



Showcasing advances and building community in modeling for sustainability

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We organized this Special Feature on “Modeling Dynamic Systems for Sustainable Development” to showcase the field’s recent advances. Much recent research in sustainability science has mobilized data and theory to better understand systems that include interacting people, technologies, institutions, ecosystems, and both social and environmental processes. A recent National Academies workshop and an Annual Review paper identified several challenges and open questions for the field, stressing the importance of developing and testing new theories to advance knowledge and guide action (1, 2). However, there has been less attention in sustainability science toward integrating modeling with theory and data-focused approaches. Modeling is necessary for making projections about the dynamical implications of our present understanding of nature-society systems—which is essential to determine whether long-term trends in nature-society interactions are consistent with sustainable development goals and to analyze whether particular interventions (e.g., technologies, policies, behavior) are likely to change those interactions in ways that promote such goals.

Many papers, through several decades, have called for better modeling tools to address the connections and feedbacks between natural and social processes (3–6). Much of this work emphasizes shortcomings of models in areas important for sustainability analysis, including capturing multiscale complexity, tracking long-term dynamics, incorporating human agency, and accounting for the generation of novelty. Although this literature highlights significant and persistent gaps in current models, there has been growing interest and action in many research communities to advance science through simulating these aspects of nature-society systems. For example, there has been renewed attention to modeling-related issues in collective efforts to address climate and global change (7, 8), macro-energy systems (9), and social-ecological systems (10). Communities focused on environmental and societal modeling have also increasingly addressed integrated systems (11–13).

Recent advances in computational tools and techniques mean that today’s state-of-the-art models and analyses look very different from, for example, perceptions of integrated assessment models typically introduced decades ago but still used to address topics such as climate change (14). New state-of-the-art models build on a broader variety of research traditions, are informed and evaluated by novel data sources (including qualitative and quantitative data), make extensive use of growing capacities for data acquisition and analysis, and engage a greater diversity of decision-relevant topics and stakeholders. Many advances are being applied to challenges within specific domains—e.g., to energy systems, food systems, and transportation systems. Others are well-known within some disciplines—e.g., ecology, economics, or

engineering—but not widely adopted in others despite having much to offer there. At the same time, there is much potential for those developing and implementing similar methods to communicate and build community across their respective disciplines and domains.

The papers in this Special Feature highlight advances in simulating coupled nature-society systems. We believe that these techniques, if they were more widely adopted, could significantly improve the capacity of sustainability science researchers to test theory, mobilize data, and inform action. Each contribution to the Special Feature addresses a specific area in which novel modeling approaches have demonstrated the capacity to advance theory and insight more broadly. The contributions were selected to be illustrative rather than comprehensive and to facilitate connections across the communities they represent. The process by which we invited and curated papers for this Special Feature reflected this community-building aim. We first conducted a virtual workshop in June 2021, in which roughly 40 invited participants shared their recent modeling advances relevant to sustainable development. We focused on recruiting a diverse cohort of authors, including multiple early-career scholars who have developed or used models in a variety of domains relevant to sustainability. Through that process, we refined our proposal for the Special Feature, and conducted an online workshop and weekly virtual seminar series in spring 2022, in which participants presented their papers for comments by the broader group. A number of the papers in the Special Feature represent work catalyzed by connections and ideas generated through this process, with collaborations from authors who had not met prior to the workshop. We hope that similar connections are further facilitated by the publication of the papers in this Special Feature.

An opening Perspective by Selin et al. (15) gives an overview of recent progress in this area, arguing that recent work has begun to address longstanding and often-cited challenges in

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bringing modeling to bear on problems of sustainable development. The paper draws on submissions from workshop participants of key examples of excellent work in their respective fields and collective discussions among Special Feature contributors. It highlights illustrative examples of innovative modeling methods and associated advances, together with specific examples from applications in recent research that illustrate how they inform sustainability-relevant questions. Selin et al. differentiate modeling work with respect to two (interlinked) approaches toward developing knowledge and informing action: 1) harnessing sector- and location-specific

insights and 2) advancing theories of nature–society systems. They organize this summary of innovative methods and recent advances by reference to four stages of modeling practice: defining the purpose of modeling, selecting components, analyzing interactions, and assessing interventions.

