainty prevents us from capturing the sizable contribution of variably saturated zones in numerical models used to predict water quality. Such capabilities are profoundly important to watershed modeling efforts nationwide.

Although the detailed linking of microbial and geochemical signatures to processes requires highly advanced data from in-depth measurements, indicator porewater constituents can provide a rich means for deducing operative biogeochemical processes. For example, indicative constituents for assessing the redox state and dominant microbial functions include dissolved iron [Fe(II) and Fe(III)], sulfate, sulfide, organic carbon, bicarbonate, nitrate, nitrite, ammonium, phosphate, chloride, and metals (i.e., major base cations and any trace metals that are present). Access to porewater data of these critical constituents becomes even more telling if it is obtained across saturation and/or biogeochemical process thresholds (e.g., redox gradients), changes in soil/sediment properties, and, especially, spatial resolution capable of detecting rapid transitions that may have a major influence on groundwater quality.

Currently, individual research groups are collecting this type of data at many sites across the country, through a variety of methods and at variable temporal and spatial resolutions. However, no national databases exist for compiling and searching these data, in spite of the highly valuable information about biogeochemical triggers and thresholds that could be gained by comparative studies of such data across sites and over time. Particularly valuable would be the ability to couple porewater data to hydrological and groundwater quality data, as well as microbial omics data from the same sites.

Scientific and Technical Objectives

We envision that a national subsurface water composition (including both porewater and groundwater) database would significantly enhance the progress of building a predictive understanding of the processes that govern groundwater quality. Thus, to increase the possibilities to compare porewater and groundwater data across sites and over time, we propose that:

1. Guidelines are developed for standardized porewater sampling and analytical methodology, to facilitate comparisons across sites and among different datasets. Options should include both off-site analysis of extracted porewater and *in situ* measurements via sensors and probes. Guidelines should also include requirements for specific analytes and spatial (lateral and vertical) and temporal resolution of data acquisition needed to capture process dynamics.

2. Steps are taken toward developing a national database for archiving soil/sediment porewater data in a standardized manner. The database should be built to allow cross-study searches and not be dependent on downloading individual datasets. However, it is essential that the data owners (contributors) are appropriately defined and referenced in any publications based on data extracted from the database.

3. The database is either linked to and leveraging data in existing groundwater and hydrological databases (e.g., NGWMN, NAWQA, GGIS, DOE-LM GEMS, and NHD), if this is feasible and relevant, or a minimum data requirement for groundwater chemistry and hydrology is added to upload the porewater data.

4. Efforts should be taken to ensure that sites included in the database span climatic regions and ecosystems (e.g., Arctic, boreal, temperate, arid, arable land, grassland, and forests).

Deliverables and Leveraging

The development of a national coupled soil porewater and groundwater database would enable nationwide and regional cross-correlation studies to unravel processes that drive groundwater quality in response to hydrological perturbations. Such meta-analyses are essential for developing a broader predictive understanding of the processes that control groundwater quality and critical biogeochemical functions within the near surface of watersheds. Thus, this effort would benefit many of the DOE Subsurface Biogeochemical Research (SBR)–funded research programs, including the Lawrence Berkeley National Laboratory Science Focus Area (SFA), Argonne National Laboratory SFA, and SLAC National Accelerator Laboratory SFA, and would leverage existing datasets collected within these and other programs, as well as infrastructure already in place at many field sites across the country. It could build on existing database and model initiatives, such as ESS-DIVE, NGWMN, and the IDEAS-Watersheds Reaction Network activity.

Referenced Databases

DOE-LM GEMS. Genome Engineering for Materials Management. U.S. Department of Energy Office of Legacy Management. [https://gems.lm.doe.gov]

ESS-DIVE. Environmental Systems Science–Data Infrastructure for a Virtual Ecosystem. U.S. Department of Energy Office of Biological and Environmental Research (maintained by Lawrence Berkeley National Laboratory). [https://ess-dive.lbl.gov]

GGIS. Global Groundwater Information System. International Groundwater Resources Assessment Centre. [https://www.un-igrac.org/global-groundwater-information-system-ggis/]

NAWQA. National Water-Quality Assessment, U.S. Geological Survey. [https://water.usgs.gov/nawqa/]

NGWMN. National Ground-Water Monitoring Network, sponsored by the Advisory Committee on Water Information's (ACWI) Subcommittee on Ground Water (SOGW). [https://cida.usgs.gov/ngwmn/index.jsp]

NHD. National Hydrography, U.S. Geological Survey. [https://www.usgs.gov/core-science-systems/ngp/national-hydrography/]

9. The Importance of Small-Scale Biogeochemical Processes in Predicting and Understanding Larger-Scale Watershed Function

Ken Kemner (Argonne National Laboratory)

Holistically understanding and predicting small-scale biogeochemical processes and function within the context of larger-scale hydrological phenomena are critical aspects of understanding watershed function. Although an understanding of smaller-scale (i.e., molecular to meter scale) processes can, at times, be developed, understanding their importance and controls on larger-scale environmental processes is important for gaining insights into watershed function.

Smaller-scale physical, chemical, and biological molecular processes are known to be major drivers for environmental system function, and understanding them is necessary for predicting watershed function. However, the frequency of occurrence and magnitude of these dominant small-scale processes often are controlled by larger-scale phenomena such as water saturation and flow. Most small-scale physical, chemical, and biological processes must be understood before, during, and after perturbations to a system's hydrology. Hydrological exchange zones can be particularly important in developing an understanding of system function.

High-frequency, long-term monitoring of the movement of water (and its biological and chemical characteristics) within an environmental system will provide the critical information needed to scale the magnitude of the small-scale biogeochemical reactions that are the direct drivers of environmental system function. This information will be critical for many models that are focused on larger-scale phenomena.

In terms of data collection, a broad and distributed science approach could be particularly valuable in providing supporting datasets that could be used by many different researchers, if the collected data are not *a priori* considered to be the sole data needed to provide new understanding to environmental system function.

Strategies to energize the scientific community to share data and ideas as part of a distributed, open watershed research effort might include ensuring scientists see direct benefits to their own research and providing new funds for them to set up the data collection. Funding for such efforts would have to be separate from the funds that cover the related research, rather than this data collection being a synergistic activity. A requirement of project support should be that the data are made available immediately. Datasets with unique DOIs are also needed, and dataset users should include the DOIs in all publications and presentations.

10. Coordinated Characterization of Watershed Response Times to Biogeochemical Disturbances

Ate Visser, Mike Singleton, Erik Oerter, Amanda Deinhart, and Richard Bibby (Lawrence Livermore National Laboratory)

Disturbances in the biogeochemical cycle at the land surface cause watershed responses in streams and rivers that are delayed by subsurface travel times of water and solutes. This delay is particularly consequential in highly impacted and agricultural watersheds (Hrachowitz et al. 2016) that suffer from legacy nitrogen (Van Meter et al. 2018) and phosphorous in streams long after surface loads have been reduced (Vero et al. 2018). It also impacts the delayed export of dissolved carbon from carbon-dense watersheds in response to global warming (Zwart et al. 2017).

How water and elements are transferred from subsurface storage to streams and rivers is one of the main questions in watershed science (McDonnell 2017). Within the last decade, a revolutionary new framework was developed to address this question (van der Velde et al. 2012; Harman 2015; Botter et al. 2011). The key concept is that the age of a parcel of water in a watershed is the primary factor predicting the probability that this parcel is transferred to streamflow or evapotranspiration. It acknowledges that hydrological conditions control whether younger or older water is able to connect with streamflow. The approach has been successfully tested in watersheds around the globe against observed concentrations of isotopic tracers (Benettin et al. 2017) and solutes (Harman 2015; Benettin et al. 2015; van der Velde et al. 2015), in field- and laboratory-scale experiments (Kim et al. 2016; Queloz et al. 2015), and in numerical models (Danesh-Yazdi et al. 2018; Kaandorp et al. 2018).

We now need to understand which characteristics of the critical zone control how watersheds select water from storage. These characteristics include both the subsurface architecture (Grant and Dietrich 2017) and the vegetation and land cover responsible for evapotranspiration (Fatichi et al. 2016). For example, the shape of the age-ranked storage-selection function is controlled by the subsurface architecture under steady-state groundwater flow (see Box 1, p. 90). It is expected that these elements are equally important across the watershed, although riparian vegetation may impose a stronger influence. The dynamic character of storage selection demands that we monitor the watershed under varying hydrological conditions, ideally capturing yearly extremes.

Characterizing the storage-selection characteristics of a real-world watershed often involves collecting samples for isotopic analyses (Benettin et al. 2017). High-resolution temporal variability of stable isotopes of hydrogen and oxygen in water molecules has proven successful in estimating the fraction of very young water in streamflow (Benettin et al. 2017; Jasechko et al. 2016). Tritium is an excellent tracer to capture stream-water age distribution on the order of tens of years (Michel et al. 2015). Newly developed techniques to analyze short-lived cosmogenic isotopes like sulfur-35 (Urióstegui et al. 2015, 2017) and sodium-22 (Kaste et al. 2016) are promising tools to support our understanding of streamwater ages and constrain storage-selection functions (Visser et al. 2019).

The proposed framework for understanding watershed response and linking the biogeochemical disturbances at the land surface to streams and rivers is inherently scalable. The storage-selection characteristics can be evaluated for a small headwater catchment, part of a watershed, or an entire river system. Once we understand how storage selection depends on landscape and subsurface characteristics, it is possible to incorporate the framework in Earth system models, such as the Energy Exascale Earth System Model (E3SM) at any scale or any grid cell size.

Physics-based distributed numerical watershed models have been applied to study storage-selection characteristics of hillslopes (Danesh-Yazdi et al. 2018) and lowland watersheds (Kaandorp et al. 2018). Physics-based distributed models are available for many more watersheds and can be used to predict storage-selection characteristics. The results of the model experiments can guide the timing and tracer selection for field sampling that is critical to understanding the response of the real watershed. In turn, the results from the field-sampling and isotopic analysis will inform the model on the appropriate implementation of subsurface architecture, vegetation structure, and plant-water strategies.

Box 1. Storage Selection and Subsurface Architecture

Consider two hillslopes with identical recharge and permeability: the slope of the bedrock controls the flow pattern in the saturated zone. On a steep slope, the thickness of the saturated zone increases with distance downslope. On a shallow slope, the saturated zone thickness decreases, leading to strongly increasing flow velocities (arrows).

As a consequence, the steep slope has a shorter mean travel time in storage and discharge than the shallow slope. However, on the steep slope, the residence time of discharge is older than that of storage. In contrast, on the shallow slope, the residence time of discharge is younger than that of storage.

Watersheds on steeper slopes have a preference to discharge older water from storage, while shallower slopes have a preference to discharge younger water from storage.

These differences are enhanced in real-world dynamic watersheds where storage selection is found to depend on the wetness of a catchment.

