MULTISECTOR DYNAMICS

Scientific Challenges and a Research Vision for 2030

MultiSector Dynamics

A Report by the MultiSector Dynamics Research Community for the U.S. Department of Energy's Office of Science, Earth and Environmental Systems Modeling Program

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Preface

This report outlines a vision for MultiSector Dynamics (MSD) as an emerging transdisciplinary field that seeks to advance our understanding of how human-Earth systems interactions shape the resources, goods, and services on which society depends. The core objective of this MSD Vision Report is to clarify core definitions, share research questions, highlight scientific opportunities, and provide steps for improving the MSD community's capacity to support needed scientific progress.

The report has several technical audiences in mind. These include current MSD researchers, scientists working in complementary fields who wish to learn more about opportunities for engagement, and research program managers at the US Department of Energy (DOE). Additionally, the research-to-operations (R2O2R) and community building elements of the report hold value for a broad array of US federal agencies as well as other governments and international organizations. As a transdisciplinary endeavor, the vision presented here should have elements that directly interest sectoral analysts engaged in energy, water, agriculture, transportation, health, etc. We hope these audiences will find the report a helpful reference and a source of opportunities for shaping the future of MSD science.

The report incorporates ideas and insights from the members of the recently established MSD Community of Practice (CoP). MSD finds its roots in a number of research fields and communities, including integrated assessment; impacts, adaptation, and vulnerability; Earth system science; and complex adaptive systems. However, the MSD CoP draws its conceptual basis from a 2016 workshop sponsored and led by the DOE, "Understanding Dynamics and Resilience in Complex Interdependent Systems: Prospects for a Multi-Model Framework and Community of Practice," organized with other federal agencies and hosted by the US Global Change Research Program (Moss et al., 2016). The rationale for the CoP is that research on understanding risks and opportunities arising from tightly connected human and natural systems is fragmented across several fields, requiring improved collaboration and synthesis to accelerate needed scientific advances. A CoP Facilitation Team and a Scientific Steering Group (SSG) were launched in 2019 to advance the needed collaborations and scientific synthesis. Since that time, an initial core group of projects supported by DOE's MSD research program has provided input to the development of the CoP through activities including a community questionnaire to identify current tools and research interests, regular meetings of technical working groups (WGs), MSD community briefings, research workshops, and the MSD CoP website.

The members of the MSD SSG and Facilitation Team are responsible for drafting this report, based on the above community inputs as well as a formal review of recent research within related fields such as Earth system science, integrated assessment modeling, economics, decision science, socio-ecological systems, socio-environmental systems, complexity science, systems engineering, energy transitions, urban systems, and coastal dynamics. Members of the major projects in the DOE MSD research program provided extensive comments on a first draft of the report (see Chapter 2.2 for descriptions and links to projects' websites for additional information). Robert Vallario, program manager for the DOE Earth and Environmental Systems Modeling MSD research program area, has provided insights, perspectives, and comments that have been critically important throughout the process. The SSG and the Facilitation Team thank these individuals for their many contributions and ongoing support. In addition, the Facilitation Team thanks the DOE Office of Science, Earth and Environmental System Modeling program for financial support of its activities through the Integrated Multisector Multiscale Modeling (IM3) project.

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Executive Summary

MultiSector Dynamics (MSD) is the study of how complex Earth, environmental, infrastructure, governance, and socioeconomic systems co-evolve in response to current and rapidly changing influences and stressors (Figure ES.1). MSD is a transdisciplinary research area that seeks to advance our understanding of how human-Earth system interactions and feedback shape pathways of societal change across scales and uncertainties. This report, developed collaboratively by the recently established MultiSector Dynamics Community of Practice (MSD CoP), presents opportunities and a vision for MSD research to advance our understanding of the local to global systems and processes that shape interdependent risks and the welfare of our modern world. This report summarizes current MSD research, synthesizes insights from these early investments, defines key concepts, identifies areas for further research, and proposes a collaborative research strategy based on open science principles and growing a diverse workforce to accelerate progress. The report grows out of several years of interactions and dialog among participants in the MSD CoP while also drawing on a breadth of reviewed research literature, reports as well as white papers, and input from the broader research community. It is targeted at technical audiences including the MSD community itself, potential collaborators in related research communities, as well as broader research programs in the United States and other countries.

Motivation: Managing Risks and Transitions in Complex Systems

The next decade represents a tremendous opportunity for the United States to address the many societal and environmental challenges we face, such as climate change and energy security. The impacts of a wide range of stressors (e.g., wildfires, floods, droughts, sea-level rise) and influences (e.g., advances in education, economic development, and technology transitions) highlight the importance of understanding how critical societal systems (i.e., infrastructure, governance, and socioeconomic systems in Figure ES.1) are shaped by and also shape Earth and environmental systems. These systems are interdependent through flows of materials, energy, water, land, human capital, and other resources, as well as through networks of markets, formal governance structures, and other socioeconomic institutions and processes. Human-Earth system feedback has profound implications for societal and environmental well-being.

Energy, including potential energy transitions, serves as a primary example of the complex interdependence between the human, Earth, and environmental systems. Energy is central to the operation of most human systems, impacting water supply, agriculture, transportation, industry, communications, and most aspects of everyday life. The strong interconnections and interdependence of energy with other sectors and the Earth and environmental systems pose unique scientific challenges for evaluating ambitious transition plans for energy production, transmission/transportation, and use.

Neglecting these interdependencies can increase risks and vulnerabilities to essential goods and services, or lead to unrealized synergies and co-benefits. A better quantitative understanding of how sectors and systems interact and co-evolve can increase adaptivity and innovation, improve societal and economic returns on investments, and strengthen local to national decisionmaking, resilience, sustainability, and competitiveness.

The US Department of Energy (DOE) is supporting the development of the field of MSD research through critical investments in fundamental research that leverages a rich legacy of science, modeling, and analytical capabilities to inform the next generation of US infrastructure decisions and deliver critical decision-relevant scientific insights into major societal challenges.

Figure ES.1: Sectors are complex systems-of-systems that shape themselves through their dynamic interactions and feedback with broader Earth, environmental, infrastructure, and socioeconomic systems.

MSD: the Science of Complex Adaptive Human-Earth Systems

The field of MSD explores the dynamics and co-evolutionary pathways of human-Earth systems with a focus on critical goods, services, and amenities delivered to people through interdependent sectors such as energy, food, transportation, health, housing, and recreation. MSD research focuses on how these sectors interact as they incorporate inputs, processes, influences, and constraints as well as feedback across Earth, environmental, infrastructure, governance, and socioeconomic systems (Figure ES.1). MSD has a distinguishing central focus on developing the next generation of open-source models and analytical tools needed to trace how major societal transitions influence—and are influenced by—environmental, technological, and socioeconomic risks and resilience. MSD seeks to specifically illuminate the emergent effects of complex interactions across sectors, systems, and their path-dependent processes.

To date, ongoing MSD research efforts have addressed science questions about the interactions of energy, water, land, food, ecosystems, climate, the economy, and demographics, primarily relying on coupled human-Earth systems modeling frameworks. They have focused on radiative forcing, land-use change and biogeochemical cycles, changes in climate and extreme weather events, and related conditions such as hydrology and sea level, and the implications of these changes for ecosystems and human systems. There is also a growing focus on the interactions and feedback of these phenomena. Scientific results have been leveraged to provide insights into issues such as how infrastructure investments in the next decade will shape the resilience of sectors, systems, and communities over the next 10–100 years. MSD research has identified opportunities and risks for regional and global economic development in the

face of changing weather patterns and extremes, major technological shifts, constraints on the availability of natural resources, and feedback to and from natural systems.

Opportunities for Advancing MSD Science

The scientific challenges highlighted in this report involve modeling interconnected human-natural systems and are thus among the most complex problems in science. The emergent complexity of the processes and outcomes that MSD addresses, varying from planned societal transitions (e.g., deep decarbonization) to coping with shocks (e.g., economic, climate, and/or social), creates a tremendous need for accelerating the scope and depth of knowledge required to advance scientific understanding. Advancing our understanding requires capturing and developing high-resolution representations of a wide range of environmental and socioeconomic processes. The processes and behaviors that govern human systems are often not well understood, and the uncertainties associated with factors such as future emissions trajectories and climate impacts are larger than the uncertainties associated with how the Earth system will respond, thus placing large methodological and computational demands on uncertainty quantification and characterization. The developed high-resolution representations of these processes need to be integrated into the complex regional-to-global contexts to capture the many co-evolving interdependencies and interactions that are shaping emergent risks and vulnerabilities. Many interdependent sectors and systems are involved through feedback that lead to co-emergent properties that shape risk, resilience, vulnerability, equity, and other measures of societal consequences. The unique characteristics of landscapes and geographies across the globe (e.g., coastal, urban, and Arctic) alter these processes and dynamics significantly, adding to MSD research and modelling challenges.

Advancing MSD science requires improving the scientific capacity of the MSD research community to understand and model complex interactions, interdependencies, and co-evolutionary pathways of coupled human-Earth systems. It requires taking advantage of innovations in data analytics, uncertainty quantification methods, artificial intelligence (AI), scientific visualization, and leadership class computing. It will require a commitment to open science and improved mechanisms for training a growing collaborative community. Advancing MSD science presents the following key scientific opportunities:

- **Strengthening foundational research capabilities:** Expand MSD's commitment and capacity for open science to continue developing interoperable and more easily reusable data, models, and analysis methods; leverage emerging computational innovations (e.g., AI, natural language processing, reinforcement learning (RL), and interactive visual analytics); and grow and diversify the MSD workforce to broaden the backgrounds, technical skills, and expertise/experiences available to advance our understanding of societal risks.
- **Advancing the science of human-Earth system interactions:** Identify and model human-Earth system dependencies and interactions at multiple scales, sectors, and systems; improve our understanding of how extreme and high-impact events propagate in systems-of-systems with thresholds, discontinuities, and tipping points; diversify approaches for representing human systems and adaptive behaviors; consider how human responses (both positive and negative) contribute to risks through interactions with hazards, exposures, and vulnerabilities; explore interactions of the key properties that characterize systems in nested and hierarchical relationships; and expand regional-scale human-Earth system modeling experiments; and many others.
- **Providing scientific and decision-relevant insights under uncertainty:** Create new opportunities for sustained collaboration and learning to ensure that MSD research is relevant to decisionmaking challenges; evaluate model performance and fidelity by incorporating user-relevant metrics and uncertainty analytics; employ exploratory modeling, scenario discovery, and other approaches that can be exploited to better understand interdependent actions across sectors under deep uncertainty; and capture and communicate the complexity and uncertainties of human-Earth systems while still delivering decision-relevant insights.

Teaming in an Open Scientific Environment to Confront Complexity

DOE's Earth and Environmental Systems Sciences Division (EESSD) is a core partner and critical source of support, shaping MSD research in terms of its scope, tools, and ambitions over the next decade. Current topical areas of focus across DOE's MSD portfolio include: multimodel, multiscale frameworks; interdependencies among energy, water, and land; direct coupling of human systems models with Earth system models to represent drivers and feedback; infrastructure, sectoral interactions, and resilience under rapid change; urban morphologies, population dynamics, and landscape evolution; capturing complex regions under stress in simulations (e.g., coasts, Arctic, and urban); scenarios, sensitivity studies, and uncertainty characterization; and data science and analytics, data fusion methods, and machine learning (ML). At the time of this report, the DOE MSD program has 10 major funded projects, comprising national laboratory science focus areas and university cooperative agreements. DOE also supports a cross-cutting community of practice (CoP) that provides a framework for growing and accelerating peer interactions, collaborative research, and engagement with other relevant research communities, and the MSD Living, Intuitive, Value-adding, Environment (MSD-LIVE), a flexible and scalable data and code management system combined with a distributed computational platform.

MSD research requires long-term collaborations with other research communities, both domestic and international. These include communities such as Earth system modeling, systems engineering, sustainable transitions, socio-environmental and socio-ecological systems, urban complexity science, and decisionmaking under deep uncertainty. In addition, other federal agencies beyond DOE have strong and interrelated research capabilities for advancing scientific understanding of the complex dynamics of Earth, environmental, socioeconomic, and infrastructure systems relevant to MSD. An ambition of the MSD community over time is to develop an open catalog and linked repositories of models, data, analysis, and decision support capabilities that can be shared to study the co-evolution of interdependent sectors and systems. This will provide a modeling and learning environment in which researchers can more easily identify and select data and models from a larger collection of resources and use them as a starting point for new analyses. As collaborations expand, the MSD CoP will continue to develop the conceptual MSD framework by creating additional resources to support collaboration, including coordinated experiments, community approaches to manage computational tradeoffs and data availability, and analysis of approaches to address shared methodological challenges.

Chapter 1.
Introduction: Critical Pathways of Societal Change

This chapter introduces the varied stressors and influences that shape pathways of societal change, the emerging research questions that drive the need for the emergence of the MSD CoP, and examples of scientific breakthroughs from early investments in MSD research. The next decade represents a tremendous opportunity for the United States to address climate and energy challenges and to realize the modernization of our infrastructure systems to be more resilient (ASCE, 2021; BERAC, 2017). These challenges are fundamentally tied to the United States' competitiveness and leadership in the global community. Near-term prioritized investments in clean energy transitions and strategic actions that address climate risks are vital first steps (National Laboratory Directors' Council, 2021). They are foundational to creating pathways to the future that enhance our national economic well-being and overall capacity to meet future challenges.

A wide range of stressors and influences, endogenous or exogenous to the coupled human-Earth systems of interest, are increasing the importance of developing insight into the ways that human choices and systems interact with changing Earth and environmental systems (USGCRP, 2018). Acute stressors include extreme precipitation, floods, wildfires, pollution, storms, and heatwaves (Figure 1.1.1). Longer-term climate stressors include changes in average land surface and ocean temperatures, sea-level rise, ocean acidification, and increasingly persistent droughts. In addition, and often less evident, a range of other influences, such as human population movements, health disparities, economic cycles, and the expansion of settlements and infrastructure, which can be caused by climate stressors in some cases, add to and dampen stresses across geographies and time. Not all of these changes are "negatives"—advances in education, economic development and growth, and improvements in technology can reduce infant mortality and birthrates, create employment opportunities, and increase societal resilience (Rosling, 2018).

Achieving a resilient future requires a careful accounting of these influences and their effects on increasingly complex, interconnected, and interdependent societal systems (e.g., infrastructure, governance, and socioeconomic) and their feedback with Earth and environmental systems (Helbing, 2013). For example, transitions in energy systems have considerable implications that cascade throughout systems of infrastructure, governance, economy, Earth and the environment (Andersen et al., 2020; Levi et al., 2019; Trutnevyte et al., 2019). For this reason,

Figure 1.1.1: Acute stressors and risks are present in the contiguous United States. Normalized information for temperature stress, flood risk, water stress, land environmental quality, and population density was retrieved from the Massachusetts Institute of Technology's Socio-Environmental Systems Risk Triage visualization platform at https://est.mit.edu/. Temperature stress and water stress are calculated based on the ERA5 dataset. Flood risk information is based on the original dataset by the First Street Foundation Flood Lab. Land environmental quality data represents the Environmental Protection Agency's Environmental Quality Index for the land domain. Population density data is from the US Census Bureau. All datasets are normalized based on each county's percentile rank of the raw data. The wildfire risk map is based on each county's percentile rank of its housing-unit weighted mean of risk to potential structures, retrieved from the Wildfire Risk to Communities dataset, developed by the US Forest Service. The data shown are relative normalized indicators and are used to illustrate the presence of multiple sources of stress or risk throughout the contiguous United States. More information about how these indicators were estimated can be found in their respective original sources.

energy transitions and climate challenges must be studied within the complex mix of human and natural systems that they shape and are, in turn, shaped by (see Box 1.1). Natural extremes are compounding each other and increasing the potential for long-lived cascading societal effects (Mora et al., 2018; Raymond et al., 2020). Societal change pathways encompass global supply chains; strained natural resources; aging infrastructures; infrastructure investments; growing, migrating, and increasingly vulnerable populations; and intensifying natural hazards. Human

decisionmaking and actions have significant feedback effects that can alter global-to-local environmental changes and their consequences (Dolan et al., 2021). There is a need for scientific innovations that can aid in navigating and prioritizing tradeoffs across candidate multisectoral actions.

Box 1.1: Energy Transitions and MSD – A Transportation Sector Example

The energy sector is critical to the operation of most human systems, impacting water supply, agriculture, transportation, industry, communications, and most aspects of everyday living. Historical energy transitions (see Figure B1.1.1) have been dominantly shaped by major changes in human systems technologies and demands. The pace of transitions is strongly controlled by the time required to transform the sector's underlying infrastructure systems (Suits et al., 2020). The accelerated pacing of current energy sector transitions and their connections to climate risks poses a unique scientific challenge. Understanding current and ongoing transitions such as the deployment of variable renewable energy sources, energy storage, and flexible demand-side technology poses a marked difference relative to their historical predecessors (Markard, 2018). The current degree of interconnectedness and interdependence on the energy sector varies significantly across regions, scales, sectors, and systems. This heterogeneity when combined with ambitious plans to rapidly transform the energy sector make evaluations of growth and transition opportunities highly complex and difficult to plan across sectors due to co-dependent risks and uncertainties.

B1.1.1 Periods of transition in the dominant fuels used in the transportation sector marking biomass to coal in 1871–1881, coal to petroleum 1921–1948. The transitions show the effects of the Great Depression as well as World War II. This figure has been created using data from Suits et al. (2020); the original figure can be found in the supplement of the same report.

The energy sector can be described at a high level around three stages of service delivery: production, conversion and transport, and use. Energy uses are typically categorized into residential, commercial, industrial, and transportation. These uses and their associated decisionmaking connect to other sectors that are co-evolving with the energy sector.

