Unraveling complex causal processes that affect sustainability requires more integration between empirical and modeling approaches

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Scientists seek to understand the causal processes that generate sustainability problems and determine effective solutions. Yet, causal inquiry in nature–society systems is hampered by conceptual and methodological challenges that arise from nature–society interdependencies and the complex dynamics they create. Here, we demonstrate how sustainability scientists can address these challenges and make more robust causal claims through better integration between empirical analyses and process- or agent-based modeling. To illustrate how these different epistemological traditions can be integrated, we present four studies of air pollution regulation, natural resource management, and the spread of COVID-19. The studies show how integration can improve empirical estimates of causal effects, inform future research designs and data collection, enhance understanding of the complex dynamics that underlie observed temporal patterns, and elucidate causal mechanisms and the contexts in which they operate. These advances in causal understanding can help sustainability scientists develop better theories of phenomena where social and ecological processes are dynamically intertwined and prior causal knowledge and data are limited. The improved causal understanding also enhances governance by helping scientists and practitioners choose among potential interventions, decide when and how the timing of an intervention matters, and anticipate unexpected outcomes. Methodological integration, however, requires skills and efforts of all involved to learn how members of the respective other tradition think and analyze nature–society systems.

social–ecological systems | coupled human–natural systems | nature–society systems | socio-environmental systems | social-ecological-technological systems

Significance

Understanding causation in nature–society systems is fundamental to advancing sustainability science and addressing sustainability problems, such as climate change, pollution, natural resource collapse, and the spread of infectious diseases. To study causation, sustainability scientists rely on modeling or on empirical analyses but rarely combine the two approaches. This lack of integration is problematic because nature–society interdependencies and the complex dynamics they create pose conceptual and methodological challenges that cannot be addressed by each approach in isolation. Using four studies, we demonstrate how integration between empirical analyses and modeling can reduce uncertainty in empirical estimates, improve the design of empirical analyses, uncover causal mechanisms, enhance understanding of the drivers of complex temporal patterns, and elucidate unexpected outcomes.

To enhance the sustainability of nature–society systems, scientists and practitioners seek a causal understanding of these systems. They may be interested in the impact of environmental change or the effect of a policy, or want to identify the factors or mechanisms that cause environmental degradation. Broadly speaking, sustainability scientists pose two types of causal questions: What are the effects of change in a system variable, process or structure (effects of causes), and what are the causes of change in system state or behavior (causes of effects)? For example, in evaluating the effects of causes, scientists may seek to assess the extent to which drought affects poverty or a new fishery policy affects the sustainability of the fishery. They may also be interested in how the effects vary by context or whether to expect unintended side effects. In explaining the causes of effects, scientists may seek to identify the interacting causes or causal pathways that bring about fisheries collapse, as well as the conditions under which this phenomenon may be observed. Answers to both types of causal questions enhance system understanding and thus contribute to the development of theory and to governance.

To answer causal questions, sustainability scientists use both empirical and modeling approaches (*SI Appendix*, Table S1). We use the word "empirical" to refer to studies that evaluate causal relationships and identify causal mechanisms by collecting and analyzing quantitative or qualitative data. Examples of empirical approaches are a randomized experimental design to assess whether community-based monitoring improves groundwater management (1), a quasi-experimental design to assess whether an antipoverty program increases deforestation (2), and a process-tracing design to identify the empirical mechanism that links the need for joint action and collaborative output in flood risk management (3). In contrast, "modeling" refers to studies that build and use process- or agent-based models to investigate the effects of changes in causal variables or structures, or to identify causal mechanisms through simulating system states and trajectories. An example of process-based modeling is an air quality model that, based on atmospheric chemistry and transport relationships, can simulate air quality changes

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resulting from COVID-19 lockdowns (4). Examples of agent-based modeling are a spatial model of resource users' decisions that can simulate the effects of a fuel subsidy on spatial poverty dynamics (5), and a model of interactions between fishers, traders, and fish stocks that can be used to investigate how and under which conditions cooperative forms of self-governance emerge (6).

Whether scientists use an empirical or a modeling approach, they will find that collecting and evaluating evidence in support of causal claims is challenging because complex interdependencies between social and biophysical processes create adaptive, nonlinear, path-dependent, and coevolutionary dynamics. In empirical studies, these dynamics may violate key assumptions required for statistical causal inference, which can introduce bias into empirical designs (7). While qualitative studies that trace a causal process in a particular case can provide insights into such interdependencies in particular contexts, the evidence needed to disentangle multiple mechanisms and to generalize is often costly or inaccessible. In addition, complex dynamics created by adaptive human or ecosystem responses can make it difficult to decide what and when to measure in empirical studies. Modeling approaches can capture some of the structural and dynamic complexity of nature–society systems. Yet the validity of any causal claims from process-based and agent-based models depends on the realism of the model assumptions and structure, which is particularly challenging when it comes to representing social dynamics and nature–society interdependencies (8, 9).

In the presence of complex nature–society dynamics, advances in causal understanding require more frequent integration of empirical and modeling approaches (10–13). To make causal claims, each approach employs different strategies that can complement each other. Yet, these complementarities are rarely observed in the sustainability literature. There are many reasons for the lack of integration. They include a) challenges of bridging epistemologies across communities and combining qualitative and quantitative methods (14, 15), b) the resources required for deep cross-community collaborations that can overcome difficulties in translation between what is measured empirically and what is modeled, c) a lack of incentives to invest in integrative work, d) more difficult review processes, and importantly, e) a lack of guidance on how to achieve integration. As a consequence, communities remain separate. For example, in energy policy research, scholarship that uses data for ex post empirical evaluations and scholarship that uses modeling for ex ante predictions are largely disconnected (16–18). In climate change research, the flagship modeling programs rarely incorporate insights from empirical analyses of social processes, in part because these insights are not well suited for the intensive computational methods used in the modeling (11, 19). In social–ecological research, insights from rich empirical place-based studies are rarely incorporated in social–ecological models (20).

Empirical and modeling approaches can be integrated in different ways (*SI Appendix*, Fig. S1 and Table S2). The simplest form of integration is to compare the results from each approach and assess whether the approaches support the same causal claim (8, 16, 18). Going further in the integration, models can also be used to expand on data-based insights about causal effects or causal mechanisms (9, 21–24), or to inform an empirical study in the presence of complex dynamics (7, 25–27). Similarly, empirical studies can inform the design of a model (28–31). Moving toward greater integration, scholars can codesign an empirical and modeling study in order to develop and test causal explanations through an iterative process that provides a structured way to identify causes, develop causal hypotheses, and test these hypotheses using both empirical and modeling evidence (32). Despite some examples of integration in the literature, there is little guidance on how to do such integration or when, and for what purposes, it is useful.

Here, we elaborate on what can be learned when these two methodological traditions are brought into dialogue and show how integrating them can improve causal understanding of complex nature–society systems. We use the word "integration" to refer to a variety of possible ways of combining the two traditions that go beyond the use of empirical data to parameterize, build, or validate a model or the use of modeling results to inspire hypotheses for empirical analysis. We present four studies that illustrate how modeling can i) improve empirical causal inference by simulating nature–society interdependencies and their influence on the estimation of causal effects, ii) elucidate whether the coevolution of human and biological adaptation is a cause of observed temporal patterns in infections, and iii), when codesigned with an empirical study, unravel complex dynamics that explain natural resource policy adaptation and environmental outcomes. By illustrating how one can integrate modeling approaches with empirical ones, and by documenting the insights that can be gained, we show how integration ultimately can support the development of better theories of nature–society dynamics, as well as future governance for sustainability. We conclude with ways forward to address some of the challenges of integrating empirical and modeling approaches.

