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Progress in modeling dynamic systems for sustainable development

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This Perspective evaluates recent progress in modeling nature–society systems to inform sustainable development. We argue that recent work has begun to address longstanding and often-cited challenges in bringing modeling to bear on problems of sustainable development. For each of four stages of modeling practice—defining purpose, selecting components, analyzing interactions, and assessing interventions—we highlight examples of dynamical modeling methods and advances in their application that have improved understanding and begun to inform action. Because many of these methods and associated advances have focused on particular sectors and places, their potential to inform key open questions in the field of sustainability science is often underappreciated. We discuss how application of such methods helps researchers interested in harnessing insights into specific sectors and locations to address human well-being, focus on sustainability-relevant timescales, and attend to power differentials among actors. In parallel, application of these modeling methods is helping to advance theory of nature–society systems by enhancing the uptake and utility of frameworks, clarifying key concepts through more rigorous definitions, and informing development of archetypes that can assist hypothesis development and testing. We conclude by suggesting ways to further leverage emerging modeling methods in the context of sustainability science.

modeling for sustainability | place-based approach | sector-based approach | theory-building approach | theory-testing approach

Calls for better modeling of nature–society dynamics have been with us since the emergence of concerns about global environmental change and sustainable development a generation ago (1, 2). Recently, Elsawah et al. (3) identified “grand challenges” for socio-environmental systems modeling including integrating human dimensions, capturing systemic change, and dealing with multiple interacting scales. A recent National Academies report setting out a vision for studying Earth’s systems highlights the need for different disciplinary communities to collaborate on models for understanding, exploring, and projecting changes resulting from the complex interconnections and feedback between natural and social processes (4). Peng et al. (5) proposed that integrated assessment models used for climate policy should better incorporate social realities. Schlüter et al. (6) note a lack of modeling tools that account for social–ecological relations and feedback. Consistent themes that emerge in these assessments of the shortcomings of models relate to difficulties in capturing important elements of complexity relevant to long-term dynamics, representing spatial heterogeneity, incorporating generation of novelty, including the influence of actors with unequal power and agency, and dealing with uncertainty. Modern arguments that improving modeling of nature–society dynamics is needed largely echo those from decades ago, suggesting a lack of progress.

At the same time, there has been a recent surge in interest and ambition among those who develop and use models of nature–society systems. A growing number of researchers are applying their tools to inform the pursuit of sustainable development. Proposals for new capabilities, fields, and communities of practice, shifting disciplinary priorities, and an increase in interdisciplinarity aim to leverage modeling approaches to transcend system-specific understanding. For example, the Multisector Dynamics effort examines “complex systems of systems that deliver services, amenities, and products to society” (7). Donges et al. (8) suggested new taxonomies for organizing connected models of human societies with Earth systems. The emerging field of macroenergy systems aims to understand the dynamics, benefits, costs, and impacts of large-scale energy systems and transitions and defines simulation, abstraction, and modeling as fundamental to its work (9). Biggs et al. (10) highlight several modeling approaches in a recent handbook of methods for analyzing social–ecological systems, including dynamical systems modeling, state-and-transition modeling, and agent-based modeling. Bauer et al. (11) summarize efforts to develop “digital twins” for Earth that link modeling and observational capacity with the goal of informing a green transition. Concurrently, data and computational advances are enabling new techniques for integrating understanding across fields (12).

One driving factor behind the recent surge in modeling ambition is practical: The acceleration of human impacts on the Earth means that incorporating nature–society interactions in analysis is increasingly vital for reliable understanding of how to promote sustainable development (13, 14). Models

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of such interactions incorporate a variety of approaches: formal or informal, qualitative or quantitative, equilibrium or dynamically focused, and with solutions achievable analytically or through numerical computation. A broad range of models can be tools toward an overall objective of building knowledge and informing action toward the problem of sustainable development. Efforts toward that objective involve two interconnected approaches: harnessing sector- and location-specific insights and advancing theories of nature–society systems. Following the first approach, much research builds from case studies of detailed processes supporting human well-being in specific places or sectors. Understanding the sector- and location-specific challenges of sustainable development often requires making projections based on the present understanding about the dynamics of nature–society systems, which include interacting people, technologies, institutions, and ecosystems, and both social and environmental processes. Quantitative modeling is especially important for understanding the behavior of these complex adaptive systems, where intuition can often be misleading. In parallel, following the second approach, there is an increasing acknowledgment of the need to build a body of knowledge that transcends individual cases. Empirical studies have shown that the pursuit of sustainable development does not follow universally consistent patterns; so-called "middle-range" theories that lie between working hypotheses in day-to-day research and all-inclusive systematic efforts to develop unified theories of behavior can enable learning and harness knowledge across contexts (15). Related to advancing theory, dynamic system models can address questions related to the emergence of novelty, path dependencies, and distributional outcomes.

