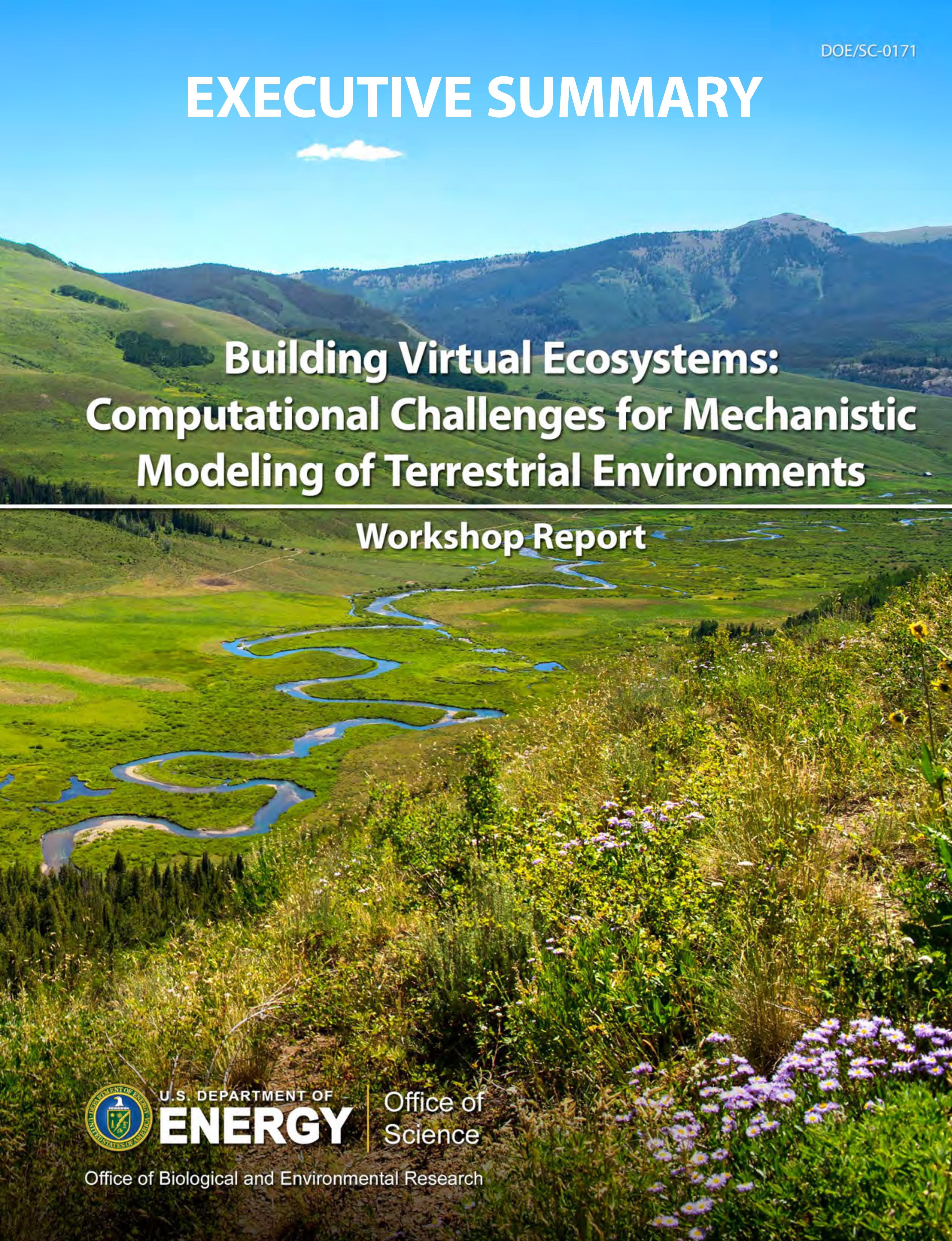
DOE/SC-0171

EXECUTIVE SUMMARY



Building Virtual Ecosystems: Computational Challenges for Mechanistic Modeling of Terrestrial Environments

Workshop Report

U.S. DEPARTMENT OF ENERGY | Office of Science

Office of Biological and Environmental Research

Executive Summary

The mission of the Climate and Environmental Sciences Division of the Office of Biological and Environmental Research (BER) within the U.S. Department of Energy's (DOE) Office of Science is "to advance a robust, predictive understanding of Earth's climate and environmental systems and to inform the development of sustainable solutions to the nation's energy and environmental challenges." This formidable challenge requires quantification of stocks and controls on states, fluxes, and residence times of water, carbon, and other key elements through all components of the terrestrial system. These components include vegetation, soils, the deep vadose zone, groundwater, and surface water. To achieve this level of predictive understanding, a new generation of multiscale, multiphysics models is needed for terrestrial systems—models that incorporate process couplings and feedbacks between various "pools" (i.e., vegetation, soils, subsurface aquifers, and surface waters) across wide ranges of spatial and temporal scales.