Four Exemplary Studies of Integrating Empirical with Modeling Approaches

Because of its multidisciplinary nature, sustainability science includes a variety of conceptualizations of causation, different ideas about causes, and different norms of what is considered an appropriate inferential practice and sufficient evidence for making a causal claim. Consequently, the methods and types of data used within empirical and modeling approaches are diverse, as are the reasons and possibilities to combine them (33). We illustrate some of this diversity with the help of four studies of complex nature–society systems in the contexts of environmental pollution, disease spread, and natural resource management. The studies differ in their causal questions (effect of causes vs. causes of effects), methods and data (quantitative vs. qualitative), and the ways in which empirical and modeling approaches are combined. Two studies are situated within what is often associated with the term "causal inference." These studies typically focus on a well-defined cause, such as an intervention or a natural event, with the aim to evaluate the size of its effect using (quasi-) experimental designs and statistical methods (Studies 1 & 2). The other two studies aim to identify causal mechanisms that can explain observed empirical patterns in contexts where knowledge and data about complex dynamic nature–society interdependencies are limited. These studies intend to shed light on the causal structure and complex temporal dynamics of the nature–society system in order to inform future data collection (Study 3) or develop theories of nature–society phenomena (Study 4).

Modeling to Support Causal Inference in the Presence of Nature–Society Interdependencies (Studies 1 & 2). For empiricists who seek to estimate the effects of causal variables in nature–society systems using (quasi-)experimental designs, nature–society interdependencies can lead to spillovers that pose challenges for causal inference. In statistics, this phenomenon is known as "interference among units" (34), where the units of analysis could be species, ecosystems, communities, or households exposed to a change in the value of a causal variable. In most studies that estimate causal effects in nature–society systems, analysts assume, either implicitly or explicitly, no spillovers among the units. That assumption implies that the outcomes (e.g., fish stocks, pollution) in one unit do not depend on the value of the causal variable in other units. For example, for a marine protected area, spillovers from zone i to zone j exist when changing i's protected status changes j's outcome when j is protected or unprotected. Zones i and j may interact via natural mechanisms (e.g., larval dispersal) or human mechanisms (e.g., displacement of fishing activity).

Widespread interdependencies in nature–society systems make spillovers the rule rather than the exception. For example, in the simple case in which an expected causal effect is estimated through contrasting average outcomes in treated and control groups, this estimator would be biased if the control units' outcomes depend on whether they are near a treated unit. Moreover, spillovers not only create an estimation challenge but also an interpretation challenge: Defining a single expected causal effect is no longer possible because a unit's outcome under treated and control states depends both on its own treatment status and the treatment status of other units. Models of nature–society systems that explicitly account for interdependencies provide insights into understanding spillovers and point scholars to appropriate empirical designs. We illustrate this potential in two studies that focus on air pollution regulation (Study 1) and marine conservation (Study 2).

Study 1: Using a process-based air quality model to inform policy experiment designs to control air pollution in the presence of spatial spillovers. Atmospheric transport of air pollutants exemplifies how spillovers complicate the causal evaluation of policies in nature–society systems. Emission reductions at one location can lead to changes in air pollutant concentrations hundreds of kilometers away. These spatial spillovers complicate any attempt to estimate the causal effect of an emission reduction policy on air quality. However, these spatial spillovers can be described by process-based air quality models, which simulate the spatial distribution (e.g., the range of atmospheric transport) of air quality changes due to emission reductions at any combination of locations.

Here, we illustrate how these models can help researchers design policy experiments. We consider a potential policy experiment aimed at reducing Nitrogen Oxide (NO_x) emissions from natural gas power plants in the western United States. NO_x is an important precursor to fine particulate matter ($PM_{2.5}$), which is the target outcome in the policy experiment.

We demonstrate how empirical researchers can use simulations from an air quality model to inform their decisions about 1) how best to randomly assign power plants to an experimental intervention (the treatment), and 2) how best to link measurement locations (air quality monitors) to the power plants. The western United States comprises 294 natural gas power plants and 625 air quality monitors (Fig. 1*A*). Importantly, monitors are not typically co-located with the plants. We assume that, in the experiment, half of the power plants will be assigned to receive the intervention (which reduces its NO_x emissions). We use an air quality model, Intervention Model for Air Pollution (InMAP) (35), to simulate the changes in $PM_{2.5}$ observed at the air quality monitor locations due to reductions in NO_x emission from power plants (Fig. 1*B*). The difference between the average $PM_{2.5}$ in the treatment and control groups is the estimated average impact of the intervention on $PM_{2.5}$. See *SI Appendix* for more details.

Insight 1a: The treatment assignment should be clustered at a spatial level that contains the spatial spillovers, and clusters should account for the atmospheric transport structures.

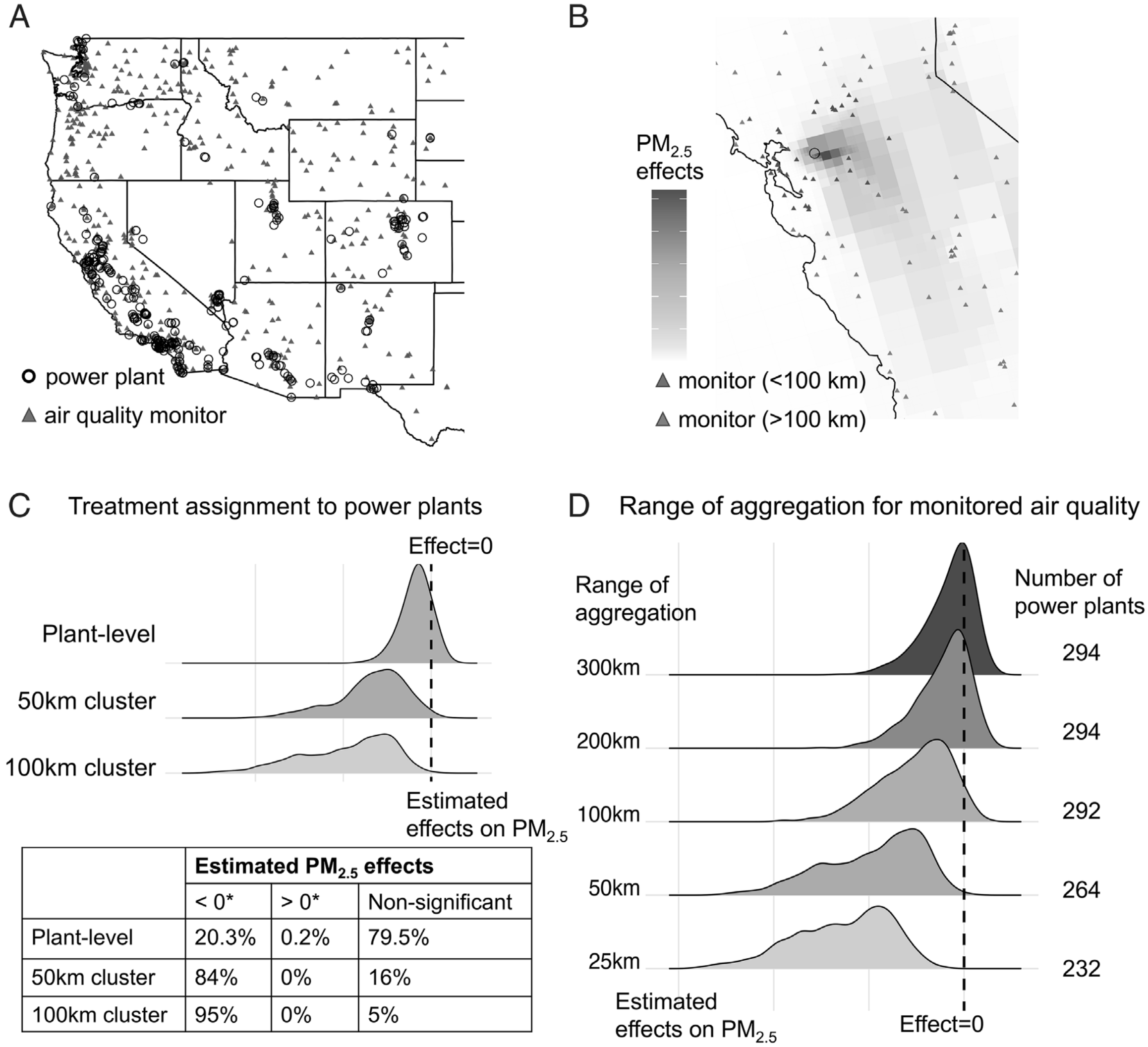
In randomized or natural experiments, the intervention is often assigned at the power plant level, but in the presence of spillovers these designs can be biased. We consider two randomized assignments: simple randomization at the plant level and clustered randomization. The spatial clusters are rectangles of 50 km or 100 km. Plants in the same cluster are always assigned to the same condition (treatment or control).