Have emerging efforts made any real progress in modeling nature–society systems in recent years? What explains the apparent disconnect between the persistence of longstanding arguments that suggest models remain as insufficient as they were decades ago, and the increasing ambition of communities who are engaged in modeling? In this Perspective, we take stock of recent progress and identify substantive advances toward better modeling of nature–society systems. We focus on an area where we see much recent work in novel and exciting approaches to modeling dynamic systems for sustainable development: developing and applying mechanistic models through computational means. Such computational models are a principal means of building and testing theory as well as using theory and empirical data to make and test projections in large-scale, complex systems (16). Recent work builds upon longstanding efforts in economics, engineering, natural resource management, energy systems, climate science, water resources, computer science, and many other traditions that have contributed to better understanding and decision-making for sustainability-relevant problems. We posit that recent advances are not widely appreciated across the broader community of researchers because they are largely drawn from specific sustainability-relevant sectors (e.g., energy, water, air pollution, transport, agriculture, fisheries, rangelands) or location-specific case studies and are mostly reported in disciplinary journals.

Our goal in this Perspective is to highlight some of the most exciting of these advances, for researchers who are interested in applying modeling techniques toward the goal of building knowledge to inform action toward sustainable development. We synthesize across and build upon recent work in this area, identifying selected methods and advances associated with four stages of modeling practice. We then discuss emerging lessons that illustrate progress in efforts to build knowledge to inform action by harnessing sector- and location-specific insights and by developing and testing theories in nature–society systems. We conclude by identifying modeling methods under development with as-yet untapped potential to advance understanding.

Methods and Advances in Modeling for Sustainability Science

To illustrate potential applications of modeling methods to research in support of sustainable development, we consider four stages in modeling practice: 1) defining the purpose of a model, 2) selecting its components and their relationships, 3) analyzing the dynamical interactions of those components, and 4) assessing the consequences of potential interventions. Disciplines related to sustainability science define the modeling process in distinct ways, but many that address dynamic systems follow similar logic that includes these four fundamental stages (e.g., ref. 17). Further, the concepts of elements (or components), interconnections (or interactions), and a purpose parallel definitions of a system itself (18). Feedback and iteration are central to modeling, and thus these stages are interdependent and interacting. Model evaluation, including incorporating views of stakeholders and users, occurs throughout all stages and involves developing targeted metrics, benchmarking with data, and testing assumptions and sensitivities.

For each of the four stages, we identify modeling *methods*—techniques drawn from a variety of disciplines and domains—that have high potential to contribute to building knowledge and informing action toward sustainable development. We then highlight *advances*, specific examples from applications in recent research that illustrate how these methods inform sustainability-relevant questions. In selecting these methods and advances, which are intended to be illustrative but not comprehensive, we draw on recent reviews of the core questions of sustainability science (19) and of systems-oriented sustainability research (13), together with topical workshops, seminars, and contributions to a Special Feature we organized for PNAS. We focus on selected papers published in the last several years (from peer-reviewed journals in the English language) that we believe provide particularly useful examples and references for researchers across different fields. Fig. 1 summarizes these modeling methods and related advances. Each of the following subsections focuses on one stage of modeling practice and expands on the summary in each quadrant of Fig. 1. Further details and examples, including references drawn from different applications, are in *SI Appendix*, Table S1.

Defining Purpose. Sustainability science is a problem-oriented field that aims to build knowledge to inform efforts to promote sustainable development: fostering equitable improvements of human well-being on multigenerational timescales. Models can be used in sustainability science for a variety of purposes, including exploring ideas, concepts, and mechanisms, building understanding about system interactions, or examining future

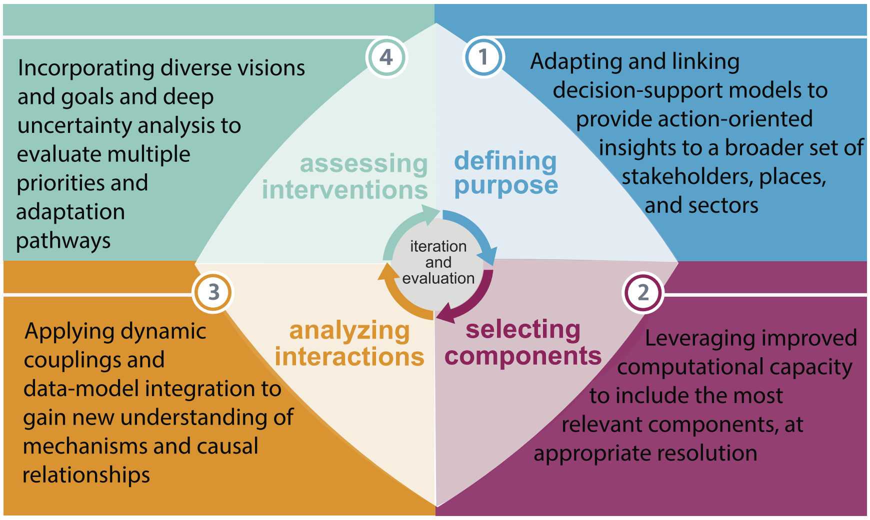

Fig. 1. Summary of methods and advances in four stages of modeling dynamic systems for sustainability science.

scenarios (20). One way to view computational modeling is as a process that integrates theory, concepts, and empirical data in ways that can directly test theories that involve dynamics (21). Modeling can also be used in combination with empirical synthesis together with stakeholders to help build mid-range theory of complex nature–society systems (22). Beyond building and testing theories, additional roles that models can play in policy and management design and implementation for sustainability include exploratory scenario simulation, goal-oriented modeling, ex ante and ex post assessment (23). Efforts to adapt existing models, and link them across sectors and places, have enabled inclusion of a wider range of stakeholders, informing different places and sectors.