Understanding how the energy sector's three stages of service delivery co-evolve to meet each use is at the center of energy transitions. Any transformation in energy production, conversion/transport, and use will propagate to the other stages and thus require close coordination and an understanding of key feedback. Conventional fuel production includes extracting, processing, and manufacturing activities around oil, coal, natural gas, biomass, geothermal, and nuclear fuels, while renewable energies directly connect to the conversion and transport stage. Over the last decade, technology innovation and policy have significantly changed the shares of each fuel and the industries that support fuel production. This transition in the United States has resulted in a significant change in the fuel portfolio, substituting 50% of coal's contribution with mostly natural gas and a doubling of wind and solar production (LLNL, 2021). Energy transitions are important across non-energy sectors because the conversion and transport of energy, whether through the electric grids, pipelines, or other methods, are strongly connected to other sectors as well as their dependencies on broader human and Earth systems. In 2021, there were clear examples of this connectedness in the low temperature-driven electricity outages in Texas and the cybersecurity-driven outage on the Colonial Pipeline. The energy sector's connection to other sectors and systems provides both a mechanism for cross-sectoral transformations as well as interdependent risks.

Navigating these complex challenges requires fundamental scientific advances to understand risks and opportunities for economic and societal development in the face of changing weather patterns and extremes, major technological advances, changing needs for and supplies of natural resources, and feedback to and from natural systems, including regional and global climate. Diverse perspectives are needed to incorporate the full depth and breadth of multisectoral systems and uncover opportunities to address clean energy transitions and climate risks. Embracing this challenge, MSD provides a framework for making fundamental advances in the necessary human and natural systems modeling as well as the analytical tools needed to accelerate our insights from it. The DOE National Laboratory Directors' Council highlights that multisectoral human and natural systems modeling offers "a powerful capability to evaluate and prioritize investments and programs that address multiple policy-related goals and outcomes simultaneously" (National Laboratory Directors' Council, 2021) . The Council highlights that these capabilities are central to our national ability to develop effective "resilience strategies that also meet our nation's energy and environmental equity objectives."

Emerging Societal Questions Call for MSD Science Advances

MSD addresses scientific needs that align with the Biological and Environmental Research Advisory Committee's (BERAC) Grand Challenges report (BERAC, 2017) by exploring the "greatest scientific challenges DOE faces in the long term (20-year horizon)." For this reason, the BERAC report reinforces the need for and value of MSD research. For example, the report highlights:

- The need to advance hierarchical modeling of complex human and natural systems while improving its value through improved diagnostic model evaluation and uncertainty analysis.
- The need to improve our modeling and understanding of extreme and high-impact events.
- The opportunity to train the future workforce in integrative complex systems science, strategically increasing interactions across disciplines, and ensuring leadership in leveraged advancements of emerging computational innovations (e.g., exascale computing and AI).
- The need for diverse disciplinary WGs to address human-Earth system research and sustainability analyses.
- The benefits of fostering coordination and collaboration within DOE, other US agencies, and beyond.

MSD directly addresses the above BERAC grand challenges while aligning with DOE's mission to advance our fundamental understanding of energy transitions and climate risks. Developing the scientific capacity to support decision-relevant scientific modeling at the needed physical and temporal scales poses many additional challenges (see Boxes 1.2 and 1.3). Advancing our understanding of societal changes (positive and negative) requires science that engages broader perspectives that are multisector and multiscale in their scope (Clarke et al., 2018).

Changing global-scale climate dynamics can have profound effects down to the scale of individuals coping

with their consequences. The goal of MSD research is to improve our ability to represent and understand the interdependent dynamics between human and natural systems, particularly under future change. Advances are needed to better resolve legacy as well as projected environmental impacts and to trace the factors that shape equity. MSD science is focused on advancing our use of emerging data, innovations in modeling human and natural systems, and intelligent analytics to capture how sectors and systems co-evolve in response to environmental, technological, and societal transitions and shocks, with a particular focus on contributing decision-relevant science insights. Progress in MSD science offers the opportunity to support DOE's mission and broader scientific objectives. We highlight four groups of challenging societal questions that require new methods and perspectives, as well as synthesis across studies and projects (Figure 1.1.2).

Figure 1.1.2: The four groups of challenging societal questions that can guide MSD research.

From Science Questions to an MSD CoP

Moss et al. (2016) summarizes the key findings of a DOE initiated workshop exploring how to accelerate scientific progress to better understand the dynamics and resilience of US connected infrastructure systems. The workshop brought together diverse perspectives from a broad range of academic disciplines and included participation from 10 federal agencies. A key recommendation and outcome of the workshop was the establishment of a conceptual framework for MSD research that would enable researchers supported by DOE, other federal agencies, and those working in other institutional contexts to coordinate their work. The framework emphasizes flexible and interoperable data sets, models, and analysis methods.

The DOE MSD program area has established the MSD CoP to facilitate the realization of the collaborative

framework proposed in the 2016 workshop. The MSD CoP emphasizes open science, advancing our understanding of complex adaptive human-natural systems and promoting translational science breakthroughs consistent with the needs of the agencies and participants in the 2016 workshop. The MSD CoP provides a framework for growing and accelerating peer interactions, collaborative research, and engagement with other relevant research communities so that we are better positioned to confront the complexity of multisectoral science questions intrinsic to the field, including (but not limited to) energy transitions and climate risks. To date, the MSD CoP has been focused on promoting progress through the following activities:

- Accelerating communication within the CoP (through a website, newsletters, and a blog) and with the broader scientific community (for example, through one of largest sets of thematically coordinated sessions at the 2020 and 2021 Fall Meetings of the American Geophysical Union)
- Establishing technical bodies to facilitate collaboration on key challenges (a Scientific Steering Group and six working groups)
- Scientific advancement and synthesis (through sponsorship of a special section of the journal Earth's Future)
- Encouraging the development of resources to facilitate sharing community data, models, and tools (e.g., MSD-LIVE), and
- Supporting a diverse scientific workforce with opportunities for early career scientists, including attention to MSD-related education.

Chapter 4 of this report describes the activities of the CoP at greater length, including opportunities for engagement through technical bodies and the development of the conceptual framework to facilitate communication and collaboration.

Box 1.2: Cities Concentrate the Effects of MSD

Cities may be humanity's most profound invention. They enable the circulation of people, goods, and ideas; yielding influences that extend well beyond physical urban boundaries. Cities are created by and are composed of interacting social, technological, and natural systems. Forms of urban life emerge from individual and collective behaviors, interactions, and choices. Innovation and economic production are more concentrated in larger cities while being reliant on a high density of connected infrastructure. The diversity of local and regional ecological contexts of cities, as well as their historical pathways of development, are critical for understanding their current vulnerabilities. Urban processes create and constrain supply chain networks, economic flows, and disease, and are the major drivers of technological innovation. The world's 300 largest cities comprise about half the nominal gross domestic product, a quarter of the global population, and a substantial share of global energy use. As illustrated in Figure (B1.2.1) urban centers across the United States are highly diverse in their geographies and heterogeneous in their infrastructure design.

B1.2.1 Composite image of the continental United States, at night, 2016, and the Chicago skyline. Image credits: NASA Earth Observatory, image by Joshua Stevens; Library of Congress collection, image from Carol M. Highsmith.

The inherently closely coupled socioeconomic, technological, and natural aspects of cities also enable the development of novel solutions. Innovations around technological mitigation of stresses and hazards, infrastructure design and use strategies, economic drivers, and social innovations are all also facilitated by their strongly interacting multi-sectoral dynamics and demands. Cities are keystones for important multiscale feedback in human-Earth systems. Different human processes operate at the full range of social scales, from individuals to cities, nations, and the planet (Figure B1.2.2). Individuals typically make decisions based on the physical, social, and economic context as exogenous. These choices include decisions like transportation mode choice within an urban environment, energy use in buildings, crop choices by farmers, and household level choices about water and energy demand. Collective social processes pose significant modeling challenges. Collective human processes can be highly nonlinear and heterogeneous, making modeling difficult. So too may be the distributional effects of influences and stressors, such as weather extremes on community infrastructures and services, resource allocations, and contributors to urban heat stress. But these processes are not fully random. There are patterns and theories for how groups of people make choices and ultimately create the long-term agglomerations of people, and the infrastructure in service that becomes cities.

B1.2.2 Social scales that shape the co-evolutionary human-natural dynamics of urban systems highlighting parcel-level individual actions (Allen-Dumas et al., 2020), city-scale heterogeneity in infrastructure access (Brelsford et al., 2017), and the nation-scale distribution of infrastructure across cities (Brelsford et al., 2020).

Scientific Breakthroughs to Inform Complex Pathways of Change

Understanding how interdependent global-to-local challenges are shaping critical pathways of societal change presents a scientific grand challenge (Clarke et al., 2018; Helbing, 2013; Moss et al., 2016). This challenge cannot be addressed fully by current research frameworks and methods because of the complexity of the myriad of Earth, environmental, engineered, and socioeconomic systems that are intertwined and the interactions that shape emergent risks and vulnerabilities (see Box 1.4). Keeping pace with the accelerating complexity of existing and future pathways of societal change requires a deep integration of diverse perspectives, technical capabilities, and rapid innovations in our modes of scientific inquiry (Elsawah et al., 2020; Moallemi and Haan, 2019; Trutnevyte et al.,

2019). Moreover, MSD seeks these new modes of inquiry to yield tools and insights for transforming the benefits and resilience of societal systems. Given their complexity, candidate pathways of change, and diverse sources of uncertainty, there is a need to rethink our traditional disciplinary approaches to science as well as the modes of science itself (Funtowicz and Ravetz, 1993; National Research Council, 2014; Rittel and Webber, 1973; Saltelli et al., 2020; Szostak, 2017).

As highlighted in Box 1.3 below, regional context is critical to our understanding of key vulnerabilities and their influence on broader global teleconnections. For example, the Mississippi River Basin in the central United States is another example of a uniquely different regional complex system with interacting land, water, ecosystems, and food systems (see Box 3.3). The stressors in this case can include droughts but also extreme precipitation and floods. Many types of teleconnections link agricultural productivity in the upper and central parts of the basin to water quality, fisheries, and ecosystem impacts in coastal areas and the Gulf of Mexico. There are clear tradeoffs between upstream and downstream outcomes, and this creates the need to balance multiple objectives across jurisdictions that lack mechanisms to coordinate these issues.

Box 1.3: Water-Energy Connections – Multisectoral Interactions of California Droughts

The droughts occurring over the last two decades in California highlight the interconnections and interdependencies between humans, Earth system extremes, sectors, scales, and systems (Clarke et al., 2018; Diffenbaugh et al., 2015). Energy, water, and land are inextricably linked in California. During the droughts, hydropower generation in California and imports from the Pacific Northwest supplied 15% of the total electricity consumption in the state in an average year (Christian-Smith et al., 2015). Environmental concerns and highly valued land have served to limit the construction of new major reservoirs causing hydropower generation capacity in California to be largely fixed. Consequently, the state has addressed its growing energy demands using other sources of energy such as natural gas, which accounts for more than 40% of the total electricity consumption. Natural gas has functioned as the primary substitute for hydropower during climatic swings, which also ties carbon emissions to drought dynamics (Kern et al., 2020). Over the period from 2002–2016, statewide droughts have substantially impacted much of California's agriculture, where local groundwater has been critical to buffering most agricultural impacts by replacing surface water deficits (Figure B1.3.1). Xiao et al. (2017) note that over the last two decades, increased groundwater pumping has led to a loss of more than 20 km^3 groundwater (>3 times the capacity of Shasta, the largest reservoir in California). During the 2012–2016 drought period, there was approximately 30% less surface water available for agriculture statewide, but about two-thirds of this loss was replaced by additional groundwater pumping, which added $600 million per year in pumping costs (Lund et al., 2018).

Figure B1.3.1 Groundwater depletion dynamics as captured by NASA's Gravity Recovery and Climate Experiment satellite mission from 2011–2013 (taken from Famiglietti, 2014).

The remaining 10% shortage in statewide agricultural water use was accommodated by fallowing half a million acres (6% of statewide irrigated crop area), stress irrigation of crops, shifting crops, and improving irrigation efficiencies (Lund et al., 2018). California's groundwater backstop buffered supply chains and enabled California to continue to send agricultural and food commodities to the rest of the nation and world during the drought (Marston and Konar, 2017). The groundwater embodied in agri-food products (Figure B1.3.2) increased over the course of the drought, despite significant declines in rainwater and surface water supplies. In this way, drought amplifies the teleconnections between water use and distant consumers of virtual water. Groundwater has the ability to buffer agricultural production and supply chains during droughts, but there is a significant tradeoff in sustaining equitable use of this resource (Escriva-Bou et al., 2020; Ghasemizade et al., 2019).

Figure B1.3.2 Change in virtual green water (soil water available to plants), surface water, and groundwater exports (m^3) over the course of the California drought between 2011 and 2014. The countries are shaded by their percent change in virtual water receipts. Rainwater and surface water embodied in exports from the Central Valley decreased, while virtual groundwater from the Central Valley increased (taken from Marston and Konar, 2017).

There is a need for scientific breakthroughs that accelerate our understanding of how feedback and interdependencies across complex adaptive human-Earth systems can shape existing risks or lead to new threats (see Box 1.4). Modeling frameworks are rapidly evolving in how they capture dynamic and adaptive representations of agents, infrastructures, and natural systems, as well as a broadening array of uncertainties (Filatova et al., 2013; Herman et al., 2020; Morris et al., 2018; Taberna et al., 2020; Trindade et al., 2020; Turner et al., 2020). These advances are providing access to new scientific hypotheses, diversifying theoretical problem framings across a broader array of disciplinary perspectives, and allowing quantitative analyses of a broader suite of societal objectives (e.g., reliability, resilience, vulnerability, robustness, economic efficiency, financial risk, stability, equity). Augmenting these recent advances, the emerging frontier of computational modeling and analytics is now beginning to embed AI and agent-based modeling into adaptive software development processes and scientific workflows. Embedded intelligence facilitates rapid iterative exploration of competing hypotheses and problem framings to accelerate scientific insights within the complex adaptive systems of interest to the MSD field (Atkinson et al., 2017; Brown et al., 2020; Deelman et al., 2019; Yilmaz, 2019). The MSD CoP envisions that such advances can also be applied to carefully evaluating the effects of model representations of scales, interactions, and path dependencies (Filatova et al., 2016; Iwanaga et al., 2021; Levi et al., 2019).

Box 1.4: Feedback and Interdependencies across Human-Earth Systems Shape Risks

Figure B1.4.1: Risk as it emerges through interactions across multiple drivers of hazard, vulnerability, exposure, and response. Adapted, redrawn, and following the lexicon from Simpson et al. (2021)

Systemic failures, extreme events, and "hyper-risks" emerge as a result of the highly complex and highly interconnected human-Earth systems (Helbing, 2013). Dynamic relationships between agents, systems, and sectors transmit risk from one to another, leading to new risks or amplifying (or buffering) existing threats (Rinaldi et al., 2001; Vespignani, 2010; World Economic Forum, 2021; Zscheischler et al., 2020). For example, one can consider some of the risks present in the water, food and energy sectors. Water shortages in the form of droughts can lead to food insecurity and volatile commodity prices as the impacts ripple through markets. Agricultural land-use changes due to drought feed back to the climate system, with both regional as well as global implications. Water-intensive energy production can also be imperiled, leading to insecurity and higher prices. Inversely, energy-intensive water production can also become more costly. National and international governance, economic disparities, aging infrastructure, population growth, and climate change all act as exacerbating drivers to these risks, inhibiting effective response. This inexhaustive list highlights just some of the increasingly globalized risks shaping human-Earth systems.

The growing complexity of these types of risks requires fundamental innovations relative to the current state of risk assessment (Field et al., 2012; Kron, 2005; Shukla et al., 2019; Society for Risk Analysis, 2018). Simpson et al. (2021) introduces a promising framework for the assessment of complex risks that expands on the traditional definition of risk as emerging from the interaction of hazard, vulnerability, and exposure, by explicitly recognizing that human responses are also determinants of risk (Figure B1.4.1). They also further distinguish that risk can emerge through interactions among multiple risk drivers present across the different determinants of risk (as opposed to a single driver of each hazard, vulnerability, exposure, and response interacting). Consider, for example, the concurrent hazards of a hurricane and pluvial flooding that compound the severity of risk. These hazard drivers interact with multiple drivers of vulnerability (poverty, race, etc.), drivers of exposure (land cover, urban stormflow systems, houses built in floodplains, duration of the flood event, etc.) and response drivers (evacuation plans, disaster relief, floodplain property insurance, etc.) to shape how risk will manifest. From the MSD perspective, this framework can be used to formalize qualitative mappings and quantitative assessments of risk as they emerge from these driver interactions. Drivers of risk stem from and operate within different sectors, and the resultant risk potentially propagates from one sector to another through their dynamic interactions. Finally, Simpson et al. (2021) additionally proposes the consideration of interactions between multiple risks and the presence of aggregate risk (the accumulation of multiple risks), compound risk (the interaction of multiple risks), and cascading risk (causal relationships between multiple risks). This understanding of risk is inherently multisectoral and places focus on interactions across human-Earth systems. It emphasizes how traditional single-sector risk analyses are prone to underestimate both overall risk and multisectoral capacities to buffer it (Harrison et al., 2016; Lawrence et al., 2020; Raymond et al., 2020).

This report contributes to a vision of MSD as an emerging field. This holds tremendous promise for advancing our understanding of the local-to-global systems that fundamentally shape the interdependent dynamics, risks, and

welfare of our modern world. This report introduces the transformative research contributions, opportunities, and advances that MSD offers as a long-term community investment.

Chapter 2.
MSD: Definition and Current Research Frontier

2.1 What is MSD?

This chapter establishes what MSD is, develops a conceptual framework for MSD as a field, describes emerging MSD research themes and science questions, summarizes current DOE MSD research thrusts, and maps MSD's research gaps.

A key charge for the MSD CoP is to provide a framework for formalizing the field's core terminology and higher-order science questions. Formally, MSD is defined as:

The study of how complex Earth, environmental, infrastructure, governance, and socioeconomic systems co-evolve in response to current and rapidly changing influences and stressors. MSD is a transdisciplinary research area that seeks to advance our understanding of how human-Earth system feedback shapes interdependent pathways of societal change across scales and uncertainties. These insights provide a basis for advancing a more resilient, adaptive, and sustainable society.

