

1 **Uncertainty analysis in multi-sector systems:**
2 **Considerations for risk analysis, projection, and**
3 **planning for complex systems**

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17 **Key Points:**

- 18 • Uncertainty is an inherent part of multi-sector systems analysis;
- 19 • Approaches to addressing uncertainty involve deliberate tradeoffs;
- 20 • Best practices involve standardizing communication and improving transparency

Abstract

Simulation models of multi-sector systems are increasingly used to understand societal resilience to climate and economic shocks and change. However, multi-sector systems are also subject to numerous uncertainties that prevent the direct application of simulation models for prediction and planning, particularly when extrapolating past behavior to a nonstationary future. Recent studies have developed a combination of methods to characterize, attribute, and quantify these uncertainties for both single- and multi-sector systems. Here we review challenges and complications to the idealized goal of fully quantifying all uncertainties in a multi-sector model and their interactions with policy design as they emerge at different stages of analysis: (1) inference and model calibration; (2) projecting future outcomes; and (3) scenario discovery and identification of risk regimes. We also identify potential methods and research opportunities to help navigate the trade-offs inherent in uncertainty analyses for complex systems. During this discussion, we provide a classification of uncertainty types and discuss model coupling frameworks to support interdisciplinary collaboration on multi-sector dynamics (MSD) research. Finally, we conclude with recommendations for best practices to ensure that MSD research can be properly contextualized with respect to the underlying uncertainties.

1 Introduction

Simulation models of multi-sector systems are increasingly used to understand societal resilience to climate and economic shocks and long-term change. To faithfully represent societal systems across spatiotemporal scales, such multi-sector system representations need to account for dynamic and endogenous interactions between sectors, rather than treating other sectors as exogenous boundary conditions and forcings. This approach is at the heart of the emerging field of MultiSector Dynamics (MSD). However, this growing complexity increases the number and types of uncertainties that affect both the inverse problem (calibration and inference) as well as the forward projection of system dynamics and resilience into the future, which is critical for decision support. This paper identifies and reviews the key challenges involved in uncertainty analysis for MSD. We discuss why they arise (or are made more acute) in the multi-sectoral modeling context, the current state of the art, and what research opportunities may help address them going forward.

Our focus is on quantitative aspects of multi-sectoral modeling. However it is important to note that there are also many semi- and non-quantitative aspects of multi-sector modeling and risk analysis. These considerations, which are critical in the development of the conceptual model of the system (S. Robinson et al., 2015) and the use of uncertainty analysis to inform policy and governance of complex, multi-sector systems in the face of systemic risk (Renn et al., 2020; Hochrainer-Stigler et al., 2020).

We begin with definitions of several key terms:

- *Sector*: a complex system-of-systems that delivers services, amenities, and products critical to a subdivision of society. Components of sectors may include infrastructure, environmental systems, governing institutions (public and private), labor force capacity, finance, and a range of actors (*e.g.*, firms, regulatory agencies, investors, consumers) involved in producing and consuming services and products (Reed et al., 2022);
- *Multi-sector system*: a set of interacting sectors that yield emergent dynamics beyond that which could be predicted from each sector alone (Reed et al., 2022);
- *Uncertainty*: “a departure from the (unachievable) ideal of complete determinism” (Walker et al., 2003) in any aspect of the system.

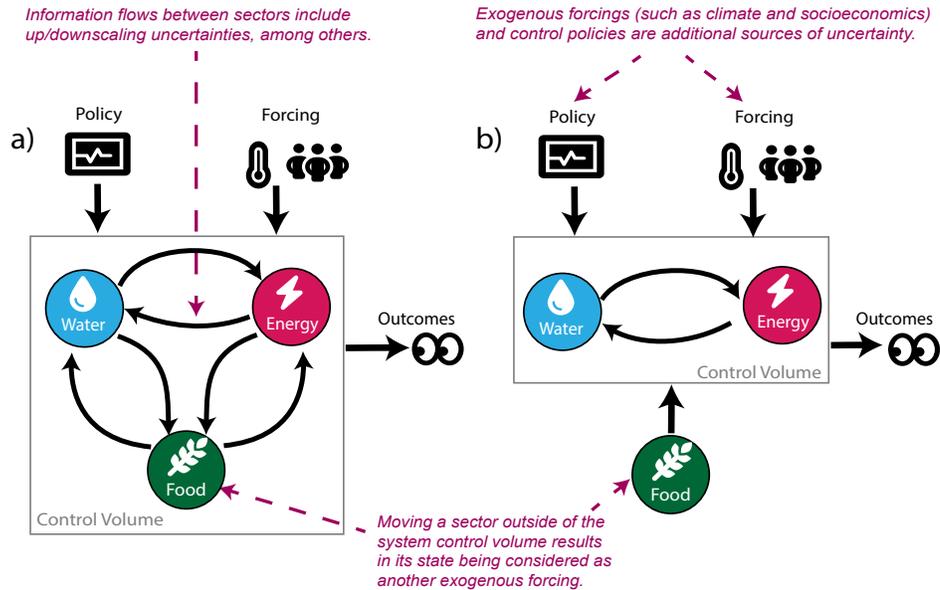


Figure 1. Schematic of a multi-sector system model. Two conceptual examples of how a food-energy-water system can be represented by coupled models of each sector. In panel a), the control volume includes all three sectors, allowing feedbacks between the food system and the water and energy system(s) that are not possible when the food system is outside of the control volume (panel b)) and is therefore treated as exogenous. The endogenous dynamics within the control volume can be further influenced by exogenous forcings, such as socioeconomic and climate inputs, and policies, which determine how sectors respond to changes in the internal system state and external forcings.

69 These definitions highlight the fact that each sector alone is a complex system of
 70 agents, institutions, and infrastructure interacting with the natural environment, and
 71 each other. A useful notion is the idea of the *control volume* of an analysis, which is a
 72 concept borrowed from thermodynamics. We use “control volume” to refer to the por-
 73 tion of the analyzed system(s) whose dynamics are modeled endogenously, as contrasted
 74 with any exogenous inputs and the model outputs. The shift to studying a multi-sector
 75 system-of-systems adds complexity by expanding the control volume under analysis to
 76 encompass feedbacks between systems, potentially across different characteristic spatial
 77 and temporal scales, and across different resolutions of the system (*e.g.*, individual agents
 78 vs. aggregations). These dynamics are represented in Figure 1, which is a schematic of
 79 a coupled multi-sector system-of-systems. Many of the challenges that we review in this
 80 paper are present in the single-sector case, but are amplified in the multi-sector setting.

81 One of the main strategic goals of MSD research is the identification and analy-
 82 sis of key uncertainties influencing the evolution of a particular system-of-systems. These
 83 analyses are often conducted using simulation models, which are a set of coupled numer-
 84 ical equations and/or agent-based rules describing the time evolution of the system state(s),
 85 given inputs of forcing variables that are external to the system. In general, multi-sector
 86 system models are subject to several sources of uncertainty, as illustrated in Figure 1.

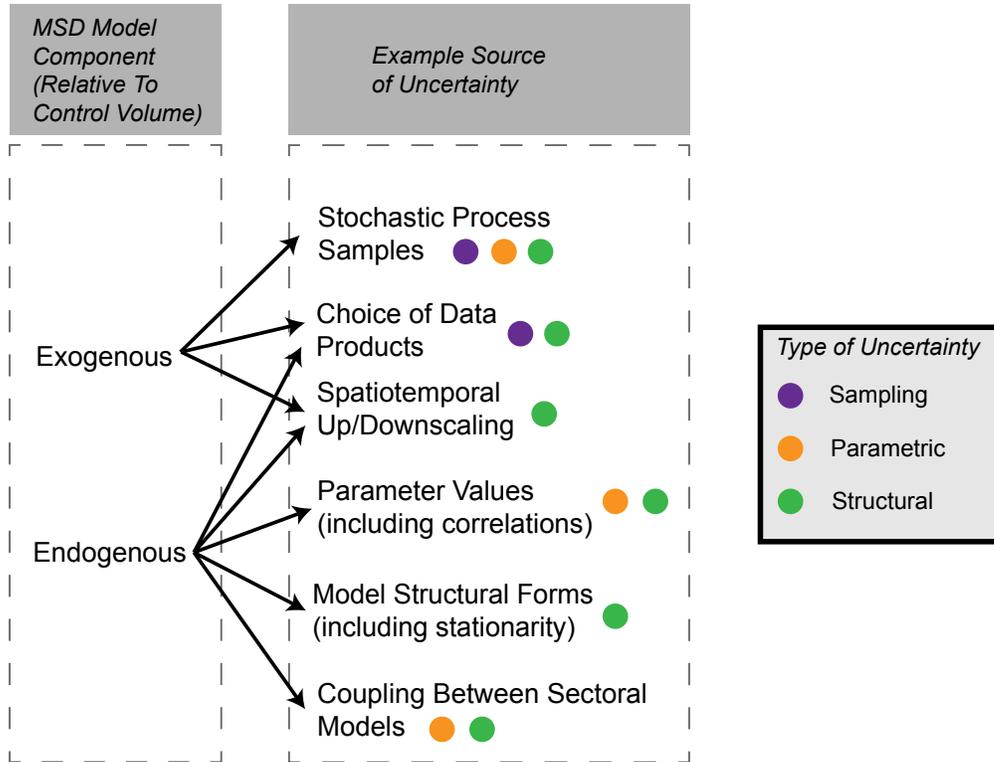


Figure 2. Example sources of uncertainty that are relevant to model components that are exogenous and/or endogenous to the control volume under analysis. Sampling, parametric, and structural uncertainties can enter the system through both exogenous and endogenous components of the system. This demonstrates some of the many ways in which MSD researchers can make choices which affect how uncertainty influences their analyses. Many of these specific examples are further discussed in the subsequent sections of this paper. The colored circles relate the uncertainty sources to the uncertainty classification in Table 1.

87 These can stem from exogenous or endogenous model components, as shown in Figure
88 2.

89 Exogenous model components can be classified as either forcings or policy inputs.
90 By forcings, we refer to inputs which serve as boundary conditions, representing char-
91 acteristics of the external environment that are relevant to one sector and/or the cou-
92 pled system within the control volume. Many variables could either be an exogenous forc-
93 ing or an endogenous component of the modeled system, depending on the boundaries
94 of the control volume. For example, global temperature would be considered a forcing
95 if it is input into the modeled system as an exogenous factor. However, if instead tem-
96 perature is generated within the control volume, it would be considered an endogenous
97 component of the multi-sector coupling.

98 By policies, we mean rules which dictate actions taken by humans or institutions.
99 Such policies influence how the sector or coupled system responds to changes in the in-
100 ternal state or external environment. Analogously to forcings, while policy rules can change
101 endogenously in response to system dynamics, we focus here on policies (or meta-policies)
102 which are supplied exogenously. Figure 2 illustrates some of the uncertainties which can
103 influence these exogenous components.

104 Uncertainties related to endogenous system dynamics include model structure and
105 parameters describing each sector as well as those describing interactions between sec-
106 tors. In combination. All of these uncertainties interact and propagate to influence the
107 modeled outcomes of interest, which could include error metrics (if observations are avail-
108 able for calibration) and/or performance metrics in the case of planning for future sce-
109 narios.

110 Accurate representation of state changes and variability within multi-sector sys-
111 tems requires careful consideration of interactions and feedbacks within the coupled sys-
112 tems. Coupling multiple sectors in a unified modeling framework creates two broad chal-
113 lenges that will be recurring themes throughout this paper: 1) scaling, and 2) the complexity-
114 uncertainty tradeoff. First, the relevant scales at which each sector is modeled may not
115 align with each other, or with influential climate and weather conditions. This creates
116 a need for upscaling or downscaling to adequately model responses and the feedbacks
117 between sectors, which introduces additional uncertainty beyond the dynamics alone.

118 As shown in Figure 1, the choice of control volume for an analysis is critical for es-
119 tablishing what sectors will be treated endogenously, and therefore what feedbacks, in-
120 fluences, and interactions are possible. We note that a broader control volume (with more
121 endogenous sectors) is not necessarily “better”, as the introduction of additional link-
122 ages and dynamics may make it correspondingly more difficult to analyze and trace the
123 uncertainties which are most relevant to the research question.

124 Second, with a fixed computational budget, there is a tradeoff between the com-
125 putational complexity of a model and the number of feasible model evaluations (Helgeson
126 et al., 2021). Accounting for endogenous interactions within and between multiple sec-
127 tors adds computational and parametric complexity. This can result in a more accurate
128 representation of observed dynamics when appropriately calibrated, but can also result
129 in unrealistic behavior when extrapolating beyond the data used for calibration due to
130 overfitting. Added complexity only improves the representation of uncertainties if the
131 primary contributors to those uncertainties were missing mechanisms in the original model
132 (Figure 3).

133 When newly added model mechanisms include missing components which help ex-
134 plain variability in outcomes, added model complexity can decrease uncertainty despite
135 the addition of new parameters and equations (the blue scenario in Figure 3). For ex-
136 ample, the addition of equations allowing the Antarctic Ice Sheet to rapidly disintegrate
137 in response to increased warming reduces uncertainty in ice sheet volume hindcasts (Wong
138 et al., 2017). This effect is the result of other unrelated parameters no longer compen-
139 sating for the missing structural dynamics. However, the inclusion of additional model
140 complexity can increase uncertainty if additional parameters which were not related to
141 the underlying sources of variability need to be calibrated (the green scenario in Figure
142 3). If these two outcomes are mixed, so that some missing mechanisms are included, but
143 the net effect on uncertainty is dampened by additional calibration needs, the result will
144 be a more moderate reduction or increase in total uncertainty (the orange scenario in
145 Figure 3).