Methods for defining purpose. Incorporating nature–society interactions into sectoral decision-support models allows a broad range of existing models that may not have been designed to address human well-being explicitly to be adapted for the purpose of sustainability-relevant analysis. Decision-support systems and associated models apply a diverse range of qualitative and quantitative approaches and incorporate social factors in order to simulate realistic options and outcomes and fully address the priorities of a broader range of users and stakeholders increasingly concerned with promoting sustainability (24). Models of natural resources and technical (engineered) systems have thus advanced substantially in their ability to incorporate nature–society interactions, including human behavior and responses to environmental change, as well as social interactions such as learning and collective action (25). Modern sector-focused models capture these interactions in ways that are credible and legitimate for their decision support applications, though they usually do not focus on inclusive well-being as a formal objective function.

Methods for simulating cross-sector connections and differing contexts can help decision-makers more effectively draw lessons that address complex sustainability challenges. So-called "nexus" approaches, linking models across sectors such as water, food, and energy, have been characterized as still in their infancy, but quantitative methods have been used to identify related synergies and trade-offs (26). Work in multisystem dynamics bridges nexus approaches with advances in formal modeling techniques (7). Advances in machine learning can enable using remote sensing information in regions where on-the-ground data are sparser (27).

Advances in defining purpose. Results from decision-support models that have been adapted to incorporate a broader scope of nature–society interactions have shown promise in providing action-oriented analysis relevant to multiple stakeholders. For example, Fletcher et al. (28) highlight how water systems models for East Africa and California were extended to better capture equity-based considerations in the context of stakeholder-engaged decision-support processes. Bremer et al. (29) engage with participants in watershed management programs in Brazil to identify how models can better meet their needs. Hess et al. develop recommendations to make air quality health effects modeling more useful to policy-makers, including using common scenarios to facilitate comparison (30).

Utilizing models across different contexts has enabled decision-relevant insights across sectors and places. Reed et al. (7) identify methodological connections involving adaptive responses, uncertainty and risk, resilience, and tipping points across detailed sectoral models. Doelman et al. (31) use a global multimodel scenario approach to quantify synergies and trade-offs associated with interventions in water, land, food, and climate. Pastor et al. (32) examine food and water linkages with international trade using a model framework accounting global water availability, crop production strategies, land use, and socioeconomic change. Nhamo et al. (33) use an integrative model for the water–energy–food nexus to provide decision-support toward the Sustainable Development Goals in South Africa.

Selecting Components. Frameworks in sustainability science provide an extensive "checklist" of the components that have been found important in shaping many nature–society interactions (19). These comprise resources (e.g., natural and human-made capital), actors who can make choices or decisions, and institutions that channel those decisions. Within any modeling effort, it is important to establish transparent criteria to determine what components are necessary and sufficient to inform the stated purpose of the analysis. This is particularly difficult in nature–society systems, where "everything is connected to everything else" (34). Related to component selection are decisions about their resolution—the aggregation of real-world detail including over time and space for analytical tractability. This is closely connected to questions of how to understand and account for heterogeneity across actors and places. Methods that leverage improved computational capacity and data availability have helped researchers simulate a set of necessary and sufficient components for sustainability analysis, at more appropriate resolution.

Methods for selecting components. Approaches for capturing diverse societal actors and agency extend beyond previous efforts that often treated people as rational actors. Growing work in computational social science has contributed to theory and associated models of human behavior (35). Agent-based modeling, which can capture heterogeneity among different agents, is increasingly applied to nature–society systems (e.g., refs. 36 and 37). Integrated assessment modeling is attempting to better capture how policy actions create winners and losers and to better account for incentives and trade-offs with knowledge from sociology, psychology, and organizational behavior (5). Several approaches to incorporating actors, decision-making, and institutions in quantitative systems modeling are ready for implementation without major changes in model structure (24). Generalized modeling approaches (38) address the challenge of incorporating components that would otherwise be omitted because of incomplete process knowledge.

The development of computational frameworks that facilitate model interoperability is addressing the technical challenge of modeling the full range of components that affect outcomes in nature–society systems. Models used by different disciplines make practical choices that are difficult to reconcile, including computational implementations such as programming language and temporal and spatial resolution. Efforts to harmonize models capturing different components such that they can be more easily run in tandem from a computational perspective have a long history. Relevant standards date back decades in some areas, such as the Earth System Modeling Framework (39). Further standardization and automation are made possible through application programming interfaces (APIs), AI, and cloud-based applications. However, while model coupling is becoming easier, much innovative method development has eschewed full coupling in favor of ad hoc, purpose-built links, facilitated in part by computational advances and new ways of thinking about architectures. System-of-systems approaches provide methodologies for linking models from different domains, which view system representations as multitier structures with differing levels of abstraction (40). Network approaches have also been used to represent systems with different types of components in a common framework (41).