Compared to the plant-level assignment, the cluster-level assignment significantly reduces potential biases due to spillovers (Fig. 1*C*). If treatment is randomly assigned at the plant level, 79% of the assignments generate misleading results. The policy would appear to be either ineffective (no significant changes in $PM_{2.5}$ compared to the control group) or even harmful to the air quality (increases in $PM_{2.5}$). These misleading results arise because, if a control group plant is next to a treatment group plant, the air quality monitors near the control plant may be downwind of the treated plant and thus measure a decrease in $PM_{2.5}$. However, if the treatment assignment is randomized at the cluster level, the chances of significantly detecting a decrease in $PM_{2.5}$ increases to 84% (50 km cluster) or 95% (100 km cluster) from 20% (plant-level assignment). Of course, when choosing the size of the cluster, experimentalists must consider potential tradeoffs—the cluster size needs to be large enough to contain much of the spillovers but not so large that the effective sample size is too small (i.e., the design is underpowered). While our modeling example does not identify an optimal cluster design (in terms of the radius or shape of the cluster), it implies that the choice of a cluster should account for the physical structure of atmospheric transport, which can be characterized by simulations using process-based air quality models.

Insight 1b: Air quality model simulations inform the decision about the spatial aggregation of the measurement at monitor locations.

Air quality monitors are not often co-located with power plants, and thus empirical researchers must determine how best to link air quality monitors to power plants. One common approach is to calculate the average pollution measurements from all air quality monitors within a certain distance of a power plant (36) and then quantify if the air quality measured near the treated plants differentially changes compared to the control plants. This radius is often chosen without careful consideration.

Using model simulations, we tested different distances (25 km, 50 km, 100 km, 200 km, and 300 km) to see how they impact the estimated effects on $PM_{2.5}$ (Fig. 1*D*). We find that there is a tradeoff in choosing the radius. A small radius (e.g., 25 km) yields the largest estimated impacts, in terms of $PM_{2.5}$ improvement, and avoids misleading estimation results due to the spatial transport (i.e., an erroneous conclusion that the intervention increases $PM_{2.5}$). However, a 25-km radius fails to capture the complete effect of the intervention because not all power plants have a monitor within that radius (only 232 out of 294 do). In contrast, a larger radius (e.g., 200 km) ensures all power plants are associated with a monitor, but that radius yields misleading evaluation results because the spatial aggregation range is too large. Within a 200-km radius of a power plant in the control group, there may exist monitors that are also close to treated units. Spillovers may thus generate misleading results. Choosing the range for spatial aggregation is thus a context-dependent decision, and this study



	Estimated $PM_{2.5}$ effects		
	< 0*	> 0*	Non-significant
Plant-level	20.3%	0.2%	79.5%
50km cluster	84%	0%	16%
100km cluster	95%	0%	5%

Fig. 1. Impacts of design and evaluation choices on the estimated effects of an air quality policy. (*A*) The location of natural gas power plants (black circle) and surface air quality monitors (green) in the western United States. (*B*) Simulated $PM_{2.5}$ changes (shown by the colors) due to emission reduction at a selected power plant (black circle) and the surrounding air quality monitors (monitors that are <100 km are shown in green color). (*C*) The range of estimated effects on $PM_{2.5}$ under three treatment assignments. The table shows the percentage of assignment cases in which one could detect a statistically significant decrease in $PM_{2.5}$ (<0*), a significant increase in $PM_{2.5}$ (>0*), or a nonsignificant result (statistical significance level at $P = 0.05$). (*D*) The estimated impacts on $PM_{2.5}$ under different ranges of spatial aggregation and the number of power plants that would be included in the analysis.

demonstrates that process-based air quality models can inform this decision.

Study 2: Using an agent-based fishery model to estimate causal effects of a gear restriction regulation in the presence of spatial spillovers. Like atmospheric processes, human mobility can lead to spillovers in nature–society systems. Greater mobility implies more potential spillover, and the nature and severity of the resulting statistical challenges will depend in complex ways on the whole system. To demonstrate this point, we extend the spatial-dynamic bioeconomic model of a fishery in ref. 7. The simulation model captures key interactions among human (fishers) and natural (fish) elements that are subject to dynamic, spatial processes and feedback, such as harvesting-induced changes in fish stocks that trigger mobility of fishers. The seascape is divided into three discrete fishing zones, and fishers make decisions about whether to fish and, if so, in which zone to fish (see *SI Appendix* for model details).

Suppose an empirical researcher seeks to estimate the average effect on fish stocks from the imposition of a spatial gear restriction, i.e., a legal restriction on the type of gear that fishers can use in specific zones. Regulators impose the gear restriction in Zone 3 to increase the zone's fish stock. The researcher can observe Zone 3's pre- and postrestriction stocks. To estimate the counterfactual stock in Zone 3 in the absence of the gear restriction, the researcher uses Zone 1 and Zone 2 as comparison (control) zones and estimates the gear restriction's effect via the popular Before-After-Control-Impact (BACI) design (a.k.a., difference-in-differences). The zones are identical in terms of their deterministic and stochastic processes. Thus, in the absence of spillovers, the BACI design would perform well: The average trend in fish stocks in Zone 1 and Zone 2 is a valid estimate of the expected counterfactual trend of Zone 3 in the absence of a gear restriction. With spillovers, however, the BACI design may perform poorly. The bioeconomic model allows us to simulate the true effect of the gear restriction and contrast it with the estimate an empirical researcher would get in the presence of spillover.

The study generates two key insights about estimating the causal effect of the gear restriction from observable data when nature–society interdependencies lead to spillovers. Both insights would be difficult for a researcher to anticipate in the absence of a model.

Insight 2a: When the causal variable decreases the ability of fishers to harvest, empiricists should expect: a) the true causal effect on the stock in the treated zone to increase when the study context moves from zero human mobility to modest mobility (Fig. 2*A*); and b) when the preintervention resource exploitation is high, the true causal effect may decrease when the study context moves from modest mobility to high mobility (i.e., for some contexts, the empiricist should expect nonmonotonic changes in the size of the causal effect as mobility increases due to compensatory effects) (Fig. 2*B*).

Insight 2a implies that modeling can help empiricists understand the dynamics that will moderate the magnitude of the expected treatment effect and whether this moderating effect is monotonic or not. The nonmonotonic pattern in Fig. 2*B* is not observed when the causal variable is hypoxia (low dissolved oxygen in the water column), which is the causal variable studied in ref. 7. The modeling reveals why. With a gear restriction, the causal variable is "assigned" to the human component of the human-nature system (i.e., the harvesting technology), whereas with hypoxia, the causal variable is assigned to the environmental component (i.e., stock growth rate and carrying capacity). That contextual difference leads to different feedback and dynamics. When the stock is treated with a negative shock in the case of hypoxia, potential biomass is taken out of the system in the treated zone with no compensating biomass added in the nontreated zones. When humans are treated with a negative shock (a gear restriction that lowers instantaneous profitability), no potential biomass is removed, and human responses trigger a compensatory effect that allows biomass to increase both in the treated and in the nontreated zones.

The moderating effect of mobility is not easily discerned in the absence of a model that incorporates the dynamics and feedback inherent in a nature–society system, yet it is important for assessing the quality of an empirical design, such as the likely statistical power (i.e., how much information about the causal effect can the design provide?). A small amount of spillover can be good for power, in the sense that the minimum detectable effect goes up dramatically, making the treatment effect easier to detect. Yet, in cases where the causal effect is nonmonotonically affected by spillovers, too much spillover makes it harder to detect the causal effect (in addition to potential bias, which is described in Insight 2b).