146 If this is not the case — for example, if future forcing scenarios dominate the to-
147 tal uncertainty in the outcomes — increased complexity in model representation may
148 be a detriment to understanding the range of potential system dynamics, as the com-
149 putational cost will limit the ability to evaluate an ensemble of scenarios. In other words,
150 finer scales and/or increased complexity do not improve model performance if there are
151 key processes missing that control variability within the coupled system. Increasing model
152 complexity may also result in negative learning or poor inferences if inadequacies in model
153 structure persist or are poorly constrained by observations (Draper, 1995; Oppenheimer
154 et al., 2008; Small & Fischbeck, 1999). Therefore, it is critical to analyze the sources of

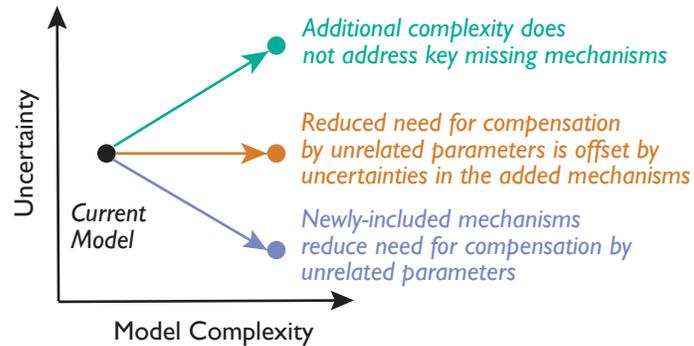


Figure 3. How adding model complexity can change model uncertainty. If the additional complexity causes key missing mechanisms to be included (blue), overall uncertainty can be reduced, as parameter distributions have less need to compensate for the missing components. If the additional complexity does not include representations of the missing mechanisms which were related to system uncertainties, overall uncertainty can increase due to the inclusion of parameters and interactions which need to be calibrated (green). In some cases, these two effects may partially cancel each other out (orange), leading to more moderate or no net changes to the total uncertainty.

155 uncertainty in multi-sector models to ensure that any additional complexity is appro-
 156 priately targeted.

157 As a consequence of these challenges, studies of single- and multi-sector systems
 158 have developed several approaches to analyzing and representing uncertainty:

- 159 • *Uncertainty Characterization (UC)*: Mapping how alternative representations of
 160 the stressors and form and function of modeled systems influence outcomes of inter-
 161 est (Moallemi, Kwakkel, de Haan, & Bryan, 2020; Walker et al., 2003);
- 162 • *Uncertainty Quantification (UQ)*: “the full specification of likelihoods as well as
 163 distributional forms necessary to infer the joint probabilistic response across all
 164 modeled factors of interest” (Cooke, 1991);
- 165 • *Sensitivity Analysis (SA)*: The study of how uncertainty in the output of a model
 166 (numerical or otherwise) is influenced by different sources of uncertainty in the
 167 model input (adapted from Saltelli et al. (2004)).

168 The goals of these methods are multifaceted: (a) to improve the accuracy of the
 169 models by identifying missing components; (b) to improve understanding of system dy-
 170 namics, risks, and vulnerabilities; and (c) to design policies or infrastructure. These ap-
 171 proaches to uncertainty analyses are not mutually exclusive, and are often combined. For
 172 example, initial studies of uncertainty characterization and system sensitivity may con-
 173 clude with a formal quantification of uncertainties related to a specific decision problem
 174 (e.g. Shortridge & Zaitchik, 2018; Taner et al., 2019). In general, sensitivity analysis may
 175 be employed for either UC or UQ, depending on the mathematical description of the in-
 176 puts and outputs. Uncertainty characterization approaches such as exploratory model-
 177 ing may be more appropriate than UQ in situations where well-defined probability dis-
 178 tributions over the sets of possible outcomes do not exist or cannot be agreed upon, a
 179 situation known as deep or Knightian uncertainty (Knight, 1921; Langlois & Cosgel, 1993;

Lempert, 2002). These steps may also be iterative and not always sequential. Specific methods for SA and UC are reviewed in detail by Pianosi et al. (2016) and Moallemi, Kwakkel, de Haan, and Bryan (2020), respectively.

Given the breadth of applications of uncertainty analysis in multi-sector systems modeling, we focus this review on key challenges related to the chain of uncertainty propagation throughout a multi-sector system. In Section 2, we discuss how choices made in the MSD modeling process exchange model and computational complexity for the ability to capture feedbacks and other dynamics, with implications for uncertainty representations. In Section 3, we discuss uncertainties in inference and calibration of multi-sector models, which can be both structural and parametric in nature. In Section 4, we discuss uncertainty in forward projections of multi-sector dynamics. In Section 5, we discuss how the increase in parametric and structural complexity associated with multi-sector analyses can result in high-dimensional outcomes that are difficult to attribute to particular sources of uncertainty, complicating the identification of scenarios of interest for further analysis or communication. Finally, we conclude by identifying some recommended best practices and cross-cutting research targets of opportunity which can help navigate some of these analytic trade-offs and complexities.

2 Types of Uncertainty and Model Coupling Regimes

In discussing the three key challenges we review in this paper, it is important to define the lexicon we will be using. MSD research is inherently interdisciplinary, and different communities of researchers focusing on different sectors often have different vocabularies, which is a fundamental challenge for interdisciplinary research teams (Bracken & Oughton, 2006; Henson et al., 2020; J. J. Cohen et al., 2021). MSD research, however, necessarily involves coupling and integration of simulation models and research outputs that may reflect differing disciplinary norms about the treatment of uncertainties. In this section, we classify key types of uncertainty and model coupling structures to help interdisciplinary teams communicate their research plans and outcomes.

2.1 Overview of MSD-Relevant Uncertainties

Simulation models are subject to several different types of uncertainty. From the perspective of multi-sector system analyses, we classify these uncertainties into three categories:

- *Structural uncertainty*: uncertainty in the mathematical and/or rule-based representation of processes within a simulation model;
- *Parametric uncertainty*: uncertainty in the numerical values of internal parameters representing endogenous model processes, given a fixed model structure; and
- *Sampling uncertainty*: uncertainty arising from the finite sampling of a stochastic process (including coverage of an output space).

Table 1 provides a brief overview of these types of uncertainty, along with examples. Parametric and structural uncertainties can be aleatory (stemming from irreducible randomness) or epistemic (stemming from a lack of knowledge about the “truth”), while sampling uncertainty typically reflects aleatory uncertainty (O’Hagan, 2004). One way to distinguish sampling uncertainty from parametric and structural uncertainty is that while sampling uncertainty relates to sampling from a stochastic process (represented exogenously or endogenously), parametric and structural uncertainties refer to uncertainty in how a simulation model responds to changes in external inputs, policies, and boundary conditions. For example, one might consider uncertainties related to model-data residuals (Brynjarsdóttir & O’Hagan, 2014) to be structural when those discrepancies are the result of choices or ignorance related to the representation of system com-

Uncertainty Type	Associated Uncertainties	Examples	Sample Method of Exploration
Structural	Model inadequacy, (epistemic) residual uncertainty	Choices of which physical processes to include and the equations used to represent them	Multi-model ensembles, multi-physics ensembles
Parametric	Parameter uncertainty	Choice of parameter vector between alternatives producing similar results, strength of coupling between models	Perturbed-physics ensembles, posterior predictive samples
Sampling	Natural variability, (aleatory) residual uncertainty, observation error	Sample realizations from a fixed stochastic process, internal variability, uncertain boundary conditions or forcings	Initial conditions ensembles, forcing scenarios

Table 1. Categories of uncertainty relevant for multi-sector models, including associated uncertainties from the taxonomy in Kennedy and O’Hagan (2001) and examples.

228 ponents (in this case, they would represent epistemic uncertainties). Alternatively, these
 229 model-data residual uncertainties could be considered sampling uncertainty when they
 230 represent particular realizations of “true” underlying stochastic processes (hence they
 231 would represent aleatory uncertainties).

232 Structural uncertainty can be defined as the consideration or inclusion/exclusion
 233 of one or more relevant structural variants. This could include different sectoral model
 234 representations, different policy or decision rules, or different choices of data products
 235 and statistical representations for exogenous forcings or model calibration (Bojke et al.,
 236 2006). Another consideration is the alignment (or lack thereof) of modeling paradigms,
 237 or formalisms, across sub-components of the system (Davis & Tolk, 2007). Decisions about
 238 how to couple models with different formalisms (*e.g.*, co-simulation, translation into a
 239 common formalism, or construction of a super-formalism) adds another level of struc-
 240 tural uncertainty (Vangheluwe et al., 2002).

241 The line between structural and parametric uncertainties can be blurry. For ex-
 242 ample, a parametrized regression model with at least one zero coefficient is the same as
 243 a simpler regression model with the relevant variable omitted. Whether this should be
 244 classified as a case of structural or parametric uncertainty is highly contextual, and de-
 245 pendent on the broader analysis, *i.e.* is there a more formal variable selection procedure,
 246 or is zero included as one element of the possible coefficient values?

247 In many cases, the same conceptual uncertainties can be classified differently ac-
 248 cording to this taxonomy depending on the control volume of a particular analysis. Fig-
 249 ure 2 shows example uncertainties which are relevant for exogenous and/or endogenous
 250 system components and how they might be classified. While there is a large amount of
 251 overlap, the nature of how uncertainties are represented can differ. For example, the Rep-
 252 resentative Concentration Pathways-Shared Socioeconomic Pathways (RCP-SSP) sce-

253 narios of future global change (O'Neill et al., 2016; Gidden et al., 2019) can be treated
 254 as a representation of sampling uncertainty when used as exogenous inputs or bound-
 255 ary conditions for a model of future climate or socioeconomic change. However, these
 256 same scenarios also reflect parametric and structural differences that may be relevant
 257 for a model or model component with feedbacks to global emissions or economic growth.
 258 Thus, it is important for MSD analyses to be transparent about not only which uncer-
 259 tainties they are treating, but how those uncertainties are represented in the context of
 260 the analytic control volume.

261 2.2 Coupling Frameworks and Control Volumes

262 Structural uncertainty is an essential feature of any modeling exercise, as all mod-
 263 elers necessarily make choices about what system dynamics will be modeled endogenously
 264 and at what resolution(s). Multi-sector modeling activities also necessarily involve cou-
 265 pling representations of multiple systems together, as in Figure 1. Model coupling can
 266 take a number of forms, even for a fixed system-of-systems, as illustrated in Figure 4.
 267 These choices have impacts on uncertainty propagation and analysis. We provide a brief
 268 overview of the types of coupling regimes and their implications for the resulting anal-
 269 yses.

270 An essential modeling decision is the selection of the control volume through the
 271 choice of endogenously- and exogenously-represented system components. Model struc-
 272 tures with a greater share of exogenous components are typically less computationally
 273 expensive than those that feature more endogenous dynamics (assuming similar spatiotem-
 274 poral resolutions). However, this comes at the expense of being able to analyze the feed-
 275 backs and interdependencies between subsystems, such as uncertainties and hypotheses
 276 related to the strength and patterns of influence of one sector on another. Whether this
 277 is acceptable depends on the research question and control volume. For example, many
 278 climate impact studies consist of one or more sectoral models forced by a climate model
 279 ensemble to produce a set of outcomes of interest (Grogan et al., 2020; Piontek et al.,
 280 2014; van Vliet et al., 2016). This choice might be reasonable if there is no clear path-
 281 way for the system contained within the control volume to dynamically influence green-
 282 house gas emissions trajectories.

283 Another critical structural distinction involving coupled models is whether a given
 284 coupling is *unidirectional* or *multidirectional*. Unidirectional coupling involves chaining
 285 models together in series, with no feedbacks between the modeled subsystems. The re-
 286 sulting wiring diagram (the directed model graph) is acyclic. Conversely, multidirectional
 287 coupling allows two model components to interact with each other, creating the possi-
 288 bility for feedbacks. Models involving multidirectionally-coupled components can have
 289 richer dynamics, but have an increased number of uncertain parameters due to the ad-
 290 ditional couplings. The potentially nonlinear dynamics introduced by the multidirectional
 291 couplings can also complicate analyses of uncertainty propagation. To date, most exam-
 292 ples of coupled multidirectional frameworks come from the multi-sector Integrated As-
 293 sessment Models (IAMs), rather than from the coupling of independently-developed sec-
 294 toral models. Examples of coupled multidirectional modeling frameworks include Yoon
 295 et al. (2021), Mosnier et al. (2014), and Walsh et al. (2019).