The increasing availability of high-resolution data and associated simulation capacity have made modeling possible at ever-finer detail. At the same time, this is prompting new ways of thinking about how to balance model fidelity with uncertainty and computational cost. Global Earth system models can now be run for multiple century-long simulations at ~10-km spatial resolution (42). High-resolution, bias-corrected climate model data are increasingly broadly available and widely applied to better understand impacts (43). New highly resolved social data, often near-real-time and at unprecedented levels of disaggregation, have prompted new applications to sustainability science (44). These data can be leveraged to better understand and simulate diverse actors' diversity of goals, access to resources, and circumstances, and their unequal degrees of agency. Data are newly available in undersampled regions due to satellite coverage, and satellite-based data products require models to interpret relationships between remotely sensed quantities and sustainability-relevant on-the-ground information. The combination of data availability and computational capacity has prompted new ways to simulate the heterogeneity that is a core element of nature–society systems. Relatedly, there is a long history in Earth system and climate modeling of applying model hierarchies or spectrums to address questions which need different degrees of resolution (45).

Advances in selecting components. Recent work has led to improved guidance on how and why to incorporate multiple actors with differential agency in modeling. Jafino et al. (46) identify concrete ways in which disaggregation of actors and associated costs and benefits could be improved in integrated assessment modeling toward assessing distributive justice, summarizing applications from model-based climate planning studies. Basheer et al. (47) use what they refer to as a "coevolutionary" modeling framework; they apply it to show that accounting for both the Nile River system and Egypt's macroeconomy better simulated the effects of coordinated strategies to manage the Grand Ethiopian Renaissance Dam. Zaniolo et al. (48) design a method using automated learning to represent different policies and their objectives and tradeoffs and show that it results in improved information for operational regulation in a case of reservoir management characterized by heterogeneous objectives and conflict between users.

The ability to account for a larger variety of model components through connected models contributes to better knowledge about the components of most importance to sustainability. The inclusion of different components in a practical modeling application can help integrate knowledge across different domains, as Lade et al. (49) describe in an example of a model that investigates the importance of social–ecological feedback for an ecological regime shift (the collapse of the Baltic cod). Barnes et al. (50) use multilevel network modeling to identify aspects of social organization that influence responses to climate change among Papua New Guinea islanders. Enahoro et al. (51) link agricultural and food system models in an integrated assessment framework to show how diversified farming practices minimize losses in ecosystem services. Mayfield et al. (52), using air pollution, climate, and employment impact modeling, are able to identify spatial differences in the economic and environmental effects of the shale gas boom in the United States. Agutu et al. integrate cost of capital values into an electrification model to identify how off-grid finance influences electrification costs (53).

As the capacity for ever-greater resolution increases, best practices for weighing the trade-offs of resolution choices in contexts relevant to sustainability have begun to be developed. Merrick and Weyant (54) summarize guidance for choosing resolution in models used for policy analysis, strategic planning, and system analysis with examples from energy and climate, noting the links of choice of resolution across space, time, and with respect to different outcomes with uncertainty analysis. Brown-Steiner et al. showed in an application to air quality that choosing coarser model resolution can decrease fidelity but increase the ability to explore uncertainty spaces with the same computational resources (55). Marcy et al. (56) examined the impact of temporal and spatial resolution decisions in energy system modeling, identifying best practices for selecting resolution. Giuliani et al. (57) use parameter exploration to identify regions where simulating highly resolved processes is important in a case of water reservoir operation.

Analyzing Interactions. The process of modeling interactions involves simulating systems' dynamic behavior over time. The nature–society system that researchers and decision-makers seek to understand for pursuing sustainability is coevolving, complex, and adaptive. Dynamics associated with complex adaptive systems include novelty, feedback, discontinuities, path dependence, and threshold behavior. Two-way interactions between natural and social components are especially important on sustainability-relevant (generational) timescales. Quantitative modeling can illuminate nonintuitive and unpredictable dynamics, especially when feedback loops are operating, and where decision-makers' mental models may be unreliable (58). Systems analysis and stylized models have also been used to identify properties of interest, including resilience, robustness, and vulnerability, which may be associated with outcomes relevant to sustainability. Dynamic couplings of models simulating integrated systems, and integration of data and modeling, have been applied to gain new understanding of important mechanisms and causal relationships in nature–society systems.

Methods for analyzing interactions. Calls to improve model representation of the dynamics of integrated systems often suggest incorporating all relevant feedback into a single model—that is, endogenization of model representations of different types of components. Full endogenization, however, may not always be necessary or desirable. Linking models through purpose-built approaches to model couplings can instead provide rigorous information without the difficulty and complexity of developing a comprehensive model that includes all linkages and feedback. These techniques also can help mitigate the risk of creating integrated models that are mechanistically coupled but not useful for advancing understanding (59). Partial couplings can isolate and thus inform understanding of mechanisms of key interactions and avoid computational and resource expense (60). Reduced-complexity models can be used to accurately describe a system using numerical techniques that make running the model simpler and more efficient. Applications of reduced complexity models enable researchers from other disciplines to better incorporate realistic feedback, retaining important detailed representations in a way that does not sacrifice too much realism. Generalized modeling approaches allow for rigorous analysis of dynamics under conditions of limited data and knowledge (38).