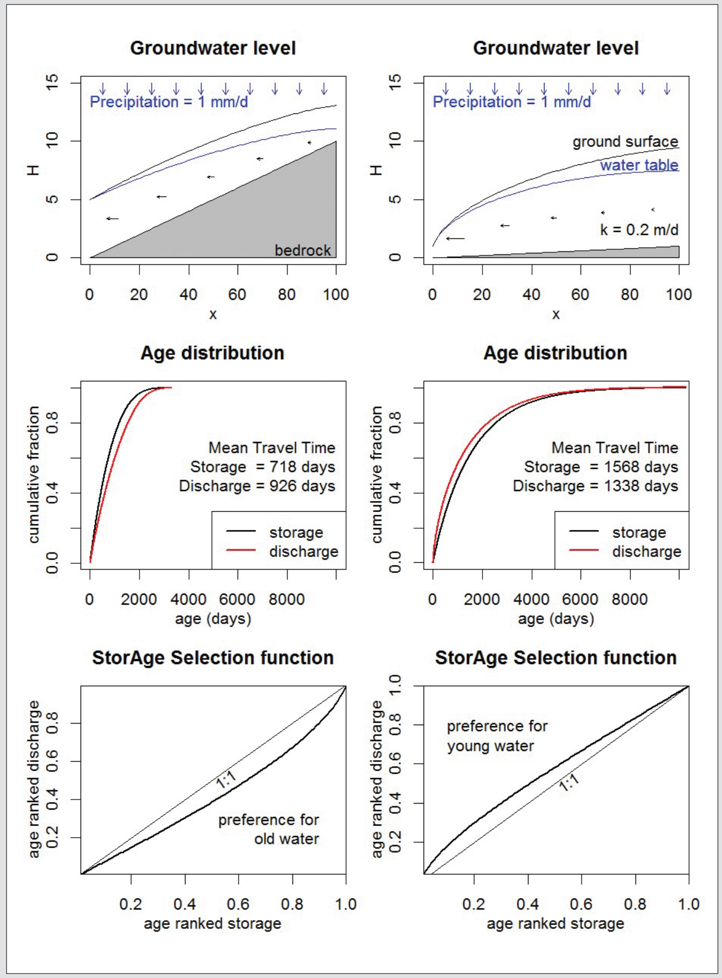

Fig. 1. (**Top**) Conceptual hillslope models, (**middle**) age distribution in storage and discharge, and (**bottom**) storage-selection functions for steep and shallow hillslopes. [Lawrence Livermore National Laboratory]

A broad-scale effort to characterize watersheds in terms of storage selection can leverage the unique national research and data infrastructure in watersheds across the continent. The distributed science approach involves engaging networks of research watersheds to collect samples for isotopic analyses. Many research institutes have the capability to perform analysis of stable isotopes (deuterium and oxygen-18). DOE can encourage the analysis of radioactive cosmogenic age-tracing isotopes at one of its unique laboratories by supporting collaborative research grants. The effort can be gradually ramped up by expanding outward from DOE Subsurface Biogeochemical Research (SBR) watershed test beds to include NEON and CZO watersheds (Brantley et al. 2017). Experimental forests and watersheds operated by the U.S. Forest Service (Safeeq and Hunsaker 2016) provide well-characterized ecosystems with supporting data on streamflow and precipitation. Simultaneously, the USGS National Water Information System database (NWIS) contains a wealth of valuable isotopic data from streams and rivers to be retrospectively analyzed in terms of storage-selection and watershed characterization (Michel et al. 2015). Extending further, the International Atomic Energy Agency Global Network of Isotopes in Rivers provides a global opportunity to consistently evaluate isotopic data to understand watershed functioning (Jasechko et al. 2016).

Analyses for single-watershed studies can be performed on desktop computer resources using newly developed open-source software (Benettin and Bertuzzo 2018). Calibrating these simple functional models on a national scale requires high-performance computing resources, either at DOE facilities or those commercially available, and a storage infrastructure like ESS-DIVE.

The proposed approach increases the predictability of biogeochemical response in rivers and oceans to anthropogenic land-use and land-cover disturbances. Combined with biogeochemical reaction kinetics, the age-ranked storage-outflow probability framework can link carbon and nutrient cycling at the land surface with the biogeochemistry of rivers and oceans. Once we understand how storage-outflow probability and biogeochemical parameters relate to climate, landscape features, and geology, we can implement the approach into E3SM. This avoids the computational cost and unrealistic data demands of a subgrid numerical flow and transport model. It expands on multipool biogeochemical cycling models by incorporating the dynamic time scales of water cycling in the subsurface. [Prepared by LLNL under Contract DE-AC52-07NA27344, with funding from LDRD project 15-ERD-042. LLNL-MI-782112.]

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11. Understanding Nonstationary Hydrologic Response from Local to Global Scales

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Nonstationary hydrologic response, represented by significant trends in annual runoff ratio (discharge/precipitation), is controlled by complex interactions among variability in climate forcing (e.g., precipitation and temperature), changes in physiological and structural responses of vegetation to elevated carbon dioxide (CO_2), and landscape characteristics such as topography and soil properties. Among these factors, the most difficult to predict, at large scales, are changes in vegetation physiological response and structure in response to climate variability, drought, and fire. Growing evidence suggests increases in CO_2 will increase plant water-use efficiency and decrease transpiration rates. Thus, there is an urgent need to address the challenge of predicting watershed-scale hydrologic response caused by changes in vegetation productivity and changes in ecosystem structure [e.g., leaf area index (LAI) and species composition]. Understanding this "compensating response" (Kergoat et al. 2002) is important because evapotranspiration accounts for about 70% of total precipitation globally (Good et al. 2015). Therefore, characterizing and quantifying changes in water-balance partitioning have important implications for predicting streamflow, groundwater recharge, water-resources management, and planning from *annual to decadal time scales*.

Scale of Investigation

Characterizing and quantifying natural vegetation response to changes in climatic forcing and elevated CO_2 from a *tree up to hillslope and watershed* scales are important for understanding watershed function due to significant impacts of vegetation on water-balance partitioning. Achieving this understanding requires establishment and/or extension of existing Critical Zone Observatories (CZO) and benchmark watersheds to measure important environmental variables for long-term monitoring under dynamic steady-state equilibrium, during and after perturbation. Most existing observational networks focus on characterization of land surface properties and fluxes. However, characterizing subsurface properties and structure remains limited despite their importance in storing and releasing of water from the catchment storage (i.e., soil and groundwater).

Limitations of Existing Numerical Codes

Several numerical codes exist that couple subsurface hydrologic processes to land surface and atmospheric dynamics using different coupling schemes such as ParFlow-CLM [a three-dimensional variably saturated flow model coupled to a Common Land Model (CLM; Kollet and Maxwell 2008) and HydroGeosphere (Therrien et al. 2010). However, in such models, vegetation is often assumed to be a static component of the hydrologic system, or prediction of vegetation dynamics is not well captured against observation. On the other hand, dynamic vegetation models consider detailed ecological processes while simplifying representation of hydrologic processes. Despite this progress, the main limitations are parameterization of such models, scaling up of small-scale processes to larger scales suitable for management and planning, as well as computational demand. To move the community forward, a team of ecologists, hydrologists, biogeochemists, microbiologists, soil physicists, and computer scientists should work together to link their modeling frameworks and develop community-level, open-source modeling systems suitable for predicting terrestrial hydrologic system response across multiple scales while considering important ecohydrologic processes.

Path Forward

In a recent study on characterizing watershed-scale response in 223 anthropogenically unaffected catchments in Australia, the authors proposed a new ecohydrologic catchment classification framework using *in situ* (e.g., streamflow, precipitation, and temperature) and remotely sensed vegetation data for characterizing watershed-scale hydrologic response (see Fig. 1; Ajami et al. 2017). However, characterizing exact causes of nonstationary catchment response was not possible given limited observational data such as soil properties, nutrient contents, and vegetation properties, as well as modeling frameworks suitable for capturing relevant hydrologic and ecological processes.

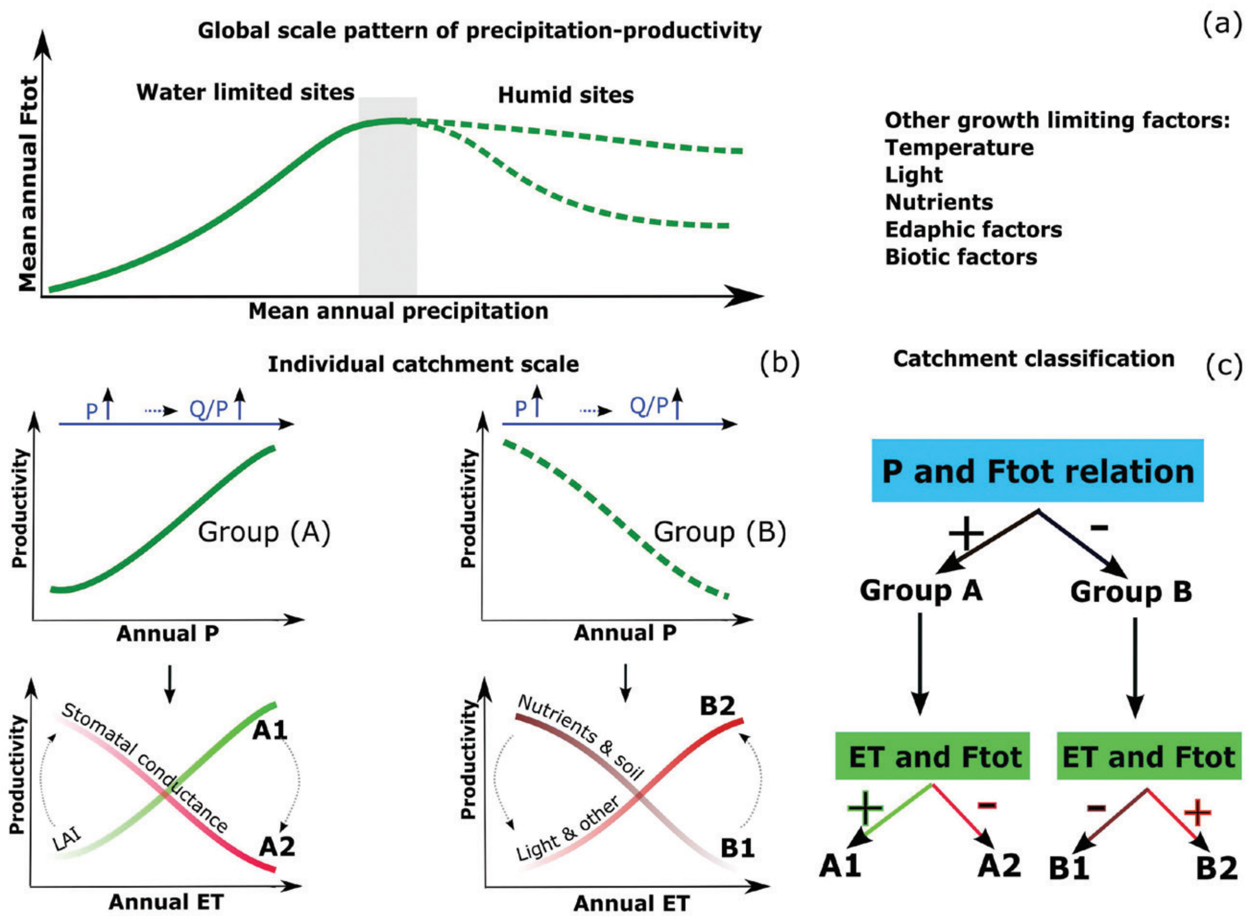

Fig. 1. Ecohydrologic Catchment Classification Framework. (a) Global pattern of annual productivity (Ftot) and mean annual precipitation relationship. **(b)** A conceptual ecohydrologic classification framework for predicting changes in runoff ratio in response to annual precipitation and vegetation productivity (Ftot) changes. In **Group A** or water-limited catchments, productivity depends on the dominance of structural control [increases in leaf area index (LAI), class A1] versus physiological control (decreases in stomatal conductance, class A2). In **Group B** catchments, productivity is likely limited by biogeochemical factors. **(c)** The flowchart shows the classification procedure [Published via a Creative Commons license, CC-BY-3.0 from Ajami et al. 2017].

Perhaps frameworks such as that described and illustrated above could serve as a guideline to highlight important data and models needed to understand watershed functions (e.g., water-balance partitioning and water storage and release) across a distributed network of observations and predict terrestrial ecosystem response to various disturbances, from watershed to global scales.

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12. Systematic Approaches to Atmospheric Forcings on High-Altitude, Mountainous Watersheds

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Recommendation

There are substantial challenges in determining the distribution of the connection between atmospheric forcing processes and surface and subsurface processes. Therefore, this white paper recommends that the watershed science community consider closer interactions with the atmospheric science community. There are mechanisms that can be considered for this cross-program collaboration, including through the concept of an integrated field laboratory (IFL), which was recommended by the Biological and Environmental Research Advisory Committee (BERAC). However, the ultimate rationale is twofold: the collaboration can (1) develop observational strategies for atmospheric forcing terms to establish the strengths and weaknesses of a sparse observational network for forcing watersheds and (2) determine the value of limited or, alternatively, intensive atmospheric observation campaigns.