296 For a concrete example of the implications of the choice of model coupling regime
 297 and control volume design, consider the coupled agricultural-hydrological system depicted
 298 in Figure 4. In the unidirectional example (Figure 4a), local hydrology, crop production,
 299 and crop prices are modeled endogenously, allowing farmer income to reflect the coupled
 300 hydro-agricultural-economic dynamics (some analyses that use similar modeling frame-
 301 works include Davies et al. (2013), Ma et al. (2016), and Stevanović et al. (2016)). There
 302 are already large uncertainties in this unidirectional case: for example, how to construct
 303 the impact of production shocks on prices (Nelson et al., 2014). However, additional in-

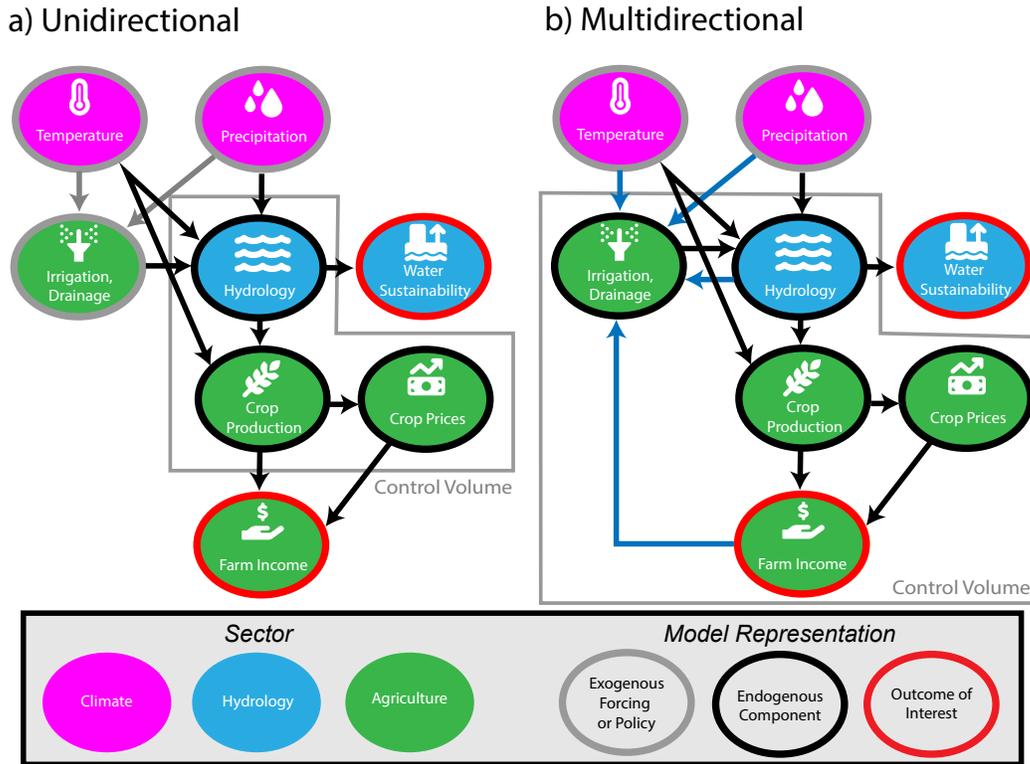


Figure 4. Simplified examples of possible model coupling configurations for a linked agriculture-water system. Panel a) represents a unidirectional coupling scheme between local hydrology, crop production, and crop prices, prohibiting the presence of feedback loops. Decisions about irrigation are supplied exogenously, either as forcings or policy rules (and may or may not be correlated or influenced by the climate forcings; those optional connections are shown with gray arrows). In panel b), the control volume has been expanded to include irrigation decisions, which allows for a multi-directional coupling scheme and feedbacks between the hydrological and economic systems and irrigation choices. Additional model couplings and dependencies in the multi-directional case represented in panel b) are represented by blue arrows. While the switch from unidirectional to multi-directional coupling makes it possible to represent richer and more realistic dynamics, the additional complexity may create computational and/or conceptual challenges for uncertainty analysis.

304 come from the joint agricultural-economic system is not allowed to directly feed back and
 305 induce changes in irrigation and drainage infrastructure. As a result, these influences on
 306 the local hydrology must be treated exogenously. In Figure 4b, which features multidirectional
 307 feedbacks through the introduction of a cycle, farm income is allowed to be invested
 308 into expanded irrigation and drainage, allowing farmers to alter the local hydrology
 309 to their benefit (with potential consequences for the broader hydrological system).
 310 This allows the analysis to more accurately capture the influence of agricultural decision-
 311 making and economic dynamics on the hydrological system and future production, but
 312 at the expense of additional data requirements and model complexity, since the relationships
 313 between farm incomes, investment decisions, irrigation operations, and local hydrology
 314 needs to be parameterized and (ideally) calibrated (Holtz & Pahl-Wostl, 2012).

315 Although Figure 4 portrays only a simple and stylized example, it nonetheless illustrates
 316 many of the important implications of the (linked) choices regarding control volume design
 317 and coupling regime for model complexity, the associated data and computational requirements,
 318 and how the results of the analysis can be interpreted with respect to relevant uncertainties.
 319 MSD investigators should hence make these choices as transparent as possible when reporting
 320 results, including by presenting a wiring diagram illustrating the coupled model structure.
 321

322 One further consideration when coupling models of different sectors is that their
 323 characteristic scales may differ with respect to space and/or time. This can require up-
 324 and/or downscaling model structures and forcings to adequately model the dynamics within
 325 and across sectors. Coupling models with different spatiotemporal scales introduces new
 326 uncertainties in how the output of one model is translated to another, which should be
 327 accounted for in model calibration. We discuss implications of scales as they relate to
 328 forcings in Section 4.2, as this is a key issue when making forward projections, though
 329 some of these considerations may also be relevant for calibration.

330 **3 Uncertainty in Model Calibration and Inference**

331 The first step in uncertainty analysis is to determine the space over which the analysis
 332 will be conducted (including input and subsystem model structures and/or parameter values),
 333 as well as ranges or distributions for the parameters which are treated as uncertain. We
 334 refer to the selection of model parameters and structures to maximize the fidelity of the
 335 system model to observational data given model and computational constraints as *calibration*
 336 (Oreskes et al., 1994). Model calibration methods can span a range of techniques from
 337 hand-tuning model parameters until the output looks “right” to fully probabilistic
 338 approaches (Helgeson et al., 2021). With sufficient data, the uncertainty in these inputs
 339 can be estimated through statistical calibration. When calibration is conducted using
 340 statistical methods, it can be considered a backward estimation of uncertainty (Kennedy &
 341 O’Hagan, 2001). While calibration aims to approximate observations of the modeled
 342 system with model output, statistical inference focuses on obtaining estimates, probabilistic
 343 or summary, of the system parameters to learn about their values. Statistical calibration
 344 and inference are closely related, but have different (if complementary) goals.
 345

346 Not all MSD analyses will require model calibration. For example, certain UC and SA
 347 studies may focus on understanding how a particular model structure responds to varying
 348 inputs over ranges or samples, rather than trying to select among model structures or infer
 349 probabilities. However, whether we are engaged in UC, UQ, or SA, we necessarily make
 350 some assumptions about parameter ranges and distributional forms (particularly in the case
 351 of UQ). These assumptions have implications for which variables we find to be most
 352 influential on the outputs and which decision alternatives we find to be most robust to
 353 that uncertainty (Quinn et al., 2020; McPhail et al., 2020; Reis & Shortridge,
 354 2022). Moreover, a model calibrated to match observations with respect to one

355 output may not sufficiently capture the dynamics of another (Efstratiadis & Koutsoyian-
 356 nis, 2010). This is unsurprising given the choices made in the modeling process, but high-
 357 lights the fact that “model calibration” is not a single method: different calibrations and
 358 calibration approaches are needed for different research questions.

359 As such, many questions surround how to best infer uncertainties through calibra-
 360 tion, even in single-sector systems. These choices, whether they involve the selection of
 361 input data, the choice of model structures, or whether to calibrate system components
 362 independently or jointly, must be made with the goals of the research in mind, as they
 363 involve tradeoffs from the perspective of uncertainty analysis. We briefly discuss these
 364 challenges to uncertainty analysis here, consider how they are magnified in multi-sector
 365 systems, and discuss open research questions for how they should best be addressed. An-
 366 swering these questions will be a critical first step before estimating how these uncer-
 367 tainties propagate forward to influence outcomes in multi-sector systems.

368 **3.1 Exogenous Uncertainties**

369 Model-based projections of outcomes in multi-sector systems require forcing multi-
 370 sector models with exogenous variables. These are often climate variables, such as pre-
 371 cipitation and temperature, but may represent the output of other linked processes and
 372 systems, depending on the specified control volume of the analysis. How these inputs are
 373 modeled has implications for the resulting projections and output analysis. Ignoring un-
 374 certainty in the marginal and joint distributions of these forcing variables can bias pro-
 375 jected system outcomes. This raises questions about 1) how to identify the structure and
 376 parameters defining the joint distribution of system inputs given limited data and 2) whether
 377 data from the past that must be used for this estimation will be representative of the
 378 future. In this section, we discuss how backwards uncertainty analyses can help address
 379 these questions and how choices in data sets and modeling can influence subsequent re-
 380 sults.

381 **3.1.1 Observational Data**

382 Observational climate data plays an important role in model calibration. Several
 383 model parameters typically need to be calibrated by relying on historical data of clima-
 384 tological variables, which may take the form of (interpolated) station data or reanaly-
 385 sis products (Auffhammer et al., 2020), or streamflow observations (Kiang et al., 2018).
 386 There are observational uncertainties associated with the measurements underlying each
 387 of these, as well as parametric and structural uncertainties in any data assimilation pro-
 388 cedure that might be used (Zumwald et al., 2020). In some cases, different choices of ob-
 389 servational datasets can lead to significantly different estimates of endogenous model pa-
 390 rameters (Parkes et al., 2019), although such uncertainties are typically neglected dur-
 391 ing model construction and parameter calibration. It may be difficult to know *a priori*
 392 whether observational uncertainties are important relative to endogenous and/or forc-
 393 ing uncertainties, and solutions such as explicitly modeling measurement errors (Schnnach,
 394 2016) or using a “dataset ensemble” (Zumwald et al., 2020)] may be computationally ex-
 395 pensive.

396 Observations of socioeconomic data are subject to uncertainties which are unique
 397 to the specific product, and these observational uncertainties could be accounted for in
 398 the calibration process via the probability model (see the discussion of likelihood func-
 399 tion specification in Section 3.2.1).

400 **3.1.2 Statistical Modeling of Correlated Events**

401 Within the risk analysis literature for individual sectors, challenges in answering
 402 these questions have been acknowledged and researched (Stedinger et al., 1993). How-

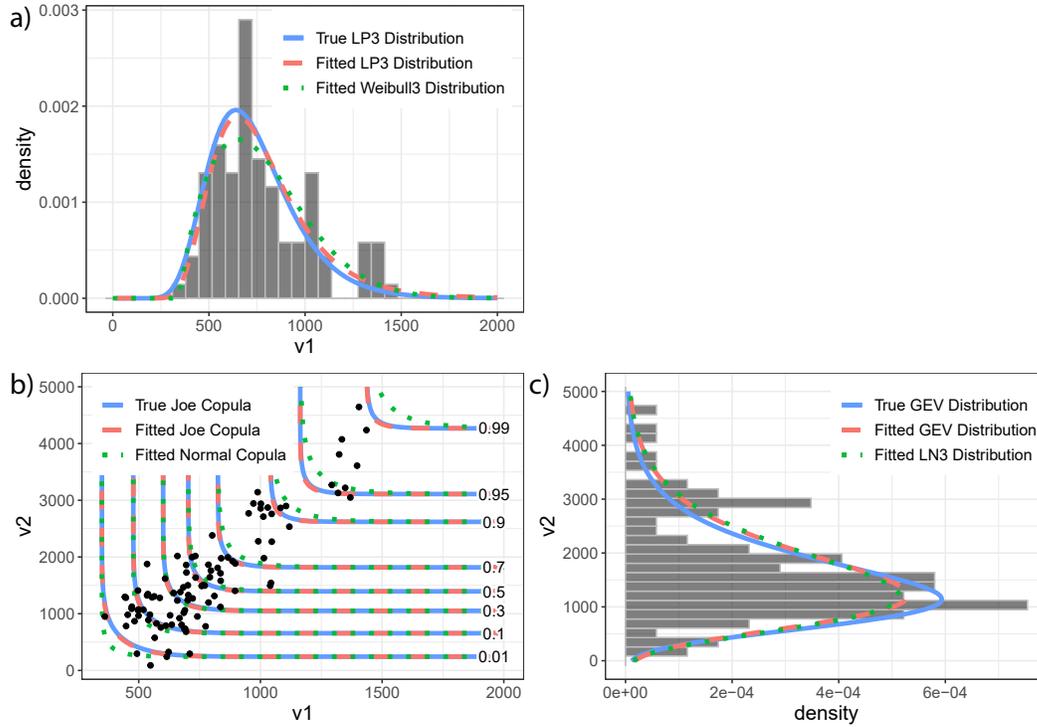


Figure 5. Example of parametric and structural uncertainty in estimating the joint distribution of exogenous variables. (a) Uncertainty in estimating the marginal distribution of variable v_1 . (b) Uncertainty in estimating the copula describing the joint distribution of variables v_1 and v_2 . (c) Uncertainty in estimating the marginal distribution of variable v_2 .

403 ever, explicitly modeling the linked dynamics of multi-scale, multi-sector systems may
 404 reveal additional vulnerabilities due to the interactions between sectors and correlations
 405 across spatiotemporal domains (Su et al., 2020; Dolan et al., 2021). This emphasizes the
 406 importance of accounting for joint extremes and compound events in multi-sector risk
 407 analyses.

408 Figure 5 shows a stylized example of this challenge: estimating the structure and
 409 parameters defining the joint distribution of two exogenous variables. In this example,
 410 synthetic observations of these two variables were generated from the joint (Figure 5b)
 411 and marginal (Figure 5a,c) distributions shown by solid blue lines in the figure. In the
 412 real world, we do not know these underlying distributions but have to estimate them from
 413 observed or modeled data. If we correctly assume the structure of these distributions and
 414 simply estimate their parameters through statistical approaches such as maximum like-
 415 likelihood estimation, we might estimate that the data came from the dashed pink distri-
 416 butions. If we incorrectly assume the structure, we might estimate they were generated
 417 from the dotted green distributions.

418 All of these fits rely on point estimates of the parameters of each distribution. The
 419 implications of errors in these point estimates are most prominent in the tails of the dis-
 420 tribution, where impacts are generally greatest, and data is most limited, resulting in
 421 the greatest uncertainty in estimation. In the example in Figure 5, both fitted distri-
 422 butions have fatter upper tails than the true distribution, which could lead to overestima-
 423 tion of the frequency of extreme events, and hence alter the resulting risk analysis. For
 424 example, if these variables represented rainfall volumes and peak storm surge or drought

425 intensity and duration, we might overestimate the impacts of floods on coastal infras-
426 tructure or droughts on agricultural production. These errors could influence decision-
427 making processes, resulting in overinvestment in stormwater infrastructure or irrigation
428 reservoirs. Underinvestment is similarly likely if we underestimate the occurrence of these
429 joint extremes. Alternative parameter estimators may result in a higher, equal, or lower
430 probability of underdesign than overdesign. If one is more risk averse, a Bayesian prior
431 can initiate the parameter estimates such that the probability of underdesign is less likely
432 (Stedinger, 1983).