Model techniques for capturing realistic dynamic behavior in sustainability-relevant systems address the interacting scales of key processes, threshold effects, rapid changes, and path dependence. Though well-established existing sectoral models often account for only a subset of the complex adaptive dynamics that occur in real-world systems explicitly, strategies that can address their implications include scenarios, limit testing, or uncertainty analyses. Promising approaches to modeling "tipping points," for example, include agent-based modeling and modeling of social dynamics (61). Methods can also be drawn from underlying mathematical toolboxes for dealing with complex systems with nonlinear dynamics, such as control theory. The ability to formulate sustainability-relevant situations as complex control problems with multiple decision-makers and multiple often conflicting goals can enable improved rigor in conducting simulations that capture feedback behavior, threshold processes, and adaptive responses.

Related to the availability and accessibility of more detailed and highly resolved data sets discussed above, data–model integrations that leverage advanced computational methods can be used to better understand dynamics and ultimately the determinants of well-being. Researchers have begun to use novel data-driven causal methods to address sustainability-relevant questions using Earth system data (62). The use of exploratory modeling techniques can inform robust inferences in coupled nature–society systems (63). Earlier work leveraging AI techniques applied to big data sets focused on prediction, but newer methods are being developed that can provide causal insights. So-called "digital twins" (11) combine two-way interactions of modeling and data analysis in a common framework.

Advances in analyzing interactions. Several studies have leveraged different coupling approaches of various complexities and degrees of endogenization to provide improved understanding of behavioral and societal interactions in nature–society systems. Tong et al. (64) combine models of power plant fleet turnover with integrated assessment modeling and air quality modeling to quantify the relative influence of retiring power plants and the application of pollution controls on human health. Muneepeerakul and Anderies (65) use stylized dynamical models to capture the interaction between the day-to-day operational management of shared natural resources (day-to-day operations) and collective action, exploring how governance emerges endogenously. Kamal Chowdhury et al. link a power system model with a hydrological power management model to show how climate variability modulates power system behavior and resultant costs and emissions (66). Beckage et al. (67) use a reduced-complexity climate model together with a simplified model of human behavioral change, to identify behavioral interactions with the largest influence on global temperature rise. Nordhaus developed equations that mimic behavior of an ice sheet model to assess the economic damage associated with scenarios of climate warming (68).

Advances in understanding of the creation and propagation of novelty and its impacts, drawn in part from long-standing research programs in evolutionary biology and economics, are beginning to inform sustainability-relevant applications to adaptation and transformation. Novelty emergence is a type of dynamic behavior that has historically proven particularly hard to capture in models, as it often depends on simultaneous, synergistic propagation of different and related innovations in different contexts. Mercure et al. (69) show how different theoretical assumptions about innovation applied in models lead to different outcomes in projecting low-carbon transitions. Meng et al. (70) assessed the performance of technology cost forecasts for energy transitions, finding that existing models outperformed expert assessments, but both approaches underestimated technological progress. Batinge et al. (71) use a system dynamics model to explore how gendered innovation affects energy security in poor urban environments.

Applying mechanistic modeling together with a broader toolbox of quantitative and qualitative methods has led to identification of previously unknown mechanisms and causal relationships. Orach et al. linked process-tracing of an empirical case with agent-based modeling to identify and test causal mechanisms to show how interest group behavior can delay or prevent fishery collapses (72). Qiu et al. combined retrospective analyses including difference-in-difference regressions with atmospheric chemical transport modeling to diagnose firm-level heterogeneity in production processes, policy responses, and air quality outcomes as a result of energy policy (73). Morris et al. (74) paired Monte Carlo analysis with scenario discovery techniques applied to large uncertainty ensembles, finding that many patterns of energy and technology development are possible for various long-term environmental pathways. Banitz et al. (75) use the example of cod fishing to show how the use of different model assumptions can identify different causal mechanisms for the same system; they suggest that ensemble modeling, statistical frameworks, or structured discussion could help resolve model disagreements.

Assessing Interventions. Modeling can provide a means to assess the potential of interventions—and updating such assessments, considering system responses and other actors' responses to them. There is increasing recognition that effective interventions must "fit" particular contexts (76) and that actors engaged in interventions have different goals and power. Combining policies and strategies such as regulations, market approaches, and persuasion to effectively promote sustainability requires better understanding of their strengths, limitations, and potential complementarities. Much modeling practice is increasingly focusing on providing decision-support for interventions. Methods that can incorporate diverse visions and goals, as well as deep uncertainty analysis, have been leveraged to evaluate multiple stakeholders' priorities and understand adaptation pathways.