A central concern of sustainability science with respect to informing action involves equitable distribution of well-being, and thus all papers in the Special Feature specifically address the cross-cutting theme of how distributional issues are considered in modeling. To further highlight the importance of equity in modeling, we highlight this issue in our second

Table 1. Modeling stages: Methods, examples, applications from the literature, and applications in this Special Feature, extended from ref. 15

Modeling stages	Methods	Specific examples	Applications from the literature	Applications in this Special Feature
Defining purpose	Incorporating nature–society interactions into sectoral decision-support models	Large-scale engineering simulations adapted for decision support	Air quality (17, 18), built environment (19), earth system modeling (20), watershed management (21), land systems (22), water and energy (23)	Fletcher et al. (24) and Venier-Cambron et al. (25)
	Simulating cross-sector connections and differing contexts	“Nexus” approaches, multisector dynamics, transfer learning	Water–food–energy (26), climate–health (27), agriculture (28), water resources (29)	Burney et al. (30) and Siddiqi et al. (31)
Selecting components	Capturing diverse societal actors and their agency	Generalized modeling, agent-based modeling, computational social science methods, integrated assessment, network models	Global change (32), natural resource management (33), water systems planning (34, 35), earth systems modeling (20)	Sparks et al. (36), Siddiqi et al. (31), and Davidson et al. (37)
	Computational frameworks that facilitate model interoperability	Modeling framework standardization, system-of-systems approaches, network approaches	Earth system modeling (38), land systems (39), fisheries (40), air quality (41), transportation (42)	Sparks et al. (36)
	High-resolution data and simulation capacity	Data assimilation, digital twins, parameter exploration, model spectrums	Earth system modeling (43), energy systems (44, 45), water resources (46), air quality and health (47), transportation (48)	Fletcher et al. (24), Sparks et al. (36), and Venier-Cambron et al. (30)
Analyzing interactions	Purpose-built approaches to model couplings	Reduced-complexity models, partial couplings, generalized modeling	Air quality (49), climate change (50), and natural resource management (51, 52)	Fletcher et al. (24), Davidson et al. (37), and Sparks et al. (36)
	Techniques for capturing realistic dynamic behavior	Agent-based modeling, scenarios, limit testing, dynamic and adaptive control techniques	Innovation (53) and energy (54, 55), water resources (56–58), socioenvironmental systems (59)	Taberna et al. (60), Noll et al. (61), Edwards et al. (62), Sparks et al. (36), and Siddiqi et al. (31)
	Data-model integrations that leverage advanced computational methods	Causal inference, digital twins, explainable AI	Energy systems (63), fisheries (64, 65), water resources (66), built environment and infrastructure (63, 67).	Schlüter et al. (62) and Taberna et al. (60)
Assessing interventions	Computational and statistical approaches that evaluate decision scenarios under uncertainty	Decision-making under deep uncertainty, exploratory modeling, scenario discovery, model ensembles	Natural capital (68), water resource planning (69), air quality (70), integrated assessment (71), land use (72)	Noll et al. (61), Fletcher et al. (24), and Burney et al. (73)
	Ways to incorporate different perspectives and normative visions in dynamic modeling	Multiobjective optimization, fuzzy cognitive mapping, participatory modeling, metrics	Climate adaptation (74), water system planning (21), inclusive wealth analysis (75–77)	Venier-Cambron et al. (30) and Siddiqi et al. (31)

Perspective. In that Perspective, Giang et al. (16) discuss how modelers engage with distributional, procedural, and recognitional dimensions of equity in all four stages of modeling practice, with examples drawn from topical case studies including those related to water resources, energy systems, air quality, and conservation.

Here, we summarize the papers in the special feature, organized by the framework outlined in the two Perspectives. Although many of the papers showcase advances in multiple stages of the modeling process, below, we highlight one core contribution for each. See Table 1 (extended from ref. 15) for additional coverage of each step in the Special Feature.