433 Risks of under-design can be compounded when considering joint drivers. The most
434 common approach to fitting joint distributions of stochastic variables is through copu-
435 las (Nelsen, 2007), which model the dependence between variables in quantile-space. First,
436 marginal distributions are fit to the individual variables and then the observations are
437 transformed into quantiles of these distributions through inversion, where their depen-
438 dency is modeled. There are many families of copulas that can capture this dependency,
439 some of which exhibit tail dependency, meaning the variables are more highly correlated
440 in the tails (upper, lower or both) than in the middle of the distribution (Schmidt, 2005).
441 Fitting a copula that does not exhibit tail dependency when the observations do can lead
442 to underestimation of the probability of joint extremes (Poulin et al., 2007). This occurs
443 in Figure 5 when assuming the two variables come from a normal copula, which does not
444 exhibit tail dependence, as opposed to the true Joe copula (Joe, 1993), which exhibits
445 upper tail dependence, meaning high values of v_1 are more highly correlated with high
446 values of v_2 than in the middle of the distribution.

447 The consequences of errors in marginal distribution estimation have been well-documented
448 in the literature on single-sector systems, most predominantly with respect to floods (Wong
449 et al., 2018). The negative consequences of incorrectly estimating the joint distribution
450 of exogenous variables, particularly in the tails, or worse, assuming independence, have
451 recently been raised in the literature with respect to coastal flooding (Moftakhari et al.,
452 2017), agricultural production (Haqiqi et al., 2021), and wildfires (Brown et al., 2021),
453 among others.

454 These consequences can be mitigated by not only using point estimates of the
455 most likely distribution parameters, but accounting for parametric uncertainty, such as
456 through sampling from frequentist confidence intervals or Bayesian credible intervals (Sadegh
457 et al., 2017, 2018). Bayesian approaches have the advantage of explicitly encoding prior
458 knowledge about parameter values as prior distributions, which can be updated using
459 Bayes' Theorem with information from data to obtain posterior distributions (P. M. Lee,
460 1989). This allows researchers to be transparent about these assumptions, which facil-
461 itates exploration of alternative hypotheses and sensitivities. Generating realizations from
462 the distributions parameterized by multiple posterior samples results in draws from the
463 posterior predictive distribution, which combines parametric and sampling uncertainty.

464 Bayesian estimation approaches can be applied to capture structural uncertainty
465 as well through Bayesian model averaging (Madigan et al., 1996; Hoeting et al., 1999).
466 However, depending on the complexity of the statistical and process models, propagat-
467 ing samples of exogenous variables through a multi-sector model to quantify output un-
468 certainty can become computationally challenging or intractable if those samples are gen-
469 erated from the posterior distributions of multiple model structures. Another option is
470 the use of principled model selection techniques, which we discuss further in Section 3.2
471 — the key point is that each approach to model selection reflects different modeling and
472 epistemic goals, and care should be taken to align the selection criteria with the goals
473 of the analysis.

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3.1.3 Nonstationarity in Exogenous Processes

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The example illustrated in Figure 5 assumes the stochastic process being estimated is stationary, meaning its distribution does not change over time (Koutsoyiannis & Montanari, 2015). For many exogenous variables, this may not be true, particularly in the context of climate change. For example, we are confident that increasing global carbon emissions have resulted in nonstationary temperature time series, but are more uncertain on how this has impacted precipitation and other climate variables (Arias et al., 2021). Assuming these other climate variables are stationary when they are not could exacerbate over or under-estimation errors, particularly in the tails (Milly et al., 2008; Wong et al., 2018). However, modeling them as nonstationary introduces greater uncertainty in the structure of that nonstationarity, as well as uncertainty in the parameters of that structure. For example, a modeler must determine which variables are non-stationary, what covariates influence those non-stationary variables, and the form of that dependency, *e.g.*, linear, log-linear, quadratic, or some other functional form (Grinsted et al., 2013; Wong et al., 2018; Wong, 2018). Time is a common choice of covariate, but loses ties to physical processes (Koutsoyiannis & Montanari, 2015), however conditioning on other covariates requires projecting how that variable will change in the future as well. With limited data to constrain the additional parameter estimates required to model these dependencies, particularly in the tails of concern, uncertainty can balloon to levels uninformative for decision-making (Serinaldi & Kilsby, 2015). Thus, modeling these processes as stationary vs. nonstationary is often a tradeoff between bias and variance (Ceres et al., 2017), and the decision about which to favor should depend on the consequences of each type of error (Rosner et al., 2014), which may differ across sectors.

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Another issue is that the models used for projections may operate on scales that are misaligned with decision processes. Returning to the temperature and precipitation example, flood managers and urban planners are often concerned with daily, local-scale projections which climate models are not designed to generate. Statistical bias correcting and downscaling based on historical observations generally ignores the physical process reasons why projections misrepresent history, and so may propagate unjustifiable physical distortion into the future (Steinschneider et al., 2015). An alternative is stochastic weather generation (Steinschneider et al., 2019), wherein small scale weather realizations are simulated through a stochastic model that ties weather conditions to observable weather regimes (Robertson et al., 2015) that are better represented by climate models (Johnson & Sharma, 2009; Farnham et al., 2018). Thus temperature and precipitation realizations can be obtained at decision-relevant scales, leveraging climate models' strengths, conditional on deeply uncertain emissions trajectories. The advantage of such an approach is the ability to produce large samples of future climate or weather conditions. Indeed, such exploratory methods can be useful for multi-sector planning studies in order to identify critical uncertainties and design adaptive monitoring systems (Quinn et al., 2020). In the broader MSD context, analogous approaches hold promise where model and decision scales are misaligned.

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3.2 Endogenous Uncertainties

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In addition to quantifying uncertainty in the exogenous forcing to our models, it is crucial to consider uncertainty in the relationships between model components themselves, both within sectors and between sectors. While individual systems, considered in isolation, may primarily face risk from extreme, tail-area events, the nonlinear dynamics associated with coupled systems-of-systems could result in more moderate stressors simultaneously affecting multiple parts of the system. An illustrative example is the impact of Winter Storm Uri on the Texas infrastructure system in February 2021. While the severity of the triggering cold snap had precedent (Doss-Gollin et al., 2021), its impact on the natural gas and electric power systems was disproportionate due to the tight

525 coupling between these systems and socioeconomic stresses such as increased heating de-
 526 mand (Busby et al., 2021).

527 *3.2.1 Addressing Uncertainty in Model Parameters and Structures*

528 Uncertainty in endogenous model components can be both parametric and struc-
 529 tural. Conceptually, it is not always easy to untangle these two different types of uncer-
 530 tainties. Within single-sector models, it is well-known that multiple combinations of pa-
 531 rameters and structures can produce dynamics similar to observations. From a Bayesian
 532 perspective, this reflects a posterior distribution over the space of joint structural and
 533 parametric combinations which does not have a unique maximum. In the hydrological
 534 literature, this non-uniqueness is typically referred to as equifinality (Beven, 2006). In
 535 such cases, Bayesian methods that explicitly estimate the posterior probability of dif-
 536 ferent parameter combinations are recommended over single-objective calibration approaches
 537 that provide parameter point estimates that minimize an objective function, such as the
 538 sum of squared errors between observed and modeled output variables (Vrugt et al., 2008).
 539 Uncertainty estimates from bootstrap replications (Efron & Tibshirani, 1986; Efron, 2014)
 540 are a reasonable alternative to Bayesian methods, though care should be taken to ac-
 541 count for dependence and potential non-stationarities.

542 Additional uncertainties come from the choice of model structures under consid-
 543 eration, as all models are necessarily just approximations to the “truth” (Oreskes et al.,
 544 1994) (or, in the common phrasing, “all models are wrong” (Box, 1979)). In general, a
 545 preferred structure is as parsimonious as possible while accurately reproducing held-out
 546 observations. There are a number of important considerations when deciding on a model
 547 selection or averaging approach, with different choices being more or less appropriate for
 548 different modeling goals (Höge et al., 2019; Bojke et al., 2006). Computational constraints
 549 may also play a role in whether a single model is selected (as opposed to averaging an
 550 ensemble of model structures), but care should be taken to acknowledge the ambient struc-
 551 tural uncertainty in the interpretation of results.

552 Potential nonstationarity in endogenous dynamics further complicates model se-
 553 lection. Model selection and averaging techniques based on optimizing out-of-sample pre-
 554 dictive performance (Gelman et al., 2014; Vehtari et al., 2017; Yao et al., 2018) may help,
 555 but still require the model structures under consideration to be capable of capturing ap-
 556 propriate changes to dynamics. Bottom-up modeling methods, such as those from the
 557 generative social sciences, can be used to explore the impacts of structural and paramet-
 558 ric uncertainties related to alternative theories of human and institutional behavior, in-
 559 cluding potential nonstationarity (Epstein, 1999). For example, several different agent-
 560 based models of flood risk have explored different theories of human behavior within a
 561 consistent modeling framework (Haer et al., 2017; de Koning et al., 2017; Magliocca &
 562 Walls, 2018). These bottom-up methods can also be used to identify the emergence of
 563 new regimes of behavior (see Section 5.2.3 for discussion of these methods). Addition-
 564 ally, The critical transitions literature provides tools for modeling and empirically de-
 565 tecting shifts in endogenous dynamics (Lade et al., 2013; Scheffer et al., 2009). Models
 566 incorporating human and institutional decisions may also be able to incorporate data-
 567 driven generation of model structure (Ekblad & Herman, 2021) coupled with dimension
 568 reduction to support feature engineering for dynamic multisector datasets (Cominola et
 569 al., 2019; Giuliani & Herman, 2018) to generate structural and parametric variants which
 570 are consistent with past observations.

571 It is unclear whether multi-sector models mitigate or exacerbate this challenge. On
 572 one hand, the models become more complex: the more complex the model, the greater
 573 the number of parameters that need to be calibrated and the more challenging this es-
 574 timation problem becomes, as more data is needed to constrain the likely parameter space
 575 (Srikrishnan & Keller, 2021). On the other hand, data from another sector might help

576 constrain the likely parameter set. For example, a set of soil parameters that perform
 577 well in simulating hydrologic behavior, may not simulate crop yields well, and that might
 578 only be discovered through a coupled agro-hydrological model. This is an example of how
 579 adding model complexity could result in less uncertainty, as depicted in Figure 3.

580 Another challenge is the specification of a likelihood function. Calibration that does
 581 not properly account for the statistical structure of model-data discrepancies can result
 582 in biased inferences and hence projections (Brynjarsdóttir & O’Hagan, 2014). This like-
 583 lihood function should ideally include different sources of uncertainties, such as both model-
 584 data discrepancy and observational errors. When these can both be modeled as inde-
 585 pendent errors with no correlation, they can be combined into a single error term. Srikrishnan
 586 et al. (2022) and Ruckert et al. (2017) provide examples of likelihood specifications which
 587 mix autocorrelated model-data discrepancies and independent observation errors.

588 For particularly complex models, the likelihood function may be mathematically
 589 or computationally intractable. Likelihood-free methods, such as precalibration (Edwards
 590 et al., 2011), Generalized Likelihood Uncertainty Estimation (GLUE) (Beven & Binley,
 591 1992), and approximate Bayesian computation (ABC) (Sisson et al., 2018) can be used
 592 in these settings to obtain a representation of “behavioral” parameter sets. However, care
 593 should be taken when interpreting these results: Stedinger et al. (2008) notes that pre-
 594 calibration and GLUE parameterizations should not be treated probabilistically, and ABC
 595 results can show strong sensitivity to the choice of summary statistics and distance thresh-
 596 olds.

597 **3.2.2 Addressing Computational Expense**

598 Even if multi-sector models can constrain the domain of likely parameter sets and
 599 structures, calibration problems could still be more challenging computationally, both
 600 because the greater number of parameters increases the dimension of the search, requir-
 601 ing more model simulations to fully characterize the posterior distribution, and because
 602 the multi-sector model itself takes longer to run. Additionally, some model components
 603 may be more trusted than others, either in terms of model fidelity or quality of calibra-
 604 tion data, and there might be concerns about “contaminating” the calibration of one mod-
 605 ule through these interactions. One approach to this problem is to calibrate the single
 606 sector models separately. However, combining the parameter sets from separate calibra-
 607 tions could yield unrealistic multi-sector dynamics by neglecting correlations. Alterna-
 608 tively, one could calibrate the multi-sector model for performance in a single sector first
 609 and then fix those parameters for a second calibration of parameters controlling another
 610 sector. This approach is common in the hydrological literature, *e.g.*, calibrating for stream-
 611 flow and then nutrients (Arnold et al., 2012), but it is still likely to neglect correlations
 612 and may underestimate multi-modality. Jacob et al. (2017) provides some guidance on
 613 navigating this problem, but the implications of these choices for MSD calibration are
 614 not well understood in general.