Methods for assessing interventions. Computational and statistical approaches that evaluate decision scenarios under uncertainty have further advanced the capacity of models, including existing decision-support tools, to evaluate the likely outcome of potential interventions relative to different metrics in particular situations, and for modelers to provide that information to a broad range of stakeholders and user groups. Techniques drawn from applying theories of decision-making under deep uncertainty, uncertainty quantification techniques, and scenario planning are being used in combination to better assess outcomes and their probabilities (77). Methods can address pathways of sequential decision-making in ways that can inform strategies beyond traditional adaptive management approaches. Exploratory modeling has been used to examine responses to management decisions along adaptive pathways (78). This can help identify unintended consequences of interventions. Computational and statistical approaches have combined ensemble simulations and deep uncertainty techniques to provide new insights targeted toward decision-making.

Recent efforts have identified ways to incorporate different perspectives and normative visions in dynamic modeling. Previous generations of decision-relevant models were often designed to serve a narrow audience and prioritized certain problem definitions, often based on the status quo. One example is the inclusion of certain social sciences such as economics, and exclusion of other social sciences and humanities that address questions about values, in models of global environmental change (79). Emerging techniques allow modelers to grapple constructively with pluralism, ambiguity, and values, engaging different users' viewpoints and perspectives as well as problem definitions. One example is the application of multiobjective optimization methods to explore tradeoffs across alternative candidate solutions (capturing objectives from different stakeholders) (80). Participatory modeling has been used to promote learning amongst stakeholders, by facilitating dialogue (81) or informing transition governance (82). Improved metrics that address different goals can also help evaluation of system progress toward sustainability goals. A growing literature connects domain-focused modeling with sustainable development goals, illustrating outputs with metrics increasingly relevant to stakeholder communities (83).

Advances in assessing interventions. Better knowledge of how decision and adaptation pathways evolve over time has been enabled by the application of decision science and option analysis in modeling, including modeling techniques drawn from the field of decision-making under deep uncertainty. The Natural Capital Project has developed and applied a suite of spatially explicit planning and assessment models to support decision-making about managing environmental resources at local to regional scales (84). Fletcher et al. (85) applied a scenario planning framework, drawing from planning approaches and climate uncertainty analysis to inform robust designs while incorporating learning, to a reservoir planning problem in Kenya. Bojórquez-Tapia et al. (86) summarize cases where modeling was used to identify adaptation pathways under deep uncertainty applied to climate uncertainty and large-scale infrastructure planning. Hadjimichael et al. paired exploratory modeling with global sensitivity analysis to enhance the ability to make inferences on water scarcity vulnerabilities in institutionally complex river basins (87). Lucena et al. (88) used multiple models to assess the interaction between climate adaptation and mitigation strategies in a case of hydropower generation in Brazil. Saari et al. (89) used an ensemble-based approach together with an integrated modeling framework to quantify the influence of natural variability in air quality and related health responses to climate policy.

Evaluations of interventions against multiple objectives and priorities are made possible through attention to different goals and normative visions. Nock et al. (90) show how maximizing social benefit, rather than cost-minimization approaches, changes allocation decisions for electricity generation infrastructure and energy access in developing countries. Bremer et al. (29) used semistructured interviews and focus groups to better understand the role that hydrologic modeling plays in supporting a range of stakeholder needs and perspectives. Devisscher et al. (91) used fuzzy cognitive mapping to incorporate environmental, social, economic, and policy factors in the context of fragmented data availability, in a case study of adaptation to wildfires in Bolivia. Edwards et al. showed that goal-inspired metrics for emissions could inform climate policies better than typically used global warming potentials (92). The concept of inclusive wealth provides a promising way of designing a limited 'dashboard' of outcomes theoretically consistent with sustainability; Ikeda and Managi (93) simulate it to project regional sustainability in Japan.

Lessons from Advancing Modeling in Sustainability Science

In this section, we highlight emerging lessons based upon the modeling methods and initial advances discussed above. Specifically, we return to the two interacting approaches that implement efforts to develop knowledge and inform action: 1) harnessing sector- and location-specific insights and 2) advancing theories of nature–society systems. We identify three lessons relevant to the former, and three lessons relevant to the latter, together with related methods and advances. We summarize these in Fig. 2.

Harnessing Sector- and Location-Specific Insights. First, for researchers who aim to build knowledge to inform action through research focusing on specific sectors and locations, a sustainability-related focus on changes in inclusive well-being as an overall "objective function" draws attention not only to the connection between different sectors but also prioritizes outcomes that can deliver equitably shared well-being improvements across present and future generations. Many of the modeling applications described in the previous section address sectors closely linked to sustainability transitions, including climate, energy, food, and land use. Modeling and analysis to better understand these systems is necessary, but not sufficient, for sustainable development. To that end, by incorporating human behavior and social dynamics into existing decision-support models, and linking across sectors, modelers increase their capacity to examine well-being in ways that inform multiple actors and interests. The importance of adaptation pathways in many such systems warrants increased attention to accounting for related dynamics in decision-relevant applications.