Broadly, MSD seeks to understand the dynamics and co-evolutionary pathways of human and Earth systems with a focus on critical goods, services, and amenities delivered to people through interdependent sectors such as energy, food, housing, transportation, health, and recreation. MSD research focuses on how these sectors interact as they incorporate inputs, processes, and constraints as well as feedback across Earth, environmental, infrastructural, and socioeconomic systems (see Figure 2.1.1).

The key words "sector" and "dynamics" in the name of MSD capture this focus. The term sector has a long history and has been the focus of many efforts to clarify and classify its definition across a wide range of contexts (Fisher, 1939; Intelligence, 2018; Kenessey, 1987; MacKinnon et al., 2019; Rosenbloom, 2017; Wolfe, 1955). As used here, the definition of sector draws on the elements of prior taxonomies, but does not adopt any single approach to maintain flexibility in application across the variety of domains that compose the MSD CoP. **"Sectors"** are defined as:

Complex systems-of-systems that deliver services, amenities, and products critical to society. Examples of components of sectors include infrastructure, governing institutions (public and private), labor force capacity,

markets, natural resources, ecosystem services, supply and distribution networks, finance, and a wide range of actors (e.g., firms, regulatory agencies, investors, consumers) involved in producing and creating demand for the services and products the sector provides.

The proposed definition of sectors is broader than many typical classifications. The field of economics, for example, defines sectors across four levels: primary (natural resources), secondary (manufacturing), tertiary (services), and quaternary (knowledge pursuits). Alternatively, investment-oriented classifications focus on categories such as utilities, telecommunications, healthcare, energy, and others based on shared risk profiles affected by, among other things, the stage of the business cycle (e.g., Global Industry Classification Standard (GICS)). For example, the water sector provides water as a commodity to a variety of users, encompassing infrastructure (e.g., dams, levees, pipes), environmental systems (e.g., aquatic habitats, rivers), governing institutions (e.g., US Army Corps of Engineers, US Environmental Protection Agency, municipal water providers), and socioeconomic systems (e.g., water pricing, water rights). As another example, the energy sector is complex systems-of-systems involved in the exploration, production, storage, transportation/transmission, and consumption of energy. In the Global Industry Classification System (https://www.msci.com/our-solutions/indexes/gics), the sector components include oil, gas, and consumable fuels along with related equipment and services, but in MSD research, the system comprises additional energy sources (nuclear, renewables) and influences (e.g., transitions to low/no carbon energy systems). The food sector is another example, comprised of complex supply chains that dynamically link production and consumption of many different types of agricultural commodities and products. It encompasses agents and systems, including farms, processing industries, equipment and amendment manufacturers, transportation systems, economic systems, water resources, and other components. The MSD framing of sectors focuses on the services and products that emerge from the interdependent and interconnected dynamics of the underlying systems-of-systems from global-to-local scales that shape their resources, demands, and impacts (see Box 2.1).

The term **"Dynamics"** in MSD refers to:

Pathways of change that result from the ongoing interactions of the components of sectors as well as from geophysical, biophysical, economic, and socio-technical transitions and shocks. The emergent complexity of these pathways is shaped by their interdependence-interconnectedness, irreversible lock-ins, contested perspectives, cross-scale influences and effects, as well as the deep uncertainties that shape their evolution.

Returning to the examples in the prior paragraph, water sector dynamics are shaped by several Earth system processes (e.g., precipitation, surface and subsurface movement of water, evaporation) as well as by human institutions such as water rights, markets, and environmental regulations. Energy system dynamics are affected by influences that cause short-term fluctuations in energy demand (e.g., economic cycles and weather) and that affect long-term decisions and transitions in production and distribution of energy (e.g., technology change and government energy policies). The dynamics of the food sector are shaped by socioeconomic forces such as wealth, culture, labor supply, freight and shipping, and economic institutions, as well as a variety of environmental factors such as hydrological impacts on production, processing, and transportation. These components interact to affect vulnerabilities in national (and even global) food supply chains as illustrated in recent research that identifies how disruptions might impact the delivery of food in the United States (Lin et al., 2019).

As illustrated by the example above, the pathways of change are affected by a wide range of stressors and influences that arise from cross-cutting infrastructure, Earth, environmental, governance, and socioeconomic systems (and their interactions, see Figure 2.2.1). MSD prioritizes the role of infrastructure systems that are responsible for the production and operation of services, including technologies, inputs, outputs, and technical characteristics of production systems (e.g., core process operations and management, labor, and capital requirements). Earth systems capture processes and cycles in the Earth's atmosphere, hydrosphere, cryosphere, and geosphere. Environmental systems are associated with biotic elements and processes in the Earths' biosphere and the provisioning of a variety of essential goods and services. Governance systems include institutions, national and international agreements, procedures, and operations through which sectors are managed. Finally, economic, political, and social systems are

Figure 2.1.1: Conceptual illustration of MSD highlighting the Energy, Water and Agricultural sectors. Although not labeled, other sectors shown in grey circles also exert influences through their interactions, dynamics, and feedback.

central to the behavioral dynamics that emerge from societal actors and their actions across scales (from individual to collective) and drive changes in consumption, migration, demography, and evolving value systems (e.g., growing expectations for reliable, resilient, and equitable services). Modeling of economic activity and the factors that influence consumption, production, investment, trade, growth, and supply and demand for the goods and services that sectors provide has received wide attention because of its importance for understanding the ongoing dynamics of change across coupled human-Earth systems. In short, all of these systems exert complex cross-scale and cross-sector influences that are critical to understanding pathways of change and transformation for technologies, infrastructure, as well as institutions (Andersen et al., 2020; MacKinnon et al., 2019).

Extremes of weather and climate (e.g., temperature and precipitation), climate phenomena that influence the occurrence of extremes (e.g., modes of climate variability), and environmental processes affected by weather and climate (e.g., floods, droughts, and landslides) (Seneviratne et al., 2012) are priorities for MSD research. These acute and long-term stresses are closely inter-related and affected by observed alterations in Earth's systems, such as changes in climate, land use, and sea level (USGCRP, 2017). Stresses can occur either individually or as a compound of extreme events (Zscheischler et al., 2020). Climate stresses can precipitate infrastructure or socioeconomic shocks such as outages, supply disruptions, and price spikes, and shocks at smaller scales can have cascading effects that are transmitted to a larger system via tipping points that trigger critical changes (Holdschlag and Ratter, 2013). These stresses in turn produce responses, both autonomous and planned, which affect system dynamics by dampening or amplifying feedback. For example, drought conditions induced by cyclical variations in the climate, anthropogenic climate change, and unsustainable use are leading to reduced water allocations in the Colorado River Basin. The restrictions are producing varied responses, leading some farmers to intensify groundwater pumping, further depleting future water resources and amplifying future shortages. In contrast, cooperative water transfers, coordinated fallowing, or planting crops with lower water use, offer responses to dampen negative drought feedback (Mankin et al., 2021).

Better representing stresses and influences in modeling is a major challenge for MSD science and a focus of ongoing work. For example, it is a challenge to improve representation of climate stressors, especially extreme events, in modeling to avoid misrepresenting potential consequences and responses (Schewe et al., 2019). Modeling of climate extremes typically considers individual, not compound, stressors and fails to account for interactions and interdependencies among them (Zscheischler et al., 2018).

Box 2.1: Multisector Dynamics Emerge from Complex Adaptive Systems-of-Systems

Building on literature related to complex adaptive systems, system dynamics, socioecological systems, resilience, and adaptive change (Anderies et al., 2013; Berkes et al., 2008; Holling, 1985; Holling and Gunderson, 2002; Sundstrom and Allen, 2019; Walker et al., 2004; Zu Castell and Schrenk, 2020), systems can be defined as sets of interacting elements that operate to form a unified whole that yields emergent behaviors and dynamics outside of any of its elemental parts. Systems can be composed of built, natural, and societal components and operate across spatial and temporal scales. In the context of the MSD science focus on human-Earth systems and their feedback, Figure B2.1.1 conceptualizes a complex adaptive system in terms of its interacting cycles of growth and disruption (Holling, 1985; Holling and Gunderson, 2002) for natural and human-built capital resources. The growth phase of the adaptive cycle emphasizes the dynamics of exploitation and accumulation of resources or capital. The second phase, disruption, represents the occurrence of a system shock and its reorganization into a transformed set of interactions between its elements (Figure B2.1.1a). Depending on the kind of disturbance, resources available (natural or built), human actions, as well as co-evolving natural elements, the system may transform to into another system all together during its reorganization stage (represented by the stylized fracture arrows, Figure B2.1.1a). As an example, consider a coastal region power system: investments supporting its establishment (e.g., infrastructure and service demands) grow to accumulate more capital and resources. A high-intensity hurricane shock can trigger transformative physical and institutional reorganization.

Figure B2.1.1: (a) Adaptive cycles of growth and disruption of a complex system. Adapted from Holling (1985); Holling and Gunderson (2002). (b) Properties of systems as they increase or decrease as a system moves through different stages of the adaptive cycle. The schematic shown presents one example of how these properties can be aligned, but the system can also be found in other configurations.

Three key system properties are central to the dynamics of an evolving system: connectedness, capital, and resilience (Figure B2.1.1b). Connectedness reflects the strength and number of interactions between a system's elements, as well as the degree of control that can be exerted on the system and its operations. Connectedness increases as the system grows, accumulates more capital and resources, and becomes more organized and aggregated. Inversely, low connectedness is a property of systems with loosely associated and diffuse elements. For instance, when thinking of an air transportation network, connectedness can be used to reflect the degree to which airline flights connect different cities. Capital can be thought of as system potential and reflects the natural and human resources, monetary assets, or other capacities that accumulate as the system develops and grows. In the air transportation example, capital may reflect the number of passenger planes and other assets owned by an airline. The shock stage triggers a release of this capital (e.g., the occurrence of an event like the eruption of the Eyjafjallajökull volcano in 2010 affecting air travel to 20 European countries) to be reorganized and utilized in a different system configuration. Finally, resilience definitions vary, but resilience is often described as the capacity of a system to absorb a shock and adapt to maintain function, structure, identity, and component interactions (Walker et al., 2004). The three properties of complex adaptive systems are not static and do not monotonically increase or decrease. Rather, connectedness, capital, and resilience ebb and flow as the system moves through its growth and disruption phases and as it interacts with other systems across scales and across sectors (Figure B2.1.1b).

Multiscale feedback is critical to our understanding of how co-evolving systems, nested processes, and interactions shape path dependencies, amplify (or dampen) dynamics, or lead to emergent behaviors (Figure 2.1.2a). One may consider the operation of a large system, for example, the Earth system, where processes span millenia in the temporal dimension and continents in the spatial dimension. Those processes shape the function and properties of smaller systems, such as national infrastructure, the temporal scale of which lies within decades or centuries, and its spatial extent covers a continental region. Lastly, utility-level systems of operation and control, which can adapt and change quicker, operate at much smaller spatiotemporal scales. With specific regard to adaptive capacity and the manifestation of connectedness, capital, and resilience, two types of cross-scale processes become fundamental. Long-term memory processes shape how smaller systems (re)organize by drawing from the potential and experience

accumulated by a larger and slower system. Shocks happening at smaller scales can have cascading effects that are transmitted to a larger system through tipping points, triggering critical changes (Holdschlag and Ratter, 2013).

Figure 2.1.2: (a) Adaptive system cycles and interactions across scales. Modified from Holdschlag and Ratter (2013). (b) Hazards as they propagate through different systems and across scales. Modified from Pescaroli and Alexander (2016).

Through these cross-scale processes, hazards (Figure 2.1.2b) can also cascade between systems and interact with drivers of vulnerability, exposure, and response (see Box 1.4) acting within systems and sectors. Figure 2.1.3 shows how the three system properties (resilience, connectedness, and capital) relate to the four determinants of risk and their drivers. System organization and aggregation (reflected by the connectedness property) can shape resilience to hazards in both positive and negative ways, through the presence of drivers and their interactions.

For example, increased connectedness between drivers of vulnerability can produce cascading effects on how a hazard manifests. Conversely, increased connectedness in the response determinant can reflect more options for flexible adaptation to the hazard. Similarly, the capital property may be a measure of more exposed assets (exposure) but also more capacity to divert said assets to other management options. Resilience is therefore a resultant property of system interactions and comes about in how hazard drivers are amplified or buffered by drivers of exposure, vulnerability, and response. Effects from lack of system resilience to a specific hazard can trigger hazards to other systems across scales and sectors (Figure 2.1.2b).

Figure 2.1.3: System properties as they interact with determinants of risk. The capital and connectedness properties relate to the presence of and interactions between drivers of vulnerability, exposure, and response. The interactions between these drivers shape the resilience property and how hazards manifest as risk.

Box 2.2: Coupled Human-Earth System Models are Critical to Understanding Feedback Across Scales
As emphasized in Figure 2.1.2, multiscale feedback between global and regional dynamics are important to our understanding of the interdependence of climate risks, energy transitions, and the broader societal pressures that are straining the sustainability of our natural resources (e.g., land, forest, water, etc.). Recent coupled human-Earth systems modeling literature emphasizes the need to better capture regions at higher sectoral, temporal, and spatial resolution (Braunreiter et al., 2021; Calvin, Bond-Lamberty, et al., 2019; Fisher-Vanden and Weyant, 2020; Monier et al., 2018; Peng et al., 2021; Trutnevyte et al., 2019). Likewise, the studies emphasize the importance of connecting improved regional representations to their global-scale effects on climate and trade dynamics. Multiscale economic framings play an important role in MSD for understanding the global-to-regional (and vice versa) feedback. This is particularly important for understanding the effects of regions responding to a growing array of influences (climate and non-climate) such as technological changes, evolving resource demands, and compounding extremes. As a specific example, the Global Change Analysis Model (GCAM, see Figure B2.2.1a) is a market equilibrium model that resolves 32 geopolitical regions, which allows it to capture broader international socioeconomic and energy dynamics (Calvin, Patel, et al., 2019). The model further resolves water and agriculture dynamics through 384 land-water regions.

Figure B2.2.1: (a) GCAM linkages across energy, water, land, socioeconomics, and climate [adapted from Calvin, Patel, et al. (2019)]. (b) Change in terrestrial carbon storage in 2071-2090 due to GCAM coupling with an Earth System Model (ESM) in gC/m2/yr for the 4.5 Watts/m2 Representative Concentration Pathway [adapted from Calvin, Patel, et al. (2019)]. Green colors indicate increases in terrestrial carbon and purple colors represent decreases.

Overall, GCAM captures interactions and interconnections across energy, water, land, socioeconomics, and climate. GCAM is representative of the broader class of coupled human-Earth systems models that aid our exploration and understanding of human-Earth systems feedback. Human and Earth systems are strongly linked by climate influences from global markets, agricultural production, energy transitions, and competition for limited natural resources. Anthropogenic emissions from industry and land-use change to alter global temperature and precipitation. This feedback is central to our exploration of how potential future pathways of change shape risk and resilience across sectors, systems, and scales. Fig. B2.2.1b shows how bi-directional coupling between GCAM and an ESM can substantially change estimates of regional terrestrial carbon storage projections. These types of feedback and dynamics are central to advancing the field of MSD and the field's broader value for exploring the implications of human activities to climate risks (e.g., changes in carbon due to land use/land cover).

In Chapter 1, Box 1.3 and Figure B1.3.2 show the observed virtual water exports that occurred during the California drought between 2011 and 2014. The complex global trade-based exports of green water (soil water available to plants) and groundwater from declining regional aquifers represent another important example of regional-to-global teleconnections. Coupled human-Earth systems models have an important role in transitioning our analysis of embedded natural resources in global trade from historical extreme events to how they may change given plausible scenarios for the future. Figure B2.2.2 shows GCAM midcentury projections for virtual green water and nonrenewable exports for a middle-of-the-road Shared Socioeconomic Pathway (SSP 2) in combination with the 6.0 Watts/m2 Representative Concentration Pathway (Graham et al., 2020). The embedded water demands and transfers in agricultural commodities in this study are shown to substantially increase from the present and put pressure on already strained global aquifer systems. More broadly, multiscale human-Earth system modeling has a fundamental role in improving understanding risk and resilience to aid our navigation of shocks, technological breakthroughs, and potentially transformative multisectoral transition pathways.

Figure B2.2.1: (a) virtual green water exports and (b) virtual blue water exports (adapted from Graham et al. (2020).

2.2 The Current Frontier of MSD Research

The MSD field is situated to exploit and help to advance frontiers in climate science, Earth system modeling, human systems modeling, AI, and exascale computing. The MSD CoP and its corresponding DOE program are uniquely focused on advancing our fundamental knowledge of how humans shape environmental, technological, and societal transitions. Put simply, the MSD field seeks to expand the frontier of complex adaptive human and natural systems science that is multiscale and multisector in its focus. As noted by the DOE Office of Science, models, analytics, and insights contributed by the field are intended to have actionable real-world decision relevance by engaging with the complexities of critical pathways of societal change (e.g., evolving energy and energy-dependent infrastructures, services, amenities, and their influence on a broadening suite of societal objectives, DOE (2021)).

MSD Research Themes and Science Questions

To date, ongoing MSD research efforts in the United States and internationally have focused on energy, water, land, food, ecosystems, climate, the economy, and demographics (e.g., recent highlights, Di Vittorio et al., 2020; Dolan et al., 2021; Jiang et al., 2020; Khan et al., 2021; Lee, 2020; Rhoades et al., 2020; Sun et al., 2020; Turner et al., 2019). Influential work in the area has focused on interactions between economic processes and environmental

change, radiative forcing, land-use change, and biogeochemical cycles, changes in climate and related conditions such as hydrology and sea level, and the implications of these changes for ecosystems and human systems (e.g., Clarke et al., 2018; Hejazi et al., 2015; Li et al., 2021; Monier et al., 2018; Riahi et al., 2017; Vega-Westhoff et al., 2020). Research has sought to provide insights into issues such as how infrastructure investments in the next decade shape the resilience of sectors, systems, and communities over the next 10–100 years. MSD research advances are necessary to understand vulnerabilities and risks for regional and global economic development in the face of changing weather patterns and extremes, major technological advances, constraints on natural resource availability, and growing human pressures on sensitive ecosystems.