615 Bayesian (or approximately Bayesian) calibration methods such as Markov chain
 616 Monte Carlo can require many thousands to millions of model evaluations, potentially
 617 making them computationally prohibitive for models that are too expensive for a suf-
 618 ficient number of runs on a given computational budget. There exist a suite of methods
 619 for speeding up Bayesian inference (Robert et al., 2018), but these may not be gener-
 620 ally applicable to MSD calibration exercises. For example, Hamiltonian Monte Carlo meth-
 621 ods (Betancourt, 2018), which are implemented in the Stan probabilistic programming
 622 language (Stan Development Team, 2019) and language-specific packages such as Julia’s
 623 Turing.jl (Ge et al., 2018) and Python’s pyMC3 (Salvatier et al., 2016), are extremely
 624 efficient, but require information about the gradient of the posterior, which can be dif-
 625 ficult to obtain from simulation models that are not written to be parsed by an auto-
 626 matic differentiation package. Another approach can be to exploit parallelization in a

high-performance computing environment, which is taken by sequential Monte Carlo-like algorithms like FAMOUS (B. S. Lee et al., 2020).

One approach to managing computational expense is reducing the number of parameters which need to be calibrated through *factor fixing*. In factor fixing, sensitivity analysis is used to identify groups of parameters or model components which are not influential and might be fixed without substantially impacting the analysis (Saltelli et al., 2008). This allows the analyst to focus their computational resources on simulating from the distributions of influential factors by justifying the deterministic treatment of non-influential factors. Different sensitivity analyses can be used for factor fixing. An important consideration is that a factor may not be influential when varied individually, but may exhibit significant influence through interactions (*e.g.*, the sensitivity analysis in Srikrishnan et al. (2022)). Consequently, the Method of Morris is commonly used for factor fixing (Cariboni et al., 2007) because it efficiently provides estimates of total order sensitivities that include individual and interactive effects (M. D. Morris, 1991). Other methods can be used for factor fixing (for instance elementary effects), but the key feature of any approach is that it should approximate total sensitivity (*i.e.* individual and interactive effects (Campolongo et al., 2007)), and be computationally efficient.

When the original model does not need to be used directly, surrogate models (or emulators) can be employed to reduce computational and parametric complexity. A number of different surrogate model structures can be used, including Gaussian processes (Kennedy et al., 2006), support vector machines (Bouboulis et al., 2015), and artificial neural networks (Eason & Cremaschi, 2014). These methods have different pros and cons; for example, Gaussian processes can only handle a limited parameter space, which can have implications for resulting risk analyses (B. S. Lee et al., 2020), while the machine-learning methods may be easy to overfit to data if not tuned carefully and may limit learning about system dynamics due to their black-box nature if not accompanied by careful diagnostics and sensitivity analyses. In many cases, a primary limitation in training good surrogate models is the number of available model evaluations (due to computational constraints), particularly as MSD outcomes of interest are likely to emerge from the interactions of a relatively large number of parameters and exogenous forcings. More sophisticated sampling strategies, such as adaptive designs of experiment (Burnaev & Panov, 2015; Gramacy & Lee, 2009; Chang et al., 2016) may be useful to maximize computing budgets, allowing surrogates to be trained on a larger subset of the parameter space. Evolutionary approaches to co-tune and select surrogate models have been proposed (Gorissen et al., 2009), which may be useful if building the surrogate model itself requires a large number of model runs to capture the dynamics of the model response surface, so surrogate modeling alone does not fully solve the problem of computational expense.

Another approach is the use of simple models to act as emulators of more complex models. This results in emulators which are mechanistically-motivated and can provide more direct insight into system dynamics and parameter values, but which may be less flexible in fitting the original model's response surface. For example, reduced-complexity climate models have been calibrated and used instead of more computationally-expensive models (Dorheim et al., 2020; Nicholls et al., 2020). While these simple models may lack the full richness and mechanistic detail of the complex models they're emulating, their increased ability to capture uncertainties may make their use more appropriate for certain research questions than the original models would have been (Helgeson et al., 2021).

However, there may be cases when emulation is insufficient due to the large number of parameters which need to be considered or the complexity of the system response surface, and full model evaluations are required for projections and scenario discovery. In this case, advances in efficient model calibration are necessary to facilitate uncertainty quantification and propagation. For example, B. S. Lee et al. (2020) demonstrate how a parallelized sequential Monte Carlo algorithm can treat a relatively large number of

679 parameters of a complex Antarctic ice sheet model as uncertain, resulting in higher po-
 680 tential contributions to future sea levels.

681 An interesting approach is the application of machine learning methods for uncer-
 682 tainty quantification. Klotz et al. (2021) demonstrate how deep neural networks, typ-
 683 ically thought of as black-box models, can be used to estimate uncertainties for a hydro-
 684 logical system, while also showing an example of how to obtain some measure of inter-
 685 pretability with a *post hoc* interrogation of fitted machine learning models. The power
 686 of careful implementations of machine learning methods, which embed mechanistic in-
 687 sights into the model structure, as an alternative for learning and uncertainty quantifi-
 688 cation for complex systems, rather than explicitly process-based modeling, is starting
 689 to be explored in the hydrological literature (Kratzert, Klotz, Herrnegger, et al., 2019;
 690 Kratzert, Klotz, Shalev, et al., 2019). These approaches may be a promising alternative
 691 to the use of computationally-expensive, mechanistic models for broader multi-sector anal-
 692 yses when large training data sets are available.

693 4 Uncertainty in Forward Projections

694 After calibrating a multi-sector model, we can use that model to project future out-
 695 comes. Analyses projecting outcomes for MSD systems involve uncertainty in two sep-
 696 arate but overlapping ways: a) accounting for uncertainty in exogenous forcings and b)
 697 understanding the relative influence of various sampling, parametric, and structural un-
 698 certainties on model projections. Due to the number of relevant uncertainties, several
 699 of them deep, forward projection exercises in MSD are typically exploratory in nature
 700 (Bankes, 1993; Moallemi, Kwakkkel, de Haan, & Bryan, 2020), which is why we use the
 701 term *projection* rather than *prediction* (MacCracken, 2001; Bray & von Storch, 2009).

702 In this section, we focus primarily on the influence of the treatment of exogenous
 703 forcings and up- and downscaling on uncertainties in projections. This focus is informed
 704 by the existence of several comprehensive reviews on techniques for SA (see *e.g.* Pianosi
 705 et al. (2016)). However, the role of computational expense, as discussed in Section 3.2.2,
 706 is a major consideration for developing projection ensembles and SA with MSD mod-
 707 els, as it is for calibration. One additional challenge here for emulation is the presence
 708 of spatiotemporal teleconnections due to the complex dynamics of cross-sectoral and re-
 709 gional connections (Helbing, 2013; Dolan et al., 2021). Mismatches between the “true”
 710 and emulated response surfaces could result in very different dynamical patterns and bias
 711 estimates of sensitivity, risk, and policy effectiveness. A related challenge is the use of
 712 a resulting ensemble to understand how uncertainties propagate through and interact
 713 within the system; we discuss these issues in the context of scenario discovery in Sections 5.2.1
 714 and 5.2.3.

715 4.1 Exogenous Forcings and Joint Extremes

716 As we discuss in Section 2.2, control volume design, including the decision of which
 717 components to treat endogenously, is centrally important to uncertainty analysis. Increas-
 718 ing the number of components that are treated endogenously can facilitate a more com-
 719 plete uncertainty analysis, since model structures, parameters, and dynamic interactions
 720 can be more systematically varied and tested. However, it is important to recognize that
 721 in practice, computational constraints and/or issues of scale and scope lead modelers to
 722 externalize much of the system dynamics into fixed, exogenous boundary conditions. For
 723 example, it may be computationally intractable to include the impact of MSD system
 724 evolution on emissions to endogenously represent changes to the climate system. These
 725 external forcings are often outputs from a separate set of models, for example one or more
 726 climatological variables simulated by an ensemble of climate models or a set of socioe-
 727 conomic projections produced by an IAM. Uncertainties surrounding exogenous forcings
 728 can often exceed the uncertainty associated with endogenous dynamics. Several stud-

ies across hydrology (J. Chen et al., 2011; Chegwiddden et al., 2019; Vetter et al., 2017), agriculture (Asseng et al., 2013; Rosenzweig et al., 2014), health (Sanderson et al., 2017), and energy (van Ruijven et al., 2019; Bloomfield et al., 2021; Deroubaix et al., 2021) find that uncertainty arising from climate models can represent a substantial fraction of the total. Similarly, many studies find large uncertainties surrounding socioeconomic inputs, including emissions scenarios (Paltsev et al., 2015), population growth (Veldkamp et al., 2016), energy costs and demand (Lamontagne et al., 2018; Su et al., 2020), economic growth (Gillingham et al., 2018), and parameterization of damages (Errickson et al., 2021).

Biased or low-coverage realizations of these uncertainties could interact with errors in the emulated response surface to compound failures to identify potential teleconnections. This section hence discusses uncertainties associated with exogenous forcing. We distinguish between climate forcing (Section 4.1.1) and socioeconomic forcing (Section 4.1.2) with further breakdowns given in each section. We provide a brief overview of how each type of forcing is typically employed in single sector models and discuss the challenges and opportunities of moving to the multi-sector case.

4.1.1 Climate Forcing

Perhaps the most common type of climate forcing data takes the form of gridded simulation outputs of meteorological variables from global climate models (GCMs). GCMs are subject to the same types of uncertainties outlined previously (structural, parametric, and sampling) and the climate modeling community typically probes each of these through ensemble frameworks. As different ensemble outputs address uncertainty differently, the choice of climate product influences how climate uncertainty is treated in the resulting MSD analysis.

Multi-Model Ensembles (MMEs), such as the Coupled Model Intercomparison Project (CMIP) (Eyring et al., 2016; Taylor et al., 2012), are the most commonly used framework. MMEs do not represent a systematic sampling of any one type of uncertainty but instead represent an “ensemble of opportunity” (Tebaldi & Knutti, 2007). That is, they are collections of models from various institutions that often share code and expertise (Abramowitz et al., 2019), with parameters tuned in complex ways (Mauritsen et al., 2012) and simulations reported without an estimate of internal variability (Maher, Power, & Marotzke, 2021). MMEs thus combine all three sources of uncertainty into one ensemble (which may or may not be desirable depending on the specific research question), but are typically framed as focusing on structural uncertainty.

In contrast to MMEs, Single Model Initial condition Large Ensembles (SMILEs) are designed specifically to estimate the effects of internal variability, which here we classify under sampling uncertainty. SMILEs are constructed by perturbing the initial conditions of a single GCM to produce varying climate and weather trajectories (Hawkins et al., 2016). The number of publicly available SMILEs (Deser et al., 2020) and the number of studies employing SMILEs (Maher, Milinski, & Ludwig, 2021) have increased considerably in recent years. One advantage of SMILEs is an improved sampling of extreme events (Wiel et al., 2019; Haugen et al., 2018) relative to MMEs.

Finally, single-model Perturbed Physics Ensembles (PPEs) are designed to sample parametric uncertainty (Murphy et al., 2004). In PPEs, the parameters or configurations of each ensemble member are systematically varied while keeping other factors fixed (Sexton et al., 2019). This framework isolates the impact of parametric uncertainties, which are typically neglected in the other frameworks, on model projections (L. A. Lee et al., 2011). PPEs may also be used to produce probabilistic projections (conditioned on model structure) if employed in a Bayesian framework (Sexton et al., 2012).

Each of the above ensemble frameworks exhibits distinct advantages and disadvantages for sectoral modeling. The different representations of uncertainty in each frame-

work may render some ensembles particularly useful for a given research question. For example, the interpretation of ensemble spread in SMILEs as arising from irreducible or aleatory uncertainty (and therefore as a representation of sampling uncertainty) makes them uniquely well-suited as decision-making tools; each ensemble member represents a plausible real-world outcome that could be included in a robust risk management strategy (Mankin et al., 2020). However, any single GCM used to produce a SMILE is still subject to structural and parametric uncertainties which may bias its representation of internal variability. Multi-model large ensembles have been proposed as one method to address this limitation (Deser et al., 2020). Utilizing both SMILEs and MMEs concurrently can help quantify what fraction of uncertainty is irreducible (Lehner et al., 2020), a metric with important policy implications (Palutikof et al., 2019). Additional considerations include ensemble configuration and data access. Given the large number of simulation members in a typical SMILE (on the order of 20 to 100), their use may exacerbate challenges related to computational tractability of MSD uncertainty analysis.

The main disadvantage of global, gridded, process-based Earth system models is their high computational cost. In contrast, simple climate models (SCMs) are generally much faster to run and thus might be preferable in a variety of modeling setups, particularly for uncertainty analyses. SCMs, which for our purposes include all climate models other than full-scale Earth system models, span a large range of structures and complexities, from one- or few-line models that aim to emulate global responses of selected outcomes (for example, global mean surface temperature or sea-level rise), to intermediate complexity Earth system models that might be spatially resolved but with very coarse resolutions and highly parameterized representations of physical dynamics (Weber, 2010). Examples of prominent SCMs include MAGICC (Meinshausen et al., 2011), FAIR (Leach et al., 2021), and Hector (Hartin et al., 2015).

The reduced computational burden of SCMs allows a better sampling of uncertainty, including the ability to produce probabilistic simulations. SCMs can also be tailored to specific, possibly novel research questions more easily than gridded climate products from GCMs (Forster et al., 2020). As noted, these advantages typically come at the expense of spatial resolution and the variety of available output variables. Given their increased reliance on parameterized processes, care must also be taken to avoid overfitting the model to calibration data; the main value of SCMs is their ability to give reliable out-of-sample estimates.

4.1.2 *Socioeconomic Forcing*

Sectoral and multi-sectoral analyses typically require exogenous assumptions about broader socioeconomic dynamics. Key socioeconomic variables generally revolve around demographics, economics, land-use, and emissions, but certain sectoral modeling efforts also require relatively more obscure quantities such as price trajectories of specific technologies (Auping et al., 2016), or local government structures (Andrijevic et al., 2020).