Background

The mountains in North America constitute a quarter of the continent's land area, but they store 60% of the snowpack (Huss et al. 2017). However, these water towers of the world are threatened by many factors contributing to elevation-dependent warming (Barnett et al. 2005; Mote et al. 2005; Mountain Research Initiative EDW Working Group. 2015; López-Moreno et al. 2017; Musselman et al. 2017), which potentially can impact water resource availability adversely (Clow 2010; Barnhart et al. 2016; Li et al. 2017; McCabe 2017). Therefore, Earth system models (ESMs) need to provide robust predictions of how water resources in watersheds in complex terrain will evolve over time. Nevertheless, across many generations of development, ESMs have shown persistent problems in their ability to capture the temporal dynamics of mountain snowpack in the western United States (Frei et al. 2005; Rutter et al. 2009; Essery et al. 2009). ESMs, even when forced by re-analyses, exhibit a common failure mode in the date of peak snowpack timing and in spring snowmelt rate within both the California Sierra Nevada and Colorado Rocky Mountains (Chen et al. 2014; Wu et al. 2017; Rhoades et al. 2016, 2018a, 2018b).

However, efforts to address these errors in ESMs are hampered by questions of which process representation(s) are contributing to this error, processes which have given rise to the community-wide efforts like the ESM-Snow Models Intercomparison Project (SnowMIP) to understand how snow processes impact ESM performance (Krinner et al. 2018). Potential explanations for the errors include: (1) the model does not prognose the correct precipitation phase, intensity, and spatial (including elevational) distribution; (2) the model exhibits biases in other atmospheric forcings such as aerosols, moisture, radiation, and wind; (3) the land surface model has structural errors; or (4) some combination of these effects. To discern which of these potential explanations drives the common failure in ESMs, the mountain hydrometeorology community has repeatedly requested the simultaneous atmospheric measurements of energy and water fluxes within complex terrain (Lundquist et al. 2003, 2016; Bales et al. 2006; Henn et al. 2018a, 2018b). They also have indicated the importance of those comprehensive observations for model testing, because of persistent questions regarding the representativeness of discrete station data in the presence of significant spatial heterogeneity in atmosphere and land-surface processes across complex terrain (Oyler et al. 2015).

A complete set of observations of the atmospheric forcings on a mountainous watershed would consist of the temporally and spatially varying distribution of (1) surface precipitation amount and its thermodynamic phase, (2) surface downwelling shortwave and longwave radiation with contributions from clouds, (3) sensible and latent heat fluxes, (4) vertically resolved wind vectors, and (5) aerosol surface deposition and its optical and biogeochemical composition.

There are a number of practical challenges associated with making these observations of atmospheric forcings in complex terrain including, but not limited to, issues associated with site access, environmental impact, maintenance of observations, power, personnel safety, and costs. These considerations have led to the reliance on sparse networks of atmospheric observations. Still, with a sparse network of discrete instruments, there are fundamental, unanswered, and controversial questions as to how to interpolate between these observations reliably. In fact, there is a strong potential for biases from point observations since steep slopes and high elevations are underrepresented (Henn et al. 2018b; Sevruk 1997; Frei and Schär 1998), and the true heterogeneity of mountainous regions may not be represented by the current measurement network (McAfee et al. 2019). Interpolating between point observations has been found to depend strongly on the number, type, and spatial/elevational distribution of observations (Zhang et al. 2017) and possibly to be the most important source of rainfall/runoff model errors (Moulin et al. 2009).

The rise of remote-sensing technologies may be able to address many of these challenges, but the strengths and weaknesses of remote sensing of atmospheric forcing in complex terrain should be acknowledged. The spatial coverage of one or a small number of remote-sensing instruments can produce comprehensive maps of complex terrain and can provide unique insights into the importance of various atmospheric processes on the watershed. The type of remote-sensing technique varies by the atmospheric forcing variable under consideration.

Precipitation Amount and Thermodynamic Phase

Polarimetric radar systems can cover large areas and provide direct information about precipitation amount and its thermodynamic phase. Unfortunately, at present, the detailed characterization of precipitation from radar in mountainous environments is extremely poor in comparison to less topographically complex parts of the United States (Maddox et al. 2002). The operational weather radar coverage in the mountainous regions of the continental United States is exceedingly sparse due to radar beam blockage (Maddox et al. 2002). The actual time-varying precipitation amount and phase in complex terrain currently can only be estimated from the few operational radars sited at or near commercial airports. Satellite radars, such as the tropical rainfall measuring mission (TRMM) and global precipitation measurement (GPM) mission, are also of limited utility for retrieving precipitation in complex terrain. Unfortunately, these satellite precipitation estimates in complex terrain can also have significant biases (Prat and Barros 2010), particularly for winter orographic precipitation.

A dedicated ground-based polarimetric radar system deployment would provide very detailed precipitation information across the majority of a watershed in complex terrain. Measurements across a representative sample of cold and warm season events would then help clarify the appropriate approaches for interpolating between sparse observations, since the spatial variability in precipitation depends on the processes that are controlling that precipitation. There are several different potential facilities that could achieve this need: DOE has considerable radar instrumentation and associated expertise as part of its Atmospheric Radiation Measurement (ARM) and Atmospheric System Research (ASR) programs. ARM regularly solicits proposals for field campaigns through the ARM Mobile Facility (AMF) and has scanning radar systems including C-band, X-band, Ka-band, and W-band radar, with the C-band being the most capable for comprehensive precipitation observations covering a radius of at least 60 km with a spatial resolution of at least 500 m and a temporal resolution of ~15 minutes. The NOAA National Severe Storm Laboratory maintains dual-polarized X-band mobile radar, and other systems maintained by other organizations including, but not limited to, Colorado State University's CSU-CHILL National Radar Facility and National Center for Atmospheric Research (NCAR) could be used. Finally, other federal and local agencies can procure a weather radar system, since commercial radar solutions can be commissioned with performance specifications related to their range, spatial resolution, minimum precipitation sensitivity, ability to discriminate the thermodynamic phase of precipitation, and duty cycle that are generally superior to existing Next Generation Weather Radar (NEXRAD) systems.

Radiative, Sensible, and Latent Heat Fluxes

Accurate estimations of distribution of shortwave and longwave atmospheric radiation in complex terrain cannot be easily accomplished with a single or small set of measurements. However, the physical processes controlling atmospheric radiation in complex terrain are well understood: solar insolation, scattering by clouds and aerosols, absorption by water vapor and other trace gases, and absorption and reflection from three-dimensional interactions with the terrain itself and surface features such as vegetation. If the time and space variations of these features can be estimated across a watershed in complex terrain, then the shortwave and longwave radiation fields can be calculated. There generally are computational limitations, which necessitate the development of parameterizations that span the parameter space of the watershed in question.

The distribution of sensible and latent heat across a watershed can also impact the surface and subsurface and affect processes such as snow ablation. These quantities can be determined from surface meteorological stations, but their distribution across complex terrain is challenging to obtain. Advanced Raman light detection and ranging (LIDAR) technologies, though of considerable expense, could be used to derive sensible and latent heat fluxes, but generally these quantities must be modeled.

Winds

The understanding of wind on a watershed represents a particularly challenging frontier. Wind may rearrange snow (Mott et al. 2018), in particular, and has been implicated in the surprisingly variable spatial distribution of snow measured by the NASA Airborne Snow Observatory (Painter et al. 2016). Winds are measured at surface weather stations and derived from the movement of weather balloons. The spatial distribution of winds can be sensed with Doppler LIDAR or radar wind profilers, but results from these instruments degrade where condensates are present, and neither fares well in precipitating events. Wind also can be derived from the movement of cloud fields from geostationary satellite observations, though the movement of clouds is a convolution of winds and the processes that control the formation and dissipation of clouds. There are challenges to deriving winds from clouds' complex terrain, because of the mechanical nature (e.g., orographic forcing) of cloud formation in the cold season.

Aerosols

Because aerosols can significantly impact snow albedo, it is important to understand their deposition amount and their optical properties. The contribution of black carbon can have a very large impact on snow albedo and is, at least in the western United States, generally limited to anthropogenic contributions, which have a more significant local component. The contribution from dust events can have local and nonlocal effects and can have watershed-scale impacts on the albedo of snow (Skiles et al. 2015). The deposition of aerosols requires detailed understanding of the distribution of winds and, consequently, turbulent fluxes across complex terrain. This information can be very difficult to obtain, but retrospective analysis on aerosol surface deposition can be performed observationally with snow pits, since snow acts as a passive recorder of aerosol deposition events. Detailed snow surveys from the NASA Airborne Snow Observatory can complement these observations. There are ground-based aerosol observations that are of high accuracy for aerosol optical depth and speciation, but these are only point measurements.

Connection to Process Models

The use of atmospheric and surface process models is necessary to interpret the observations and provide context for ESM development. They provide an integrated and physics-based framework for uprooting the sources of ESM errors. The coupling of surface and atmosphere process models is nontrivial at many levels, especially from scale mismatch. Downscaling may be required (Winstral et al. 2014).

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13. Anthropogenic Processes Profoundly Influence Watersheds

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For decades, it has been widely recognized that anthropogenic processes have transformed large shares of the Earth's surface (Vitousek et al. 1997) and reduced terrestrial water storage enough to become a significant contributor to global sea level rise (Gornitz et al. 1997; Pokhrel et al. 2012). The importance of anthropogenic influences on hydrological processes at the watershed scale have also been widely recognized (Felfelani et al. 2017; Sivapalan et al. 2014). Humans, when acting collectively, can harness the energetic and technical capacity to change nearly any aspect of a watershed. Indeed, humans have dammed (Yang et al. 2011), channelized (Amissah et al. 2018; Munoz et al. 2018), created (Heness et al. 2017), and entirely dried up (Carriquiry and Sánchez 1999) major global rivers and waterbodies. Anthropogenic changes in water demand and both surface- and groundwater withdrawal patterns lead to alterations in the basin-scale water balance. Anthropogenic changes in land use and land cover, particularly impervious surfaces, alter the speed of water movement and influence infiltration. Hydraulic infrastructure such as dams, reservoirs, and levees change river and streamflow dynamics with attendant consequences in sediment load and transport, water temperature, turbidity, and flood risk. Urban and agricultural runoff influences biogeochemistry both locally and far downstream. Anthropogenic processes now have a significant influence on watershed hydrology for a substantial share of, if not all, watersheds around the globe.

A robust ability to predict ranges of potential outcomes of the social processes that influence water storage, movement, and quality is crucial for prediction of watershed function at decadal scales or longer. As predictive time frames become longer, the social processes that must be considered become more complex and the structured manner in which people act collectively becomes more significant. For short-term predictive models of watershed function, complex social dynamics can plausibly be ignored by assuming the status quo remains in place. On seasonal to annual time scales, anthropogenic influences governed by "simple decisions" can be simulated with reasonable fidelity by assuming economically rational actors operating in a fixed social and economic context. However, as the predictive time frame becomes longer, an increasing variety of behavioral strategies become possible—both for individuals' own decisions and through collective action and institutional change. Over long time periods, collective choices are increasingly likely to cause changes in the social and economic context in which individuals make decisions about where to live, what kind of yard to have, or what kind of crops to grow.

For example, during the height of the recent California drought, residential water consumption declined by nearly 30% compared with that during the predrought peak (Kostyrko 2016), groundwater pumping for agriculture increased by 70%, and net agricultural water deliveries declined by 10% due to a broad series of anthropogenic responses to the drought (Howitt et al. 2015). For the most part, urban water-consuming behavior has now returned to about halfway between predrought levels and the maximally conserving months, while agricultural use has returned to predrought levels or higher. These behavioral changes occurred on a seasonal to annual time scale, and the agricultural changes in particular were well estimated using standard econometric models. On a multiyear to decadal time scale in Las Vegas, Nevada, long-term awareness that the city's fixed water supply must serve a growing population drove substantial institutional and infrastructural investments in water conservation. These strategies included everything from award-winning advertisement campaigns, incentives for grass replacement, and a changed regulatory structure that permitted graduated fines for water waste. These institutional changes contributed to a growing proliferation of individual choices to invest in water-conserving infrastructure (Brelsford and Abbott 2017). Large-scale legal and institutional changes can have even farther reaching effects: for several decades, the water agencies serving Las Vegas have been seeking to develop broader views of legally permissible cross-state water transfers than those delineated by the 1922 Colorado River Compact (Mulroy 2008), including supporting cross-state water-rights purchases and interstate water banking. If these strategies for allocation changes succeed, a rapid and substantial movement of water from the arid, low-population watersheds of Nevada, Arizona, and Utah into the Las Vegas metropolitan area would likely soon follow.