Figure 2.2.1: Recurring cross-cutting questions and themes identified across the current MSD project portfolio.

The themes and research questions that motivate MSD research are evolving rapidly. Figure 2.2.1 highlights four groups of cross-cutting questions that have emerged from a synthesis of past MSD studies and current projects. The underlying methodological innovations required to address these cross-cutting questions are extremely valuable for the societal challenges raised in Figure 1.1.2 as well as the BERAC grand challenges in general (BERAC, 2017). MSD research increasingly includes a broad range of disciplinary and transdisciplinary perspectives to answer scientific challenges relevant to society. Studies are broadening the range of sectors and concerns that are incorporated to include, for example, transportation, human health, insurance, industrial supply chains, financial services, and real estate. They are using higher spatiotemporal and sectoral resolutions to consider conditions, processes, institutions, and dynamics at local scales that have fundamental influences on the interactions of systems and sectors at regional, national, and even international scales, and vice versa. MSD research is representing human behaviors in increasingly diverse ways, including influences such as legal institutions, operating rules, and

non-economic drivers of preferences to more accurately capture how decisions about resource use, investment, and adaptive management are made. Interest in societal outcomes beyond economic impacts (e.g., equity, capital requirements, stability of governance, biodiversity) is broadening the need to incorporate a more holistic suite of objective measures in MSD research. Further, recognition that there are many important sources of uncertainty, some of which cannot be resolved, is driving innovation in uncertainty characterization, including the adoption of frameworks for exploratory modeling under deep uncertainty (Marchau et al., 2019; Moallemi et al., 2020) and representing the evolution of dynamically adapting systems with human actions as a core component (Haasnoot et al., 2013; Trindade et al., 2019).

Current DOE MSD Research Thrusts

The DOE Office of Science and the EESSD more specifically, are core constituencies and sources of support that are shaping MSD research in terms of its scope, tools, and ambitions over the next decade. DOE's Earth and Environmental System Modeling program includes a MSD program area that has the goal of exploring the complex sectoral interactions and potential co-evolutionary pathways within the integrated human-Earth system, including natural, engineered, and socioeconomic systems. Scientific insights and tools emerging from DOE's Earth and Environmental System Modeling program hold significant potential to inform next-generation US infrastructure decisions and new development pathways for improved energy and economic security, including the implications of technological innovations.

Figure 2.2.2: Cross-cutting themes that have emerged across the current MSD project portfolio. Near term refers to 10-20 years, mid term is 20-50 years, and long term 50-100 years.

Current topical areas of focus across DOE's MSD portfolio include: multimodel, multiscale frameworks; interdependencies among energy, water, and land; direct coupling of human systems models with Earth system models to represent drivers and feedback; infrastructure, sectoral interactions, and resilience under rapid change; urban morphologies, population dynamics, and landscape evolution; capturing complex regions under stress in simulations (e.g., coasts, Arctic, and urban); scenarios, sensitivity studies, and uncertainty characterization; and data science and analytics, data fusion methods, and ML. As reflected in a recent analysis by the CoP, the DOE MSD program area portfolio Figure 2.2.2 shows a strong emphasis on human-Earth system modeling, focusing on infrastructure, economic, and governance systems across a diversity of scales. The projects have a strong emphasis on regional and local modeling. Likewise, the planning horizons considered across the projects vary from near term (2030), mid term (2050), and long term (2100). There is a particular emphasis on understanding the energy-water-land nexus under a range of radiative forcing scenarios for climate risks. The multisector needs, risks, and vulnerabilities across these co-evolving systems are large and growing in the face of shifting temperature and precipitation patterns, water supplies that depend on increasingly limited groundwater, energy transitions, transitions in regional economic development (including land use), as well as US population shifts. Beyond the sectors highlighted explicitly in Fig. 2.2.2, other emerging sectors of focus include transportation, health, forestry, finance, and ecological services. Box 2.3 Lists example capabilities developed by the DOE MSD projects.

Box 2.3: Example Highlights and Capabilities Developed by DOE MSD Projects
DOE-funded MSD research projects are developing data sets; a hierarchy of models, including high-resolution representation of local scale processes and reduced-form emulators of global systems; model coupling tools; new ways of representing human responses and adaptivity; approaches for applying high-performance computing to represent complexity; and other capabilities. There are many ways of cataloging these advances—the framework for MSD research continues to evolve an approach that can be used to facilitate extensibility and reuse of these resources with problem-specific adaptations. This brief and incomplete static listing uses the cross-cutting MSD research themes identified in Figure 2.2.1 above. An updated, curated list of DOE MSD research highlights is found here.

Interdependencies, Interconnections, and Complexity

- Urban scaling as validation for imperviousness predictions based on population (Brelsford et al., 2020)
- Power sector detail and flexibility represented in a multi-sector model (Wise et al., 2019)
- Improving consistency among models of overlapping scope in multi-sector studies: The case of electricity capacity expansion scenarios (Iyer et al., 2019)
- The interplay between changing irrigation technologies and water reuse (Zuidema et al., 2020)

Stressors and Influences

- Identifying and describing the nonlinear interactions of tide, storm surge, and river flow in the Delaware Bay Estuary (Xiao et al., 2021)
- A permafrost implementation in the simple carbon-climate model Hector (Woodard et al., 2021)
- A spatial population downscaling model for integrated human-environment analysis in the United States (Zoraghein and O'Neill, 2020)
- Using AI to understand key wildfire controls (Wang et al., 2021).

Human Systems' Representations

- Identifying emergent agent types and effective practices for portability, scalability, and intercomparison in water resource agent-based models (Kaiser et al., 2020)
- A multiscale framework for the integration of economic and biophysical determinants of sustainability (Baldos et al., 2020)
- Global agriculture market integration critical for modeling land-use change (Zhao et al., 2021)
- The effects of neighborhood morphology on microclimate and building energy use (Allen-Dumas et al., 2020)

Evaluation of Uncertainties, Data, and Models

- Statistically bias-corrected and downscaled climate models and underestimates of the adverse effects of extreme heat on US maize yields (Lafferty et al., 2021)
- How structural differences influence cross-model consistency: an electric sector case study (Cohen et al., 2021)
- Calibrating simple climate models to individual Earth systems models: lessons learned from calibrating Hector (Dorheim et al., 2020)
- Small increases in agent-based model complexity and large increases in the required calibration data (Srikrishnan and Keller, 2021)

At the time of this report, the DOE MSD program has 10 major funded projects comprising national laboratory science focus areas and university cooperative agreements (Figure 2.2.3). Collectively, these projects encompass a large-scale multi-institutional exploration of key MSD challenges, including a broad array of DOE laboratories and academic institutions that are central to the emerging CoP. The brief synopses and activity highlights below provide a snapshot of the current frontier of MSD research in fully funded or co-funded DOE MSD projects. They do not capture the full scope of these projects, nor additional work co-sponsored by DOE's MSD programs such as project collaborations with US Geological Survey and the National Oceanic and Atmospheric Administration (NOAA) and other projects such as MSD-LIVE (see Box 4.1 below).

Coastal Observations, Mechanisms, and Predictions Across Systems and Scales (COMPASS)

Focus: Enhancing predictive understanding of marine and freshwater coastal systems and their responses to multiple stressors that integrate water, soil, and vegetation, including processes governing carbon and nutrient cycling, representation of land-lake-atmosphere interactions, transport of nutrients, and interactions with urban systems.

Figure 2.2.3: Current multi-Institutional national laboratory-led Science Focus Areas and university Cooperative Agreements supported by the DOE MSD program.

Example Activity: Investigate the combined impact of urbanization and climate warming on summer heat stress, convective storms, and urban flooding in the Great Lakes region, with a specific focus on the Chicago metropolitan area.

CoP Themes: Coastal Observations, Mechanisms, and Predictions Across Systems and Scales is focused on human-Earth system dependencies and interactions and how stressors such as summer heat stress, storms, and flood patterns are influenced by factors including land-use and land-cover change and unique coastal climate processes.

Project website: https://compass.pnnl.gov/

Global Change Intersectoral Modeling System (GCIMS)

Focus: Improving the understanding of the complex interactions among energy, water, land, climate, socioeconomics, and other important human and natural systems at regional-to-global scales, with an emphasis on developing and applying an internally consistent, open-source, computationally efficient modeling framework that captures the evolution of the integrated human-Earth system.

Example Activity: Exploratory ensemble modeling is being used to better understand the uncertain dependencies and interactions that exist across the energy-water-land-climate change pathways. Using scenario discovery and unsupervised ML techniques, in particular, to map how human and environmental influences lead to compounding vulnerabilities in the United States and globally.

CoP Themes: GCIMS is specifically focused on better capturing interdependencies and interactions while considering deeply uncertain tradeoffs across a broader array of societal objectives.

Project website: https://gcims.pnnl.gov/

A Framework for Improving Analysis and Modeling of Earth System and Intersectoral Dynamics at Regional Scales (HyperFACETS)

Focus: Developing comprehensive frameworks for climate data assessment that incorporate process-oriented, feature-specific, and use-inspired metrics. These efforts are focused on making advances in the continental United States that (1) increase understanding of processes at the climate-water-energy-land-decision interface and (2) fundamentally improve credible climate modeling of regions.

Example Activity: Advancing the storylines approach for understanding the drivers, dynamics, and multisectoral implications of significant hydroclimate events. Organizing research around significant events (e.g., the 2018 CA wildfires or CO's Spring Miracles) and the climatology of recurring high-impact events (e.g., droughts and tropical storms) with the engagement of regional stakeholders to identify vulnerabilities and key event drivers. The goal is to broaden the suite of metrics that can be used to inform model improvements, generate salient regional scenarios, and generalize to broader classes of extreme events.

CoP Themes: HyperFACETS is specifically focused on multisectoral dependencies and interactions, improving coupled human-environment modeling, and facilitating improved uncertainty characterization via innovations in scenario exploration.

Project website: https://climate.ucdavis.edu/hyperfacets/

Integrated Coastal Modeling (ICoM)

Focus: Advancing innovations across a range of modeling tools to systematically understand and analyze coastal processes, hazards, and responses across a range of spatiotemporal scales. These efforts have a near-term focus on the mid-Atlantic region, which exhibits a wide diversity of coastal development patterns and is home to dense networks of connected infrastructure that is often stressed or disrupted by hurricanes, extratropical storms, droughts, and other extreme events.

Example Activity: Coastal development patterns can strongly shape community risk posed by extreme flood events. A modular agent-based human-natural systems model is being developed to capture key physical, demographic, economic, and institutional drivers of coastal development. The model enhances exploratory evaluations of how candidate actions and uncertainties associated with human behavior shape risk and resilience.

CoP Themes: ICoM is focused on better understanding how adaptive human actions shape coastal risk, multisectoral dependencies and interactions in connected infrastructure, and the uncertain effects of potentially compounding human-natural coastal stressors.

Project website: https://icom.pnnl.gov/

Integrated Framework for Modeling Multi-System Dynamics

Focus: Advancing a multi-system modeling framework to focus on energy-water-land-atmosphere interactions and uncertain human responses at decision-relevant scales. These efforts use a near- to long-term focus on the lower US Midwest and Gulf Coast to understand regional-to-global teleconnections given compounding human and natural influences, extreme events, and co-evolving multisectoral infrastructure systems.

Example Activity: In the Mississippi River Basin and its estuary, advancing a systems-of-systems approach to understanding how evolving flood and drought risks shape the sustainable management of resources (water, land, energy, fisheries, etc.) given competing objectives and uncertain tradeoffs across sectors and regions is crucial. Diverse sectoral interests include agriculture (fertilizers and irrigation), estuary managers (environmental impacts), fisheries managers (hypoxia and productivity), ports (navigation and trade), developers (land development), and energy (cooling water and power production).

CoP Themes: The Massachusetts Institute of Technology Joint Program on the Science and Policy of Global Change is focused on multisectoral dependencies and interactions that are intra-regional within the Mississippi River Basin and shaped by competing resource objectives and human decisionmaking. The uncertain co-evolution of the

region's resource systems as they confront technological transitions and climate risks has potential global-scale implications given their market-driven teleconnections to other regions globally.

Project website:
https://globalchange.mit.edu/research/research-projects/integrated-framework-modeling-multi-system-dynamics

Integrated Multisector, Multiscale Modeling (IM3)

Focus: Advancing open-source, process-based human and natural system interactions modeling from local to continental scales to forecast vulnerability and resilience under both short- and long-term influences. The project is studying the responses of interacting energy, water, land, and urban systems to compounding influences over the course of the 21st century (climate-driven heatwaves and drought, population change and urbanization, changing socioeconomic conditions, and technology change).

Example Activity: Advancing modeling of urban heatwaves and vulnerability by better capturing interactions between urban microclimates, heatwave adaptations, urban morphology, socioeconomic heterogeneity, and anthropogenic feedback. The model coupling effort blends dynamic urban and building morphology, adaptation strategies (e.g., white and green roofs), detailed microclimate modeling, and innovations in uncertainty characterization.

CoP Themes: IM3 is centrally focused on multisector dependencies and interactions through advancing model coupling experiments across the continental United States, regional, and urban scales to better understand vulnerabilities from compounding extremes. The project is dedicated to open-source and reproducible model coupling experiments that incorporate improved representations of adaptive human actions and uncertainty characterization.

Project website: https://im3.pnnl.gov/

Interdisciplinary Research for Arctic Coastal Environments (InteRFACE)

Focus: Advancing arctic marine biogeochemistry, shipping, and coastal change to better understand how reductions in sea-ice thickness and extent alter maritime shipping, resource extraction, and communities along the northern Alaskan coast as well as the broader Arctic. Key feedback include changing riverine fluxes influencing sea ice, ocean circulation, marine biogeochemistry, and the economic activities of coastal communities. Likewise, changes in erosion and flooding shape the economics of maintaining, relocating, and expanding coastal communities and infrastructure systems. The project is exploring how these changes affect local, regional, and global communities and economies.

Example Activity: Exploring the physical and human drivers and uncertainties that influence future arctic fossil resource extraction and the resulting shipping, encompassing a myriad of human-Earth system feedback. The timing of the availability of cheaper oil extraction technology, whether early or later in the 21st century, has the potential to substantially impact sea ice, permafrost, global market conditions, and human decisionmaking related to multisector infrastructure systems. Increased oil and gas shipping from the Arctic region has the potential for economic teleconnections as well as significant effects on climate risks on a global scale.

CoP Themes: InteRFACE explicitly engages with global-to-local dependencies and interactions resulting from the co-evolutionary pathways of human-Earth system dynamics in Arctic coastal systems. Global market conditions, sea ice, permafrost, and local-scale human systems decisionmaking are strongly entwined. Uncertain human and global physical influences as well as stressors require advances in uncertainty characterization, model coupling, and capturing adaptive human actions across sectors and scales.

Project website:
https://climatemodeling.science.energy.gov/projects/interface-interdisciplinary-research-arctic-coastal-environments

Program on Coupled Human and Earth Systems ADAPT (PCHES-ADAPT)

Focus: Understanding risk and response behaviors within the context of landscape evolution, interconnected infrastructures, and the resilience of complex systems. The frameworks of computational tools developed in PCHES-FRAME are being applied and extended through research focused on the quantification and characterization of

water stress, wildfires, and flooding. A particular focus is to identify, characterize, and compare risk management strategies, adaptive measures, and their implications for systems resilience.

Example Activity: PCHES-ADAPT will conduct two regional case studies—water stress and wildfires in the western United States and water stress and flooding in the Great Plains and Upper Midwest. These cases will be combined with additional information to form the basis of three intercomparison exercises: (1) responses and implications of water stress in the western United States and Great Plains regions; (2) flooding responses and implications in the Upper Midwest and East Coast; and (3) uncertainty characterization and quantification methods across all the cases.

CoP Themes: PCHES-ADAPT focuses on the CoP themes of stressors, influences, and adaptive human system responses. In addition, the project contributes to the development of uncertainty characterization and quantification techniques for complex, coupled, multisector modeling systems to explore their suitability for application to other modeling frameworks.

Project website: https://www.pches.psu.edu/

Puget Sound Project

Focus: Establishing a testbed for advancing transferable knowledge and modeling of coastal systems, including how the complex terrain and environment of Puget Sound interact with the large-scale climate conditions and human systems, and how these jointly contribute to the Sound's hydroclimate (including hydrological extremes).

Example Activity: Understanding and evaluating different modeling approaches for representing processes governing atmosphere-land-river-human interactions in the topographically complex Puget Sound region requires considering orographic precipitation, rain-on-snow events, and hydrologic extremes and the impacts of land and water management and use.

CoP Themes: The Puget Sound project initially contributes to two key CoP themes: stressors and extreme events (how different modes of climate variability interact with land surface features and heterogeneity) and model evaluation (the sensitivity of modeling climate and extremes to model resolution, process representations, and regional downscaling techniques).

2.3 Mapping MSD's Research Gaps

As MSD research seeks to engage with and better understand the dynamic and adaptive complexity of human-Earth systems and the implications for a broader array of societal objectives, over the next decade the field will need to work to address the gaps summarized below.

Workforce Gaps for Addressing Human-Earth Systems Complexity

- There is a dearth of programs in the United States that provide the types of transdisciplinary training and research experience needed for advancing MSD research as well as growing job opportunities at the community level.
- Junior researchers that engage in MSD research lack MSD-dedicated forums for networking, building long-term collaborations, and professional mentorship.
- Diversity, equity, and inclusion are significant challenges that are critical to framing MSD science questions, innovating technical advances, and framing societal relevance.
- Over the next decade and beyond, sustained MSD research advances will require care in retaining and promoting researchers, especially women and underrepresented minorities.