Projections of the future of the global economy and its associated socio-political dynamics are characterized by deep and dynamic uncertainties. As such, the global change research community typically relies on carefully crafted sets of plausible alternative futures known as scenarios, the canonical example being the Shared Socioeconomic Pathways (SSPs) (Riahi et al., 2017). Here, we briefly discuss the design and usage of the SSPs as well as their characterization of associated uncertainties. Our discussion can be generalized to other unrelated but similarly constructed scenario-based approaches (for example, as in Gurgel et al. (2021) and citeAwildImplicationsGlobalChange2021).

SSPs provide global trajectories of socioeconomic factors such as demographics, health, education, urbanization, economic growth and inequality, governance, technology, and policy. There are five SSPs, each reflecting qualitative global narratives that represent equally plausible future socioeconomic and geopolitical trends along axes of high or low

830 challenges to climate change mitigation and adaptation (O'Neill et al., 2017). These tra-
831 jectories are passed to IAMs that generate quantitative projections of energy use (Bauer
832 et al., 2017), land use (Popp et al., 2017), and associated emissions, among other out-
833 comes (Riahi et al., 2017). These projections may represent a “baseline” scenario with-
834 out climate policy or under various Shared climate Policy Assumptions (SPAs) that rep-
835 resent different sets of climate policy attributes (Kriegler et al., 2014). By design, the
836 SSPs are parsimonious representations of future socioeconomic conditions at the global
837 scale (Kriegler et al., 2012). As such, they often need to be supplemented with sector-
838 specific (*e.g.*, Rao et al. (2017); Graham et al. (2018)) and/or localized scenarios (*e.g.*,
839 Kok et al. (2019)).

840 There are large uncertainties both within and among the SSPs, many of which ap-
841 ply to scenario-based approaches more broadly. First, the key socioeconomic drivers of
842 a given outcome often do not obey consistent narratives, but instead arise from a mix-
843 ture of components from the narrative-driven scenarios (Lamontagne et al., 2018; Dolan
844 et al., 2021). This highlights the difficult but important task of designing suitably en-
845 compassing scenarios from which such hybrids can be drawn. Multi-model comparisons
846 often find large structural (Duan et al., 2019) and parametric (Krey et al., 2019) differ-
847 ences across IAMs that propagate into simulated outcomes (von Lampe et al., 2014; Harm-
848 sen et al., 2021). Behind any given quantitative projection in the SSP framework is an
849 assumption that the underlying IAM has produced a plausible real-world trajectory, but
850 this has been increasingly challenged, particularly with respect to energy mixes (Ritchie
851 & Dowlatabadi, 2017a, 2017b; Burgess et al., 2021; Hausfather & Peters, 2020). It re-
852 mains challenging, in general, to evaluate the efficacy of IAMs across the wide range of
853 research objectives for which they are employed (Wilson et al., 2021; Schwanitz, 2013).
854 Some authors advocate for a more holistic approach with a diminished role for IAMs (Morgan
855 & Keith, 2008). Some technical details of SSP design may also limit their utility for de-
856 cision making. As the baseline SSPs do not include climate policy or climate impacts,
857 there is no single scenario that incorporates the best estimates of impacts or the latest
858 governmental mitigation targets (Grant et al., 2020). A related concern is that scenar-
859 ios can become out of date, particularly for near-term projections, either as more recent
860 data is made available or through improvements in scientific understanding and mod-
861 eling capabilities (Hausfather & Peters, 2020; Burgess et al., 2021).

862 Scenarios such as the SSPs are also typically not accompanied by probabilistic in-
863 formation, which can make them difficult to integrate into risk assessments and may make
864 their interpretation more susceptible to typical cognitive biases (Tversky & Kahneman,
865 1974; Morgan et al., 1992; Webster et al., 2001). Alternatively, probabilistic approaches
866 can be used to systematically explore the uncertainty space and provide insight into the
867 likelihoods of both inputs and outcomes. While uncertainty quantification and the use
868 of probabilities is not always appropriate, there are cases in which it is defensible and
869 can provide useful information for risk-based decision-making, particularly when rele-
870 vant assumptions about likelihoods, data sources, and distributional forms are made trans-
871 parent (Morgan & Keith, 2008). Such an approach has particularly been used for key
872 socioeconomic drivers such as population, GDP, and emissions (*e.g.*, Gillingham et al.
873 (2018)). IAMs may also be employed in a probabilistic setting, sampling from distribu-
874 tions of key inputs to explore the uncertainty space (Webster et al., 2012; J. Morris et
875 al., 2022), although this remains a rare approach. Methods employed to develop prob-
876 ability distributions for model inputs vary on a case-by-case basis and can involve time
877 series forecasting (Keilman, 2020; Vollset et al., 2020), broader statistical approaches (Raftery
878 et al., 2017; Liu & Raftery, 2021), and expert elicitation (Christensen et al., 2018), pos-
879 sibly used alongside process-based models (Güneralp & Seto, 2013; Seto et al., 2012; Srikr-
880 ishnan et al., 2022). Employing a statistical model for exogenous forcings may offer some
881 advantages, including the ability to validate out of sample and to more completely probe
882 structural and parametric uncertainty owing to the reduced computational expense. How-
883 ever, the core difficulties lie in carefully quantifying “standard” uncertainties, including

884 specifying the relevant, possibly multivariate, probability distributions, as well as prop-
 885 erly characterizing deep uncertainties. It is also important to include the correlation struc-
 886 ture of uncertainty across outputs, even for univariate distributions. For example, many
 887 probabilistic population forecasts include 95% confidence intervals for each country, with-
 888 out explicitly specifying the correlation among countries: is the 90th percentile for US
 889 population in 2070 coincident with the 90th percentile for Canada in 2070? Such cor-
 890 relational effects have important implications for sectoral dynamics across space and time.

891 In addition to socioeconomic forcings, another important sources of uncertainty in
 892 human system modeling are socioeconomic policies, or the rules by which the model re-
 893 flects human responses to changes in the internal state or external environment. There
 894 are many theories from political science, sociology, psychology and other social science
 895 fields that are relevant to the modeling of human, firm, and government behavior and
 896 shifts. A growing and diverse literature draws on these theories to model dynamics such
 897 as the evolution or breakdown of cooperation (Stewart & Plotkin, 2014; Auer et al., 2015),
 898 the diffusion of opinions or innovation (Janssen & Jager, 2001), and the behavior of in-
 899 vestors or consumers in markets (Bonabeau, 2002). Multi-formalism modeling or multi-
 900 paradigm modeling presents the potential for integrating such dynamics into multi-sectoral
 901 models (Vangheluwe et al., 2002).

902 4.2 Changing Scales

903 Mismatches between the characteristic scales of forcing inputs and system mod-
 904 els creates challenges and uncertainties that are somewhat distinct from those discussed
 905 thus far. In this section, we discuss the impacts of downscaling climate and socioeconomic
 906 data to match the spatiotemporal scales relevant for models.

907 4.2.1 Downscaling Climate Data

908 Downscaling, and the oftentimes related process of bias-correction, has received con-
 909 siderable attention in the hydrology and climate impacts communities. There are two
 910 broad categories: dynamical, which involves running a high-resolution regional climate
 911 model forced with boundary conditions provided by a GCM (Giorgi & Gutowski, 2015),
 912 and statistical, which involves modeling a statistical relationship between large-scale at-
 913 mospheric predictors and local predictands (Hewitson et al., 2014). Both methods can
 914 involve some form of bias-correction, although typically more so for statistical approaches
 915 (Maraun, 2016). Known uncertainties, which apply equally to dynamic and statistical
 916 downscaling, include the validity of any stationarity assumptions, the physical plausi-
 917 bility of results across space and time (Maraun, 2016), and the resulting representation
 918 of (multivariate) extremes (Werner & Cannon, 2016; Zscheischler et al., 2019). An ad-
 919 ditional uncertainty that is relevant for bias-correction and statistical downscaling, and
 920 can be difficult to account for, is the choice of observational product (Lopez-Cantu et
 921 al., 2020).

922 When possible, careful consideration should be given to what information is most
 923 important for the relevant sectoral dynamics and/or decision problems — for example,
 924 methods that jointly process temperature and precipitation (*e.g.*, Abatzoglou and Brown
 925 (2012)) may be better suited for analyses where risks are driven by multivariate hazards,
 926 whereas methods that place a higher emphasis on capturing spatial structure (*e.g.*, Pierce
 927 et al. (2014)) might be preferred for sectors in which spatial heterogeneity is important.
 928 In any case, performing a hindcast test, where sectoral outcomes simulated by the orig-
 929 inal GCMs are compared to those simulated by downscaled outputs, can be useful to un-
 930 cover biases directly relevant to sectoral dynamics that might otherwise go unnoticed (Lafferty
 931 et al., 2021). Practical considerations such as the spatiotemporal domain and resolution,
 932 as well as the number of variables included, are also likely to be important factors in de-
 933 termining which datasets are widely used. Ease of access is also crucial: products that

934 abide by community standards and strive towards the FAIR principles (Wilkinson et al.,
935 2016) will better facilitate inter-comparisons and research extensions.

936 **4.2.2 Downscaling Socioeconomic Forcings**

937 Downscaling is also increasingly relevant for socioeconomic projections, with im-
938 portant differences in understanding and application relative to climate simulations. So-
939 cioeconomic dynamics are inherently multi-scale in that different national or regional poli-
940 cies can interact with the same global drivers to produce a broad and possibly diverg-
941 ing set of outcomes. Downscaling in the socioeconomic context can mean the generation
942 of additional regional/local scenarios that fit into a broader global context, or the more
943 traditional exercise of interpolating gridded data to a higher resolution.

944 For the former case, there are a number of possible approaches to multi-scale sce-
945 nario generation, each differing in the level of interconnectedness across scales (Biggs et
946 al., 2007). Downscaling, in the sense of generating regional scenarios from a set of global
947 or otherwise larger-scale contexts, should hence be understood as only one possible “top-
948 down” option. Other participatory “bottom-up” (Kok et al., 2006) or hybrid (Nilsson
949 et al., 2017) approaches may be more suitable in some situations. However, even within
950 the downscaling paradigm there is a considerable degree of heterogeneity regarding, for
951 example, the strictness of quantitative boundary conditions and the consistency of qual-
952 itative storylines (Zurek & Henrichs, 2007). Additionally, downscaling can follow a “one-
953 to-one” approach where regional storylines follow as closely as possible the global nar-
954 ratives, or a “many-to-one” approach where regional storylines are perturbed around a
955 broadly consistent larger context (Absar & Preston, 2015). The many-to-one method bet-
956 ter represents the increasing uncertainty at local scales but may quickly become chal-
957 lenging to manage (Kriegler et al., 2014). It may also be necessary to generate quanti-
958 tative trajectories of important quantities, either to reflect the results of the regional sce-
959 nario generation process or to include new factors that were previously unavailable. To
960 this end, many IAMs can be employed at regional or national scales (*e.g.*, Palazzo et al.
961 (2017)).

962 In many cases, modelers require spatially-resolved information beyond the highly
963 aggregated outputs of most IAMs. For example, the SSPs provide projections of key drivers
964 such as population structure only at the national scale and land-use at the regional/continental
965 scale. As such, a number of methods are used to downscale these scenarios into gridded
966 products. Most follow a similar framework, where statistical or process-based models are
967 calibrated on historical data and then applied to aggregated IAM outputs in the future
968 period.

969 Statistical methods are typically employed to downscale population and other de-
970 mographic factors. One rudimentary approach is to fix the spatial pattern at the cur-
971 rent distribution and scale each grid point with national factors (Caminade et al., 2014).
972 More sophisticated approaches include gravity models that assume areas with certain
973 characteristics, such as higher populations, attract more people (Jones & O’Neill, 2016)
974 and regression methods that make use of auxiliary variables likely to be important in de-
975 termining future growth (Murakami & Yamagata, 2019). Several studies jointly down-
976 scale population and GDP (*e.g.*, Wear and Prestemon (2019)). Across all methods, para-
977 metric and structural uncertainties are rarely explicitly included or examined.

978 Land-use downscaling is typically more involved than population or GDP down-
979 scaling, reflecting large uncertainties in socioeconomic and biophysical conditions. Many
980 models allocate land via profit maximization, which can be employed within a statisti-
981 cal framework (Meiyappan et al., 2014) or within IAMs reconfigured to produce grid-
982 ded outputs (Fujimori et al., 2018). As with population and GDP downscaling, para-
983 metric and structural uncertainties are typically neglected. One notable exception is M. Chen
984 et al. (2019), which examined parametric uncertainty in Demeter, a downscaling algo-

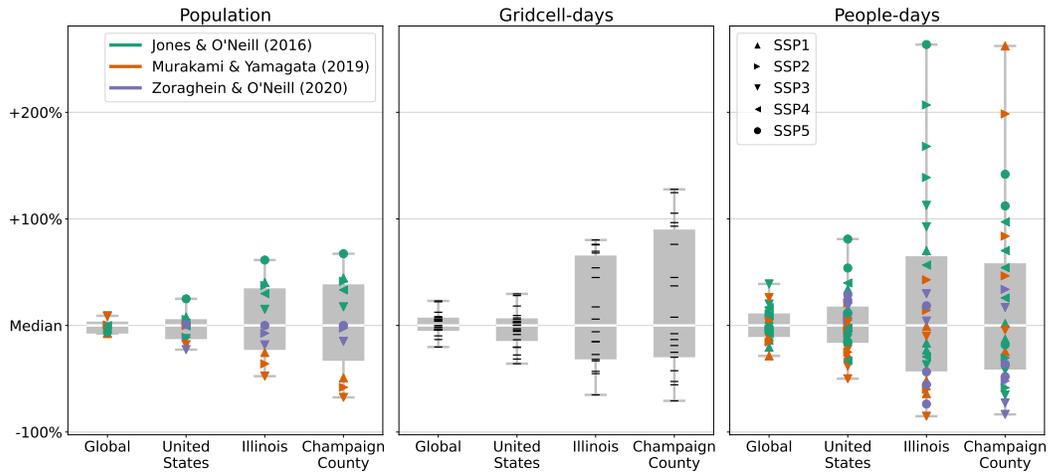


Figure 6. Exogenous uncertainty in compound extremes across scales. In each subplot, the boxplots show the distribution (relative to the median projection) of population (left), the number of annual gridcell-days above 35°C (center), and the number of annual people-days above 35°C (right), at different spatial scales (global, national, regional, and local). Boxplot whiskers extend over the full range of data and a sampling of individual points are shown by the markers, where different colors represent difference population downscaling methods and different symbols represent different SSP scenarios. Gridcell-days are calculated from the 21 models in the NEX-GDDP ensemble (Thrasher et al., 2012) as 2040-2060 averages and people-days are calculated by multiplying by the projected (2050) number of people in each gridcell; both metrics are then summed over the appropriate spatial region. Population distributions are taken from publicly available products that downscale the SSP population scenarios (Jones & O’Neill, 2016; Murakami & Yamagata, 2019; Zoraghein & O’Neill, 2020).