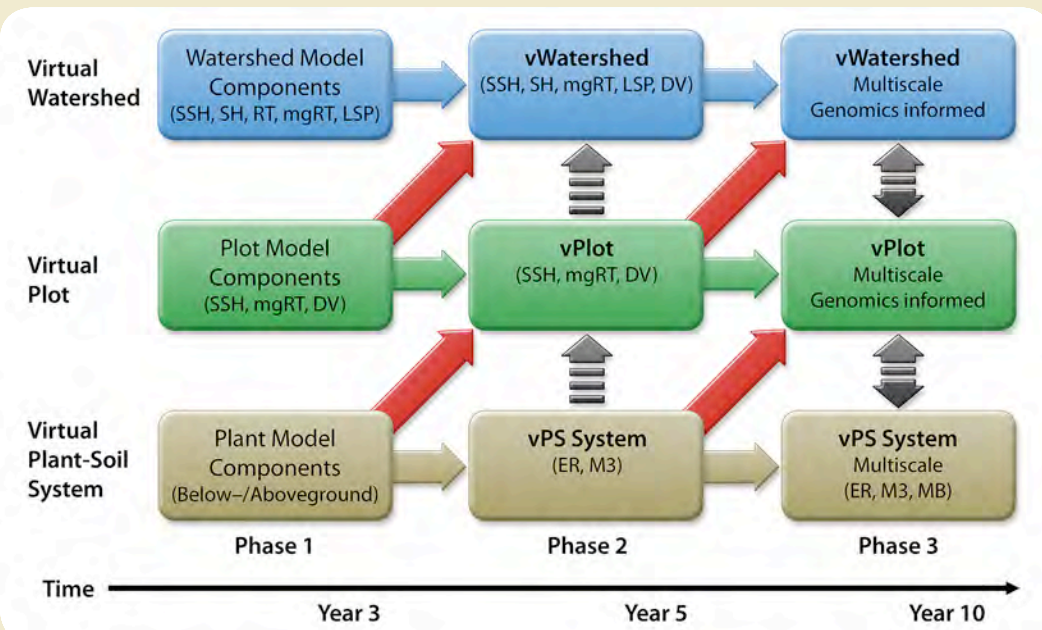
To explore the potential of a new generation of multiscale, multiphysics models for revolutionizing the understanding of terrestrial ecosystem dynamics, BER held the Computational Challenges for Mechanistic Modeling of Terrestrial Environments workshop on March 26–27, 2014, in Germantown, Maryland. The workshop brought together 29 researchers with diverse expertise, including hydrologists, environmental scientists, ecologists, microbiologists, plant scientists, and computational scientists. Through a combination of invited talks, breakout sessions, and report-back discussions, workshop attendees identified challenges and research opportunities needed to develop a more seamless and continuous framework for mechanistic modeling of terrestrial environments extending from the bedrock to the atmospheric boundary layer and from single-plant systems to fields of crops to watersheds and river basins.

Three broad scientific challenges were identified. At the scale of individual plants, a more robust, predictive capability requires greater focus on integrating, at the whole-organism level, the rapidly developing mechanistic understanding of plant growth, form, function, and interactions with the surrounding biotic and abiotic environment in the soil and rhizosphere. At the scale of catchments and watersheds, the central challenge is to develop high-resolution watershed-scale models of the hydrological, carbon, and nutrient cycles with tractable representations of the integrated vegetation-hydrological-biogeochemical systems. Cutting across the disparate spatial and temporal scales is the third challenge of improving models for biogeochemical cycling, including more realistic descriptions of microbiological communities and their function and better representations of the effects of small-scale processes and heterogeneities at field scales. These three individual challenges are interlinked, emphasizing the multiscale, interdisciplinary nature of the overarching challenge.