Workflow Gaps for Addressing Human-Earth Systems Complexity

- As MSD research considers a broader suite of human-Earth system feedback as well as their implications across sectors, systems, and scales, maintaining FAIR (Findable, Accessible, Interoperable, and Reusable)

principles for data and source codes, as well as ensuring reproducibility, are likely to become substantially more challenging.

- The complex and dynamic co-evolution of the human-Earth systems of focus in MSD poses a fundamental need to rapidly broaden our access to new hypotheses and accelerate scientific progress via improved modeling, wide dissemination of analytic tools, and enhanced mechanisms for community-level training and learning.
- New training and tools are necessary for transdisciplinary communities to support and sustain commitments to open science so that innovations can be widely and rapidly leveraged.

Methodological Gaps for Addressing Human-Earth Systems Complexity

- MSD research needs to draw on tools from the complexity field (e.g., network theory, information theory, and causality inference) to develop more powerful tools for understanding evolving human-Earth system dependencies and interactions.
- Fundamental innovations are needed to better capture the underlying behavioral uncertainties within human systems that shape the dynamics of large-scale societal transitions.
- Recent advances in RL, control, and ML have yet to be adopted to better capture highly nonlinear and uncertain "state-action" feedback within MSD systems and understand their consequences (e.g., infrastructure investments or ecological tipping points).
- Deeper collaborative connections with the statistical, mathematical, and computational sciences are needed to transition emerging uncertainty, AI, and computing architectures into MSD research efforts.

Translational Gaps for Connecting MSD Research Insights to Operations

- An emphasis on research-to-operations and operations-to-research is needed to ensure that MSD insights are able to connect to and inform real-world decisionmaking and, in turn, that applied, operational work can inform MSD research questions.
- There is a need for the MSD CoP to collaborate with communities of practice and government agencies conducting applied research (e.g., US Environmental Protection Agency, US Geological Survey, NOAA, US Army Corps of Engineers, US Department of Agriculture) to leverage complementary capabilities that can further both applied and fundamental research.
- Methodological advances are needed to push the frontiers of decision analytic tools that can simultaneously capture the complexity and uncertainties of the human-Earth systems of focus in MSD while effectively facilitating decision-relevant insights.

These gaps and challenges present opportunities for the MSD CoP moving forward. They inform a transformative research vision for the next decade. Chapter 3 describes that vision and emerging innovations that hold promise for addressing the MSD research gaps described above. Chapter 4 elaborates on opportunities for inter-agency/inter-community collaborations that can leverage the strengths of those involved to fill scientific gaps and inform R2O2R opportunities. Ultimately, addressing these gaps will put MSD in a better position to tackle the complexity of human-Earth systems through its main science questions related to dependencies, interactions, stressors, uncertainties, adaptive human actions, and model coupling. It will also accelerate the inclusion of new perspectives and access to new scientific questions and hypotheses.

Chapter 3.
MSD 2030: Transforming our Understanding of Human-Earth System Complexity

This chapter offers strategies to accelerate collaborative science insights for the MSD research community, including developing a more diverse, equitable, and inclusive workforce and transforming collaborative workflows through the adoption of open science practices to scale and accelerate MSD insights. The chapter further presents MSD research aspirations for the next decade. These include better integration with complexity science, improving human systems uncertainty research, leveraging computational advances for exploratory modeling of coupled human-Earth systems, and taking advantage of emerging opportunities in data analytics, computational architectures, and embedded intelligence in scientific workflows to overcome barriers to MSD research insights.

3.1 Going Exponential: Accelerating Collaborative Science Insights

Haimes (2018) notes that our capability to model and gain insights into complex co-evolving human-Earth systems is a rate and capacity limited process itself. Considering lead times for research and development, this presents the dilemma that models or analytics that adequately capture key dynamics, systems' elements, and their evolving relationships are often no longer relevant for decision-insight once they are actually available for use. Adding to the rate and capacity challenges, the scope of the major societal questions driving MSD research (see Chapter 1) presents a representation challenge. Understanding resilience and distributional effects, including equity, in complex human-Earth systems requires a significant investment in growing and diversifying the MSD workforce to broaden the backgrounds, knowledge, and experiences the community can draw on to advance our understanding of societal risks. As noted in Chapter 1, societal change pathways related to energy transitions and climate challenges encompass global supply chains, strained natural resources, aging infrastructures, uncertainty in infrastructure investments, increasingly vulnerable populations, and intensifying natural hazards. Moreover, we must overcome workforce and workflow gaps (see Chapter 2.2) within the MSD CoP itself as an enabling mechanism for confronting the complexity of co-evolving human-Earth systems. Fundamentally, the community needs to exponentially scale inputs to MSD science (workforce, tools, hypotheses, teams, agencies, sectors, and scales) and the resulting outputs (results, papers, insights, and translational science benefits to society).

Workforce Development Opportunities

Who constitutes the MSD scientific community is integral to the community's capacity to meet its scientific objectives. Exponentially scaling hypothesis generation and exploration requires a broader and deeper workforce developed using active commitments to diversity, equity, and inclusion (DEI). Following a number of US scientific societies, in this report, we define "diversity" as "the full spectrum of personal attributes, cultural affiliations, and professional or socioeconomic statuses that characterize individuals within society" and equity as the objective of establishing equal opportunity and representation, which implies creating opportunities for disadvantaged and historically underserved individuals and communities to facilitate their advancement in science and society (AGU, 2018). The Science, Technology, Engineering, and Math (STEM) fields that primarily compose MSD are significantly less diverse than the US population as a whole (National Academies of Sciences and Medicine, 2020).

Figure 3.1.1: Percent of employed in each occupation in 2019 versus fraction of the US population in 2019. Data are from Table 9-7 and Table 1-2, National Center for Science and Engineering Statistics. 2021. Women, Minorities, and Persons with Disabilities in Science and Engineering: 2021. Special Report NSF 21-321. Alexandria, VA: National Science Foundation. Available at https://ncses.nsf.gov/wmpd. Underrepresented Minority group is composed of response groups from the original dataset as follows: Hispanic or Latino, American Indian or Alaska Native, Black or African American, Native Hawaiian or Other Pacific Islander, or More than one race. Number is the number of employed persons in each occupation, so the size of the bubble represents the size of the occupation. Gender identity information is not available in the dataset, so we summarize by sex.

Figure 3.1.1 compares the composition of the working-age (18–64) US population in 2019 to the composition of several scientific fields that are relevant to MSD. Underrepresented minorities make up a smaller fraction of almost every scientific field than they do of the US population as a whole in Figure 3.1.1. Women are particularly underrepresented in engineering, natural, and computer science occupations. This represents a significant gap in potential (not recruiting and retaining women means missing half of the best scientists), as well as an opportunity to

grow the MSD workforce. Simply put, the MSD CoP cannot achieve its full potential for science without developing a more representative workforce (see Box 3.1 below).

Figure 3.1.2: Holistic STEM workforce career development model from Batchelor et al. (2021).

It is critical that the MSD research community diversifies and actively improves the inclusive framing of research questions. Research shows that contributions by non-majority groups within a scientific field tend to be more novel but are less recognized (Hofstra et al., 2020). Beyond inclusion, active mentorship, advocacy, and promotion of underrepresented scientists are key to growing their contributions and maximizing their recognized innovations to the MSD field. Overall recruitment and retention of women and underrepresented minorities as well as the overall aspiration of exponential growth for the MSD science community requires moving beyond the limitations of the "STEM Pipeline" analogy, which has been shown to exclude non-traditional professional career paths that severely impact underrepresented minorities and identities (Bernard and Cooperdock, 2018; Cannady et al., 2014). Batchelor et al. (2021) suggests that STEM workforce development is better captured with the Braided River analogy shown in Figure 3.1.2. They suggest that the Braided River model is a more holistic representation of "learning ecosystems" and presents a diversity of inclusive entry points to the "many paths" for scientific career development. The model also highlights the value of transdisciplinarity, lifelong learning, and sustained mentorship. DEI, recruitment, and retention must also be carefully considered as part of the community's open-science aspirations (i.e., the workflow gaps in Chapter 2.2). The MSD CoP can take concrete steps through initiating active mentoring programs, sustaining outreach to professional science or engineering societies for underrepresented groups, and collaborating with academic partner institutions for broader training and recruiting efforts. Community level support of training opportunities and improved access to emerging MSD innovations is fundamental to the goal of going exponential. Murphy et al. (2020) highlights that the collaborative structure and broader social networks of open-science initiatives have yielded more frequent high-status authorship for women relative to a narrower focus on reproducibility.

Box 3.1: Growing and Diversifying Who is MSD to Confront Complexity

Figure B3.1.1 summarizes the properties, stages, and potential outcomes to consider in the development of a CoP. The continuum from standard transmissive dissemination of science to transformative co-creation is fundamentally shaped by a community's defined membership, network relations, and the balance of power to make contributions. As noted in Figure B3.1.1, community-led co-creation is a mechanism for creating altogether new modes of framing and exploring scientific hypotheses that can potentially yield transformative changes. Institutional support of DEI has direct potential benefits for science outcomes. Nielsen et al. (2017) highlights that increasing the number of women and their leadership roles in teams has been shown to aid collaborative task completion with improved awareness of social dynamics, membership expertise mapping, and broadening the topics considered in framing research questions. Incorporating DEI in MSD will require continuously adapting to incorporate the best available information, particularly because the majority of studies so far have focused primarily on the impacts of greater representation of white women in STEM. More research is needed to understand what practices best support scientists from other underrepresented groups and the impact of intersectional identities on key outcomes. Initial steps are to create a mission statement that addresses DEI and use community resources to implement evidence-based practices that support the diverse growth of early career researchers in this community (Hill et al., 2010; Johnson et al., 2019; National Academies of Sciences and Medicine, 2020). DEI work (Tilghman et al., 2021) supports the MSD science mission and is critical to the aspiration of exponential growth to confront the complexity of human-Earth systems.

Figure B3.1.1: The Center for Scientific Collaboration and Community Engagement (CSCCE, 2020) participation model for the stages of collaborative relationships for an emerging CoP. The CSCCE Community Participation Model is shared under a CC BY-NC-ND 4.0 license, and may only be reused in its original form (which includes the CSCCE logo)

Workflow and Open Science Opportunities

As noted in Box 3.1, the aspiration of exponentially accelerating collaborative science innovations will require that the MSD CoP undergo a transformational change in the way research is done. This transformation includes (but is not limited to) expanding the breadth and scale of questions explored, making it easier for new and diverse researchers to join the MSD community, incorporating new technologies like AI and exascale computing, and facilitating collaboration across teams and projects. Open science is one strategy to enable these changes. New training and tools are necessary for MSD as a transdisciplinary community to support and sustain commitments to open science so that innovations can be widely and rapidly leveraged.

As a first step toward realizing MSD open science aspirations, the community's tools need to be developed using the FAIR data standards or open-source software principles (Wilkinson et al., 2016). The FAIR data principles aim to facilitate the reuse of datasets by enhancing the ways in which data is managed, documented, and shared. FAIR data also facilitates opportunities to apply machine- and deep-learning methods (Wise et al., 2019). FAIR data is directly related to EESSD's data-model integration Scientific Grand Challenge to *"develop a broad range of interconnected infrastructure capabilities and tools that support the integration and management of models, experiments, and observations across a hierarchy of scales and complexity"* by adhering to its fundamental value of *"effective data management, including developing community data standards and formats and sharing and preserving data, to increase the pace of scientific discovery and ensure scientific integrity"* (DOE, 2018). The code corollary to FAIR data is the practice of open-source software. Open-source software fosters creativity, wider adoption, and rapid improvements in the underlying code base (Paulson et al., 2004).

Figure 3.1.3: The growing global research community and scholarship employs GCAM since its transition to an open-access community model in 2010. NA designates periods when a given category of data is not available.

A compelling example of the benefit of transitioning toward an open science perspective within the MSD community is the transition of the GCAM from a primarily closed modeling system developed for and by researchers at Pacific Northwest National Laboratory into a community model (Figure 3.1.3). As a community model, the development of GCAM employs version control and a defined process for feature development and integration. Researchers from across the country and the world can develop their own features and improvements to the model. Additionally, there is a systematic process for potentially incorporating those changes into the core model. As a community model, GCAM is now used by a growing number of US and world-wide research groups as well as other US agencies, including the US Environmental Protection Agency. Since its transition to a community model in 2010, GCAM's influence embodies "Going Exponential" in supporting scholarship and its user base.

Overall, it is critical to grow and diversify the MSD research community while ensuring that breakthroughs are rapidly accessible through a commitment to open science.

Box 3.2: Open Science to Scale and Accelerate MSD Insights

Open science aims to accelerate scientific progress by making the data, code, methods, and products underpinning scientific research freely and easily available to downstream users. Open science is an umbrella term that describes foci ranging from open-access journals to reproducible research to open-science tools like data repositories and open-source models (Figure B3.2.1). The open-science movement has risen to the point of being recognized by the US National Academies of Science and Medicine as a fundamental means for realizing 21st century research innovations (National Academies of Sciences and Medicine, 2018).

Open science accelerates progress by reducing barriers to entry, gaining economies of scale, and avoiding duplication of effort (Allen and Mehler, 2019). Researchers that embrace open science in their own work generate more citations and collaboration opportunities compared to those who do not (McKiernan et al., 2016). There are two key tenets of open science as it relates to the going exponential theme described here: reproducibility and extensibility. Reproducibility, the ability to reproduce the results of others, is a critical component of the scientific method, and is fundamental to ensuring scientific integrity. Open science facilitates reproducibility by making it easier to repeat and confirm the findings of others (e.g., McNutt, 2014; Pfenninger et al., 2017; Wicherts et al., 2011). The concept of extensibility–the ability to quickly and easily build upon the work of others–is critical for going exponential for MSD. The extensibility of research is particularly relevant to the MSD research community, where the scope of problems being tackled is large, but there are still significant overlaps in themes and approaches across projects (e.g., see Box 2.3). Teams across the MSD community focus on problems in common sectors (e.g., energy, water, transportation) with analogous properties and characteristics (e.g., networks, capacity, flow). As such, datasets and models generated in one project often have value for another project. In a "closed" research environment, new project teams often spend a tremendous amount of time and effort on initiating complex modeling tasks when building on existing tools or approaches could dramatically accelerate their ability to explore diverse hypotheses or innovate new modes of analysis. There are large opportunity costs within the MSD CoP when models, data, and analytic tools are not publicly available or poorly documented, making it difficult for a downstream user to adapt prior scientific assets for a different purpose. Consequently, there is a major opportunity for innovation scaling through open science practices to enable MSD breakthroughs.

Figure B3.2.1: Graphical taxonomy of the interrelated aspects that shape open science ranging from access, evaluation, funding policies, and tools. Graphic redrawn from Pontika et al. (2015).

3.2 MSD Research Aspirations for the Next Decade

As noted in Chapter 1, this report formalizes a vision for MSD as an emerging transdisciplinary field, advancing our understanding of the local-to-global systems that fundamentally shape the interdependent dynamics, risks, and welfare of our modern world. The aspirations shared here seek to encourage transformative research that addresses the major methodological challenges driving MSD research (see Chapter 2.2). There are, however, methodological, data availability, and computational gaps that are at present limiting the MSD community's ability to understand the complexity of human-Earth systems and their feedback. In this section, we identify and discuss the needs for: (i) better integration with the complexity field; (ii) improved modes of analysis for capturing uncertainties in how human systems shape dynamics; (iii) computational advances that enhance representations of highly nonlinear and uncertain "state-action" feedback; and (iv) solutions to overcome computational scaling and scientific inference barriers to MSD research insights. Addressing these gaps will require deeper collaborations with the statistical, mathematical, and computational sciences. These research gaps correspond closely to the BERAC Grand Challenges (BERAC, 2017, see Chapter 1.0) and addressing them will position the MSD research community over the next decade to support DOE's mission and broader scientific objectives related to human-Earth systems feedback for energy transitions and climate risks. Figure 3.2.1, redrawn from the EESSD Strategic Plan, (DOE, 2018) broadly frames the Division's vision for integrating innovations in modeling, observations, field experiments, and computational experiments.

Although Figure 3.2.1 provides an excellent idealized aspiration, it does pose significant challenges when trying to implement this workflow to address MSD research questions. Capturing interdependent global-to-local pathways of societal change requires the exploration of deeply uncertain co-evolutionary dynamics and feedback for human-Earth systems. Pathways of change encompass a myriad of intertwined environmental, economic, engineering, and social systems. Their multisector interactions shape near-term to centennial-scale emergent risks and vulnerabilities. Understanding how emergent risks shape multisector vulnerabilities and resilience is highly non-trivial, requiring a broader framing of hazard-exposure-vulnerability-response [see Box 1.4, Simpson et al., 2021]. As an example, a retrospective analysis of the 2018 European heatwave highlights the conceptual challenge of mapping the complex interactions that generated risks to infrastructure systems (Figure 3.2.2 redrawn from Simpson et al., 2021). The mix of scales, sectors, systems, and path dependent-processes that shaped the illustrated infrastructure risks from the 2018 European heatwave poses a daunting gauntlet for forwarding model-driven projection systems. Heat extremes not only produced health effects, but they also increased energy demand and caused rail lines to buckle. Drought conditions reduced river levels, affecting shipping (an alternative to rail) and power generation, and also reduced crop yields. These types of extreme events often yield

Figure 3.2.1: EESSD's vision for an idealized strategy for integrating state-of-the-science knowledge about critical systems that effectively blends multiscale and multiprocess observations, field experiments, and modeling experiments (redrawn from DOE, 2018).

changes to human systems, including behavioral preferences, governance, institutions, and infrastructure investments, that can fundamentally reshape societal pathways of change. This level of complexity poses fundamental challenges to the EESSD's model-observation-experiment framework in Figure 3.2.1 in terms of the rate limits for modeling as well as understanding how decomposability, observability, and predictability limits shape the cycle of experimental design.

Figure 3.2.2: The emergent, complex interactions of drivers within and between each determinant of risk during the 2018 European heatwave. Here, determinants of risk refer to hazard, exposure, vulnerability, and response. Arrows designate driver interactions, and addition signs indicate the aggregating effects of drivers (redrawn from Simpson et al., 2021).