Insight 2b: When the causal variable reduces the ability of fishers to harvest, empiricists using a BACI design should expect that: a) the divergence between the true causal effect and the estimated effect will grow when the study context moves from zero mobility to higher mobility; and b) the direction of the divergence (i.e., the sign of the bias) depends on the preintervention exploitation levels (Fig. 3).

Insight 2b implies that modeling can help empiricists understand the challenge that spillovers pose in popular empirical designs for estimating causal effects from data. As in the case of a hypoxia (7), the divergence between the estimated average causal effect of the gear restriction and its true average causal effect is higher at higher levels of mobility (Fig. 3). But in contrast to the hypoxia case, the sign of the divergence—i.e., whether we are overestimating or underestimating the true effect—depends on the prerestriction conditions (contrast Fig. 3 *A*, *C* and *B*, *D*). This difference arises because of the nonmonotonic relationship between the true causal effect and mobility in the high exploitation case (Fig. 2*B*). Thus, the model demonstrates that the degree to which spillovers affect empirical estimation is determined by which element of the coupled human-environment pair is affected by the causal variable.

Integrating Modeling and Empirical Approaches to Assess Causal Implications of Complex Dynamics. Complex dynamics in nature–society systems, such as when disturbances, stochasticity, or path dependence fundamentally alter system dynamics, make causal attribution significantly more challenging from both conceptual and empirical perspectives (Fig. 4). In *A*, the parallel trend between treatment and control units means that the treatment effect is not time-varying. In *B*, the disturbance affects not only the outcome's magnitude, but also its dynamics, by reducing the amplitude of the waves in this stylized case. As a result, the magnitude of the treatment effect no longer

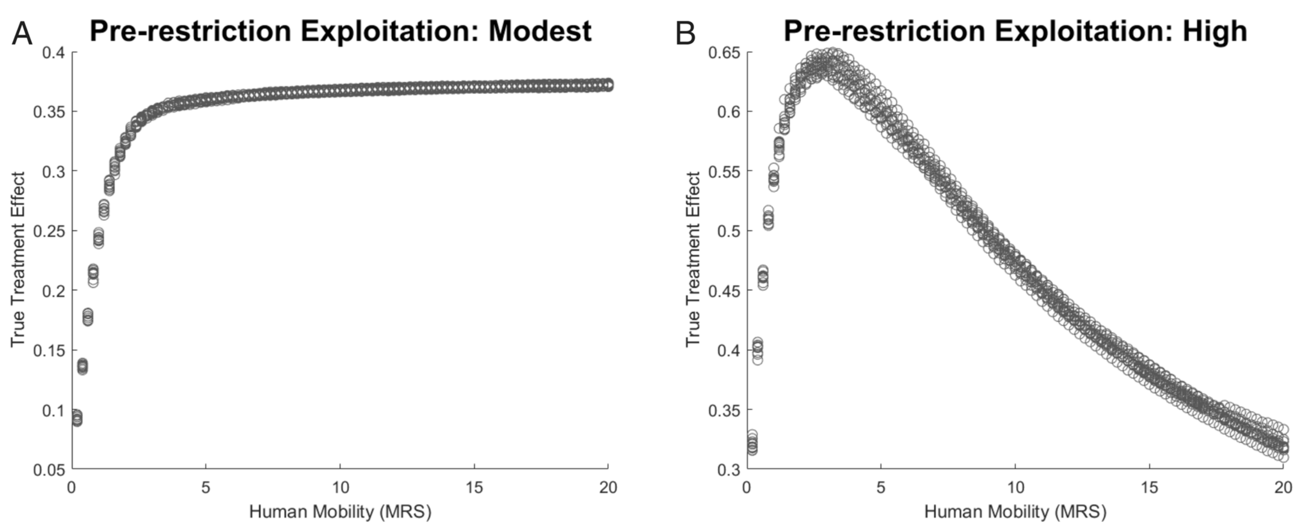


Fig. 2. Expected causal effect of a spatially designated gear restriction. The treatment effect is the percent increase in the fish stock compared to the counterfactual stock. This effect varies with the degree of fisher mobility and the level of prerestriction fishing activity. Human mobility is modeled by the marginal rate of substitution between fishing revenue and travel cost (MRS); higher values imply greater mobility. (*A*) Modest prerestriction exploitation implies that the prerestriction stock was maintained at approximately maximum sustainable yield. (*B*) High prerestriction exploitation implies the prerestriction stock was low.

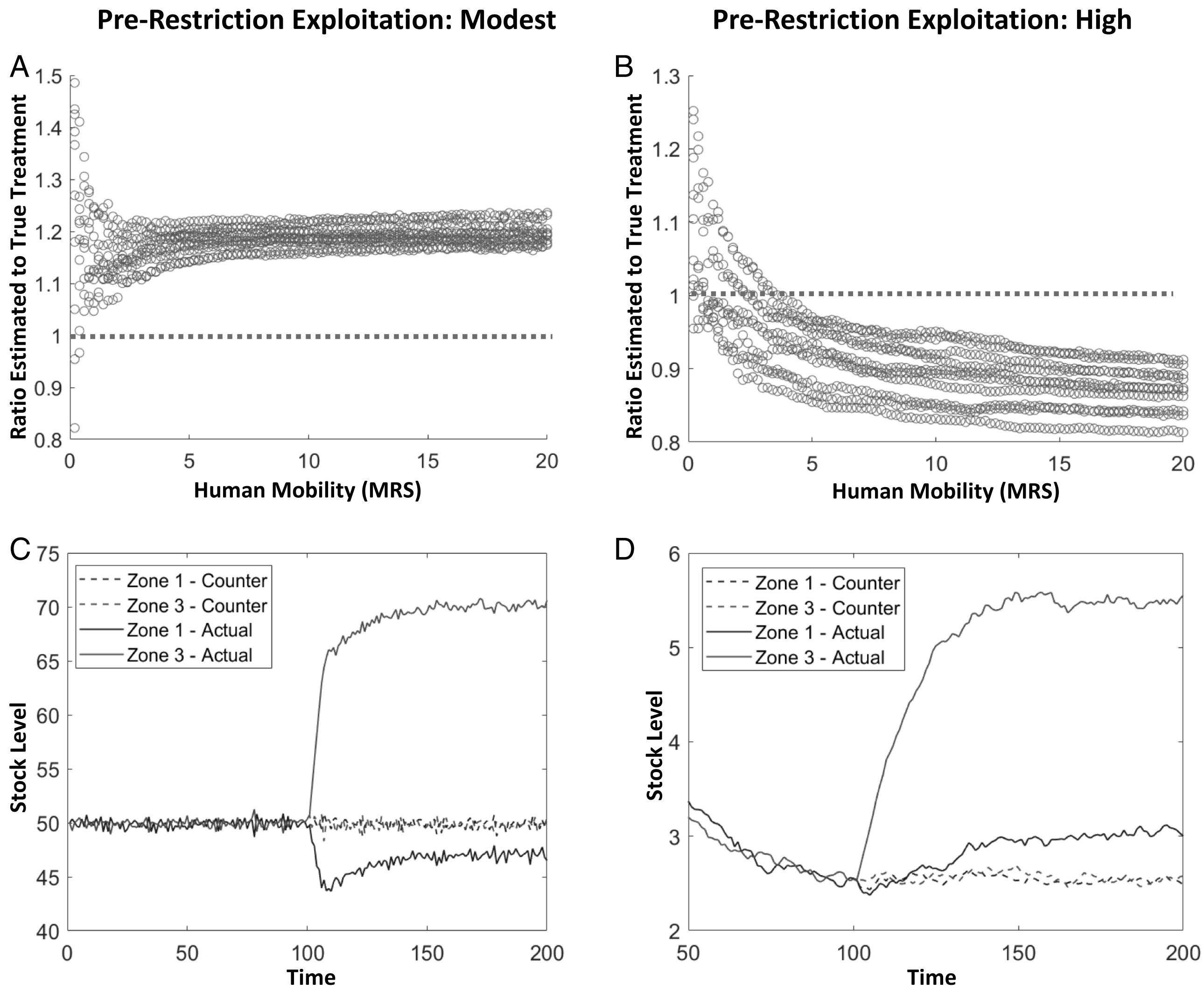


Fig. 3. Divergence of the true causal effect of a gear restriction and the estimated causal effect. The divergence depends on the degree of fisher mobility and the level of prerestriction fishing activity. (*A* and *B*) Ratio of the estimated to the true effect. Values above (below) 1 imply the design overestimates (underestimates) the effect. (*C* and *D*) Simulated fish stocks from a single model run for a high mobility case (MRS = 20) with moderate (*C*) and high prerestriction fishing activity (*D*). Zone 3 is treated with the gear restriction at $t = 100$, and Zone 1 is the comparison zone. For both zones, Actual is what happens with treatment and Counter is what would have happened in the absence of treatment.