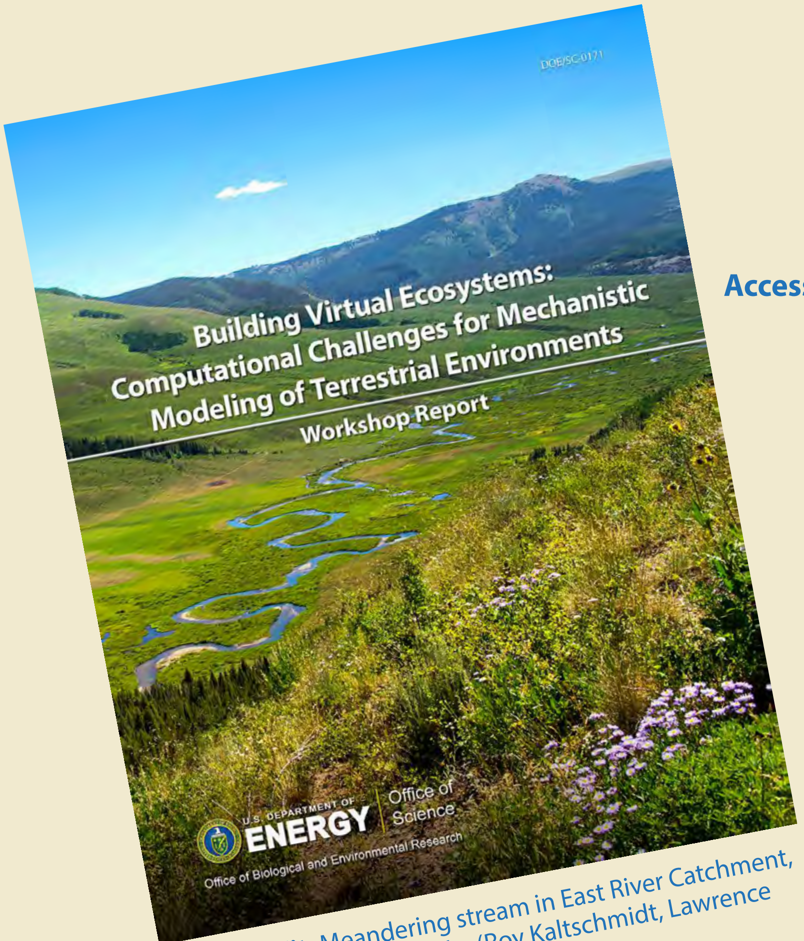
To meet these three challenges, three research opportunities were identified: (1) a *virtual plant-soil* model that combines mechanistic models of plant growth, form, and function with high-resolution models of hydrological and biogeochemical processes in the surrounding soil and rhizosphere; (2) a *virtual plot* model that combines multiple virtual plants or parameterizations of individual plants with detailed representations of belowground processes; and (3) a *virtual watershed* model that tracks fluxes and storage of water, energy, carbon, and nutrients on the surface and in a three-dimensional subsurface. The third opportunity should take into account the effects of small-scale processes and heterogeneity and employ more sophisticated and comprehensive treatments of hydrological, elemental, and nutrient cycling in subsurface and surface waters, which is mediated by vegetation and exchanges between the atmosphere and land surface.

Just as progress in experimental science depends on technological advances in instrumentation, progress in computational science requires advances in hardware, software, and algorithms. A new generation of multiscale, multiphysics models for terrestrial systems will require careful attention to software design, productivity tools, and programming models. Recent trends in hardware design raise uncertainty about programming models and the actual performance of application codes. Moreover, software development tools and programming models have not kept pace with changes in hardware, creating significant uncertainty for domain and computational scientists. This confluence of disruptive trends in computer hardware with the drive toward predictive, multiscale simulations is putting immense pressure on the scientific community to find new ways to maintain its scientific productivity. However, these challenges also create opportunities, which led the DOE Office of Advanced Scientific Computing Research (ASCR) to convene an interdisciplinary workshop, Software Productivity for Extreme-Scale Science, in January 2014. An important finding of that productivity workshop was that significant improvements in development practices and library interoperability could underpin a shift toward a more agile collection of high-quality composable components, ultimately maintaining or even enhancing productivity. This paradigm shift to an agile collection of interacting components, which the ASCR workshop participants coined a "software ecosystem," expresses the need to go beyond the modularity of traditional multiphysics codes to a higher level of interoperability.

To meet BER's programmatic goals as outlined in several recent documents (workshop reports, strategic plans, and advisory council reports), the BER scientific community will need to adopt this paradigm shift. Doing so presents an exciting opportunity to establish a new community approach to modeling and simulation, in which multidisciplinary domain scientists work closely with computational scientists to develop interoperable modules that can be assembled in flexible configurations within a common framework, making possible the simulation of the multiscale structure and function of a variety of terrestrial environments. This report concludes that adopting this new approach is necessary to overcome the challenges associated with increasing model complexity and the disruptive effects of new computer architectures. The result will be a significant improvement in the scientific productivity of a BER research portfolio that is increasingly focused on predictive simulation tools as an integrative science outcome.



Schematic of Phased Development of Multiscale Modeling Based on an Ecosystem of Interoperable Components. The spatial scale (vertical) is subdivided into the virtual plant-soil system, virtual plot, and virtual watershed. In the first phase (~ 3 years), the focus is on the collection and design of components for existing and new mechanistic models at each scale. Components include shoot and root models of plant function, subsurface hydrology (SSH), surface hydrology (SH), reactive transport (RT), microbial genomics–informed RT (mgRT), land-surface processes (LSP), and dynamic vegetation (DV). Phase 2 (~5 years) marks the initial prototype of virtual laboratory capabilities at each scale with increasing runtime configurability and use of upscaled or high-fidelity subgrid models (red and black dashed arrows). These models include environmental response (ER) plant models and multiscale mechanistic models encompassing genetic to organismic scales (M3). Finally, in Phase 3 (~10 years) the virtual capabilities reach full maturity with flexible, multiscale coupling and advanced support for data integration and analysis workflows, including integration of the plant microbiome (MB).



Cover Credit: Meandering stream in East River Catchment, Gunnison County, Colorado. (Roy Kaltschmidt, Lawrence Berkeley National Laboratory).

Access the entire report via:

http://doesbr.org/VirtualEcosystems/

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