985 rithm that uses a rules-based approach to describe land conversion (M. Chen et al., 2020).
 986 M. Chen et al. (2019) finds a considerable propagation of uncertainty into future pro-
 987 jections, with large effects on grasslands and cropland, but little influence on urban ar-
 988 eas. Demeter is a relatively simple model with few parameters, but similar effects are
 989 likely to be found in more complex downscaling algorithms.

990 In general, the uncertainties of a scenario approach, used alone or in conjunction
 991 with climate projections, are amplified at smaller scales. This is demonstrated in Fig-
 992 ure 6, which shows a simple socioeconomic metric (population), a simple climate met-
 993 ric (gridcell-days above 35°C), and a related joint metric (people-days above 35°C) at
 994 increasingly smaller spatial scales. In each case, relative uncertainty (as measured by the
 995 ensemble spread) increases at smaller scales. We also see that for population projections,
 996 the downscaling algorithm (delineated by different colors) becomes more important than
 997 the SSP scenario (delineated by different shapes) at smaller scales. At all scales, the joint
 998 metric is more uncertain than either single metric.

999 **4.2.3 Temporal Scales**

1000 The appropriate temporal scale of forcing data should be dictated by the relevant
 1001 sectoral dynamics and outcomes of interest. As such, choices should be carefully moti-
 1002 vated by the relevant scales for system dynamics of primary interest: long-term trends
 1003 or short-term stresses? Systems and outcomes that are more sensitive to transitory phe-
 1004 nomena, including tail events that are limited in time, are likely to require forcing data
 1005 generated by an alternative suite of models. For example, time series approaches can be
 1006 used to model various economic indicators at different temporal resolutions (De Winne
 1007 & Peersman, 2021; Koop & Korobilis, 2009). This contrasts with a SSP-like framework
 1008 that aims to understand decadal-scale changes in socioeconomics and thus produce quan-
 1009 titative trajectories that are typically smoothly varying and with 5-year time steps.

1010 The temporal scale of analysis may also influence other modeling decisions in non-
 1011 trivial ways. For example, most population datasets project residential populations rather
 1012 than ambient population, which accounts for daily population movements to and from
 1013 work or school (McKee et al., 2015). Ambient population is likely a more useful metric
 1014 for understanding exposure to short-lived climate or weather hazards.

1015 **5 Scenario Discovery and Characterizing Dynamics**

1016 **5.1 The Role of Scenario Discovery in MSD**

1017 From its inception, MSD has aimed to be societally-relevant by improving our un-
 1018 derstanding of the dynamics of integrated human-Earth systems and impacts on com-
 1019 plex societal changes (Reed et al., 2022). The identification and communication of key
 1020 uncertainties to other researchers, decision-makers, and the public are therefore key com-
 1021 ponents of MSD analyses. However, the high dimensionality, interconnectivity, and com-
 1022 plexity of the uncertainty space discussed in the preceding sections presents a significant
 1023 challenge to this goal. The response of the public and stakeholders to uncertainty is highly
 1024 complex and dependent on a number of factors, including how that uncertainty is com-
 1025 municated to them (Ho & Budescu, 2019; Howe et al., 2019). As such, uncertainties of-
 1026 ten are not fully accounted for in planning processes (Carlsson Kanyama et al., 2019).
 1027 To ensure stakeholders consider uncertainty in their decision-making, researchers must
 1028 supply information that is relevant to addressing their concerns, but does not danger-
 1029 ously narrow the framing of the decision problem.

1030 Our inability to predict *a priori* the leading sources of uncertainty and understand
 1031 how they impact complex outcomes necessitates large ensemble simulations, with hun-
 1032 dreds to millions of scenarios in order to capture tail risks, interactions, and key dynam-

1033 ics (Lamontagne et al., 2018). This requires a method to select a few key desirable or
 1034 undesirable outcomes, ideally representative of a broader class of dynamics, from a large
 1035 set of model runs. Scenario discovery (Bryant & Lempert, 2010) is one class of such meth-
 1036 ods, which has already seen wide adoption in MSD-related work (*e.g.*, Moallemi, Kwakkel,
 1037 de Haan, and Bryan (2020); Lamontagne et al. (2018); Dolan et al. (2021); Jafino and
 1038 Kwakkel (2021); Quinn et al. (2018); Guivarch et al. (2016); Halim et al. (2016); Wang
 1039 et al. (2013)).

1040 Scenario discovery is a computer-assisted approach to scenario development that
 1041 identifies regions of the uncertainty space that are tied to outcomes of interest (Bryant
 1042 & Lempert, 2010; Kwakkel, 2019). These methods begin by sampling possible values of
 1043 uncertain factors, which are then simulated using one or more system models to gener-
 1044 ate a large ensemble of potential future system conditions. Typically, a binary classifi-
 1045 cation is applied to designate scenarios of interest in which some notable outcome is ob-
 1046 served (*e.g.*, a satisficing constraint for objective attainment) (Herman et al., 2015). Machine-
 1047 learning classification methods are then applied to identify the leading predictors of a
 1048 case of interest (Bryant & Lempert, 2010). The most commonly used methods are the
 1049 Patient Rule Induction Method (PRIM, (Friedman & Fisher, 1999)) and Classification
 1050 and Regression Trees (CART, (Breiman et al., 2017)), though other methods can be used,
 1051 such as logistic regression (Quinn et al., 2018; Lamontagne et al., 2019). Once the lead-
 1052 ing predictors and conditions associated with the cases of interest are identified, they are
 1053 ideally translated into qualitative, comprehensible narratives to facilitate communica-
 1054 tion and interpretability (Parker et al., 2015; Trutnevyte et al., 2016; Moallemi et al.,
 1055 2017; Jafino & Kwakkel, 2021). As can be seen by its procedure, scenario discovery is
 1056 primarily focused on parametric uncertainties, which are an accessible if incomplete way
 1057 of defining the space of possible futures.

1058 Scenario discovery is often referred to as a “bottom-up” or *a posteriori* approach
 1059 because it defines key drivers and scenarios after generating and analyzing a large simu-
 1060 lation ensemble. In contrast, “top down” or *a priori* approaches begin with expert as-
 1061 sessment of key drivers and associated uncertainties to develop a small number of sce-
 1062 nario narratives, which are in turn simulated with systems models (Bryant & Lempert,
 1063 2010; Kwakkel, 2019; Maier et al., 2016). The nature of multi-sector systems, which are
 1064 characterized by a large number of uncertainties, emergent complexity, and correlated
 1065 outcomes across sectors, severely limits the ability of any group of experts to anticipate
 1066 key drivers and dynamics (Helbing, 2013; Marchau et al., 2019). In such cases, *a priori*
 1067 approaches may suffer from narrow problem framing, inadequate coverage of surprising
 1068 or paradoxical outcomes, and may be less conducive to participatory decision making
 1069 with diverse stakeholders (Bryant & Lempert, 2010).

1070 As an illustrative example, we once again turn to the impacts of Winter Storm Uri
 1071 in February 2021 (Busby et al., 2021). Despite recent precedent for similarly or more se-
 1072 vere weather conditions (Doss-Gollin et al., 2021), energy and gas operators failed to win-
 1073 terize equipment in Texas. As a result, gas production and delivery were severely cur-
 1074 tailed during the peak of the cold, disrupting electricity production from natural gas while
 1075 smaller outages from wind, nuclear, and coal generating plants also occurred (Busby et
 1076 al., 2021). At the same time, electricity demand for heating spiked, bringing the Texas
 1077 power grid to within minutes of collapse, leading regulators to curtail electricity supply
 1078 to millions of people. The days-long outage severely curtailed the delivery of basic ser-
 1079 vices such as water and wastewater, internet, medical services, food, and heat (Busby
 1080 et al., 2021; Watson et al., 2021). This is an example of a chain of events leading to the
 1081 failure of a critical infrastructure system which, in retrospect, ought to have been fore-
 1082 seen, but which seems to have been missed in scenario planning, particularly as the dis-
 1083 ruption transcended traditional sectoral boundaries.

1084 5.2 Challenges for Scenario Analysis in Multi-Sector Systems Model- 1085 ing

1086 The uncertainties that arise in multi-sector modeling often go beyond what has typi-
1087 cally been explored with Scenario Discovery. In particular, MSD analyses present chal-
1088 lenges to typical scenario discovery approaches for three reasons: (a) the high dimension-
1089 ality of the uncertainty and outcome space, (b) the challenge of defining cases of inter-
1090 est across sectors, and (c) the difficulty of interpreting *a posteriori* scenarios. MSD re-
1091 searchers should be aware of these gaps, and potential alternative methods, as they iden-
1092 tify scenarios of interest for further analysis and communication.

1093 5.2.1 High Dimensional Uncertainty and Outcome Spaces

1094 Any scenario analysis begins with a design of experiment, which is unavoidably an
1095 *a priori* narrowing of the uncertainty space to be explored. In the MSD setting this is
1096 increasingly difficult as complex systems interactions and teleconnections massively ex-
1097 pand the space that needs to be considered, while simultaneously obscuring the key un-
1098 certainties and amplifying the consequences of an incomplete representation. This presents
1099 a major challenge to scenario discovery in MSD. Incomplete representations of uncer-
1100 tainty typically manifest in three ways: the selection of factors, the number of samples,
1101 and the range of samples.

1102 In Section 3.2.2, we discussed factor-fixing through sensitivity analysis. These tech-
1103 niques may fail when confronted with path dependence, emergence, and multiple out-
1104 puts of interest. Factor influence may evolve over time and depend on earlier systems
1105 evolution, and is unlikely to be the same across output metrics (Lamontagne et al., 2018).
1106 Often, a more informal factor-fixing ensues in MSD studies, driven by “lamp-post sci-
1107 ence,” where factors are varied because existing databases, such as the RCPs or the SSPs,
1108 make them easy to include, while other factors are fixed simply because they are more
1109 difficult to sample or because existing products fail to account for their uncertainties (as
1110 discussed in Section 4). A common example is an under-representation of structural un-
1111 certainties in scenario discovery, such as model structural uncertainty or the decision prob-
1112 lem framing (Quinn et al., 2017; Rozenberg et al., 2014). Such experimental designs are
1113 often necessary to limit computational expense, but the resulting consequences for pro-
1114 jections and planning are difficult to quantify.

1115 Sparse sampling of uncertainties is one way to limit the computational cost of gen-
1116 erating ensembles of model runs, but this can severely limit our ability to identify lead-
1117 ing drivers of outcomes. As an example, Lamontagne et al. (2018) considered more than
1118 33,000 scenarios derived as hybrids of the SSPs: a marked increase over the 3-5 canon-
1119 ical SSPs considered in many analyses. This decoupling of the SSP dimensions highlighted
1120 plausible yet overlooked narratives with serious global consequences. However, the ex-
1121 perimental design in Lamontagne et al. (2018) did not disentangle, for instance, the yield
1122 improvements for different crops in each of the 285 modeled land-use regions across the
1123 globe, nor were GDP or energy technology trajectories decoupled for individual coun-
1124 tries, instead opting to vary “consistent” SSP narratives for different sectors. It is not
1125 clear that such consistency is epistemically valuable for scenario discovery. Sectoral stud-
1126 ies in water resources suggest these choices may substantially bias robustness and sce-
1127 nario discovery assessments (Quinn et al., 2020; McPhail et al., 2020).

1128 The high dimensionality of the uncertainty space often necessitates inadequate cov-
1129 erage of extreme cases that are likely to drive cases of interest. This is particularly acute
1130 in the case of deep uncertainty, where full UQ may be inappropriate. One approach is
1131 to use multiple models with varying structures instead of a single, more complex model;
1132 scenario discovery on the resulting multi-model ensemble can yield insights into differ-
1133 ent dynamical pathways leading to outcomes of interest under varying assumptions (Kwakkel
1134 et al., 2013; Auping et al., 2014).

1135 **5.2.2 Multiple Outcomes of Interest**

1136 Within a single-sector or regional analysis, defining cases of interest can be rela-
 1137 tively straightforward (*e.g.*, when is a levee overtopped, or when is there a blackout?).
 1138 Many sectoral studies have utilized satisficing criteria across several metrics, often uti-
 1139 lizing the logical connection between those metrics to identify cases of interest, followed
 1140 by binary classification on those scenarios (Herman et al., 2014). In MSD settings, this
 1141 process is more complicated as the number of sectors and regions increase, with corre-
 1142 spondingly more complex interactions and teleconnections. For these complex systems,
 1143 it is not necessarily clear *a priori* which output(s) might be correlated and simultane-
 1144 ously achieve the satisficing criteria. For instance, Jafino and Kwakkel (2021) illustrate
 1145 diverse inequality patterns in adaptive water-food management that defy binary clas-
 1146 sification. The dynamical nature of MSD systems also presents a challenge to traditional
 1147 binary scenario discovery, as the timing of failure conditions can be an important con-
 1148 sideration (Steinmann et al., 2020). Another complication is the presence of spatial and
 1149 temporal teleconnections, which may mean that outcomes of interest in different sectors
 1150 occur at different time steps or different spatial regions.