has a time-independent definition. Defining the treatment effect empirically requires a conceptual understanding of the system's dynamics.

In real systems with complex dynamics, empirically estimating a treatment effect can require a model that facilitates such understanding. This requirement also applies to the identification of causal pathways or mechanisms because the temporality of the system, such as its history, stochasticity, feedback, or path dependence, can affect if and how a mechanism plays out. Our causal understanding of dynamic nature–society systems thus depends upon our capacity to understand key drivers of system behavior, such as adaptive human behavioral responses to changes in natural systems. This can be achieved for example through improving the plausibility of the models we use to describe system behavior using empirical assessments, or through codesigning an empirical study and a model, so that the empirical study can provide insights into complex causal processes while the modeling can analyze the effectiveness and generality of found mechanisms in a dynamic nature–society context. We illustrate this potential in two studies, one from the COVID-19 pandemic in the United States (Study 3), and one from natural resource policy change (Study 4).

Study 3: Using a process-based model to improve causal understanding of the drivers of COVID waves. Complex nature–society system dynamics resulting from the spread of the COVID-19 virus make both empirical causal analysis and predictive modeling very challenging. COVID-19-associated behavior changes are among the most dramatic collective behavior changes the world has ever seen. In 2020, billions of people worldwide upended their lives in order to fight this virus with the first tool available: distance. Across the United States, typical daily travel distances dropped by 95% during the height of the "safer-at-home" phase of the pandemic (Fig. 5*A*). These changes in mobility, however, did not affect COVID spread as expected. In our empirical analysis of drivers of COVID-19 waves (see *SI Appendix* for details), we consistently observe lower mobility associated with higher COVID-19 infection and transmission rates (Fig. 5*B*). This observation is exactly opposite of expectations based on the physical process of person-to-person transmission through respiratory contact. The apparent paradox holds even after

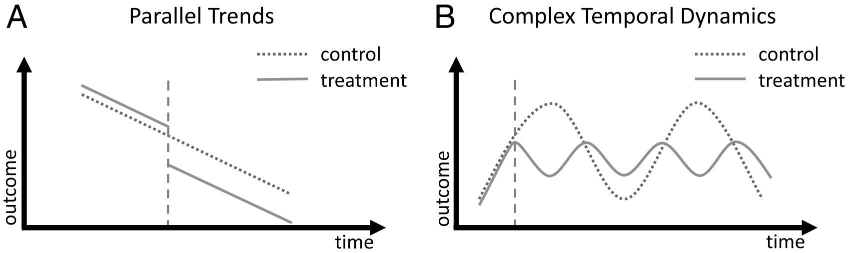


Fig. 4. (*A*) shows a stylized example of the use of parallel trends to identify a treatment effect. (*B*) demonstrates the challenges in defining a treatment effect when the intervention changes the temporal patterns of the system.

including a temporal lag between mobility and cases and across a wide range of geographies and time periods between 2020 and 2021.

Similarly, predictive models have been largely ineffective at describing the long-term (> 1 mo) dynamics of the COVID-19 pandemic in the United States, in particular, the repeated occurrence of waves (23). A characteristic wave pattern in COVID-19 cases is consistent across geographic scales, continents, income levels, and through a broad range of COVID-19 mitigation strategies and capabilities (Fig. 5*D*). A primary modeling challenge is identifying when a new wave will begin and when the current wave will recede in the absence of data on turning points (23).

Our study of the COVID-19 pandemic in 2020 and 2021 in the United States shows how dialogue between modeling and empirical analyses of a temporally complex system, such

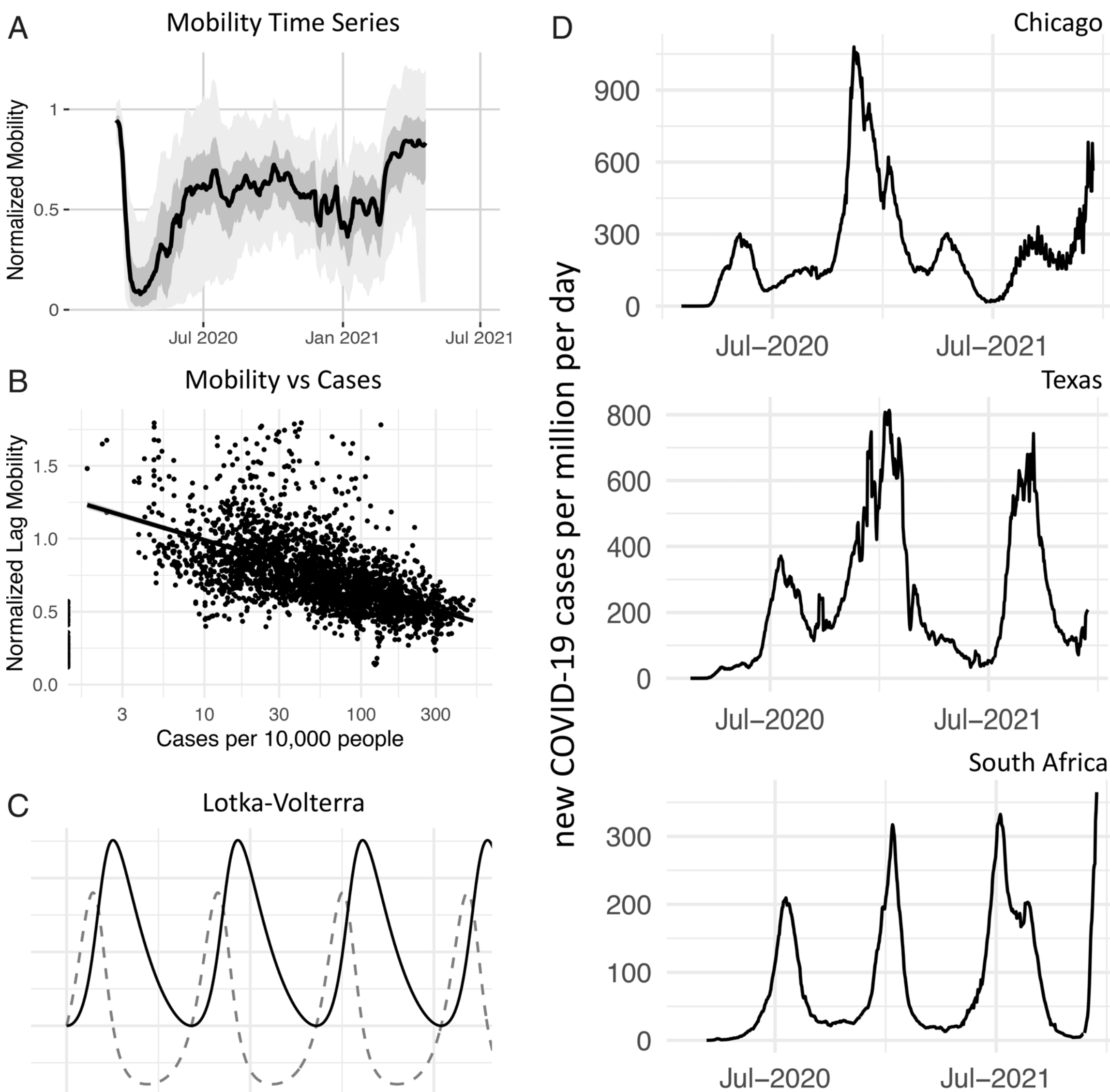


Fig. 5. Disease influences human behavior, which drives early COVID waves. (*A*) shows the median, 25th to 75th percentile, and fifth to 95th percentile distribution of mobility changes for all US counties between March 2020 and April 2021, compared to February 2020. The data are normalized by county so that 1 is median county-level mobility in February 2020. (*B*) shows the association between weekly new cases and 14-d lagged and normalized mobility in the US Northeast for July to September 2020. (*C*) shows an example result from the Lotka–Volterra Model. (*D*) shows 7 d moving average cases for the Chicago metro area, Texas, and South Africa. See *SI Appendix* for data sources.