The social processes that lead to these hydrological outcomes are difficult to predict. However, a growing subfield of hydrology, socio-hydrology (Sivapalan et al. 2014; Brown and Lall 2006; Srinivasan et al. 2012; Elshafei et al. 2014; Di Baldassarre et al. 2015, 2018a), is seeking to develop robust, empirical strategies for understanding and parameterizing interactions between anthropogenic and hydrological processes. One approach has included a careful description of the effects that human behavior and social processes have on hydrological processes, for example, through agricultural, industrial, and urban use patterns. Another approach aims to describe the effect that hydrological processes have on humans, often focusing on the consequences of floods, droughts, and contaminant or disease loads. More recent work aims to take a bi-directionally coupled feedback approach to understanding socio-hydrological systems, such as by describing a concept of "social memory" or the "'levee effect" (Di Baldassarre et al. 2018b) by which populations that have recently been exposed to some form of water-based adverse event are more resilient to that same category of event in the future, while those that have been protected become more vulnerable.

One common critique of existing work is that the majority is based on case study approaches, which can fail to contribute to a more generalizable understanding of the dynamics of socio-hydrological systems. If generalizable patterns can be identified, then our ability to describe long-term watershed dynamics would be substantially improved.

I propose considering socio-hydrological systems as *structurally co-constituted* of social, built, and natural elements. This perspective goes beyond quantification of feedbacks between the social and natural domains (still conceptualized separately) and instead encourages us to focus on the co-evolution of the systems. This approach allows us to ask questions such as: What types of innovations have successfully been used to address water-management challenges? Can we describe a relationship between hydrological conditions and institutional innovations? Which structural components of the system affect its resilience to hydrological events and through what mechanisms? Given a characteristic management challenge, which patterns—in institutional structure and in ecological and economic context and dynamics—can we observe in management strategies? This strategy would contribute to seeking generality in system response to characteristic management challenges and concerns such as water excess, water scarcity, and water quality.

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14. Where Does the Watershed End and Anthroshed Begin? A Need to Understand and Represent Shifting Human and Natural Controls on Hydrologic Systems

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The Problem

Streamflow is a fundamental water cycle variable that drives downgradient biogeochemical reactions and transport and is critical to human decision making across multiple jurisdictions. High in its headwaters, streamflow emerges via a complicated set of surface and subsurface pathways driven primarily by the biophysical properties of its catchment. As water moves farther downgradient, it interacts more frequently with increasingly complex human infrastructure expressly designed to further modify the timing and magnitude of streamflow. The integrative nature of streamflow compounds the uncertainty arising from upstream biophysical controls, but conceptualizations of the water cycle often fail to consider the influence of human modifications to hydrologic connectivity. This failure can create considerable error associated with forecasts in downstream and coastal locations where key energy and agricultural infrastructures are located. State and federal agencies depend on such streamflow predictions to manage hundreds of dams, private companies use them to optimize energy production, municipalities depend on them to plan for urban growth, and agricultural producers use them to create irrigation schedules. Across the United States, changes to critical energy and agricultural infrastructures are being assessed, depending on predictions of streamflow well into the next few decades. At seasonal to subseasonal scales, streamflow prediction is necessary to constrain interannual water planning (e.g., estimates of reservoir carryover) and improve resilience and planning for high or low flows. Incorporating the human footprint and improving streamflow predictions are necessary for updating current management plans and better evaluating risk in the face of future change. We contend that key gaps in the underlying conceptual and numerical models used to actively manage water resources lie in a relatively simplistic treatment of the critical zone, particularly in mountain landscapes, and the omission of human modifications to the retention, storage, and release of water from the landscape. To improve predictions of streamflow at the spatiotemporal scale at which it is useful for planning and decision making, we must achieve the following goals:

1. Improve the representation of the heterogeneity of the critical zone and advance our fundamental understanding of how to scale key processes that influence the retention, storage, and release of water from headwater catchments.
2. Better characterize how human activities modify hydrologic regimes as processes that can be incorporated into models.
3. Identify where in the landscape, and at what time scales, human influence supersedes first-order controls on hydrologic response to precipitation inputs.

The State of Watershed System Modeling

There have been significant advances in deploying distributed, process-oriented hydrologic models to predict streamflow in the preceding decade. Perhaps, most notably among these is the National Water Model (NWM), which has been deployed throughout the watersheds of the continental United States (CONUS) and is now used operationally by NOAA to provide streamflow forecasts for the nation. The dynamical core of the NWM corresponds to the Weather Research and Forecasting Hydrological modeling system (WRF-Hydro). WRF-Hydro consists of a column land surface model, corresponding to the Noah-MP model (Niu et al. 2011), which solves for the vertical exchanges of water and energy between the land surface and atmosphere, coupled interactively with hydrologic and river routing schemes that predict streamflow along the nation's river and stream network, which corresponds to the National Hydrographic Dataset (NHDPlus HR) provided by the U.S. Geological Survey. Vertical fluxes of water and energy are resolved at spatial resolutions of 1 km throughout CONUS with temporal resolutions of 1 hour. Horizontal routing of water over and through hillslopes is resolved at spatial resolutions of 250 m. The operational NWM is forced by a variety of weather and subseasonal forecasting products, ranging from the Global Forecasting System forecast at short lead times (10 days) to the Climate Forecasting System (CFS) data at coarse temporal scales (3 months). Despite the significant advances in developing and deploying a model as complex as the NWM, there remain considerable capability and science gaps that limit the underlying WRF-Hydro framework in accurately predicting streamflow at scales relevant to human decision making.

Our understanding of streamflow generation processes commonly begins in headwater catchments, where precipitation falls, is stored and/or routed via myriad surface and subsurface pathways downgradient. The mathematical representations of these processes used in modeling frameworks are based on small-scale physics, and models often implicitly assume that these processes scale upwards linearly and additively in space and time (e.g., Kirchner 2006). In the case of WRF-Hydro, the Noah-MP column land surface model represents dynamic interactions among components of the snow-soil-atmosphere-vegetation system and is meant to capture the way in which Earth's critical zone attenuates the flow of moisture.

Owing to its heritage as a land surface model for coupled land-atmosphere models, the Noah-MP column land surface model relies on constitutive relationships between macroscale fluxes and model states that arose due to a paucity of data or a lack of established literature to develop improved relationships. As a result, the representation of the spatial structure of the critical zone is relatively simplistic. While soils can vary in space, the depth of the soil column is treated as fixed and there is no direct representation of flow through complex pathways such as macropores and/or fractures. These preferential flow paths can be particularly important in headwater and mountain systems where landscapes are thinly mantled with well-developed soils. As such, WRF-Hydro does well at larger scales, but it necessarily oversimplifies headwater and subsurface processes.

Moving downstream, the dominant controls over the timing and magnitude of streamflow shift as the human footprint increases. Water-management infrastructure and decision making in response to previous conditions and available forecasts begin to exert greater control over the timing and magnitude of streamflow than the emergent properties of the headwater catchments. The lack of explicit representation of human modification of the landscape in the form of dams with complex operator procedures, diversions of water for irrigation, and return flows associated with runoff from irrigated systems is a critical second limitation of the NWM and WRF-Hydro framework. These human processes are complex, adaptive, and nonlinear, exerting considerable control over the characteristic spatiotemporal scales of water retention, storage, and release in many systems. The changes to hydrologic pathways and travel times imparted by human activities also must have corresponding effects on biogeochemical cycles and the export of weathering materials from the critical zone. Yet, the ways in which humans dynamically modify hydrologic pathways and connectivity are nearly completely absent from large-scale hydrologic models like the NWM/WRF-Hydro framework. There is, moreover, no clear sense of when or where in the landscape we shift from one set of governing rules (dominated by natural processes) to another (dominated by human activity), nor is it clear whether the transition is abrupt or gradual.

Opportunities for Innovation

New model developments are required that would include advancing capabilities for improved representations of multiscale processes and dynamic interactions between and among hillslopes, catchments, watersheds, and human perturbations. To incorporate human controls on streamflow, we must develop novel means by which to incorporate human decision making, and the rules governing them, into these models. These applications will require interdisciplinary work with researchers that study emergent dynamics of human systems such as communication networks and learning. At the same time, advancing representation of hillslope processes and human controls will require that we develop (1) methods to partition the landscape into process domains according to the preeminence of human versus first-order control and (2) models that can reliably represent the interactions between and among those process domains.

Improved predictions of streamflow in the anthropocene will necessarily require a distributed, open-source approach to gather enough data across scales and disciplines to incorporate into community hydrologic models. One significant advantage of the NWM/WRF-Hydro framework is its community-supported and open-source nature. As an open-source model, the community is able to innovate on the underlying process representation, use it for fundamental hypothesis-driven and/or place-specific research questions, and develop and test new methodologies for model calibration and assimilation of novel data streams into the model. Other communities, particularly the Earth system modeling community, have seen significant advances made in the model state of the art due to the willingness of the community to rally around a small set of open-source, albeit still flawed, models. Such model advancements rely fundamentally on expanded data collection. As one of the most tangible components of the water budget, streamflow has been the target of numerous citizen science initiatives that gather distributed data (e.g., StreamTracker and Crowd Water; analogously, biodiversity citizen science has resulted in up to $2.5 billion of annual in-kind contributions; Theobald et al. 2015). These data are potentially very valuable for their spatial coverage but require that we reconcile diverse and novel datasets (e.g., photos of a dry creek bed), determine how to integrate them into models, and identify locations that are currently lacking data. Automation and standardization of data integration could benefit from techniques like machine learning, but conceptual development will be a prerequisite to determine which data are most valuable and in what form.

Moreover, we must consider how participation in such distributed and open projects can be incentivized for data and model producers. Researchers' reluctance to participate in open science is often based on a fear that data will be used without credit or inappropriately, or that they will not receive sufficient acknowledgement given the work that went into its production. We must ensure that recognition for contributions is commensurate with its usage and will translate into metrics acknowledged by review boards at participating scientists' places of employment. For example, creating new public metrics of dataset or model downloads and usage in publications, or counting data production as a publication with citations (e.g., the *Earth System Science Data* journal). Individual institutions hoping to encourage their faculty or researchers to participate in such initiatives may also consider updating metrics for performance/tenure review to include participation in such open initiatives more prominently.

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15. An Integrated Suite of Sensing and Data Capabilities for Open Watershed Science

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Sensing provides (1) the critical datasets for mechanistic understandings of key watershed processes and functionalities and (2) the development of multiscale, multiphysics watershed models with improved predictive capabilities. The complex and dynamic interactions between the different compartments and components of watersheds over a wide range of spatial and temporal scales pose a significant challenge to the development of reliable models for prediction and management. Our capability to collect the right type of data at the right place and time is essential to the improved understanding of the underlying mechanisms driving watershed behavior and, subsequently, their accurate representation in models.

Modern technological progress has significantly improved our capabilities to measure and to analyze. These capabilities open up a wide range of new possibilities for sensing at watershed scales and beyond. While sensing and measurement technologies are moving forward quickly at an individual level, integrated sensing across a diverse range of watersheds, each with a unique set of conditions and functions, requires coordinated efforts that take a holistic and standardized approach to facilitate cross-watershed data sharing, comparison, and meta-analysis. Such a holistic approach requires a systematic view of the range of watersheds under study to decide where, what, and how to invest efforts. The spatial and temporal dynamics of the systems under study and the need to allocate resources efficiently require that we approach this effort with a new paradigm.

Future generations of sensing networks suitable for open watershed science must comprise diverse but compatible sensing modalities that can operate across a range of spatial scales. New approaches are needed for efficient onboard or localized data processing and communication. These sensor packages should be customized and deployed based on the type, location, and timing of data requirements, using best-available model predictions to inform these decisions. This framework should represent a circular feedback, where model-informed sensor deployment feeds back to data assimilation and/or model evaluation and refinement. Recognizing that our best-in-class models will not always represent important processes, sensing for discovery is a critical need, in which the focus comprises new sensors, new sensor combinations, new locations, and new approaches to data interpretation and translation to knowledge. This discovery aspect will initially require controllable systems to evaluate coordinated sensor performance under realistic but known heterogeneity, allowing multiple research groups to work together to evaluate new sensing approaches while leveraging information from well-developed sensor platforms.