Defining Purpose

While the overarching goal of sustainability science is to bridge knowledge and action toward sustainable development, models are designed for particular users and inform more specific purposes. While the constraints of this collective effort as a Special Feature of PNAS meant that many of the models presented had a shared purpose and audience of PNAS readers, the models involved in this work have much broader applicability. Giang et al., in their Perspective, survey opportunities and methods for incorporating procedural and recognitional equity considerations into this phase of modeling, including attention to the participants, worldviews, and knowledge systems that inform these choices.

While many models already exist that can simulate environmental and engineered systems, some of these models have been repurposed or extended to address different contexts more relevant to sustainability and human well-being, to different audiences. One example of this comes from the paper of Fletcher et al. (24), who build upon models used for water infrastructure planning, extending beyond a specific system to build middle-range theory on the relationship between climate variability and priorities in infrastructure-related climate adaptation. By applying this model together with climate model projections, nonstationary signal processing, stochastic weather generation, and reinforcement learning-based advances in stochastic dynamic control, they find that dynamic planning can help build adaptive capacity, particularly in regions that experience long-term climate oscillations.

Selecting Components

Efforts to improve modeling of nature-society systems have focused on including more model components, representing ever more detail in human activities and environmental processes. A major challenge has involved finding ways to incorporate aspects of these systems that are known to be important to sustainability, but are not typically simulated or easily quantified. These aspects include the knowledge and formal and informal rules and norms that can affect interactions between and among different actors and their surroundings. Agent-based modeling (ABM) provides one mechanism by which diverse societal actors and their agency can be simulated, and Taberna et al. (60) combine a state-of-the-art ABM evolutionary macroeconomic framework with empirical survey data to estimate household adaptation to flood and its aggregate as well as distributional impacts. They illustrate that common

assumptions of rational representative agents in such models overestimate diffusion of adaptation and underestimate damages, mainly due to omitting sociobehavioral adaptation constraints such as awareness and social influences revealed in survey data. Furthermore, they display the mechanisms through which even under a nearly complete adaptation diffusion, adaptation benefits are uneven, further exacerbating inequalities. Running ~0.5 million ABM runs, this exploratory modeling shows that behavioral uncertainty can mediate the importance of physical factors traditionally thought to be decisive for the uptake of adaptation measures.

Davidson et al. (37) identify three modeling approaches commonly used to assess climate mitigation interventions, where there is strong potential to incorporate institutions (formal and informal rules for shaping behavior): agent-based, integrated assessment, and engineering-economic optimization modeling. They compare how including heterogeneous institutions in each approach affects simulated sustainability outcomes, such as emissions reductions and costs. Results showed that including or omitting institutions can alter results, for example changing estimated costs of climate mitigation. Importantly, representing additional components does not necessarily require using a single model that can capture everything: as the analysis by Davidson et al. shows, different types of models can be used to provide insights used independently or in combination. Nor does representing components necessarily require quantitative data. Siddiqi et al. (31) show that qualitative information on systems that includes institutions and knowledge, combined with a matrix-based approach to sustainability analysis (the human-technical-environmental systems framework), can be leveraged to simulate networks over time. They use this combined qualitative-quantitative approach to identify factors contributing to food security over a decades-long history of the Indus River Basin.

Analyzing Interactions

Capturing the complex, adaptive nature of the dynamics of nature-society systems poses a challenge for modeling. Factors such as feedback behavior, threshold processes, and adaptive responses, are often uncertain. Even where they are well-characterized, these factors can pose computational challenges in complex coupled systems. As a result, many studies omit societal responses altogether, even where including them might change results. Sparks et al. (36), drawing from air quality analyses, address an example of one of these areas, involving exposure to air pollution under changing climate. While people can (in part) adapt to reduce their air pollution exposure by staying indoors on polluted days, this effect has largely been omitted in quantifications of future air quality impacts. Sparks et al. link global-scale climate and atmospheric chemistry modeling to adaptation modeling including social learning. They find that the effect of including societal response is not only substantial but also shapes the ways in which the burdens of responding to pollution are distributed, including both the costs of adaptation and the remaining impacts of those who are unable to adapt (such as outdoor workers). The paper by Edwards et al. (62) addresses a type of dynamic that has historically proved difficult to predict—the generation of