as the COVID-Society system, improves causal understanding and helps address both the empirical and modeling challenges. This dialogue identifies important drivers in system behavior, demonstrates when new models are needed, and clarifies how empirical analysis can provide conceptually relevant results.

Insight 3a: A single shift in the understanding of causal interactions in this system can address both the empirical and modeling analytical challenges. Treating human behavior as causally affected by disease explains the association between high levels of disease and high levels of mitigation, and it provides an explanation for repeated waves in COVID-19 cases that are unexpected in classical epidemiological models.

Dialogue across approaches provides the insight needed to explain both the empirical association and the wave-like dynamics. Both empirical and modeling communities explored the effect of human behavior on disease, e.g., "to what extent did mobility reductions cause reductions in transmission?." However, neither community significantly explored the causal relationship in the opposite direction "what is the effect of disease on behavior?" This gap is apparent when seeking to explain both analytical challenges. Within mathematical epidemiology, there is some history of endogenizing behavioral reactions to disease to explain waves and the long-run path of disease (37, 38), but they were not initially applied to the COVID-19 pandemic. In a review of 350 articles on nonpharmaceutical interventions in the context of the COVID-19 pandemic, only one publication explored the effect of disease on behavior, and none examined the potential for a bidirectional causal relationship between behavior and disease (22).

We argue that strong and bidirectional causal relationships between disease prevalence and disease mitigation activity result in complex features of system behavior—particularly the recurring waves in COVID-19 cases. This bidirectional causality provides an explanation for the apparent paradox observed in the empirical association between high cases and high mitigation. These characteristic waves cause a strong temporal dependence in the difference between "what is," and "what might have been" (as in Fig. 4), where some kind of mitigation changes the timing of waves in cases. This hampers our ability to estimate the causal effect of mitigation.

Insight 3b: Because disease and human behavior dynamics operate on similar timescales, modelers must account for both processes when characterizing system behavior. This requires modeling attention focused on behavioral dynamics, as well as an empirical focus on measuring and characterizing human behavior in ways that can be coupled to existing biophysical models of disease dynamics and other nature–society interdependencies.

Building from Insight 3b, we propose a model designed to explore the endogenous interactions of COVID-19 mitigation behavior and disease. With perfect data, one could define mitigation activity to include the full suite of activities aimed at reducing disease spread, from federal policy to individual choices. In practice, we can only measure a handful of these—particularly changes in movement patterns.

We propose that mitigation behavior may be equivalent in importance to the virus' innate biological properties for the course of disease outbreaks. We adapt a Lotka–Volterra model to dynamically represent interactions between viral spread and our mitigation actions, casting mitigation behavior as the "predator" (M) and infections as "prey" (I). This model captures biological characteristics of disease and adaptive behavioral responses, and it predicts waves in COVID-19 cases that we observe across cities, states, nations, and the world despite the vast range of mitigation strategies that have been employed (see *SI Appendix* for justification).

$$\frac{\delta I}{\delta t} = \alpha I - \beta IM, \quad [1]$$

$$\frac{\delta M}{\delta t} = \eta MI - \gamma M. \quad [2]$$

The basic Lotka–Volterra equations (Eqs. **1** and **2**) lead to a long-term relationship characterized by steady oscillations in the levels of new cases and mitigation behavior (Fig. 5*C*). Many new cases lead to an increase in mitigation effort, and increased mitigation results in case levels declining. As cases decline, mitigation efforts also fall, providing an opportunity for the virus to spread again.

During the first year of the pandemic, the globally dominant strain of the disease closely matched the original genome sequence, the infected population was still a small share of the total, and pharmaceuticals were not yet available, and so the oscillating features of COVID-19 case levels likely were driven by nonbiological characteristics, specifically societies' mitigation actions.

However, over the longer term, other factors will complicate this dynamic relationship for COVID-19. Immunity derived from both prior infection and vaccination has reduced the susceptible population. Genetic change in the virus has led to more infectious variants, changing the α parameter. Increased availability of pharmaceutical treatments (e.g., Paxlovid) and prevention (vaccines) may reduce effective disease severity, meriting disinvestment in economically punishing social distancing measures and other mitigation strategies. Maintaining a close dialogue between modeling and empirical analyses of disease as COVID-19 moves toward endemic conditions will support appropriate long-term biopreparedness.

Study 4: Codesigning an empirical and a modeling study to explain interest groups' success in influencing natural resource policy making and its diverse consequences for sustainable resource use. Complex dynamics of nature–society systems can be the reason why the same causal mechanism can lead to qualitatively different outcomes in similar systems. For example, interest group participation in natural resource management contributed to the collapse of the Baltic cod fishery, while it improved management of Southern Ocean toothfish fisheries (32). How a mechanism plays out in a particular context can be very different, making identification and generalization difficult. In this study, we demonstrate how an empirical approach that traces the pathway between a cause and an effect in a particular case can be combined with agent-based modeling to identify mechanisms that may explain an observed empirical outcome and to assess their performance in a dynamic social–ecological environment. Such codesign is particularly useful in contexts where nature–society interdependencies create complex dynamics for which little theoretical knowledge exists. In view of these challenges, this study aimed to identify how, that is through which mechanisms, and under what conditions, interest group participation in natural resource policy making can bring about a fishery policy change toward sustainable resource use.

Process-tracing is used to identify the causal mechanism of interest group influence, while agent-based modeling extends it further to account for interactions with the social–ecological dynamics of a fishery. The strengths of this combination are the ability of process-tracing to illustrate a detailed temporal unfolding of a causal process and the ability of ABM to explore this causal process in a dynamic nature–society system. Through analyzing and comparing simulation runs that produce different outcomes, we can investigate complex nature–society feedbacks that drives policy change and adaptation.

Process-tracing was used to analyze how environmental interest groups influenced the 2013 EU Common Fisheries Policy (CFP) reform (see details in ref. 39). Past studies have pointed to interest group interactions within the policy process such as lobbying, providing expert and technical information, building coalitions, and competing for influence, as parts of causal mechanisms that link interest group influence to policy change (e.g., refs. 40–42). While these studies have assessed interest group influence on policy change across multiple issues, institutional and nature–society contexts, quantifying the degree of influence is problematic (43), and studies typically focus on identifying influence, not explaining it.

Insight 4a: Process-tracing suggests that by building belief-based coalitions environmental interest groups are able to overcome resource disadvantages, compared to industry interest groups, and influence policy change according to their preferences.

The empirical investigation of interest group behavior was based on interviews and document analysis. It provides an in-depth understanding of the causal mechanism that links interest group participation and their influence on policy change, focusing specifically on the role interest group coalitions played in the CFP reform process. The aim of process-tracing is to identify a causal mechanism that links interest group participation in the reform, their coalition-building activities, and their influence on policy change. Model design and the empirical investigation mutually influenced each other in the search for causal mechanisms.