We see this development as a tiered approach, building sensor packages to measure "critical-to-know-everywhere" parameters for robust deployment across vast spatial scales. Parallel development of data processing and communications schema will be essential, as will the development and testing of next-generation sensors for "important-to-know-but-hard-to-measure" parameters, prior to their incorporation into robust and customized sensor packages.

We suggest that the sensing capability needed for open watershed science in a distributed research network should include four key components: (1) emerging new sensor development; (2) improved data automation, transmission, and edge computing capabilities; (3) development of data analytics/machine-learning (ML) tools; and (4) establishment of virtual observatories and a cyberinfrastructure platform (see Fig. 1). These four components interact and integrate to provide next-generation sensing capabilities as a critical support of distributed open watershed science.

The four key components are briefly discussed below.

- **Emerging sensor development:** Despite the wide number of sensors and sensing technologies available, there is still a strong limitation, in terms of our capabilities, to sensing key variables in watershed processes, especially chemical and biological parameters. Emerging sensors that expand our capability in chemical and biological sensing represent a critical need. In addition, new developments in multiple other areas also bring exciting opportunities to greatly expand our sensing capabilities. This includes, for example, quantum sensing, unmanned aerial vehicle (UAV)-based sensing, geophysical imaging, and fiber optical sensing, as well as the deployment of large-scale wireless sensor networks.

- **Data automation, transmission, and edge computing:** Autonomous data collection and transmission are key components of ecosystem sensing that can significantly increase data density while reducing cost. Technologies to solve wireless communication challenges in remote areas are essential to improving autonomous data collection and transmission that can enable the deployment of distributed wireless sensor networks. In addition, edge computing technologies that can significantly reduce data volume for transmission represent an example of developmental needs, especially for those specific data types that generate a large volume of data on daily basis.

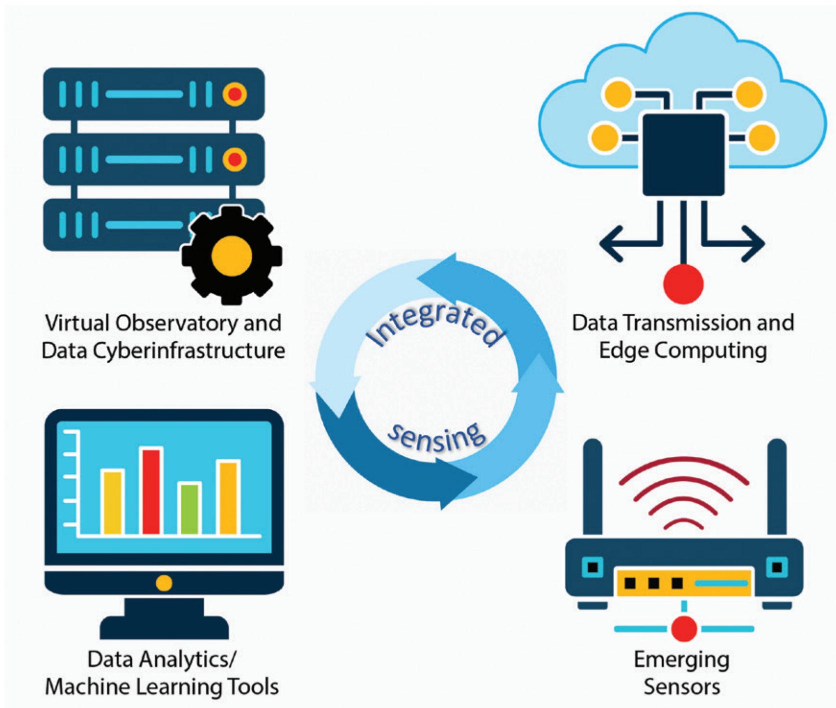

Fig. 1. Four key components of an integrated suite of sensing and data capabilities for open watershed science. [Lawrence Berkeley National Laboratory]

- **Data analytics/machine-learning tools:** Data-intensive scientific discovery requires effective data analytical tools to sift through a large volume and diversity of data, searching for regularities and patterns. In watershed studies, how to integrate heterogeneous and distributed datasets from omic to watershed scales into predictive models of watershed functioning presents a significant challenge. Developments of sophisticated ML algorithms have greatly expanded our selection of analytical techniques available to deal with complex and heterogeneous datasets and created better ways to integrate datasets from multiple sources and researchers. A challenge facing researchers is how to effectively evaluate and select practical ML tools that best fit the dimensionality and diversity of the datasets with which they are dealing. In addition, improving the ease of use of these new algorithms could help improve the turnover rate from data to knowledge in the broader community.

- **Virtual observatory and data cyberinfrastructure:** The data cyberinfrastructure is the interface between data and user. It needs to integrate automation, storage, analytics, and visualization and to play the central role in promoting collaboration and sharing where data generators, users, modelers, and stakeholders can access/analyze data, visualize/share results, and work together to improve our understanding of system dynamics to support decision making. The data infrastructure needs to support virtual observatories that allow synchronization and provide virtual connections between laboratory, controlled mesoscale, and field experiments.

16. Calibration and Coordinated Data Collection from Deployed Sensors

Don Nuzzio (Analytical Instrument Systems, Inc.)

Whether the researcher is deploying simple temperature loggers or more sophisticated multisensor systems, accurate sensor calibration is required. The models generated for a particular area are only as good as the raw data presented to the person modeling a particular environment.

Having a National Institute of Standards and Technology (NIST)–like traceable calibration check for deployed sensors will increase our confidence in the data acquired. It also will allow us to identify sensors that are out of calibration as well as ones that are just not working properly. This in itself would be time saving for the researcher and further ensure the integrity of data collected.

Sensors from standard suppliers are good and do provide adequate data, but for the best accuracy these sensors should be calibrated in the systems in which they are to be used, with some external check. Sensors can be different within manufacturing; batch-to-batch variation can exist during production. Sensors also vary, for example, with respect to temperature, pressure, humidity, and storage conditions. It is to this end that we need to ensure with the highest confidence that the outputs from these systems are accurate.

When choosing a sensor, several key points need to be addressed for the data output to be valid:

1. Types of measurements needed.
2. Type of environment sensors to be deployed.
3. Degree of accuracy required.
4. Degree of precision required.
5. Required resolution of needed measurements, in significant figures.

These are just some of the considerations to be addressed when collecting data from any sensor in any environment. At a minimum, having a *standardized set of calibration criteria* for all types of sensors will allow for a better science and better modeling.

17. Autonomous Monitoring with Real-Time *In Situ* Sensor Networks

Ruby N. Ghosh (Opti O2, LLC)

Environmental sensor networks capable of taking data quickly enough to capture minute-scale fluctuations and durable enough to capture these data for entire seasons are essential for studying the seasonal and annual effects of environmental activity across an entire watershed system. The models informed by these data are useful for predicting both short- and long-term changes to economically important watershed systems. Distributed sensors that are cost and labor effective are required for these applications. The sensor networks need to be deployable in remote locations as well as operable remotely with minimal maintenance. Rapid and open sharing of data among stakeholders necessitates autonomous, telemetered data transmission.

Opti O2 has developed and demonstrated a prototype network of dissolved oxygen (DO) and temperature probes for monitoring a river catchment to provide high-resolution data of DO dynamics associated with ground/surface water exchange in the hyporheic zone. The optical probes can be deployed in fresh/salt water or buried directly into soil/sediment for *in situ*, concurrent observations of DO and temperature. The sensor network can operate continuously without human intervention for an entire hydrological year, including several freeze/thaw cycles of the river and buried probes. The system operates autonomously and on solar power, transmitting data over wireless networks to remote servers and providing data at 5-minute intervals. To better inform models of watershed dynamics, our dataset includes meteorological parameters such as barometric pressure and air temperature. The system is scalable for extended *in situ* hydrological studies capable of operating in both river and hyporheic zones. Our goal is to enable cost- and labor-effective, watershed system–scale remote observations of DO, temperature, and other environmental parameters.

18. 4D Sensing and Data Integration for Predictive Understanding of Ecohydro-Biogeochemical Functioning at Watershed Scale

Baptiste Dafflon, Haruko Wainwright, Susan Hubbard, and SFA Watershed Function team (Lawrence Berkeley National Laboratory)

Predictive understanding of ecohydro-biogeochemical functioning is often hindered by the heterogeneous and multiscale fabric of terrestrial systems. In particular, water, carbon, and nitrogen cycling is modulated by hydro-biogeochemical processes and interactions occurring from bedrock to canopy, involving geology, soil, plants, microorganisms, energy and water exchanges, and fluid composition. These factors dynamically interact with each other across space, creating significant spatiotemporal variability and "hot spots"/"hot moments." Observing how heterogeneous terrestrial compartments—such as geology, soil, and vegetation—respond to variable atmospheric forcing and disturbances is critical to (1) identify key factors controlling water and biogeochemical cycling, (2) provide parameters and validation data for mechanistic models, (3) provide near–real time information relevant for decision making in natural and managed systems, and (4) improve predictive understanding of ecohydro-biogeochemical functioning.

Recently, our ability in modeling complex processes has been significantly advanced from a single site or hillslope to watershed scale, including complex ecohydrological and biogeochemical processes. DOE has developed a suite of high-performance computing (HPC) software for numerically simulating ecosystem behaviors, subsurface/surface flow and transport, and atmospheric processes (U.S. DOE 2015a). In parallel, advances in sensor networks, geophysics, and remote sensing have created great opportunities in characterizing subsurface and surface dynamics and their interactions in a temporally and spatially resolved manner. In particular, DOE recognized the strong value in using novel aerial sensing approaches using unmanned aerial system and/or aircraft to investigate ecosystem dynamics (U.S. DOE 2015b). In addition, the development of packages of sensors for coincident sensing of above- and belowground properties has shown promise to provide unprecedented observations and understanding of plant-soil or above- and belowground process interactions (e.g., Dafflon et al. 2017).

There are, however, significant challenges remaining to incorporate all these state-of-the-art sensing and characterization technologies into HPC-enabled simulations, and to provide actionable information in a real-time manner. A particular challenge is to adequately incorporate state-of-the-art airborne remote sensing and other point-scale datasets for providing soil, surface, and vegetation properties with sufficient spatial and temporal resolution, and for parameterizing, validating, and/or refining mechanistic models.

Within several DOE-funded projects, including the SFA watershed function and NGEE–Arctic projects, we intend to improve our ability to quantify three-dimensional (3D) distribution of bedrock-to-canopy characteristics that drive and modulate hydrothermal-biogeochemical processes, as well as to observe the spatiotemporal variability (in 4D) of critical properties and ecosystem responses to climatic perturbations in various subsystems and aggregated fluxes within water and nutrient cycles. A particular emphasis is to develop methodologies to effectively use time series of ground-based and airborne measurements. Time-series data are key to observe the system response to atmospheric forcing modulated by geology, geomorphology, and vegetation characteristics. Such information can be used to (1) detect and understand changes in trajectories and/or responses to disturbance, (2) estimate soil characteristics indirectly by ingesting data into model parameter-estimation algorithms (e.g., Tran et al. 2017), (3) improve mechanistic model parameterization and validation, and (4) evaluate the future behavior of watershed functioning.

Here we identify three areas of research that we consider crucial to improve the multiscale understanding of ecohydro-biogeochemical functioning:

1. **Above- and belowground co-variability for scaling:** Multiscale, multitype datasets (including point-scale and soil/core sample measurements, ground-based and airborne geophysics, airborne LIDAR and

multispectral imagery) can serve to build a 3D and/or 4D digital ecosystem. Because soil and other subsurface characteristics can only be measured at discrete locations across space, it is important to quantify the linkages among interacting above- and belowground properties and processes (Falco et al. 2019; Dafflon et al. 2017). The co-variability among subsurface properties and surface characteristics (e.g., geomorphology and vegetation) can then be used to estimate soil properties at the watershed scale from remote-sensing platforms using a probabilistic mapping technique or ecosystem functional zones construct (Wainwright et al. 2015). Identifying above-/belowground relationships will inherently benefit from development of novel ground-based sensors and remote-sensing techniques to improve estimation of soil, surface, and vegetation properties over space and time.