Second, while addressing sustainability challenges requires modeling processes that interact on a variety of timescales, a sustainability perspective suggests the importance of attention to decadal to generational-scale outcomes. Modelers are well equipped to identify how spatial and temporal scales interact, but the goal of informing sustainability may lead to different choices about the resolution of components, which may include increasing resolution and data fidelity, or reducing resolution to enable addressing interactions of multiple components.

Third, informing efforts toward equitably shared well-being for present and future generations foregrounds issues of power differentials among actors. This encourages modelers to grapple with the implications of power and associated issues of equity in their work, and fully addressing these issues requires further challenging underlying assumptions

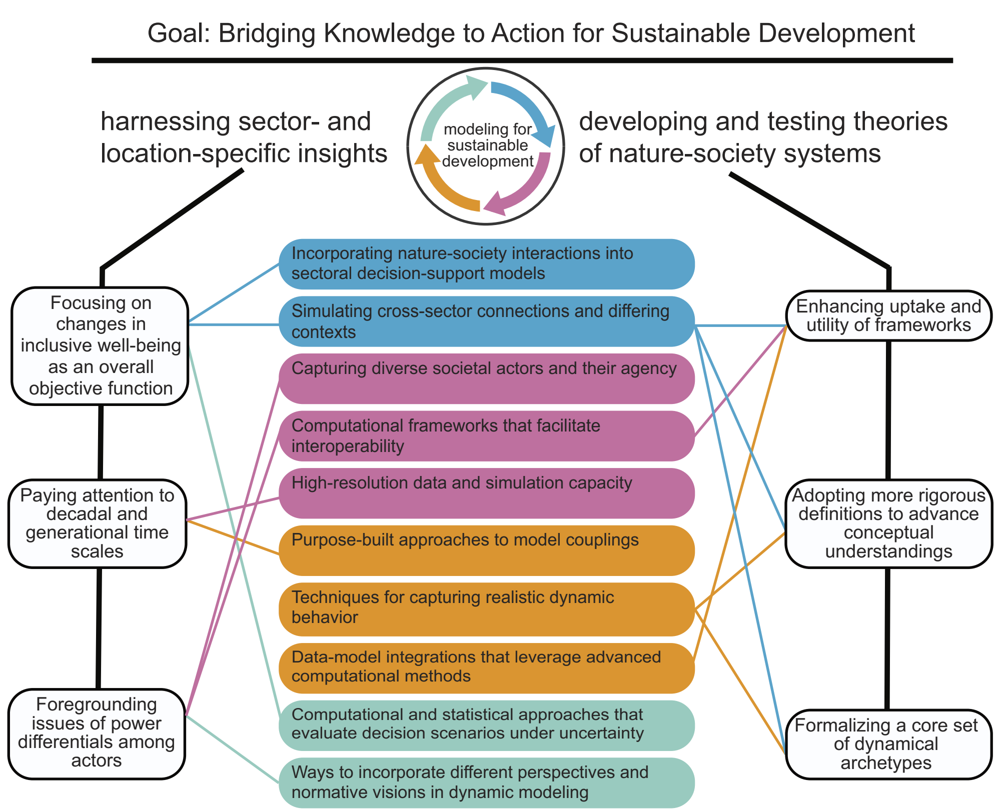

Fig. 2. Emerging lessons resulting from connecting research aiming to building knowledge to inform action that uses one of two interconnected approaches (i.e., 1) harnessing sector- and location-specific insights and 2) developing and testing theories of nature–society systems), with modeling methods identified in the text.

that may still remain unstated in modeling related applications. Leveraging approaches to capture diverse societal actions can better accommodate stakeholders' diverse values and preferences. Relatedly, incorporating different goals and normative visions of sustainability into models can inform the development of appropriate metrics. It is also closely related to efforts to better capture actors and their diverse values. Further exploration of equity in modeling is addressed elsewhere in the Special Feature on Modeling Dynamic Systems for Sustainable Development.

Advancing Theories of Nature–Society Systems. For work that aims toward advancing theories of nature–society systems, particularly middle-range theory, making better use of modeling methods enhances the utility of frameworks across the research communities contributing to sustainability science. A wide variety of systems-oriented analytical frameworks exist to help researchers identify important components and their interactions, but much sustainability-relevant research does not make use of them (13). Recent work has developed new approaches to bridge frameworks to methods in ways that can facilitate modeling (94). The modeling methods and advances described above provide a toolbox that can help analysts select and examine which of the potentially important elements and interactions are necessary and sufficient to determine outcomes in a particular case. For example, increasing computational interoperability and applying techniques such as loose couplings can help to make models usable outside the communities that developed them. Methods that link across sectors and contexts lead to understanding the application of models across cases. Efforts to apply multiple approaches in a single study such as data–model integrations also represent steps forward.