novelty, through innovation. Historically, integrated assessment models that have been used to evaluate climate change policy have been critiqued for their insufficient representation of the potential for future technologies to emerge. Edwards et al. address this critique head-on, using historical technology analogues and early adoption indicators to model feasible growth pathways for the case of carbon dioxide removal technologies, and incorporating results into an integrated assessment model. They show that this results in a more realistic analysis of the potential for such future technologies to address climate change. Schlüter et al. (61) focus on the objective, common to many fields of science, of better understanding causal relationships in interactions, identifying causal mechanisms and assessing causal effects, as well as making robust causal claims; this is a challenge given the complexity of human–natural systems. Through presenting example studies, focusing on environmental pollution, disease spread, and natural resource management, they show key pathways for, and insights gained from, integrating empirical and modeling approaches to causal analysis and inquiry.

Assessing Interventions

Ultimately, modeling that contributes to sustainable development efforts has the potential for informing potential interventions by actors. A specific challenge in assessing interventions involves the unanticipated responses that might occur through social processes, where actions by one set of actors induce responses by others. For the case of policy interventions, Noll et al. (73) address one case of this type of effect. They use a system dynamics model to simulate how public policy interventions to stimulate technology development can induce global technical change through innovation “spillovers” where incentives in one region positively (or negatively) influence the same technology’s deployment in other regions, thereby inducing further learning. Relatedly, Burney et al. (30) propose a method to decompose spatiotemporal signals of weather variation that they then apply to examine potential interventions to reduce the vulnerability of agricultural productivity in Brazil to climate shocks, considering effects on related financial institutions such as large banks. To do this, they pair empirical statistical damage estimates derived from recent weather and outcome observations with projected future climate changes and proposed responses, then apply these to future climate simulations. New metrics are also being developed to analyze the impact of interventions for different actors, with different characteristics, often with a focus on equity. Venier-Cambron et al. (25), in an examination of future scenarios of conservation, present a systematic approach to identify areas of potential tension between global conservation objectives and local food security, evaluating the outcome in terms of equity. They call for the use of multiple indicators, reflecting the diversity of land-use needs, in conservation planning.

Ways Forward

The ten research papers in this Special Feature illustrate a sampling of a very broad range of methods that exist at the cutting edge of modeling dynamic systems for sustainable

development. The papers also, collectively, make progress toward developing middle-range theory in sustainability science. There is much potential for generalizable insights across different domains, addressing fundamental questions about topics of relevance to sustainable development, such as how novelty emerges within nature–society systems, what conditions promote changes over longer-term timescales, how heterogeneous and nonlinear processes interact over spatial and temporal scales, and how unequal distributions of power and influence affect efforts to promote shared well-being. While modeling-focused analyses often have much to say about these topics more broadly, research contributing to these types of ambitious cross-cutting aims is often difficult to communicate through traditional peer-reviewed papers. We thus asked the authors of each of the papers in this Special Feature to draw out such lessons for middle-range theory, and these contributions are also highlighted through the Significance Statement speaking to a broader audience in the field of sustainability science.

While the papers in this Special Feature showcase concrete modeling advances, they also illustrate that there is still much work to be done. Modeling will always be imperfect, and future studies (including empirical and theoretical analyses) will likely identify components and interactions which are influential for sustainability but currently unknown. Many models still fall short of directly informing efforts toward comprehensive well-being, as many still focus on single sectors or output metrics. As theoretical and empirical work advances in better understanding the functional relationships between resources and human well-being, models will have an important role to play in further developing analyses that resonate with longer-term sustainability questions. Further, though there has been much progress as summarized by Giang et al. (16), many modeling efforts continue to reinforce dominant power dynamics and existing inequities. Further attention to equity and justice considerations in modeling is increasingly important if models are to be fully leveraged in efforts to promote sustainability.

All of the papers in this Special Feature are openly available without a paywall on the dedicated PNAS web page (<https://www.pnas.org/topic/555>). This methods-focused special feature complements other Special Features in the Sustainability Science section of PNAS (<https://www.pnas.org/special-features/sustainability-science>), many of which can be potential opportunities to bring modeling advances to bear on the hottest topics of the field. Through this initial effort to highlight a diversity of research in this area, we hope to inspire further development of new modeling methods and advances toward the ultimate goals of sustainability.

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