2. **Distributed continuous sensor network coupled with satellite remote sensing:** New sensing technologies —real-time sensors, telemetry, cloud computing, and remote sensing—provide enormous opportunities to better understand terrestrial systems and to better manage water and other resources. Numerous technological developments are ongoing to observe thermal-hydro-biogeochemical processes using distributed sensor networks (e.g., Oroza et al. 2016), including Lawrence Berkeley National Laboratory's EcoSENSE (see white paper, "An Integrated Suite of Sensing and Data Capabilities for Open Watershed Science," p. 106) and Distributed Temperature Profiling system (Léger et al. 2019). Similarly, remote-sensing products are becoming widely available with constantly increasing temporal and spatial resolution, which enable observation of plant and landscape signatures over space. Several spatiotemporal integration algorithms have been successfully developed, such as the Bayesian geostatistical methods, Kalman filter, and Spatio-Temporal Neural Network (Chen et al. 2013; Wainwright et al. in revision; Oroza et al. 2018; Ziat et al. 2017). For example, spatially sparse but temporally continuous data (e.g., time series from distributed sensor networks) and temporally sparse but spatially continuous data (e.g., imagery from satellites) can provide together enough spatiotemporal information on interacting processes to reconstruct spatiotemporal variability in specific vegetation or soil properties at watershed scale.

3. **Real-time data analysis and data-model integration algorithms:** Even though real-time sensor packages are becoming widely available, there have been limited applications of such real-time information effectively used for decision making in scientific research and watershed management (e.g., Schmidt et al. 2018). Currently, real-time sensor data are often used just for scientific understanding after all the data are collected and synthesized or management decisions are made infrequently such as once in a month. This limitation is due to the fact that it requires time and effort for one person or a team to synthesize all the information available. For example, plant phenology information such as the Normalized Difference Vegetation Index (NDVI) would need to be evaluated in conjunction with historical data or some trigger-level values for data-driven projections. The challenge is to integrate all the information quickly into actionable intelligence and/or a modeling framework. The back-end algorithms have to be evolved to synthesize all the datasets, such that we extract tractable and actionable measures based on a suite of real-time datasets, as well as drive large-scale ecohydrological and biogeochemical models. Improving near–real time processing and interpretation can certainly be improved by a data management system and shared workflow. For example, the API and Jupyter offer an opportunity to implement and combine various types of processing algorithms of remote-sensing datasets automatically obtained from the database (e.g., ESS-DIVE), as well as to track and visualize a workflow. The next step is to create a software ecosystem of processing and model-data integration algorithms (e.g., parameter estimation and uncertainty quantification) to bridge state-of-the-art sensing technologies and simulators.

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19. Modeling Concentrations and Evasion Fluxes of CO_2 in Rivers and Streams

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Statement of Problem

The evasion of carbon dioxide (CO_2) from surface waters to the atmosphere represents a significant flux within the terrestrial carbon cycle (Ciais et al. 2013), with early estimates on the order of ~2 petagrams of carbon (Pg C) per year (Raymond et al. 2013) that continue to increase (Sawakuchi 2017). However, due to the intensive nature of monitoring across relevant spatial and temporal scales, the true magnitude and dynamics of these fluxes remain largely uncharacterized (Duvert et al. 2018; Allen and Pavelsky 2018). Headwater streams, in particular, represent a major uncertainty in global flux budgets and may contribute a substantial and underestimated portion of global fluxes due to (1) higher turbulence and associated exchange rates with the atmosphere (Raymond et al. 2012) and (2) partial pressure of CO_2 (pCO_2) that is more reflective of subsurface environments on the order of 10^3 to 10^5 parts per million (ppm) (Marx et al. 2017). This uncertainty remains a significant gap in both conceptual models of the natural carbon cycle and the ability to monitor and predict changing fluxes into the future. Since the processes that control stream pCO_2 and evasion rates span a wide array of disciplines within the watershed science community and vary across environments, the development and application of scalable, mechanistic models depend on the ability to leverage existing research infrastructure such as the DOE Subsurface Biogeochemical Research (SBR) watershed test beds and the NSF Critical Zone Observatories (CZO) and NEON sites.

Scales and Processes

River and stream pCO_2 reflect a continuum of watershed processes that vary across spatiotemporal scales. Specifically, measured pCO_2 integrates the balance of high-pCO_2 groundwater inputs (reflecting soil respiration and chemical weathering), organic carbon respiration via hyporheic exchange, in-stream metabolism (the balance of respiration and primary production; Vannote et al. 1980), downstream transport, and the progressive evasion of CO_2 to the atmosphere. Current observations and conceptual models contend that the importance of these inputs and outputs varies broadly as a function of watershed scale (Duvert et al. 2018; Marx et al. 2017; Hotchkiss et al. 2015). Groundwater inputs dominate concentrations and fluxes at small-stream orders, with subsurface-level pCO_2 decaying rapidly as surface waters equilibrate with the atmosphere. The length scales over which this equilibration occurs have not been fully described, though discrete groundwater seepage zones have been shown to affect stream pCO_2 over as little as tens of meters of stream length (Johnson et al. 2008). At larger spatial scales where surface waters approach equilibrium with the atmosphere, in-stream carbon processing is thought to increase in importance (Hotchkiss et al. 2015). Again, however, there is yet no framework through which to predict where these transitions from upland to in-stream controls occur.

The processes that control stream pCO_2 and CO_2 fluxes also vary across temporal scales. Studies have demonstrated diurnal oscillations in stream pCO_2, reflecting cycles of stream metabolism (Schelker et al. 2016). Pairing pCO_2 with dissolved oxygen sensors may offer the potential to disentangle these diurnal drivers (Duvert et al. 2018; Hotchkiss et al. 2015). Storm and snowmelt events affect stream pCO_2 through a range of processes including (1) mobilization and flushing of high-pCO_2 upland soil- and groundwaters; (2) reductions in subsurface transit times that affect the extent of water-rock interactions; (3) the potential initiation of overland flow such that waters do not experience subsurface pCO_2 levels; and (4) increased stream turbulence and advection velocities that promote transport and evasion, among others. On seasonal scales, in-stream metabolism is controlled by temperature, light, and nutrient availability. Additionally, seasonal hydrologic shifts such as snowpack accumulation/melt or transitions between wet and dry seasons may alter subsurface flow regimes, groundwater inputs, and stream discharge and turbulence. Depending on subsurface water transit times, seasonal shifts in soil respiration and subsurface pCO_2 may also be translated to streams, particularly in small watersheds.

Challenges and Opportunities

The fundamental challenge in characterizing these processes is the fact that CO_2 is not conservative in surface waters and rapidly exchanges with the atmosphere. Thus, the ability to monitor streams at the necessary spatial and temporal resolutions to estimate integrative fluxes is often cost prohibitive. This problem is particularly pronounced for headwater streams, of which millions of systems exist across the continental United States. Currently, the only viable method for quantifying global headwaters' CO_2 budgets and for predicting and monitoring changes into the future is through the development and application of scalable models. A number of efforts to date have upscaled statistical distributions of measured stream pCO_2 by stream order and have employed empirical relationships among stream morphology, landscape characteristics, and discharge to model fluxes to the atmosphere (Raymond et al. 2013; Butman and Raymond 2011). Given the advances in conceptual models of watershed processes afforded by distributed research networks over the last decades, the community is now poised to develop a new generation of physically based models of stream pCO_2 and CO_2 evasion.

Reactive transport models, which allow for the integration of processes over the entire length of a stream network, are particularly promising based on their potential to overcome sampling limitations at low-order and ephemeral streams. New models should prioritize flexibility in incorporating complexity across CO_2 input and output parameterizations, including stream metabolism, groundwater concentrations and input fluxes, gas transfer coefficient parameterizations, and in-stream inorganic carbon speciation (Stets et al. 2017). Reactive transport codes of stream pCO_2 should also be developed to interface with existing distributed subsurface hydrologic models, some of which incorporate subsurface biogeochemistry (Beisman et al. 2015), at the sub-watershed to continental scale (Maxwell et al. 2015). This will facilitate the upscaling of watershed-validated models for larger-scale prediction and monitoring efforts. Additionally, pCO_2 evasion models along with distributed subsurface hydrologic models should be used to guide field monitoring designs to target "hot spots"/"hot moments," including predicted zones of groundwater seepage and the stream-length scales over which to optimize sensor spacing.

The development and application of stream CO_2 reactive transport models will require coordination across watershed science disciplines and the leveraging of existing research sites that target a broad range of environments. Common datasets collected at sites such as SBR watershed test beds, CZOs, and NEON sites, including stream discharge, soilwater/streamwater/groundwater geochemistry, soil respiration rates, and subsurface pCO_2 provide a foundational database for model calibration and evaluation. The recent availability of *in situ* pCO_2 sensors for stream and hyporheic zone monitoring also provides the opportunity to expand existing watershed research site infrastructure to specifically target these measurements. Communication will be necessary in developing community-level standard operating procedures and QA/QC to produce comparable data between sites, as neither of these currently exist for pCO_2 sensors. Additionally, ongoing efforts to characterize subsurface hydrology and groundwater/surface-water interactions at high resolution through near-surface geophysical methods and in-stream distributed temperature sensors may guide model development and validation at sub-watershed scales.

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20. Looking Within and Beyond Individual Watersheds for Integrated Hydro-Biogeochemistry Theory

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Watersheds are the fundamental units that support river networks, the blood vessels of Earth's surface that ultimately drain into the ocean. Watersheds are complex hydro-biogeochemical systems. They receive water, mass, and energy; transport them to distinct compartments; and transform them into various forms. These processes couple physical flow and chemical and biogeochemical processes. The process interactions and feedbacks are dictated not only by hydroclimatic forcings, but also by the architecture of a watershed, in particular aboveground characteristics such as land cover and surface topography and belowground structures such as soil depth, soil type, and root systems. These external forcings and internal idiosyncrasies govern the magnitude, timing, and distribution of water flow and chemicals (Chorover et al. 2011; Brooks et al. 2015), giving rise to nonlinear emergent behaviors at the watershed scale.

Understanding feedbacks and nonlinearity requires process-based models that integrate multiple interacting processes to decipher convoluted water and chemistry signatures encoded in water data (e.g., precipitation, discharge, and groundwater) and water chemistry data (e.g., carbon, nitrogen, phosphorus, and metals). Such integration, however, does not come easily with traditional boundaries of water- versus biogeochemistry-relevant disciplines. Relevant model development has been advancing along two separate lines: (1) hydrology models that have mostly focused on simulating surface- and groundwater processes at the watershed scale and beyond (Fatichi et al. 2016) and (2) reactive transport models that have primarily pivoted on transport and biogeochemical reactions in "closed" groundwater systems without as many interactions with the "open" surface water systems (Steefel et al. 2015; Li et al. 2017a). These approaches come along with a history of hydrologists, often trained as physicists with expertise in fluid mechanics, and biogeochemists and environmental engineers trained as chemists and biologists.

There are, however, critical needs to reach beyond disciplinary boundaries and integrate the two lines to develop watershed reactive transport models, not only to gain fundamental understanding of watersheds as complex systems, but also to solve today's pressing global environmental challenges. Natural systems such as watersheds, however, could not care less about artificial disciplinary boundaries; processes relevant to different disciplines all occur simultaneously. Research questions at the interfaces or "ecotones" of different disciplines can reveal fundamental mechanisms that shed light on puzzling observations arising from nonlinear emerging behaviors. In addition, it is important to possess the capabilities of forecasting not only for water quantity (flow), which is well under way with the National Water Model, but also for water quality (chemistry). Such capabilities are essential as the pace of climate change and human perturbation accelerates. A wide spectrum of water-related hazards (e.g., hurricanes, flooding, and droughts) looms (IPCC 2013). Large hydrological events bring out excessive water and disproportionally large pulses of "stored" contaminants that deteriorate aquatic and ecosystem health (Raymond and Saiers 2010; Huntington et al. 2016). On the other hand, droughts induce water-borne diseases (Perez-Saez et al. 2017) and deteriorate water quality (Ejarque et al. 2018). Problems related to excessive nutrient export, including eutrophication and hypoxia in rivers, lakes, and coastal areas worldwide, have lingered for decades and will continue to do so, calling for advanced tools for prediction and for management (Royer et al. 2006; Seitzinger et al. 2010; Van Cappellen and Maavara 2016; Van Meter et al. 2017).