Keeping pace with the accelerating complexity of existing and future pathways of human-Earth system changes requires a deep integration of diverse perspectives, technical capabilities, and rapid innovations in our modes of scientific inquiry (Elsawah et al., 2020; Moallemi and Haan, 2019; Trutnevyte et al., 2019). Moreover, MSD seeks these new modes of inquiry to yield tools and insights for transforming the benefits and resilience of human and natural systems. Given their complexity, candidate pathways of change, and diverse sources of uncertainty, there is a need to rethink our traditional disciplinary approaches to science as well as the modes of science itself (Bai et al., 2016; Funtowicz and Ravetz, 1993; Geels et al., 2016; National Research Council, 2014; Rittel and Webber, 1973; Saltelli et al., 2020; Szostak, 2017). This holds tremendous promise for advancing our understanding of the local-to-global systems that fundamentally shape the interdependent dynamics, risks, and welfare of our modern world.

Complex Adaptive Systems-of-Systems Opportunities

As illustrated in Figures 3.2.2 and 3.2.3, Simpson et al. (2021) highlights the need for modeling advances that can better cope with the reality that interacting risks can emerge from complex mixtures of determinants (hazards, exposures, vulnerabilities, and responses) and drivers (climate, socioeconomic, environmental, infrastructure conditions, etc.). Of note is the role of human "responses" where actions, such as investments or operational changes, can be strong determinants of risk, potentially degrading or improving conditions, as well as drivers of other dependent risks (see Figures B1.4.1, 3.2.2, and Box 1.4). Moreover, combinations of multiple risks (Figure 3.2.3) pose challenges based on how their interactions manifest (e.g., linear aggregation, compounding feedback, or highly nonlinear cascades).

Figure 3.2.3: Illustration of how multiple risks can interact, ranging from additive aggregations to unidirectional or bi-directional compounding and sequential cascading (redrawn from Simpson et al., 2021). The risks, as illustrated, can be different from one another. Interactions can emerge across different measures of risk defined across diverse objectives, scales, sectors, and systems.

As an example, the February 2021 Texas power outage resulting from Winter Storm Uri illustrates how human responses are central determinants of risks as well as how risks can yield cascading impacts across complex networks of cross-sectoral exposure and vulnerability pathways (energy, water, human health, finance, housing, insurance, etc.). As a hazard, Winter Storm Uri was not unprecedented in Texas as the temperature extremes and energy demands during the event were less severe or equivalent to winter storms in 1951, 1983, and 1989 (Doss-Gollin et al., 2021). Moreover, the cold snap in 2011 caused rolling blackouts in Texas and highlighted clear systemic vulnerabilities. Human responses, characteristics of the regulatory system, markets, and lack of winterization of

key infrastructure systems strongly shaped the emergent cascade of interacting risks (Smead, 2021). The February 2021 Texas power outage also highlights the complex interplay of diverse societal objectives (reducing loss of life, reliability of services, resilience of services, equity of impacts, minimizing financial volatility, cost, etc.) across a broad range of actors, scales, systems, and sectors.

As a transdisciplinary endeavor, MSD research offers the opportunity to diversify model-based human-Earth systems problem framings across a broader array of perspectives, enabling detailed quantitative analyses of a broad suite of societal objectives (see Box 3.3). MSD has a distinguished central focus on developing the next generation of open-source models, analytical tools, and theoretical insights that enhance our ability to trace environmental, technological, and societal transitions. As defined in Chapter 2.1, understanding multiple sectoral perspectives requires care in capturing the dynamic co-evolutionary pathways of the underlying systems-of-systems governing them. Over the last century, many diverse scientific disciplines (e.g., socio-ecological systems, systems engineering, complex systems, and Earth science) have been drawn to the formal framing of their research through the systems-of-systems perspective, (Anderies et al., 2013; Gorod et al., 2008; Haimes, 2018; Holling and Gunderson, 2002; Iwanaga et al., 2021; Pescaroli and Alexander, 2018; Simpson et al., 2021), all of which emphasize the importance of capturing the hierarchy of systems' structures and their interdependent state dynamics. These traits are central to the challenges posed in trying to understand path dependencies, lock-ins, and the potential for emergent behaviors (natural, engineered, and socioeconomic).

Box 3.3: The Competing Objectives and Complexity of Estuaries

Figure B3.3.1 Visualization of runoff from farms (green areas) and cities (red areas) draining into the Mississippi River, delivering nutrients into the Gulf of Mexico and shape the dynamics of hypoxia (courtesy of NOAA, https://oceanservice.noaa.gov).

The Mississippi River Basin in the central United States, the Mekong River Basin in Southeast Asia, and the Chesapeake River Basin in the Mid-Atlantic United States are examples of complex estuarine systems with interrelated resource challenges. Careful management of key resources, such as land, water, energy, food, and ecosystems, is essential to

a sustainable future that meets both human and environmental needs. However, resource management is becoming increasingly difficult due to complicating factors directly related to MSD challenges, such as: competing objectives and tradeoffs between different sectors; deep uncertainties related to climate risks, population dynamics, economic outcomes, infrastructure development, technological innovation, and governance; local to global teleconnections from agriculture productivity and shipping impacts; as well as long infrastructure lifetimes where there are growing vulnerabilities to extreme events. Modeling to understand these complex interconnected ecosystems is particularly challenging, requiring representations of land, ocean and freshwater processes as well as how their feedback with human systems shape the emergent risks and sustainability of their ecosystem services.

The lower Mississippi River Basin (from the lower Midwest to the Gulf Coast) is a prime example to demonstrate the MSD approach to this class of systems. Like many estuaries, the Mississippi River Basin includes an important agricultural region—the lower Midwest produces grains that are consumed domestically and exported globally. The river, and its system of barges and levees, is used to transport fertilizers from the Gulf region upstream to agricultural producers, while grains travel downstream to ports in the Gulf for shipment to their final destinations. The river itself also carries fertilizers and agricultural runoff downstream to estuaries, causing hypoxia and creating ecosystem risks, including threatening the ocean food web and reducing fishing productivity for coastal communities. In complex estuaries and their connected river basins, there are clear tradeoffs between upstream and downstream outcomes related to water, land, and ecosystems, and a need to balance multiple objectives (Kling et al., 2014; Rabalais and Turner, 2019). MSD research advancements are needed for capturing these complex, adaptive systems-of-systems (Haimes, 2018) integrating different types of data and analytic tools, including those focused on hydrology and water quality, agriculture and land use, energy, transportation systems, economics (including local-to-global markets), population dynamics, governance, climate and extreme events, ecosystems, and actions across diverse social scales. Open-science workflows are needed to facilitate rapid depth and dexterity in modeling and analytics to allow researchers flexibility in their science questions and ability to rapidly shift their emphasis across sectors, scales, and systems of focus.

The systems-of-systems perspective is a fundamental and emphasized feature in the definition of MSD. As illustrated in Chapter 2.1 (see Box 2.1 and Figure 2.1.3), three key properties characterize systems in nested and hierarchical relationships: (1) connectedness, (2) capital, and (3) resilience. Very similar taxonomies and traits have emerged within the engineering literature (Boardman and Sauser, 2006; Gorod et al., 2008; Helbing, 2013). These traits provide a helpful lens for scientifically framing MSD explorations of risk, adaptivity, and sustainability and how they emerge as system properties. From a transdisciplinary perspective, there is a rich array of opportunities for engaging with and advancing complexity science within MSD (e.g., network theory, feedback and control, deep uncertainty, stochastic adaptivity, path dependency, regime transformation, self-organization, emergence, compound, and cascading risks).

Human Systems Uncertainty Research Opportunities

The representation of dynamic and adaptive human actions in human-Earth systems models represents a core challenge for MSD research (see Box 3.4), particularly given uncertainties regarding human actors and their interactions with the physical environment (Bland and Schaefer, 2012; Osman, 2010). Human systems uncertainties have many dimensions. A few examples include: identification of key individual, collective, and institutional actors; capturing diverse objectives and tolerances to risk; and functional representation of actors and their actions in models. As noted by Trutnevyte et al. (2019), at present, multisectoral modeling approaches typically represent human development trajectories in the form of exogenously defined assumptions such as consumption intensities and rates, end-use technologies, and so forth. However, such approaches implicitly ignore potential human-Earth system feedback, assuming that the land, energy, and water-utilizing activities of human actors (and the beliefs, preferences, and institutions underlying those activities) are rigid in the face of changing environmental and socioeconomic conditions. As noted in Box 2.2, most global coupled human-Earth systems models used to evaluate long-term energy, land, and water trajectories adopt a neoclassical economic paradigm that assumes rational actors with

complete knowledge operating within the context of efficient global commodity markets. These models represent possible changes in sectors that produce energy, food, manufactured products, and many other goods and services. They have been central to ongoing efforts to understand how climate change and efforts to address it interact to affect future environmental conditions and human welfare. Strengths of these approaches include consistency in different inputs and outputs and including feedback from the effects of environmental changes on economic development. However, these economic frameworks are often limited to capturing local-scale facets of the natural and built physical environment. Advances across disciplines over the past several decades have enabled models of human actors to exhibit real-world myopia, bounded rationality, incomplete knowledge, and dependence on past experiences (Ajzen, 1991; Kahneman and Tversky, 2013; Simon, 1972; Weber, 2006). Additionally, there is merit in incorporating behavioral heterogeneity among individuals, such as differences in risk tolerance, and shaping preferences (Barsky et al., 1997; Chan et al., 2020; Koning et al., 2019).

Box 3.4: Uncertainty, Adaptivity, and the Dynamics of Human Systems

There is a strong divergence of empirical and theoretical approaches that have been adopted across disciplines for capturing dynamic and adaptive actions in models of human systems (e.g., Axelrod, 1997; Bertsekas, 2019; Harou et al., 2009; Lempert, 2002; Powell, 2019). This divergence speaks to the structural and parametric uncertainties in how MSD models represent human systems. These uncertainties potentially confound the effective analysis and diagnosis of vulnerability, risk, and resilience (see Figure 2.1.3). Accounting for the interacting effects of uncertainties and decisionmaking can drastically change projected dynamics and risks. The levee effect provides a poignant example in which the simplistic assumption of rational, forward-looking, all-knowing actors in a flood-prone housing market leads to a pronounced misdiagnosis of evolving risk. As levee construction bolsters a community's sense of security from floods, the presence of the levee paradoxically induces further urban development, leading to a magnification of flood risk relative to pre-levee conditions (Di Baldassarre et al., 2013; White, 1945). Neglecting this feedback can result in biased projections (Figure B3.4.1). This decision-making feedback can interact with different representations of physical-system uncertainties in nontrivial ways.

Figure B3.4.1: Illustration for how capturing human response dynamics reshapes determinants of risk (Hosseini-Shakib et al., 2021). Panel (a) illustrates climate change shifting water level hazards toward more extreme cases. Panel (b) shows the potential shift exposure to water level hazards with and without accounting for the levee effect. Lastly, panel (c) demonstrates the potential cumulative differences in projected risks.

Agent-based models of urban development are being used to better represent individual and collective actions related to flood risks, particularly in coastal regions. Recent modeling efforts (De Koning and Filatova, 2020; Haer et al., 2019; Löwe et al., 2017; Rauch et al., 2017) have focused on representing urban development in coastal environments as a complex interplay between human action and adaptation amid a dynamic natural landscape that is prone to both acute system shocks (e.g., floods, hurricanes) and long-term system change (e.g., sea-level rise).

Such efforts have been driven by a recognition that coastal environments comprise tightly intertwined human-Earth systems, with coastal urban development pathways emerging as the outcome of complex interactions among household preferences and risk tolerance, natural system stressors, infrastructure changes, and land-use policy decisions. Despite these burgeoning efforts, current approaches are largely simplified or ignored:

- The complex physics of flooding processes, including the distribution, frequency, and severity of floods over time (e.g., tail events) and the spatially heterogeneous characteristics of inundation during such events.
- Human responses and institutional changes that distinguish how flood types (extreme events, nuisance flooding, and sequential flooding events) shape short-term responses (e.g., dislocation and housing price signals) as well as long-term actions (e.g., levee construction and zoning policy).
- The potential complexities in system behavior (nonlinearities, tipping points, etc.) that arise when accounting for the interactions of these detailed processes.

As with all models, agent-based modeling must be carefully considered in terms of its underlying data, complexity of representations, and ability to capture key dynamics of interest (Srikrishnan and Keller, 2021). Moreover, given the growing interest in capturing novel dynamics outside of available historical observations, there has been an increasing focus on ensemble-based exploratory modeling frameworks to discover emergent outcomes of interest (Bankes, 1993; Lempert, 2002; Moallemi et al., 2020).

Figure B3.4.2: Agent-based abstraction of coastal urban morphological evolution balancing flood, water supply, land use, infrastructure expansion, and changes in residential housing. Figure courtesy of the ICoM project.

To address some of the issues described above in Box 3.4, agent-based modeling could be integrated more fully with larger scale human-Earth system models to coherently represent human system dynamics across scales, from global to local. For example, a coupled human-Earth system model could be used to simulate global scale population dynamics, land-use changes, and other macroeconomic outcomes under future scenarios of climate and socioeconomic change. Such simulations would provide a locale-specific agent-based model, such as the coastal flooding urban development model described above, with physical, economic, and demographic boundary conditions including population controls, commodity prices, and land-use changes. In turn, the agent-based model could be used to simulate urban development patterns that take into account local environmental, institutional, and infrastructural

elements of the system that are not represented in the global economic model. Basheer et al. (2021) demonstrate such a two-way iterative procedure between a regional computable general equilibrium economic model and a regional sector-specific water systems model.

Capturing how human systems shape the determinants of risk (hazards, exposure, vulnerability, and response) even for a single extreme event poses a major scientific challenge (see Figure 3.2.2). However, there is, at present, a dearth of modeling and analytic tools for better understanding how the co-evolutionary dynamics of multisectoral systems-of-systems shape risk. Formally, the scientific framings of rapidly changing human systems, their multisectoral demands, and their feedback with Earth systems are themselves deeply uncertain (Quinn et al., 2018; Quinn et al., 2017). Co-evolutionary pathways of change in human-Earth systems over the coming decades have irreducible uncertainties where it is impossible to perfectly define and represent systems of focus, their boundaries, and interactions (Kwakkel et al., 2016; Walker et al., 2003). Moreover, there is a broad range of plausible futures where there is no clear consensus on their likelihoods and consequences, often yielding complex tradeoffs across diverse MSD objectives (Dolan et al., 2021; Lamontagne et al., 2018).

Given these challenges, the MSD research community should exercise caution when employing explicit or implicit predictability assumptions over long-time scales and for complex human-Earth system dynamics. Recent literature advancing scenario analyses via exploratory modeling under deep uncertainty (Marchau et al., 2019; Moallemi et al., 2020) highlights a need for scientific framings that focus on generating a diverse ensemble of plausible futures. This shift away from deterministic single future predictions moves the focus to exploratory studies that support the discovery of what futures, actions, and outcomes are the most consequential.

Human-Earth Systems Exploratory Modeling Opportunities

As noted in Chapter 2.2, there is a need over the next decade to foster deeper collaborative connections with the statistical, mathematical, and computational sciences to transition emerging uncertainty, AI, and computing architectures into MSD research. This research gap and opportunity has been widely acknowledged in recent DOE strategic reports [e.g., the Grand Challenges report (BERAC, 2017), the EESSD Strategic Plan (DOE, 2018), and the Advanced Scientific Computing Advisory Committee (DOE ASCAC, 2020b)]. Given the large and long-lived capital investments associated with energy transitions, managing climate risks, and improving our national infrastructure systems, it is important to avoid myopic lock-ins and unintended amplifications of risks by actions that fail to meet engineered, economic, and social requirements across many plausible futures. A core benefit of the MSD research aspirations presented here is the transformation of the community's ability to advance broader exploratory modeling applications and analytics.

The DOE is in a unique position to initiate exploratory modeling experiments for co-evolving human-Earth systems at computational scales and resolutions beyond historical tractability limits (DOE ASCAC, 2020b). Exploratory modeling efforts at the interface of ESM and regional scale MSD research present an opportunity for leadership-class computational experiments that can provide fundamental insights. Hawkins and Sutton (2009)) explains the importance of understanding the relative balance of climate projection uncertainty between internal variability, model structure, and scenarios for human systems. Over the last decade, modeling and computational innovations have allowed for the emergence of single model initial condition large ensemble experiments that have been run across multiple ESMs [(Deser et al., 2020)]. Building on these innovations, Lehner et al. (2020) has been able to capitalize on work by Hawkins and Sutton (2009) to further explore the balance of how internal variability, model structural uncertainty, and human systems forcing scenarios shape climate projections of temperature and precipitation scales (long-term, global vs. decadal, and regional).

A clear implication of Figure 3.2.4 is that the transition to finer regional scales and decadal mean states can significantly shift the relative effects of how internal variability, forcing scenarios, and ESM structural differences shape projections. These results are relevant to how MSD research can provide support for understanding pathways

of human-Earth system change. For example, the winter season is when Seattle currently gets approximately 65% of its annual rainfall on average, and the region is highly dependent on snowpack. Clearly, changes in mean winter precipitation for Seattle have large multisectoral implications given the broad dependence on the region's water supply. Changes in the timing and magnitude of snowpack melt rates represent a key human-Earth system feedback. However, there are far broader implications for the results in panel (d) of Figure 3.2.4 than limitations in understanding changes in mean precipitation. Floods, droughts, heatwaves, as well as other extremes are generally of interest and shape regional development and infrastructure investment pathways. There are two pertinent concerns: (i) near-term prioritized capital investments must contend with significant irreducible uncertainties and (ii) the interplay of internal variability with single or multi-state extremes (e.g., persistent hot or dry droughts) in shaping the path dependent dynamics of the impacted human systems is not well understood. Broadly, the limitations of the observed record and its ability to capture internal variability as well as extreme events in the water cycle remain an area of significant concern and need research (e.g., see Dettinger and Ingram, 2013; Pendergrass, 2018; Quinn et al., 2020).