Second, models provide a common ground on which to compare, critically assess, and synthesize multiple perspectives on key concepts such as adaptation, transitions, transformations, vulnerability, and resilience. Formal modeling provides a way to transparently compare the purposes, components, interactions, and interventions that different traditions apply to similar phenomena, even where increasing complexity addresses realistic rather than stylized systems. Researchers have noted that diversity and openness in definitions for the concept of resilience, for example, may impede their application to complex systems modeling (95). Conversely, adopting more rigorous definitions can help advance conceptual understandings through referring to system components, their relationships, and their dynamical interactions. One test of an effective definition is whether it is consistent across different modeling choices. An example of this is efforts to better understand adaptation, identified as a capacity necessary to support sustainable development (19). Formalizing adaptive mechanisms in models, especially agent-based models, has used detailed data from case studies to explore causal claims. In contrast, efforts to advance theory on adaptation have been hampered by a lack of definitional clarity, with much effort spent on differentiating whether adaptive responses occur with relevance to internal or external shocks. A modeling perspective reveals that this differentiation depends on subjective boundary definition, suggesting that efforts to advance theory might more usefully focus on characterizing specific types of dynamical behavior.

Third, formalizing a core set of dynamical archetypes in modeling could assist efforts to develop and test mid-range theory across sustainability science. In system dynamics modeling, archetypes are defined as basic modes of system behavior and their associated feedback structures; introductory texts build from the understanding that the behavior of systems arises from their structure and their combinations form the building blocks for complex system behavior. Archetype analysis is increasingly used as an approach to understand recurrent patters of variables that affect sustainability-relevant outcomes (96). Reference to common archetypes enhances efforts to simulate cross-sector connections and differing contexts. While there is a need for going beyond stylized systems, defining archetypes can help efforts to leverage methods drawn from other fields that can capture complex dynamics. A core set of widely understood modeling archetypes in sustainability could be leveraged to explore theories and hypotheses (97).

Emerging Techniques and Ways Forward

In summary, there have been repeated calls for improved models of nature–society systems to be used in support of sustainable development. Many, even most, recent examples of these exhortations echo themes identified decades ago when modeling and computation, data availability, and understanding of nature–society systems were substantially less advanced. Here, we argue that recent modeling advances have begun to address these longstanding challenges. These advances often lack visibility outside particular application domains but are addressing common questions, and their insights can be harnessed to advance open questions in sustainability science.

A focus on modeling and related methods clarifies the relationship between the two interrelated approaches to building knowledge to inform action in sustainability science: 1) harnessing sector- and location-specific insights and 2) advancing theories of nature–society systems. Many modeling advances draw from research that primarily applies the former approach, though both are indispensable in efforts to achieve an overall goal of bridging knowledge to inform action toward sustainable development. For research focused on specific locations and sectors, modeling requires categorization and abstraction of elements and interactions. The process of simplification can thus help derive hypotheses to advance theory. For efforts focused on advancing theory, formalizing a model representation can provide conceptual clarity and enable hypothesis testing. More formal acknowledgment of the importance of both approaches and their interrelationship, for example through future synthesis efforts or through targeted journal keywords (a set is suggested for this paper), may help researchers better situate contributions to this rapidly growing field.

Models will also be most effective in the context of these interconnected approaches when they are applied considering best practices and when used in combination with empirical data and theory development. Researchers in sustainability transitions have welcomed increasing efforts to apply modeling but drawn attention to its limits (98). Others have argued that researchers ought not to even attempt modeling certain aspects of uncertain human–natural systems (99).

Given the fast-moving frontier of emerging methods, it is important to recognize that modeling has dramatically advanced in recent years and that what once seemed to be fundamental limitations of modeling methods could potentially be addressed with new innovative ideas (5, 99). However, every scientific method, including modeling, is associated with limitations and uncertainties. Applying best practices such as identifying objectives, documenting data, and testing key assumptions should be standard expectations for models in any field (17). Researchers would also be well-advised to remember that modeling is one of many methods that can help further understanding and that its potential for supporting advances is enhanced when used in combination with other methods.

The examples we cite here illustrate how modeling can be applied to draw robust conclusions meaningful to an audience interested in advancing sustainable development. However, further work is required to fully leverage the modeling methods and advances described above toward broader understanding. Publication and review processes, as well as disciplinary norms for tenure and professional advancement, still largely discourage researchers from drawing broader lessons across sustainability-relevant cases. While an increasing number of outlets have emerged for such work, the challenge of ensuring fair and thorough review across disciplines can discourage researchers from fully leveraging the potential of newer modeling methodologies. Interest in common themes, as noted above, has prompted numerous calls for new disciplines and specializations. While emerging communities often need new structures and organizations, we see greater utility in broadening existing forums for sharing methodological advances and empirical results. Modeling advances are further enhanced, and research communities benefit from open access to publications, data, and code, including applying FAIR (findability, accessibility, interoperability, and reuse) principles, with important implications for equity .

Finally, we focused in this Perspective largely on modeling tools and techniques currently being applied. There is much potential for future improvement. Advances in computational methods, in particular, the rise of automation and AI, in combination with ever-larger data streams, have the potential to induce transformative change in modeling processes (12). Fittingly, the insights that sustainability science has developed to rigorously analyze the development and propagation of novelty and innovation may prove useful to increase the likelihood that these tools are used to advance common goals of equitable improvements in well-being within and across generations.

Data, Materials, and Software Availability. All study data are included in the article and/or *SI Appendix*.

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