Although solute and water quality models have been developed as add-ons to hydrological models (Arnold 1994; Donigian Jr. et al. 1995; Santhi et al. 2001), they typically have relatively crude representations of reactions, without rigorous formulation of reaction thermodynamics and kinetics developed in geochemistry and biogeochemistry. Reactive transport has been brought to the watershed scale only recently (Yeh et al. 2006; Bao et al. 2017; Li et al. 2017b).

Model development in both catchment hydrology and reactive transport has leaped forward without much interaction until very recently. Observations that record the integrated signature of water and water chemistry, nonetheless, have accumulated for decades. In fact, now is an exciting time marked by a deluge of data. The past decades have witnessed rapid advances in technology and unprecedented generation of Earth surface data from remote sensing from satellites (Hrachowitz et al. 2013; McCabe et al. 2017). Water and water chemistry data are collected through research networks including the CZOs, LTER, Great Lake Ecological Observatory Network (GLEON), USGS, and NEON, presenting unprecedented opportunities for integrated understanding. In that context, research sites championed by the SBR program [e.g., East River Watershed (Hubbard et al. 2018) in Colorado and the Columbia Flood Plain in Washington] offer multifaceted test beds with tremendous data in an interdisciplinary context and, therefore, platforms for integration, in a sense similar to CZOs (Brantley et al. 2007). It is indispensable in such a cross-disciplinary context to adopt diverse philosophies, perspectives, and approaches (Harte 2002).

In individual watersheds, researchers need to ask questions at the boundaries of multiple disciplines. For example, how are travel time and water age (hydrology) linked to water chemistry and biogeochemical rates (biogeochemistry)? How do they differ from theories developed in laboratory settings with simplified conditions? Functional relationships between these quantities will need to be developed. It is also crucial to go beyond individual watersheds. Because each watershed has its own hydroclimatic forcings and idiosyncrasies (e.g., land cover, soil type, lithology, and topography) that govern water flow, synthesis studies also are needed for a large number of watersheds to explore general patterns and principles and to classify: How do functional relationships vary under diverse climate, land cover, and geology conditions? What are the first-order control and watershed characteristics that can be used for prediction?

Answers to these questions are important not only for understanding watershed processes, but also for understanding cross-scale behavior [i.e., the connection between small-scale physics and large-scale behavior (upscaling)], a major challenge that has been extensively discussed in various disciplines (Beven 1989; Levin 1992; Sivapalan et al. 2003; Hrachowitz et al. 2013). Although spatially explicit hydrological models have advanced significantly over the past years, the issue of upscaling always arises when prediction is needed at larger spatial scales. An individual watershed may be one homogeneous grid block or even smaller than one grid block in large-scale models such as the National Water Model. Representing watershed reactive transport in these models requires going beyond spatial heterogeneities and process complexity that obscure results. Instead of measuring everything everywhere, efforts should focus on the end-members in distinct zones (e.g., surface water, soil water, and groundwater) that play a dominant role in different hydrological regimes. For example, studies need to focus on "hot spots" (e.g., riparian zones) and "hot moments" (e.g., storm events, snow melt, and droughts) where biogeochemical transformation rates are disproportionally high. Such efforts can guide projects toward reducing computational cost, facilitating explicit incorporation of feedback schemes, and forecasting the future, but also, more importantly, toward developing hydro-biogeochemical theory at the watershed scale.

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21. A Hierarchical, Process-Based Model as a Core Capability for Coordinating Distributed Networks of Watershed Science

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Models play a variety of crucial roles for distributed watershed science. Predictive models inform stakeholders about watershed problems, solutions, and implications of those solutions. Process-based models are unique in their ability to allow researchers to simplify and manipulate physical processes, determining causality and exploring process uncertainty. Finally, models provide a key data integration tool, filling gaps and providing context for distributed and heterogeneous data streams. Watershed science has greatly benefited from a strong modeling subdiscipline and will continue to do so in the future.

However, models are faced with an evolving challenge with increasing demands. More and more field and theoretical researchers are encouraged to ensure their science can "inform a model," and model developers are encouraged to ensure their models are driven, parameterized, and evaluated using data. In this white paper, I look to identify the key challenges facing process-based watershed models and suggest one view of what the core of a "virtual ecosystem" (U.S. DOE 2015) of watershed models would look like.

Challenges for Process-Based Models in Watershed Science

Watersheds are a critical national resource, but climate and human system changes and extremes provide unique challenges to watersheds across the nation. In addition to changing climate and land use, our watersheds are stressed by sources and transport of sediment, salinity, contaminants, and nutrients. While each watershed faces a unique climate, human, and infrastructure context, underlying each of these concerns is a common dynamical core of hydrologic flow and transport of chemical components.

Focusing then on this hydrologic core, several key features general to all watersheds make process-based modeling difficult. The hardest of these is scale. Hydrologic modeling has, as a community, identified hyperresolution models, or models that resolve full-river basins at the scale of tens to hundreds of meters, as a grand challenge and a key tool for understanding watershed function (Wood et al. 2011). However, others have noted that small-scale parameters and processes often determine key feedbacks within the water cycle, and they cannot realistically be resolved even at hyperresolution (Beven and Cloke 2012). For instance, (1) runoff generation is fundamentally altered by microtopography at the scale of centimeters to meters; (2) nutrient and contaminant processing often happens at "hot spots," and are being governed by hyporheic exchange at extremely small scales; and (3) natural and engineered systems such as fractured bedrock, impervious surfaces, and wastewater flow provide fast pathways that move water in ways not well captured by integrated hydrology models. Often the impact of these processes is measured at full-watershed or full-river basin scale—5 to 7 orders of magnitude larger than the processes themselves. The physics of these processes is difficult to measure and constrain; significant parametric and process uncertainty is ever present.

Given even a sufficient model of flow and reactive transport across watersheds, the driving, parameterizing, and evaluating of that model bring their own set of difficulties. Individual projects tend to develop "one-off" data products, such as specific meshes at one resolution for one watershed, hand-tuned and bias-corrected precipitation datasets, or point measurements of tracer experiments or river discharge that link models to data. The heterogenous nature of data products provides a key challenge for process-based models across watersheds; enabling models to tap the wide range of available datasets is a critical challenge.

The Dynamical Core of a Virtual Ecosystem of Watershed Modeling Capability

While watersheds vary greatly and individual research questions need individualized models and data, a distributed network of watershed science would be greatly enabled by a common dynamical core that is *broadly applicable but locally relevant*. Such a capability, based on integrated surface and subsurface flow and transport of chemical components, would be the core backbone of a virtual ecosystem of models and data and would provide a coordinating base for watershed scientists wanting to integrate their research with the broader community.

One way of addressing the wide range of scales needed for watershed science is through hierarchically multiscale models. The first scale jump would be from the full–river basin or full-watershed to the sub-basin or sub-watershed level, where individual catchments are decomposed in a coarse-scale domain decomposition. By leveraging the inherently weak connection of water across sub-watershed boundaries, physics is used to determine inherent parallelism, computationally exploiting a strategy used throughout watershed science history.

This decomposition would be fundamentally more scalable than existing globally coupled models, and it would enable adaptation of hydrology for leadership-class computers, which rely on graphics processing units (GPUs) and other novel architectures to provide the extreme computational throughput needed for hyperresolution simulations. This approach would be inherently performance portable, allowing investigations of individual catchments on laptops, in addition to studies of full-river basins on leadership-class computing resources. And the approach need not be less accurate than globally implicit methods; novel algorithms in nonlinear domain decomposition suggest strategies for efficiently recovering the globally implicit solution.

The second scale jump would be within individual hyperresolution grid cells to capture the fine-scale processes identified above. Subgrid models (Jan et al. 2018) would be developed and evaluated to capture microtopographic runoff generation, hyporheic exchange fluxes to drive travel time–based approaches for hot spot/"hot moment" biogeochemical models, and natural and engineered water fast paths. These models, conceptualized and calibrated using fine-scale measurements and process understanding, would be critical to address the huge range of scales integrated by hydrologic processes.

In addition to being performant for hydrology, a virtual ecosystem capability must admit and encourage the development of process components across disciplines and specific to individual research questions. Flexible software design (e.g., Coon et al. 2016) allows such components to be included through interfaces (e.g., Johnson and Molins 2015), introducing configurable hooks to allow these components to feed back on the core capability. Such software flexibility is essential for the inclusion of biogeochemical reaction pathways, ecosystem function and plant hydraulics, and coevolving social networks of institutions and individuals.

Finally, a distributed network for watershed science must focus on robust workflows for incorporating a broad set of data into models instead of the current approach of "one-off" products. The explosion of remotely sensed data products and new approaches in data science, such as machine learning and artificial intelligence for identifying, contextualizing, and generalizing data, provide an exciting new frontier for automating the process of integrating heterogeneous data into models. Integrating data centers (e.g., ESS-DIVE) with models through workflow tools would increase the impact of both data and models.

In conclusion, watershed science is in need of a broadly applicable but locally relevant, process-based modeling capability based on flow and reactive transport across scales. Such a capability would allow generalization and coordination across research projects and questions, and it would greatly improve the productivity of scientists across a distributed network of watersheds. Furthermore, thanks to advances in computational performance, physical understanding, algorithms, data sources, and data integration science, such a capability is currently tractable.

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22. Using Machine Learning to Leverage the Value of Big Data and High-Frequency Monitoring in Characterizing Watershed Sediment Dynamics

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Characterizing the transport of sediments and associated nutrients to downstream receiving waters is one of the most important functions of watershed science. Understanding the spatial and temporal patterns of sediment transport within river systems is key to effectively managing water resources for drinking water, recreational use, and ecological health. Transport is frequently episodic, occurring primarily during hydrological events triggered by rainfall-runoff processes, making detailed characterization of dynamics challenging. In the hydrology and environmental monitoring fields, we have refined the ability to measure sediment and nutrient yields through the development of a robust streamflow gauging network and reliable sampling and sensor technologies (e.g., Jones et al. 2018). This has provided important information on the amounts and, to some extent, the timing of sediment and nutrient delivery to receiving waters. A current challenge is to advance further the characterization of the dynamics within the watershed through analysis of high-frequency sensor data. How to accomplish this and what makes this the right time to invest in addressing this challenge are key questions.

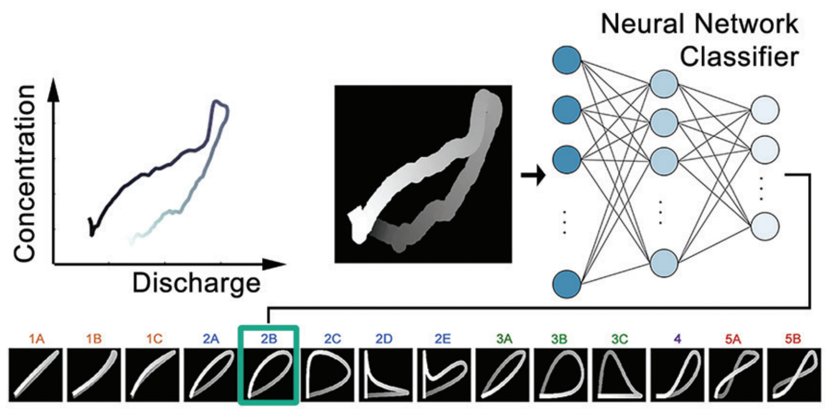

Fig. 1. Application of machine learning to analyze concentration-discharge relationships of individual hydrological events and categorize those events based on visual patterns. [University of Vermont, Burlington]

Hydrologists and environmental managers for decades have conducted routine, periodic sampling of rivers and have developed models to estimate nutrient fluxes effectively. Examples are the use of the Soil and Water Assessment Tool (SWAT) models; Hydrologic Engineering Center's River Analysis System (HEC-RAS) models; and Weighted Regressions on Time, Discharge, and Season (WRTDS) regression models to study sediment and nutrient fluxes into Lake Champlain (U.S. EPA 2013; Medalie 2016). This central landscape feature of Northern New England is under threat from excessive phosphorus and sediment loading, triggering the development of a Total Maximum Daily Load (TMDL) for phosphorus and a critical need for understanding spatial and temporal patterns of sediment transport within watersheds.