Figure 3.2.4: Time-varying variance decomposition of the relative fractions of variance contributed by internal variability (orange), forcing scenarios (green), and differences in ESMs structures (blue). This figure is from Lehner et al. (2020).

Tebaldi et al. (2021) further reinforces the opportunity for and value of collaborative ensemble modeling experiments blending advances in ESMs as well as MSD community contributions for uncertainty quantification as well as emulation-based analyses of extremes (see Figure 3.2.5). Addressing the question: "what is the lowest warming level to trigger at a 100-fold change in frequency of the present-day 100-yr ESL [extreme sea-level] event, making it at least an annual occurrence by 2100?." The results in Figure 3.2.5 are a US snapshot of the more than 7000 coastal locations globally modeled in this study. The reduced complexity of the Hector-BRICK climate model (or emulator, Hartin et al., 2015; Vega-Westhoff et al., 2019; Wong et al., 2017) enabled the exploration of 39 uncertain parameters in an adaptive Markov Chain Monte Carlo analysis that explored 10,000 parameter combinations. Figure 3.2.5 highlights the complex mixture of warming levels required for locations along the US East and Gulf coasts to be exposed to substantially more frequent ESL events. As noted by Tebaldi et al. (2021), the close proximity of coastal locations with substantially different required levels of warming (e.g., 1.5 °C versus 5 °C) highlights the need for further higher-resolution studies to better resolve the coupled human-natural system dynamics as well as their influence on the determinants of sea-level rise risks (hazards, exposures, vulnerabilities, and responses). These issues are of critical importance to the US and global coastal systems.

Figure 3.2.5: Global warming levels reached by 2100 (distinguished by colour) causing the present-day 100-yr ESL event to become at least an annual event. The + sign associated with 2 °C and 5 °C indicates projections that include Structured Expert Judgment-derived estimates of ice-sheet contribution to relative sea-level change. Figure has been redrawn with data from Tebaldi et al., 2021).

Although the insights from Lehner et al. (2020) and Tebaldi et al. (2021) both show the potential for unique and diverse regional climate futures, the studies are limited in their exploration of human systems forcing scenarios. In contrast, Dolan et al. (2021) exploit a modest set of five ESMs in an exploratory analysis of the economic implications of water scarcity for 235 global river basins across 3000 human systems scenario futures using GCAM. The study shows that water scarcity has dynamic and complex basin-to-global teleconnections depending on relative regional differences in the capacity within the modeled scenarios. Every river basin was found to have positive and negative outcomes as well as unique underlying factors (e.g., ESM climate projection, land use, groundwater access, agricultural efficiencies, transportation, and manufacturing) that control their dynamics. Some of the basins were shown to be far more economically robust if they had the capacity to draw on alternative water sources or shift economic activity. However, several of the basins also showed a vulnerability to economic tipping points where the combination of challenging climate conditions, prolonged scarcity, and limited capacity to respond caused sustained economic losses. For example, the Lower Colorado River (Figure 3.2.6) tipping point emerged for scenarios that combined low groundwater availability, low agricultural productivity, and strong economic demands within the United States and Europe. Across nearly all of the river basins of focus, runoff uncertainty as shaped by ESM projections was strongly amplified by human system responses.

Figure 3.2.6: Results from an exploratory analysis using the GCAM to evaluate the economic impacts of water scarcity over 3000 futures. The futures are generated using a broader sampling of the factors used to define the SSPs. The negative economic tipping point illustrated emerges across five ESMs' projections for hotter and dryer futures combined with SSP conditions that limit basin level water supply capacity expansions. Figure from Dolan et al. (2021).

Together, the results of Dolan et al. (2021); Lehner et al. (2020); Tebaldi et al. (2021) highlight the significant opportunity for pressing forward on regional-scale human-Earth systems exploratory modeling experiments that better capture deeply uncertain futures as well as how they shape key determinants of risks (i.e., hazards, exposure, vulnerability, and response as illustrated in Figures 3.2.2 & 3.2.3).

Opportunities in Data, Computation, and Embedded Intelligence

Exploratory modeling offers significant promise for aiding the MSD research community to better engage with the complexity of human-Earth systems dynamics and their interdependent risks. To exploit the full potential for exploratory modeling innovations, the community must position itself to take advantage of the explosive growth of emerging data resources, algorithmic innovations, and analytic advances that facilitate improved model-derived

inferences. Modeling frameworks are rapidly evolving in how they capture dynamic and adaptive representations of agents, infrastructures, and natural systems subjected to a broadening array of uncertainties (Filatova et al., 2013; Herman et al., 2020; Knox et al., 2018; Morris et al., 2018; Taberna et al., 2020; Trindade et al., 2020; Turner et al., 2020; Yoon et al., 2021). These advances are providing access to new scientific hypotheses, diversifying theoretical problem framings across a broader array of disciplinary perspectives, and allowing quantitative analyses to explore a broader suite of societal objectives (e.g., reliability, resilience, vulnerability, robustness, economic efficiency, financial risk, stability, and equity). Augmenting these recent advances, the emerging frontier of computational modeling and analytics is now beginning to embed AI and agent-based modeling into highly adaptive software development processes and scientific workflows. Embedded intelligence facilitates rapid iterative exploration of competing hypotheses and problem framings to accelerate scientific insights within the complex adaptive systems of interest to the MSD field (Atkinson et al., 2017; Brown et al., 2020; Deelman et al., 2019; Yilmaz, 2019). Such advances can be applied to carefully evaluate and trace the effects of our representations of scales, interactions, and path dependencies (Filatova et al., 2016; Iwanaga et al., 2021; Levi et al., 2019).

These issues tie closely to the Advanced Scientific Computing Advisory Committee's (DOE ASCAC, 2020a) key findings related to AI and ML, which highlight:

- US competitiveness requires substantial efforts to train a workforce able to use and advance AI/ML technologies in mission-critical areas.
- AI, growing data resources, and emerging high-performance computing platforms present a once-in-a-generation opportunity to start an ambitious AI for science initiative.
- The MSD community should explore emerging AI/ML multiscale, multisector capabilities to understand risk and resilience for changing human-Earth systems.

The value propositions for the MSD CoP are significant given the diversity and complexity of the systems-of-systems research focus, including:

- Automating or accelerating workflows that combine large heterogeneous data sources with complex model chains
- Improving the state-awareness of modeled agent-behavioral responses to capture more realistic dynamic and adaptive actions
- Enhancing exploratory modeling through better evaluative diagnostics and inference analytics for discovering consequential processes, dynamics, or consequences in large ensemble outputs
- Advancing the ability to trace path dependencies, risk interactions (compounding or cascading), and emergent dynamics through improved algorithms for control, classification, and regression.

However, recognizing these opportunities is not trivial. The explosive rates of innovation across the many subdisciplines of AI/ML have made it difficult for domain scientists to realize the full potential of scientific workflows. Moreover, application areas such as MSD are generally far more complex and computationally demanding than the standard benchmarking suites used in the computational sciences literature. Two major reasons for the discrepancies in benchmarking efforts are (i) the nontrivial effort required in resolving mathematically or computationally complex case studies and (ii) a general lack of coordination between computational and domain scientists. Teaming MSD, mathematics, statistics, and computational scientists will be a critical strategy for leveraging the relative strengths and expertise to accelerate innovative analytical insights in complex human-Earth systems. As an example, consider that the scientific community is in the early stages of major breakthroughs in natural language processing (NLP) models with the introduction of transformer neural networks (Brown et al., 2020; Hutson, 2021). There has been an exponentially scaled rate of growth in text-generating neural networks such that the full internet is now being exploited as source training (3.2.7). For example, OpenAI's Generative Pre-trained Transformer 2 and 3 (GPT-2 and GPT-3) emerged in succession in approximately a year with dramatic increases in training data scope, model complexity, and capabilities.

On its surface, the explosive growth of NLP model complexity and capabilities may seem distant from the MSD

Figure 3.2.7: The exponential growth in the parametric complexity of NLP neural network models since a key breakthrough in the use of transformers was introduced in 2017 (Vaswani et al., 2017).As measured by the models' parameters, the scale of text-generating neural networks is growing exponentially. Redrawn from Hutson (2021). * The performance of Google's 1.6-trillion-parameter "sparse" model is equivalent to that of 10-billion- to 100-billion-parameter "dense" models.

research community. Consider the recent example application of NLP by Callaghan et al. (2021) that auto-extracted evidence and attribution for climate change impacts globally in a meta-analysis spanning 100,000 studies. This study represents the beginning of a transition toward embedded intelligence in scientific workflows (e.g., transitioning from code versioning services like GitHub to services that actually produce code like OpenAI's Codex). The implications for intelligent scientific workflows are significant given that this breakthrough is still in its nascent stage. In the near term, it is expected that a large ecosystem of services and applications employing NLP models will be emerging across a very broad range of end uses. The GPT-3 platform (Brown et al., 2020) responds to plain English requests and has demonstrated preliminary results that include:

- Topical text analyses and synthesis
- Data gathering by mining the full public internet and graphical design
- Software coding tasks in multiple programming base languages
- Automated multi-algorithmic workflow generation with other ML tools.

Although at present, private commercial NLP development and applications are dominant, public sector science should both be a beneficiary as well as a source of evaluative safeguarding of the potential externalities of this type of breakthrough. Hutson (2021) note that there is significant promise and peril in how NLP models may be used, as well as how the open science research community may be affected by private versus public domain controls. Examples of societal externalities include systematic biases in datasets, using NLP to weaponize global disinformation campaigns, and the carbon footprint of the computational demands of NLP itself. In the context of MSD research, the NLP example in Figure 3.2.7 is illustrative of the types of breakthroughs that may emerge in coming years that can shape the community's ability to better engage with the complexity of human-Earth systems as well as realize recent visions for embedded intelligent services that could advance scientific workflows (e.g., Atkinson et al., 2017; Yilmaz, 2019). Beyond algorithmic advances, there is a revolution in future computing architectures (Hoppe, 2021) that are advancing beyond traditional high-performance computing systems (e.g., application-specific integrated circuits, field-programmable gate arrays, quantum computing, and neuromorphic computing). The DOE Office

of Science Quantum Information Science initiative represents a direct outgrowth of the Congressional National Quantum Initiative Act, emphasizing the importance of global leadership for harnessing emerging transformative computing breakthroughs. Over the coming decade, quantum computing has the potential to fully redefine what is scientifically tractable for MSD research by achieving unprecedented scales of simulation, optimization, and ML tasks that aid our exploration of the challenging combinatoric elements of MSD applications (e.g., path-dependent and state-aware actions for massive numbers of simulated agents).

Beyond general workflows, another key area of AI/ML innovation that holds significant promise for MSD is RL as well as its hybridization with other more commonly employed methods (e.g., deep learning). Following the terminologies of recent reviews (Bertsekas, 2019; Powell, 2019), the RL area termed "policy approximation techniques" offers the opportunity to train dynamic and adaptive agent behaviors that are state-aware using Monte Carlo-based simulation training. Herman et al. (2020) reviews how RL-policy approximation innovations can be central to innovating agent-based abstractions of infrastructure investment pathways, adaptive operations, and other complex behaviors across a range of objectives and timescales (Figure 3.2.8).

In the illustrated example in Figure 3.2.8, exploratory ensemble hydroclimatic projections are initially analyzed with trace-specific moving window automated trend detection. Trend information is combined with trace-specific Bayesian inference to then project a conditional set of futures of focus. Lastly, the RL trains policy rule networks (e.g., neural networks) where the inner loop explores alternative policy network structures and the outer loop selects indicator variable inputs (e.g., precipitation and temperature) that trigger state-aware actions to achieve measures of system performance. In short, training dynamic and adaptive agent behaviors is itself a mechanism for understanding the important candidate sources of information, preserving path dependency in actions that are appropriate to the worlds to be experienced and exhibiting different time dynamic behaviors subject to objectives informing system performance (e.g., see Quinn et al., 2018). Changes in modeling, information selection, and analytic modes of inference provide an opportunity to better understand the implications of workflow choices, their uncertainties, and the capacity of agents to adapt. This type of framework offers an approach to more fully realize the interplay of key determinants of risk (hazard, exposure, vulnerability, and response as suggested in Simpson et al., 2021; see Figures 3.2.2 and 3.2.3). It will be critical for the MSD CoP and, more broadly, DOE to accelerate effective teaming and training strategies to exploit the rapid evolution of high-performance computing architectures over the next decade and their growing specialization for supporting embedded intelligence in sensing, simulation, and algorithmic workflows.

Figure 3.2.8: This is a conceptualization for how broader statistical inference techniques and policy approximation-based RL can be combined to yield dynamic and adaptive agent behaviors. This figure is from Herman et al. (2020).

Chapter 4.
Teaming Opportunities to Confront Complexity

4.1 Motivations for an Expanded Teaming Strategy

Previous chapters present a conceptual vision for transforming our understanding of the interdependent risks and resilience in human-Earth systems. This chapter draws on this vision and describes a conceptual strategy for how the MSD community can team with others more broadly to address the complexity of human-Earth system science challenges. Open science practices are central to the proposed strategy for fostering collaboration with researchers working in other agencies and research communities.

The scientific challenges highlighted in this report involve modeling interconnected human and human-natural systems and are thus among the most complex problems in science. The emergent complexity of the processes and outcomes that MSD addresses, varying from planned societal transitions (e.g., deep decarbonization) to coping with shocks (e.g., economic, climate, and social), creates a tremendous need for scope and depth of knowledge. Advancing our understanding requires capturing a wide range of environmental and socioeconomic processes. The processes and behaviors that govern human systems are often not well understood, and the uncertainties associated with factors such as future emissions trajectories and climate impacts are larger than the uncertainties associated with how the Earth system will respond, thus placing large methodological and computational demands on uncertainty quantification and characterization. Many interdependent sectors and systems are involved through feedback that leads to co-emergent properties that shape risk, resilience, vulnerability, equity, and other measures of societal consequences. The unique characteristics of landscapes and geographies across the globe (e.g., coastal, urban, and Arctic) alter the processes and dynamics significantly, adding to the research challenge. Transforming MSD science to advance broader exploratory modeling applications and take advantage of innovations in uncertainty analytics, AI, and leadership class computing will require a commitment to open science and improved mechanisms for training a growing collaborative community (Haimes, 2018).

Collaboration not only across research teams working on projects supported by BER but also with science sponsored by other agencies and developed in other research communities can accelerate the development of insight for societal needs at the rate needed for decision relevance. Other federal agencies and DOE programs

beyond BER have interrelated research interests and capacities in research on the complex dynamics of human and natural systems. For example, the National Science Foundation, US Geological Survey, US Bureau of Reclamation, US Army Corps of Engineers, US Department of Agriculture, US Department of Homeland Security, US Environmental Protection Agency, National Oceanic and Atmospheric Administration, National Aeronautics and Space Administration, National Geospatial Intelligence Agency, and National Institutes of Health all conduct research in Earth, environmental, socioeconomic, and infrastructure systems relevant to MSD. Most of these agencies participated in the 2016 MSD workshop (Moss et al., 2016) and the published work of individual scholars working with these programs is cited throughout this report. As a recent and specific example, in November 2020, the federal interagency Coastal Integrated Hydro-Terrestrial Modeling Coordinating Group within the US Global Change Research Program and the MSD research community jointly organized a workshop focused on the challenges of modeling and evaluating coastal landscapes. The focus was on co-evolving human and natural systems subject to influences and stressors including extreme weather events, sea-level rise, natural and anthropogenic disturbances, and other impacts from climate change. The workshop highlighted the significant potential for collaboration and identified some 40 potential use cases (modeling experiments to explore a research question) across rural and urban landscapes, sectors, and themes, including landscape evolution, compound extreme events, infrastructure, land use and water quality, energy transitions, economic dynamics, and water supply and demand. This focus on coastal hydro-terrestrial modeling extends a broader interagency collaboration to integrate research performed across multiple mission agencies into a national capability to enhance knowledge, understanding, prediction, and management of diverse US water challenges (Scheibe and Stafford, 2020).

Beyond this, numerous distinct research communities, including systems engineering, sustainable transitions, socio-environmental systems, socio-ecological systems, urban complexity science, Earth systems modeling, decisionmaking under deep uncertainty, and others, are producing research literature, data, models, and analysis methods that are valuable for advancing MSD research. The MSD CoP seeks to complement and facilitate collaboration with these research communities. Related efforts in organizing large-scale scientific collaborations focused on developing community modeling systems (e.g., the Community Earth System Model and the Community Surface Dynamics Modeling System) provide examples for collaboratively advancing the development of data, models, and the capacity to integrate them to explore complex systems that build on insights from multiple disparate research traditions and communities. We encourage interested researchers who may find resonance with the themes and opportunities identified in the report to contact the MSD CoP to discuss the collaboration opportunities described below.

4.2 Conceptual Framework for Collaboration

Given MSD's objective of understanding co-evolving sectors and systems linked through interactions and feedback, MSD projects frequently bring together diverse data and models that were never intended to be used together (and hence have a patchwork quilt of scales, resolutions, programming languages, and complexity). This not only presents a series of technical challenges that must be overcome to perform MSD research, but also limits the extensibility of MSD models and analytical tools by other projects and communities. Thus, there is a fundamental need to formalize a conceptual framework of definitions, models, data, analysis, conventions, and decision support capabilities that support integration. The term "framework" refers to a modular, interoperable, and flexible approach to linking data sets and models of relevant sectors and systems. The 2016 workshop that gave rise to the MSD CoP (Moss et al., 2016) highlights that these elements include:

- A diverse suite of capabilities to represent the drivers, decisions, processes, and uncertainties, including both detailed process-based models as well as reduced-form representations of models of the relevant interacting systems;
- Shared naming conventions and vocabulary (taxonomy) for processes, variables, units, and types of coupling to facilitate efficient and accurate sharing of information;

- Improved documentation and broader access for data, models, and analysis methods so that users can identify and differentiate functionally similar capabilities to determine those that may be reused and are best suited for their needs;
- Effective provenance management to capture and credit modeling contributions, evolving input and output data sets, and new coupling strategies for MSD multimodel workflows;
- Enhanced community-scale (i.e., not project-specific) methods and tools for model evaluation and analysis of uncertainty of both individual and coupled components (see Chapter 3.2); and
- Community-building efforts such as coordinated experiments, intercomparison activities, and formal methods for sharing information about capabilities as they emerge.