The ABM formalizes the empirical causal mechanism uncovered in process-tracing, in order to test it and analyze how it performs when interest group activities are linked to a nature–society system that changes through their actions. Model simulations show how fishery policy output (e.g., fishing quota, Fig. 6*C*) is causally linked to nature–society outcomes (e.g., fishery income or state of the fish stock, Fig. 6*B*). While insight 4a provides us with a detailed and rich account of the causal mechanism in the CFP reform process, it is difficult to distinguish which contextual factors matter for outcomes. Without the model simulations, it is difficult to understand the complex causal structure that dynamically links policy and the nature–society system it is intended to govern. The ABM builds on the strengths of the in-depth empirical causal explanation provided by the process-tracing. It uses modeling scenarios to further extend and test the causal explanation.

To design the ABM, we implement three elements of the interest group influence mechanism identified in process-tracing: 1) interest groups' ability to form belief-based coalitions that can lobby policymakers with higher efficiency; 2) interest groups' mobilization in coalitions as a response to perceived economic or ecological "crisis" in the governed system; 3) link between

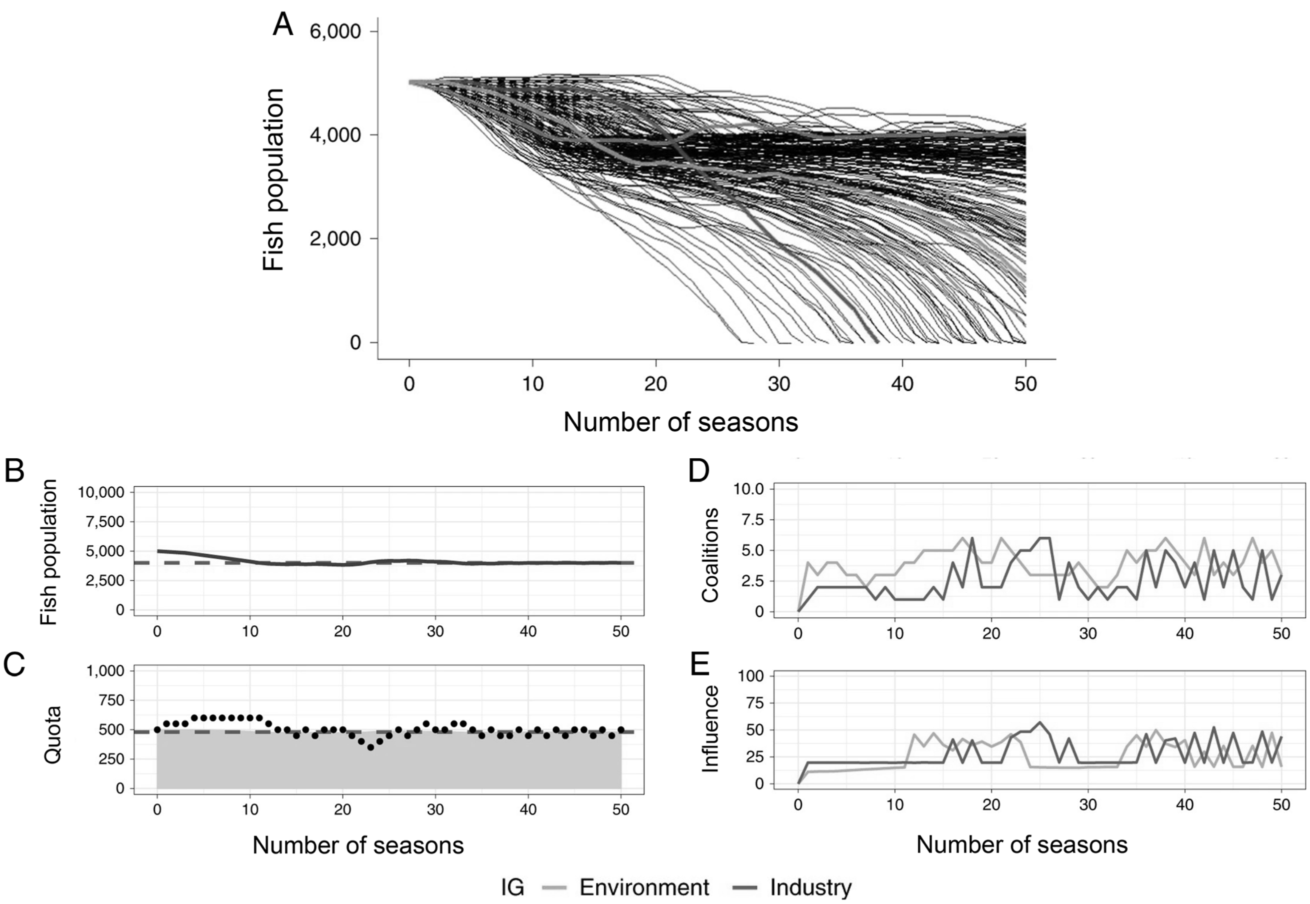


Fig. 6. The activation and timing of the tug-of-war causal mechanism determine the type of long-term outcome of the fishery. (*A*) shows changes in fish stocks over time in 200 model runs in an experiment in which both types of interest groups are able to build coalitions. (*B–E*) show results of the run displaying a balancing dynamic (blue line on *A*). The dashed line in *B* and *C* represents the concern threshold of environmental and industry groups, respectively. The light blue field in *C* shows the amount of catch that can be taken out during each respective year to maintain fish stock size. Source: Orach et al. (32).

interest group resources (funding), their perceived influence, and their lobbying success (see ref. 32 for details of model design). The ABM recreates this setting not only to see if environmental interest group success can be reproduced under such conditions but also to explore how interest coalition-building and lobbying in response to perceived changes in the managed fishery can influence the sustainability of the fishery over time.

Insight 4b: Stochasticity and timing at which the "tug-of-war" between competing interest coalitions activates can lead to path dependencies that generate different system trajectories (Fig. 6*A*). When implementing the empirical mechanism of interest group influence, ABM simulations result in three qualitatively distinct types of outcomes. These are the fast decline (red line), slow decline (green line), and balancing (blue line) trends of a fish population.

Insight 4b sheds light on a feedback mechanism responsible for the stabilization of the catch quota through consecutive mobilization of industry and environmental interest coalitions (Fig. 6 *C* and *D*).

This "tug-of-war" mechanism can slow down a collapse of the fish population or even prevent a collapse if interest groups engage in it early enough (see Fig. 6*B*—the tug-of-war shown in Fig. 6 *C* and *D* stabilizes the quota at the level that slows down fish population decline and maintains it at a relatively sustainable level further on). Path dependency helps explain these dynamics, as the initial coalition response by environmental groups and their lobbying success coincides with a relatively slow increase in quota and a high fish population, triggering the tug-of-war early on. Stochastic events play an important role in the emergence of path dependency, e.g., early presence of coalitional pressure from environmental groups can prevent quota "spikes" that are difficult to revert in time to prevent fish population collapse.

The methods used in this study are complementary: They serve different purposes while sharing a similar conceptualization of causality. Both process-tracing and ABM view causality as generative, i.e., causation involves a mechanism or causal process that links cause and effect. Here, a causal mechanism is conceptualized as a set of entities and activities that, by interacting over time, generate system-level outcomes (13). While the empirical study identified the coalition-building strategy as the core part of a mechanism explaining environmental group success, the ABM shows how the effectiveness of interest coalitions is dependent on the timing of their formation in relation to policy and ecological dynamics. The model allows us to build on the empirical mechanism and generate hypotheses that link interest group perceptions of change, coalition and policy dynamics, and long-term outcomes for sustainability of fisheries. These hypotheses could be further tested in other empirical contexts, a process that may contribute to building middle-range theories of policy adaptation that account for micro- and mesolevel policy dynamics and interest group participation in fishery governance.

Discussion

Scientists have long recognized the need for multi-method approaches to analyze complex sustainability problems (44, 45), but causal studies that integrate empirical and modeling approaches are still rare.