Currently, we can leverage two recent advances in science and computing. They are the use of high-frequency sensors to monitor rivers nearly continuously and the ability to leverage advanced algorithms and computing power to recognize intricate patterns in observed data. For instance, networks of optical turbidity sensors have resulted in a continuous time series of accurate, suspended-sediment concentration estimates for likely hundreds of rivers spanning many years and thousands of storm events. Similarly, for nutrients, high-technology optical sensors are yielding near-continuous records of nitrate and dissolved organic carbon (DOC; Pellerin et al. 2016; Vaughan et al. 2017; Snyder et al. 2018). Next, we have the advancement of machine-learning and deep-learning methods. Driven by advances in computing power, available datasets, and breakthroughs in algorithms, extensive research into applications of deep learning and machine learning has been sparked (LeCun et al. 2015). Application of machine learning such as artificial neural networks to hydrological data has taken place for decades (Abrahart et al. 2012); however, the robust application of deep-learning and advanced machine-learning techniques lags significantly behind that in other fields such as finance, autonomous vehicles, medical imaging, and social media.

An example of the potential of these techniques in applied hydrology and watershed science can be found in a proof-of-concept project we conducted that automated the analysis of hydrological events using machine learning (Hamshaw et al. 2018). Events were characterized by a restricted Boltzmann machine neural network (a foundational network of deep-learning techniques) that was trained to learn and classify the visual shapes (patterns) of data collected during individual storm events. This type of analysis, colloquially referred to as hysteresis analysis, has been utilized in hydrology for inferring watershed sediment dynamics (Williams 1989; Aich et al. 2014). The use of high-frequency monitoring data and advanced machine-learning algorithms (adapted from computer vision research) allowed us to expand the hysteresis analysis approach to larger datasets through automation and to leverage more intricate patterns for a more nuanced analysis (Hamshaw et al. 2018). The result was the ability to infer sediment dynamics within watersheds to a greater extent than was previously possible based solely on monitoring data collected at the watershed outlet.

However, the potential to leverage big data and machine learning in the hydrological sciences has not been fully realized for various factors. First, the data associated with tens of thousands of hydrological events likely monitored across the United States need to be made more accessible to a wide variety of users (Pellerin et al. 2016). Aggregation of large datasets to further develop these methods and models is hampered by fragmentation of monitoring data repositories and lack of consistency in data management and publication. Second, for robust analysis of water quality sensor data, further attention to the temporal data segmentation is warranted. *Ad hoc* methods of event segmentation are often implemented on a per-study basis and the extraction techniques often glossed over in results. Given the key episodic behavior of the majority of water quality data, there is a need to refine temporal data analysis methods and agree on standard approaches to identify what constitutes an "event." The development of a coordinated, open network of watershed monitoring programs and datasets will help to spark further advancement of big-data and machine-learning analysis of watershed systems. In addition, data-driven analysis and machine-learning methods will be especially powerful when combined with on-the-ground knowledge of watershed perturbations or synoptic monitoring programs, leading to development of a "library" of watershed responses to a changing climate.

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23. Cyberinfrastructure Requirements and "Repository of Repositories" Concept

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Currently, extensive data are being generated around watershed systems by various resources funded by DOE, USGS, NSF, and USDA. A broad cyberinfrastructure exists to serve as repositories and organizational systems for all these data. Key examples in this field include ESS-DIVE (e.g., sensor data and genomic data), KBase (primarily, genomic and multiomic data), WHONDERS (e.g., amplicon datasets, metagenomes, and metabolomes), and CUAHSI. Currently, there is minimal to no interaction/interconnection among these resources.

It is critically important that these repositories be interoperable. They should share a common set of user accounts (perhaps, based on ORCID) and user organizations (e.g., laboratories and projects), a requirement which will facilitate the ability to move even private data seamlessly between and among these resources. A user in one resource should be able to query other resources and transfer the data as needed. Because multiple data products generated from a single environment or environmental sample may be spread across multiple repositories, it is critically important that these repositories use a common sample/environment identifier (ID). Ideally, this ID should be linked somehow to a DOI; it could be created at the project level, with subdata items maintained as sub-IDs linked to a top-level DOI). Repositories must agree on standards for sample IDs, environmental IDs, name standards for geographical locations, and, ideally, even unit/format standards for certain data types.

Cyberinfrastructure is also required to enable users to run common analyses on their data. Existing tools like KBase already offer this capability, although many tools of interest to the ESS community are not currently available in KBase (e.g., PFLOTRAN, trait-based modeling, and ecosystem modeling). Many of these tools can (and already are) being ported into (or linked to) KBase (e.g., PFLOTRAN, trait-based modeling, and IDEAS). Other simulation environments also exist, many of which are built on Jupyter notebooks (e.g., KBase). An example is CUAHSI.org. The standard of using Juptyer notebooks (or similar environment) as a mechanism for preserving provenance on analyses performed by users to facilitate scientific reproducibility and transparency is essential for open science. Cyberinfrastructure should support the capture, storage, query, retrieval, and rerunning of scientific analyses, with links to all data used in each given analysis. Having a DOI for these stored analyses would probably be useful.

Also critical is that full provenance is captured for each derived data product. By this, we mean that a derived data product (e.g., a genome) should link back to the raw data from which the product was created (e.g., raw reads), as well as the algorithms and parameters used to create the product (e.g., gene callers and assemblers). This is particularly helpful when the field has yet to arrive at completely standardized workflows or ontologies (e.g., true in the case of taxonomy). If the raw data are linked to the derived product, then a user can re-analyze the raw data as needed to produce a new ontology or apply an updated workflow or technique.

One compelling idea that emerged in the meeting was to construct a "repository of repositories," which would link together datasets from many different repositories based on whether the data came from a common location, involved a common species (e.g., taxonomical term), involved a common biological function (e.g., enzymatic function), involved common vegetation (e.g., as predicted from LIDAR), or involved a common biological sample (e.g., metagenomes, metabolomes, and amplicon data, all collected from a single sample). These terms and IDs would be loaded into a relational database of metadata, with each term linking back to all data products in all repositories that involve that term. These metadata terms would not be limited to direct descriptors of a data object (e.g., location and sample ID). Terms also could be derived categorizations or classifications assigned by an algorithm (e.g., taxonomy assigned to a clustered set of amplicon reads, function assigned to a protein sequence, and vegetation assigned to a LIDAR pattern). These terms can form hierarchically organized layers (e.g., metabolite, reaction, pathway, and subsystem). Terms could also be statistical descriptors assigned to regions of spatio-temporal data (e.g., noisy, volatile, and flat). Terms could even be assigned based on phenotypes and behaviors generated by complex reaction transport models (e.g., conservative transport, essential gene, and fast-growing organism). By assigning these terms, a very complex and difficult to digitally introspect data product (e.g., a spatiotemporal simulation) can be distilled down to high-level descriptions of system properties and behavior exposed by the simulation. Terms also could be mapped to datasets by text-mining publications linked to the same datasets. We anticipate that machine-learning classifiers will be used extensively to assign these terms to raw and derived data. For these terms to be useful, it is critically important that they be pulled from a controlled vocabulary maintained and kept standardized across this metadata repository. Once created, this repository will support sophisticated queries (e.g., "show me all environments where transport is conservative"; "compare all amplicon datasets from environments with high and low redox scores, and show me the species that are significantly different"; and "which parameters/terms have the greatest impact on water quality"). Statistical hypotheses and models can also be applied to this database to test the fit systematically to all available data (e.g., how much of the variability in water quality is explained by vegetation alone). Machine-learning/model-learning approaches can be used for this last task. The data and analysis provenance cyberinfrastructure (described earlier) will be critical for this resource to be useful, because this provenance will enable users to dive deeply into the specific data/terms that are identified as important to a specific scientific question of interest.

Appendix 5. References

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Appendix 6. Acronyms and Abbreviations

1D, 3D, 4D	one-, three-, and four-dimensional
AI	artificial intelligence
AMT	audiomagnetotelluric
ANL	Argonne National Laboratory
API	application programming interface
ARM	CESD Atmospheric Radiation Measurement program
ASR	CESD Atmospheric System Research program
BER	DOE Office of Biological and Environmental Research
BERAC	Biological and Environmental Research Advisory Committee
BSSD	BER Biological Systems Science Division
CEAP	USDA Conservation Effects Assessment Project
CESD	BER Climate and Environmental Sciences Division
CO_2	carbon dioxide
CONUS	continental United States
COS	Center for Open Science
C-Q	concentration discharge
CUAHSI	Consortium of Universities for the Advancement of Hydrologic Science, Inc.
CZO	Critical Zone Observatories
DataONE	Data Observation Network for Earth
DO	dissolved oxygen
DOE	U.S. Department of Energy
DOE-LM GEMS	DOE Office of Legacy Management Geospatial Environmental Mapping System
DOI	digital object identifier
DOM	dissolved organic matter
E3SM	Energy Exascale Earth System Model
EMI	electromagnetic interference
EMSL	DOE Environmental Molecular Sciences Laboratory
EPA	U.S. Environmental Protection Agency
ERI	erosion resistance index
ESM	Earth system model
ESS	Environmental System Science
ESS-DIVE	Environmental Systems Science Data Infrastructure for a Virtual Ecosystem
FAIR	findable, accessible, interoperable, and reusable
FBA	flux balance analysis
FICUS	Facilities Integrating Collaborations for User Science
FOA	funding opportunity announcement
FTICR-MS	Fourier-transform ion cyclotron resonance mass spectrometry
GGIS	Global Groundwater Information System
GPR	ground-penetrating radar
GUI	graphical user interface
HBGC	hydro-biogeochemistry
HIS	Hydrologic Information System
HPC	high-performance computing
ICON	integrated, coordinated, open, and networked
IDEAS	Interoperable Design of Extreme-scale Application Software
I/O	input/output
JGI	DOE Joint Genome Institute
JPL	NASA Jet Propulsion Laboratory
KBase	DOE Systems Biology Knowledgebase
LBNL	Lawrence Berkeley National Laboratory

LIDAR	light detection and ranging
LLNL	Lawrence Livermore National Laboratory
LTAR	Long-Term Agroecosystem Research initiative
LTER	Long-Term Ecological Research network
ML	machine learning
MODEX	model-experimental coupling
NASA	National Aeronautics and Space Administration
NASEM	National Academies of Sciences, Engineering, and Medicine
NAWQA	National Water-Quality Assessment
NEON	National Ecological Observatory Network
NEST	network of energy sustainability testbeds
NGEE	Next-Generation Ecosystem Experiments
NGWMN	National Ground-Water Monitoring Network
NHD	National Hydrography Dataset
NIFA	USDA National Institute of Food and Agriculture
NMDC	National Microbiome Data Collaborative
NOAA	National Oceanic and Atmospheric Administration
NRCS	USDA Natural Resources Conservation Service
NSF	National Science Foundation
NWM	National Water Model
ORNL	Oak Ridge National Laboratory
OSTP	Office of Science and Technology Policy
PFLOTRAN	Massively Parallel Reactive Flow and Transport Model
Pg C	petagrams of carbon
pCO_2	partial pressure of CO_2
PI	principal investigator
PNNL	Pacific Northwest National Laboratory
QA/QC	quality assurance and quality control
S^3	Solo, Share, Synergy
SBR	CESD Subsurface Biogeochemical Research program
SFA	Science Focus Area
SLAC	SLAC National Accelerator Laboratory
TEM	transient electromagnetic
TES	CESD Terrestrial Ecosystem Science program
USDA	U.S. Department of Agriculture
USGS	U.S. Geological Survey
WHONDRS	Worldwide Hydrobiogeochemistry Observation Network for Dynamic River Systems
WRF-Hydro	Weather Research and Forecasting Hydrological modeling system

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