The framework described above is intended to support deep integration of insights and methods from diverse communities that explore dynamic and adaptive human-Earth systems as well as their determinants of risk with different perspectives and methods. The research framework can be used to identify gaps and facilitate collaborative efforts where teams-of-teams come together to tackle common problems. It offers the opportunity to reduce barriers to entry into the MSD CoP for specialists with deep domain knowledge of component systems, sectors, and processes and to facilitate the development of an ecosystem of interoperable practices and standards. Finally, such a framework for MSD research would also enable wider adoption of MSD tools and methods by other agencies and research communities—a central component of the R2O2R pipeline.

4.3 Open Science and Collaboration Management

The MSD CoP's strategy for teaming is founded on the principles of open science (see Box 3.2). Open science accelerates progress by reducing barriers to entry, gaining economies of scale, and avoiding duplication of effort (Allen and Mehler, 2019). A key focus here is on the concept of extensibility, or being able to build on the work of others. The need for extensible MSD research results from overlaps in research questions, topics, and approaches across projects, such that datasets and models generated in one project have value to another project. Consistent with DOE's EESSD data-model integration Scientific Grand Challenge (BERAC, 2017), the MSD CoP promotes the adoption of the FAIR modeling and data standards (Wilkinson et al., 2016) and open-source software principles (Paulson et al., 2004).

A key component of the MSD CoP teaming strategy is a flexible and scalable data and code management system combined with a distributed computational platform that will enable DOE MSD researchers to document and archive their data, run their models and analysis tools, and share their data, software, and multimodel workflows. With support from BER's MSD program, the community has established the MSD-LIVE to facilitate and incentivize collaboration (see Box 4.1). MSD-LIVE was designed to embody four core values/best practices in open science:

- **Living**: There should be continuous interaction with the platform throughout the data and code lifecycle rather than only storing the final product.
- **Intuitive**: Using the platform should not require a steep learning curve.
- **Value-adding**: There should be tools built into the platform that enhance the ability of the MSD community to do their work.
- **Environment**: The platform should include a computational component that delivers an integrated data-work environment as opposed to a stand-alone data repository.

Box 4.1: Advancing the MSD CoP with a State-of-the-Science Data and Computational Platform

MSD research is diverse—in disciplines, methods, tools, institutions, cultures, computational requirements, software complexity, teams, and disciplines that may not traditionally work together. The diversity of the MSD community leads to not only a wide range of data types and formats, but also a spectrum of disciplinary and institutional traditions with respect to data and software management. This makes data and code management a challenge—from finding appropriate storage to defining standards to making it easy for others to find, share, and re-use data and code.

MSD-LIVE grew out of several years of engagement with the MSD community. Through that engagement, the project identified a number of project, community-level, and technical needs with respect to data and code management. These challenges include:

- *Finding and Managing Data*: Projects have grown in size and diversity in order to address bigger and more complex problems. There is a need for data and code to be openly developed and documented in ways that promote reusability and interpretability across diverse teams.
- *Training*: Projects struggle to onboard new researchers and familiarize them with the tools available to effectively manage data and code. Similarly, they often have challenges capturing institutional knowledge from team members that leave projects.
- *Collaborating*: Projects increasingly span multiple institutions, each with their own computational environments and access restrictions. The lack of community-wide tools for documenting and sharing data limits collaboration and creates barriers to entry.
- *Versioning*: There is limited use of data, model, and workflow versioning. This limits the extensibility of MSD experiment, which often involve complex multimodel workflows.
- *Machine Learning*: Researchers are increasingly using ML/AI approaches to analyze data and simulations. Projects would benefit from easy access to physically distributed datasets and cutting-edge ML/AI resources.
- *Proprietary Data and Code*: Researchers are using more proprietary models and datasets as they simulate finer scales and more detailed processes. Projects are independently finding best practices for working with proprietary data and code.

MSD-LIVE addresses these needs with a flexible and scalable data and code management system combined with a distributed computational platform that will enable MSD researchers to document and archive their data, run their models and analysis tools, and share their data, software, and multimodel workflows. The long-term vision is to develop a world-class data and computational platform that will accelerate progress, facilitate and incentivize collaboration, and enhance the scientific impact and visibility of the MSD community.

Users of MSD-LIVE will be able to:

- Share working and final-form data and code across institutions using team-based roles and permissions that create the ability to work with proprietary data and code.
- Use an intuitive, web-based user interface to document and share datasets, set access controls, associate data with the code used to produce them, and mint data DOIs.
- Create, publish, and execute versioned workflows by linking together interdependent pieces of code and data using seamless access to local and non-local data resources.
- Deliver data-driven discoveries using technology that enables cutting-edge ML/AI by providing seamless access to data that may be physically located in different places.

4.4 Collaboration through an Expanded CoP

As discussed in Chapter 1, the MSD CoP represents an initial investment by the US DOE's Office of Science to accelerate the organization of the research community to model complex interactions of coupled Earth, environmental,

socioeconomic, and infrastructure systems that provide critical goods and services for humankind. The MSD CoP is establishing itself using a suite of strategies, including improved community-level communications (a website, newsletter, webinars, and other forms of interaction); establishment of technical bodies focused on advancing fundamental science (i.e., a SSG and topical WGs; see Chapter 1 and Sections 2.1 and 2.2); and the development of a conceptual framework for collaboration Section 4.2). Figure 4.4.1 illustrates the challenges, driving questions, activities, and outcomes of the MSD CoP.

Six initial MSD CoP WGs have been established to facilitate collaboration and accelerate scientific progress in priority areas. These are described on the MSD Community website, and individual WG websites identify opportunities to contribute to these topics through participation in webinars, intercomparisons, and collaborative research and publications. These WGs are an opportunity to collaboratively address specific technical challenges and objectives. The WGs are proposed by community members and reviewed and rechartered every two years. They are open to all interested individuals with relevant expertise, including those from outside the DOE MSD program. In addition to having open membership, WGs also convene monthly seminars and occasional workshops. For example, a recent 100-person workshop convened by the MSD Urban Systems Working Group brought together leaders in urban complexity science with DOE MSD researchers. Fine-scale urban data, ML, and cross-sectoral modeling can better inform urban planning and design. The workshop explored opportunities to harness recent advances in computational science and the explosion of data available on human system processes to explore interdependent human health, social, economic, and sustainability challenges in urban environments in the context of multiple stressors and influences. As of November 2021, the current MSD CoP WGs are:

- Urban Systems: Cities are a key focal point for addressing questions related to system dependencies, tipping points, and uncertainties. Cities are also a fruitful context to explore model coupling across sectors and scales. However, efforts to combine multi-sector urban tools and insights to examine key uncertainties, interactions, and tradeoffs are still nascent. The urban WG facilitates the development of these tools and ideas and explores several key questions: What are the risks faced by the world's urban areas as they seek to increase resilience and balance multiple objectives such as human health, economic development, and sustainable use of resources? How does urban change influence larger-scale infrastructure, economic, and Earth system processes, and how is urban evolution constrained by these larger systems? Which processes and couplings must be represented to understand multi-sector dynamics within cities?
- Multisector Impacts of Energy Transitions: Technological advancement and energy and environmental policy have driven rapid changes in the energy sector, and these developments have a pervasive influence on other economic sectors and natural systems. As these developments accelerate, there is an increasing need to understand the resulting feedback between human and natural systems. This WG advances the understanding of these multisectoral relationships by building a diverse team to identify what feedback, sectors, and societal constructs are missing from existing analytical approaches and define new research pathways toward a more holistic understanding of the multisector impacts of energy transitions.
- Human Systems Modeling: The Human Systems Modeling WG explores state-of-the art modeling methods that can improve representation of human decisionmaking and adaptation in multi-sector systems, drawing from advances in economics, social sciences, computer science, and statistics. It investigates a range of modeling techniques (e.g., agent-based, bioeconomic, and computable general equilibrium) and their integration with physical energy-water-land models for capturing human response to both natural and socioeconomic stressors under short-term shocks and long-term change.
- Uncertainty Quantification and Scenario Development: The Uncertainty Quantification and Scenario Development WG studies the propagation of uncertainties, including deep uncertainties, through multi-sector systems. It is interested in understanding how uncertainty interacts with complex system dynamics and cross-sectoral feedback mechanisms to affect the robustness and resilience of these systems. It also conducts research into the construction of scenarios to capture the range of uncertainties in outcome space in the presence of deep

Figure 4.4.1: Logic model of the MSD CoP depicts community challenges, inputs, activities, outputs, and outcomes. The CoP includes an evaluation component intended to evaluate progress in developing an MSD research framework, including shared terminology and synthesis of results around higherw-order research questions.

uncertainty.

- Open Science and FAIR Data: One component of an effective CoP is leveraging shared tools and resources. The purpose of this WG is to facilitate the reuse of models and datasets across the MSD community. The long-term vision is to foster a culture of openness and to facilitate a collaborative, resource-rich, community-driven way of doing MSD research. In this open science world, MSD datasets would be developed using the FAIR; Wilkinson et al. (2016)) data standards and open-source models would be the norm rather than the exception. If successful, this WG will accelerate progress, facilitate and incentivize collaboration, and enhance the scientific impact and visibility of the MSD community.
- Professional Development and Education for Early Career Scientists: As the MSD community is formed and begins to grow, this WG seeks to expand participation among a diverse group of early career scientists, provide professional development opportunities to graduate students and post-docs, and serve as a contact point for interdisciplinary education activities taking place in the MSD community. The overarching goal of this group is to support early career success in the field, which we believe will in turn support the scientific vision of MSD. Specific activities include planning workshops for early-career faculty and completing an inventory of MSD-related coursework at US universities.

To achieve the ambitions outlined in this report, additional investments and collaborations beyond these initial MSD WGs will need to be identified and nurtured to address the many research needs, opportunities, and challenges identified throughout this report. The collaborative strategies and infrastructure of the MSD CoP need to be expanded to provide a more diverse community of researchers access to essential transdisciplinary knowledge and a powerful environment of data, modeling, and analysis tools that accelerate idea generation and hypothesis testing through linked models of MSD. The CoP will also need to expand to provide training in the use of the framework and system of tools and resources and to develop educational opportunities for expanding the workforce needed to research and manage systems complexity.

Chapter 5.
Summary: Syntheis of MSD Research Opportunities

This chapter synthesizes the many opportunities discussed in Chapters 2 and 3 and highlights a subset of near-term opportunities for advancing MSD research. Given the large and long-lived capital investments associated with energy transitions, managing climate risks, and improving our national infrastructure systems, it is critical to rapidly improve our scientific capacity to understand the complex interactions, interdependencies, and co-evolutionary pathways of coupled human-Earth systems. Development of modeling capabilities and analytic tools for understanding complex multisectoral interactions within human-Earth systems lags those available for research focused on individual sectors or systems. Detailed and high spatial/temporal resolution data and models for different components and processes of human systems (e.g., infrastructure systems, natural resources management, and adaptive actions) have not been extensively integrated with Earth and environmental systems models to understand the feedback and effects of interacting thresholds. A core benefit of the aspirations presented in this report is the transformation of the research community's ability to understand and inform how to meet engineering, economic, and societal requirements robustly, equitably, and efficiently across many plausible futures.

Transforming our quantitative understanding of how sectors and systems interact and co-evolve holds the promise of increasing adaptive capacity and innovation, improving societal and economic returns on investments, and contributing to US competitiveness and leadership. The MSD CoP provides a framework for growing and accelerating peer interactions, collaborative research, and engagement with other communities so that we are better positioned to confront the complexity of multisectoral science questions intrinsic to energy transitions and climate risks. A number of key near-term opportunities exist to advance MSD research.

Strengthen Foundational Research Capabilities

Rapidly advancing the modeling of complex interactions between sectors and systems will depend on strengthening foundational research capabilities to enable the community to take advantage of the explosive growth of data resources and advances in computation and embedded intelligence. An associated key need is expanding and diversifying the MSD workforce to broaden the backgrounds, technical skills, and expertise/experience the community can draw on to advance our understanding of societal risks. Near-term opportunities include:

- Expand community resources for data and code management (i.e., MSD-LIVE) and promote the adoption of the FAIR data principles and open-source software to enhance the reproducibility and extensibility of MSD research.
- Provide training to support and sustain commitments to open science.
- Leverage emerging computational innovations and develop novel computing and software infrastructures to facilitate large-scale data storage and analysis.
- Expand opportunities for the teaming of MSD researchers, mathematicians, statisticians, and computational scientists to accelerate innovative analysis of complex human-Earth systems.
- Invest in exploratory modeling experiments, visualization capabilities, and AI approaches to exploit emerging computing architectures, including Exascale, cloud, and edge computing systems.
- Address DEI challenges that are critical to framing MSD science questions, innovating technical advances, and establishing societal relevance.
- Create community-level transdisciplinary training and research opportunities needed to advance MSD research as well as grow job opportunities at the community level.
- Expand national and global MSD-focused forums and include opportunities for early-career scientists for networking, building long-term collaborations, and professional mentorship.

Advance the Science of Human-Earth system Interactions

Understanding risk and resilience in changing human-Earth systems requires fundamental and rapid advances in understanding of their complex interactions, interdependencies, and co-evolving pathways. Research is advancing data, models, and analytics to capture nonlinear system behaviors, the potential for cascading failures, and feedback across deeply interconnected sectors and systems. Near-term cross-cutting research themes discussed in Chapters 2 and 3 of this report include:

- Interdependencies, interconnections, and complexity:
  - Identify and model human-Earth system dependencies and interactions across sectors and systems and advance hierarchical modeling that integrates high resolution and reduced form representations of key interactions across multiple scales.
  - Extend analytic frameworks for exploring risk and adaptivity to incorporate complex mixtures of determinants (hazards, exposures, vulnerabilities, and responses) and drivers (climate, socioeconomic, environmental, infrastructure conditions, and others).
  - Explore interactions among the key properties that characterize systems in nested and hierarchical relationships, for example, connectedness, capital, and resilience.
  - Apply methods and concepts from complex systems science.
  - Enhance representations of highly nonlinear and uncertain “state-action” feedback.
  - Increase the resolution and detail of physical and socioeconomic processes.
- Stressors and influences
  - Explore how large-scale decadal-to-centennial Earth systems and local-to-regional, sub-daily-to-weekly meteorological processes are altering climate stressors and extreme events.
  - Couple human systems with Earth and environmental systems models, both to represent human system climate drivers and feedback central to improving Earth systems models and to characterize the risk and resilience of human systems.
  - Continue to improve emulation capabilities to represent important Earth and environmental system processes using ML, observational data, and ESM projections.
  - Develop process-oriented, feature-specific frameworks to evaluate different sources of climate information for specific areas of application, given uncertainties.
  - Improve understanding of how extreme and high-impact events propagate through thresholds, disconti-

nuities, and tipping points in systems-of-systems , .
  - Conduct regional-scale human-Earth systems exploratory modeling experiments that better capture deeply uncertain futures (e.g., considering internal variability, model uncertainty, and human systems) as well as how uncertainties shape key determinants of risks.
- Human systems representations:
  - Diversify approaches for representing human systems and adaptive behaviors, including influences such as legal institutions, operating rules, and non-economic drivers.
  - Analyze how uncertainties in how human systems are represented in models (e.g., the identification of key individual, collective, and institutional actors; capturing diverse objectives and tolerances to risk; and functional representation of actors and their actions in models) shape our understanding of complex system dynamics.
  - Exploit the human systems data revolution, agent-based modeling, and other advances.

Evaluate Uncertainties, Data, and Models for Scientific and Decision-relevant Insight

Capturing higher-fidelity representations of coupled processes or sectors in increasingly complex models and workflows while also trying to rigorously make valid model-based scientific inferences presents multiple challenges to MSD researchers. An important research opportunity is advancing MSD methods and tools for uncertainty characterization that are scalable for research on complex, interdependent sectors, systems, and their component processes. A number of near-term opportunities will increase the robustness of insights and ensure that investments in basic MSD research are able to inform societal challenges such as next-generation infrastructure decisions, including:

- Create new opportunities for sustained interactions among MSD researchers and various user communities (e.g., researchers from other fields, managers/decisionmakers in sectors and systems) so that operational needs inform MSD research questions and MSD insights are made more relevant and accessible for applications (R2O2R).
- Use MSD science to explore a broader array of questions and outcomes such as risk, reliability, resilience, adaptive capacity, equity, capital requirements, stability of governance, and ecosystem health.
- Improve diagnostic model evaluation and advance understanding of best practices for coupling diverse models.
- Advance techniques for exploratory modeling under deep uncertainty to investigate the implications of a diverse ensemble of plausible future conditions to support the discovery of what futures, actions, and outcomes are the most consequential for the co-evolution of human-Earth systems.
- Improve collaborations with statistical, mathematical, and computational sciences to adapt to emerging uncertainty, AI, and computing architectures for MSD research efforts.

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The MultiSector Dynamics Community of Practice (MSD CoP) was formally established to generate a vision for MSD as a global research area, clarify key questions, establish and assist scientific working groups (WGs), shape a strategy for community development, and foster synergies across interested research, government, and user communities.

The MSD CoP is working to bridge several diverse research communities that focus on complementary aspects of complex interactions, interdependencies, stressors and influences, and co-evolutionary pathways of human and natural systems. The research programs within DOE's Earth and Environmental Systems Sciences Division represent a core constituency of the MSD CoP.

This report represents the collaborative contributions of the recently established MSD CoP and outlines a vision for MSD as its own, emerging field. There is tremendous promise for advancing our understanding of the local to global systems that fundamentally shape the interdependent dynamics, risks, and benefits of our modern world. The MSD 2030 Vision, as presented here, formally introduces the transformative research contributions, opportunities, and advances that MSD offers over the next decade.

MultiSector Dynamics