Greater integration of these complementary approaches would facilitate theory building and offer insights for governing nature–society systems. Models represent researchers' and practitioners' understanding of the causal structure of particular phenomena. They can thus serve to evaluate the quality of different empirical designs (air quality study), assess the implications of nature–society interdependencies for empirical estimates of causal effects (gear restriction study), help identify nature–society interactions that shape complex system dynamics (COVID study), and explain the multiple pathways that a causal mechanism may trigger in dynamic nature–society systems (fishery governance study). In contrast, empirical studies provide insights about causal mechanisms, the magnitudes, and directions of causal relationships, as well as contextual factors that influence these relationships and mechanisms. They can thus serve to build models, particularly those that include social dynamics, or evaluate and improve the quality of existing ones. Below, we describe four cross-cutting insights and one policy insight that highlight how integrating the two approaches can enrich causal understanding and strengthen causal claims. We also discuss ways forward to address some of the challenges of integrating both approaches.

Cross-Cutting Insight 1: Modeling can Improve Empirical Designs and Reduce Uncertainty in Empirical Estimates. In causal inference studies, scientists' decisions about empirical designs and estimation procedures (e.g., where or when to measure outcomes) should be guided by assumptions about potential interdependencies among the natural and social elements of the system. Given the dynamic nature of nature–society systems, these assumptions may be best articulated by models. For example, models allow scientists to quantify, for a specific empirical design, what divergence they can expect between the true and the estimated effect in a system, thus helping scientists determine whether the estimated effect is likely to be an upper or a lower bound on the true effect size (air quality and gear restriction studies). Modeling also sheds light on what effect size scientists can expect in a particular context or with a particular design, which helps scientists determine how much data they will need to achieve a target level of statistical power. Modeling also highlights that the timing and type of data collection can be critical for causal inference because of the underlying complex dynamics (COVID study). Importantly, because modeling allows scientists to vary the degree of interdependencies and consider implications for empirical designs, it can help empiricists to assess when the additional costs of formally addressing interdependencies with more data or more sophisticated designs may be warranted.

Cross-Cutting Insight 2: Modeling Elucidates Unexpected Outcomes and Helps to Judge the Importance of Contextual Factors and Complex Dynamics. Modeling can identify qualitative outcomes and causal pathways that are either unexpected or beyond the scope of the original empirical analysis. The gear restriction in Study 2 was expected to increase stocks in the regulated zone but not in the unregulated zone. Yet, the model revealed that when the preintervention fishery was highly exploited, the restriction could increase the stock in the unregulated zone as well. This potential effect could not have been anticipated without modeling, and it directly informs the analysis and interpretation of the empirical results. The air pollution and the gear restriction studies show how models can inform scientists about where to expect different outcomes when the same intervention is applied across contexts and what contextual features generate this heterogeneity. For COVID transmission, the bidirectional causality between mitigation behavior and the spread of disease is typically beyond the scope of empirical analysis, but modeling that includes that bidirectional relationship can explain the estimated positive associations between disease and mitigation behaviors we observe. The agent-based model of fishery governance reveals that stochasticity and the timing and conjunction of events can lead to path dependencies that generate qualitatively different outcomes in a dynamic nature–society system. Modeling indicated the importance of additional mechanisms, such as a tug-of-war process, for stabilizing the fish population. These two studies show how modeling can inform scientists about where to expect variation within a single case and what complex dynamics generates this heterogeneity. Guided by these expectations about contextual factors and dynamic patterns, scientists can better determine which variables and interactions, among myriad potential ones, should be the focus of data collection and which hypotheses or causal mechanisms should be the focus of analysis and testing.

Cross-cutting Insight 3: Integrating Empirical Approaches with Modeling Improves Causal Explanations in Absence of Prior Causal Knowledge about Complex Nature–Society Interdependencies. Integrating empirical and modeling approaches is particularly relevant when there is little a priori causal understanding of the system, few theories or models to build on, and a lack of data. These contexts are common in complex nature–society systems. The empirical approach can inform model development with insights about potential causal factors and mechanisms as well as relevant contextual details, particularly regarding human behavior, social interactions, institutions, and nature–society interdependencies. Vice versa, modeling can help focus empirical analyses on the complex interactions between causal factors or mechanisms, interactions that can then be further explored and refined through future modeling. Integration creates opportunities to account for human adaptation, which contributes to complex dynamics but is inherently difficult to include in both empirical and modeling studies. The COVID and fisheries governance studies are examples of the early iterations of this form of integration.

Cross-cutting Insight 4: Integrating Empirical Approaches with Modeling Facilitates the Development of Middle-Range Theories. Integration is useful for causal explanation—i.e., to identify the mechanisms and processes that explain observed empirical patterns—with the aim to build middle-range theories (10). Middle-range theories, or contextualized generalizations (46), are particularly relevant for complex nature–society systems whose context-dependence and complex dynamics make highly abstract theories less useful (47). For example, the combination of qualitative process tracing and agent-based modeling in the fisheries management study facilitated the integration of contextual empirical knowledge into middle-range theory building. The codesign of the empirical study and the model supported the development and testing of a mechanism-based explanation because it focused the empirical study on the micro- and meso-level interactions that explain interest group success. The model, which formalized these interactions and simulated their interplay with system level dynamics, could then be used to test whether these interactions generate the same outcome in the virtual world, and to further investigate the working of the mechanism in a dynamic nature–society context. The integration of empirical and modeling approaches can thus help to generate causal explanations and support generalizing from case studies [Fisheries management Study 4, (10)] or demonstrate when new theoretical models are needed (COVID Study).

Policy Implication Insight: Integrating Empirical Approaches with Modeling can Help Improve Governance in the Presence of Complex Nature–Society Interdependencies and Dynamics. Governance of nature–society systems is fundamentally about choosing among potential actions that will affect the natural and social components of these systems and their interactions. A better understanding of causality in contexts in which interdependencies and dynamics are the rule rather than the exception contributes to making such choices. The integration of empirical and modeling approaches provides such understanding, which is often difficult to gain from one approach alone. Our four studies demonstrate that integration can ultimately provide more accurate measurements of the magnitude of a policy effect, indicate when and how the timing of an intervention or policy evaluation matters, and help to anticipate potential unexpected outcomes. By providing policymakers with a better understanding of the interacting mechanisms that generate a problem or contribute to a solution, integration can help policymakers to design more "complexity-aware" interventions.

Ways Forward. Independent of the scientific and policy benefits from integration, engagement in multi-method scientific collaborations facilitates thinking across domains and breaks down disciplinary and methodological silos, which have long been identified as important barriers to understanding and governing complex nature–society systems.

While the benefits of integration are multiple, bringing methods from different traditions into dialogue is costly, and scientists need guidance about when and to what degree integration is most valuable. Our experience in producing this article highlighted several challenges, and pointed to some possible ways to overcome them. For example, integration requires that team members have the skill to navigate different ideas about causation, different technical terms, concepts, and methods and a willingness to communicate about them in unfamiliar ways. Successful collaborations will occur in teams whose members succeed in learning how members from other traditions think and analyze nature–society systems. Building and maintaining such teams needs sustained effort and commitment that goes beyond regular projects. Such learning can also take place in dedicated workshops, summer schools, and institutes, and be supported by tools for interdisciplinary collaboration (48, 49). Collective change will also be necessary. To establish the groundwork for broader integrative collaborations in sustainability science and provide guidance for cross-community collaborations, scientists will need to make more efforts to clarify and communicate the basic assumptions that underlie different epistemological traditions. More transparency about assumptions and the process of integration, supported by, e.g., protocols such as (50) or "behind the scenes" descriptions, will enable other scientists to learn from how teams have tackled these challenges. Another step would be that journals encourage registered reports of integrated designs (i.e., ref. 51) to reduce the risk that researchers will invest substantial resources only to have trouble finding a suitable publication outlet. Finally, efforts are needed to ensure that professional incentives, norms, publication and review structures, and funding schemes in academic and research organizations support, rather than discourage, integrative collaborations.

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