1151 One potentially promising category of techniques is multinomial classification, wherein
 1152 scenario discovery simultaneously identifies multiple different “cases of interest” (Gerst
 1153 et al., 2013). Typically, this is performed in a sequential approach, where the output space
 1154 is first partitioned into classes of interest, then classification tools are used to identify
 1155 input factors that are most predictive of individual class membership (Jafino & Kwakkel,
 1156 2021). The partition of the outcome space could be manual (Lamontagne et al., 2018;
 1157 Rozenberg et al., 2014), or utilize clustering algorithms (Gerst et al., 2013; Steinmann
 1158 et al., 2020). Manual classification has the advantage of interpretability but suffers from
 1159 the same weaknesses as *a priori* scenario development for high dimensional problems.
 1160 On the other hand, while clustering with statistical algorithms is more scalable, the re-
 1161 sulting classes can be difficult to interpret, and the results can be sensitive to a number
 1162 of choices, such as the number of classes. Standard scenario discovery is then often im-
 1163 plemented on each of the classes individually through a series of binary classification prob-
 1164 lems. One drawback of this is that the membership rules between classes might not be
 1165 easily distinguishable (Kwakkel & Jaxa-Rozen, 2016), which may hinder stakeholder en-
 1166 gagement (Jafino & Kwakkel, 2021). Because the classification is conducted independently,
 1167 the relationship between classes may also be difficult to interpret. Alternatively, a con-
 1168 current multinomial scenario discovery approach has also been proposed (Jafino & Kwakkel,
 1169 2021), which simultaneously partitions the data and predicts class membership through
 1170 the use of multivariate regression trees. This approach can reveal more detailed classes
 1171 than the sequential approach, but this comes at the expense of interpretability and com-
 1172 municability.

1173 The scale, diversity, and interconnectivity of the uncertainty space in MSD prob-
 1174 lems poses a significant challenge to traditional scenario discovery techniques. For ex-
 1175 ample, how can we identify the potential for cross-sector interactions to lead to cascad-
 1176 ing failures? One route is through the application of methods from the complexity sci-
 1177 ences to investigate nonlinear feedbacks, emergent behavior, and tipping points (Berkes,
 1178 2007). Similar to scenario discovery, these approaches aim to understand the space of
 1179 possible trajectories of a system rather than prediction of the particular system state at
 1180 a given point in time (Brugnach & Pahl-Wostl, 2008), in part reflecting the high levels
 1181 of uncertainty in MSD systems (Vogel et al., 2015).

1182 A complex systems approach to understanding parametric uncertainty can provide
 1183 more information than typical sensitivity analyses about the importance of model pa-
 1184 rameters in determining qualitative behavior. Qualitative behavior of interest, for ex-
 1185 ample, would involve regime shifts toward an unstable equilibrium consisting of a dif-
 1186 ferent set of feedbacks. Examples of regime shifts include a lake switching from being
 1187 oligotrophic to eutrophic (Carpenter, 2005), as well as the collapse of communities that

1188 are economically dependent on local natural resources (Y. Chen et al., 2009). The possi-
 1189 bility of this type of sudden, discontinuous change in equilibrium behavior does not nec-
 1190 essarily exist in all systems, but becomes more likely in highly coupled systems (Lade
 1191 et al., 2013).

1192 One example of a dynamical systems tool with potential application to MSD anal-
 1193 yses is topological data analysis (TDA) (Wasserman, 2018; Smith et al., 2021; Chazal
 1194 & Michel, 2021) to understanding the network structure of coupled model output. An-
 1195 other example is generalized modeling, which is a form of dynamical systems analysis
 1196 that does not require specifying functional forms. Instead, it allows the functional forms
 1197 and magnitudes of relationships between variables to be treated as parameters (Gross
 1198 & Feudel, 2006; Lade & Gross, 2012; Lade & Niiranen, 2017). Finally, structural uncer-
 1199 tainty in agent-based modeling can be addressed using pattern-oriented modeling, a method
 1200 that involves formulating alternative theories of agents' behavior and testing them by
 1201 how well they reproduce characteristic patterns at multiple levels (Grimm et al., 2005).

1202 **5.2.3 Scenario Interpretability**

1203 A primary goal of decision support for MSD is to identify broadly plausible path-
 1204 ways by which good or bad outcomes might occur and be influenced by changes to ex-
 1205 ogenous forcings, system dynamics, and/or policy interventions. This requires identify-
 1206 ing and articulating the patterns and mechanisms by which these changes propagate through
 1207 the coupled system. However, a typical theme in statistical learning is the tension be-
 1208 tween classification ability and the interpretability of the resulting classes. In scenario
 1209 discovery, the emphasis is to maximize interpretability, at the expense of "optimal" clas-
 1210 sification.

1211 Interpretability is particularly difficult in MSD settings given the presence of tele-
 1212 connections and emergent dynamics. While a powerful classifier may be able to identify
 1213 the experimental factors related to scenarios of interest, the resulting scenarios may not
 1214 be tied to a clear narrative explaining the circumstances and dynamics driving the out-
 1215 comes. The interpretability-prediction tradeoff is not unique to scenario discovery or MSD,
 1216 and there exists an opportunity to include emerging developments in machine learning
 1217 and visual analytics with existing scenario discovery workflows to improve interpretabil-
 1218 ity. One such direction is the use of machine learning methods to predict future vulner-
 1219 able conditions based on observed system states and fluxes (B. Robinson et al., 2020),
 1220 and to design dynamic adaptation policies to mitigate them (J. S. Cohen & Herman, 2021).
 1221 Advances in interpretable machine learning (Rudin, 2014; Rudin et al., 2021; Murdoch
 1222 et al., 2019; Molnar et al., 2020) also present opportunities to help navigate the trade-
 1223 off between interpretability and classification when analyzing model output ensembles.
 1224 Interpretable approaches to machine learning also have the potential advantage of in-
 1225 creased transparency, which might help expose systematic biases in MSD modeling which
 1226 could be relevant to decision-making.

1227 Despite challenges to interpretability, MSD model projections and analyses can be
 1228 useful in informing policy under uncertainty. For example, lower-dimensional models have
 1229 been used in social-ecological systems literature to provide broad insight into resource
 1230 management problems relevant to MSD while remaining interpretable. The robust con-
 1231 trol framework has been used to identify fundamental tradeoffs in the robustness of dif-
 1232 ferent institutional arrangements, modeled as different controllers for the system, to pa-
 1233 rameter uncertainty (Anderies et al., 2007; Rodriguez et al., 2011). This approach has
 1234 also shown how preparing for certain types of shocks may make a system more vulner-
 1235 able to novel ones (Cifdaloz et al., 2010; Carlson & Doyle, 1999, 2000; Doyle & Carlson,
 1236 2000; Manning et al., 2005). This same modeling framework has also been used to ex-
 1237 plore how policy implementation issues that result from or exacerbate uncertainty, such
 1238 as infrequent sampling or implementation delays, impact policy performance (Rodriguez

et al., 2011), especially under the possibility of regime shifts (Polasky et al., 2011). Finally, MSD models have been used to identify safe operating spaces (Barfuss et al., 2018; Cooper & Dearing, 2019; Rockström et al., 2009) and identify threats to system resilience and the importance of cross-sectoral policies (Brunner & Grêt-Regamey, 2016).

Model development is a component of uncertainty characterization and can aid the process of communication, social learning, and exploration of scenarios and solutions among diverse stakeholders (Brugnach & Pahl-Wostl, 2008). Methods for exploring structural uncertainty, especially when paired with expert elicitation and participatory processes, help identify conflicts and agreements and make explicit different problem framings and mental models (Brugnach & Pahl-Wostl, 2008; Hare & Pahl-Wostl, 2002; Rouwette & Vennix, 2020). In addition to improving the model predictions, this process also increases the likelihood of stakeholders accepting model results (Pahl-Wostl, 2007; Giordano et al., 2020). For MSD systems, scaling these participatory modeling approaches to higher levels of governance with far more stakeholders remains a challenge, though there is an emerging environmental governance literature aimed at informing these higher level processes, particularly in the context of global climate change policy (Cloutier et al., 2015; Figueiredo & Perkins, 2013; Fröhlich & Knieling, 2013).

6 Conclusions & Best Practices

MSD is an emerging area of research focused on identifying and analyzing complex systems related to critical societal questions. Conclusions based on limited analysis (for example, analyses which only account for a handful of scenarios), could harm decision-making by anchoring stakeholders to a range of outcomes which might not be representative of true risks. As a result, all MSD analyses ought to explicitly discuss how the research methods treated uncertainty (or consciously chose not to, for example in a benchmarking activity).

It is not necessarily reasonable or even desirable for every MSD analysis to account for all types of uncertainties. For example, while we have focused on quantitative aspects of uncertainty analysis for MSD systems, there are a number of other considerations which might influence an MSD research design (Renn et al., 2020). For example, governance or stakeholder concerns might reduce the range of uncertainties, system configurations, or decision alternatives under consideration. The translation of systemic risk analyses into governance strategies is also critical, and requires an interdisciplinary, layered approach (Renn et al., 2020; Hochrainer-Stigler et al., 2020). Additionally, it can often be easier to focus on specific uncertainties or dynamics with reduced-form representations or samples of less-relevant model components.

Rather, best practices in MSD uncertainty analysis should facilitate communication across interdisciplinary teams of investigators and emphasize transparency, so that uncertainties that were not considered or fully treated in a given analysis can be examined in subsequent studies. One of the key points we have tried to emphasize is that many uncertainty-relevant research decisions should be made intentionally, to ensure that they are aligned with the research question, and that the resulting interpretation of results takes place within the context of the research design. To this end, we suggest that MSD research should include the following best practices and principles, though this list is by no means exhaustive and will likely evolve as practices and methods change over time.

1. *Develop consistent vocabulary:* Differing uses of terms such as “uncertainty characterization” can hinder the interdisciplinary collaboration which is intrinsically part of MSD. Standard definitions of approaches and a standard classification of uncertainty types can help clarify how uncertainties were and will be conceptualized and treated.

- 1288 2. *Include wiring diagrams and graphical representations of modeling choices:* As dis-
 1289 cussed in Section 2.2, choices related to control volumes and coupling direction-
 1290 alities can limit how uncertainties can be represented and alter the resulting dy-
 1291 namics, such as introducing amplifying or dampening feedbacks. Contextualizing
 1292 the results of an MSD analysis can be difficult without transparent communica-
 1293 tion of these choices. We prefer the inclusion of graphical representations of cou-
 1294 pling frameworks, such as those seen in Figure 4, as they illustrate the control vol-
 1295 ume while making cycles and other connections clear.
- 1296 3. *Deliberate selection of methods and data products for uncertainty analysis:* Almost
 1297 every choice about the treatment of uncertainty, from calibration through scenario
 1298 discovery, involves tradeoffs affecting the ability to address the driving research
 1299 question. As a result, these choices should be justified based on the aims of the
 1300 analysis. Documenting the motivation behind these choices, and their limitations,
 1301 helps to contextualize the results and defines clear opportunities for future research.
- 1302 4. *Test sensitivities to UQ assumptions about deep uncertainties:* In Section 3, we
 1303 discussed the importance of the prior ranges and distributions used in an uncer-
 1304 tainty analysis. When deep uncertainties are present and could influence calibra-
 1305 tion results through data or constraints, the use of a single input distribution to
 1306 produce probabilistic projections could be misleading. When computationally tractable,
 1307 one approach could be to re-calibrate the model under various realizations of deeply
 1308 uncertain factors (*e.g.*, Srikrishnan et al. (2022)), but in general, a sensitivity anal-
 1309 ysis should be conducted to explore the dependence of the obtained projections
 1310 on the choices made in quantifying inputs.
- 1311 5. *Make model code and configurations open-source and open-access:* One category
 1312 of uncertainties mentioned in Kennedy and O’Hagan (2001) that we do not ex-
 1313 plicitly account for in our taxonomy (though it is a subset of structural uncertainty
 1314 in our framework) is “code uncertainty,” as the specific implementation of model
 1315 code can create uncertainty in outcomes. Well-documented and open-source code
 1316 increases transparency around this class of uncertainties. Moreover, MSD mod-
 1317 eling frameworks are complex, and potentially highly sensitive to specific choices
 1318 of parameter values. Configuration files can be easily shared in public reposi-
 1319 tories along with the model code used for the analysis and documentation. Align-
 1320 ment with the FAIR principles (Wilkinson et al., 2016) for data and code shar-
 1321 ing should also be encouraged.

1322 Throughout our discussion, we have also identified several challenges and poten-
 1323 tial research opportunities, some of which cut across the different stages of MSD uncer-
 1324 tainty analyses. One always-present challenge is created by the increased computational
 1325 complexity of MSD models relative to single-sector models. Further advances in statis-
 1326 tical computing via emulation or parallelized calibration methods can help navigate this
 1327 tradeoff and leverage high-performance computing environments. Innovation applications
 1328 of machine-learning methods could be particularly fruitful, either for use as emulators
 1329 or as a direct replacement for mechanistically-motivated models (though this requires
 1330 careful model construction and *post hoc* UC and SA exercises to avoid overfitting a black-
 1331 box model). Advanced machine learning methods, particularly those that feature increased
 1332 interpretability, could also be fruitful when applied to high-dimensional scenario clas-
 1333 sification and identification. Methods from closely-related disciplines, such as complex-
 1334 ity science and network analysis, should also be tested for suitability in MSD applica-
 1335 tions, to further address these challenges.

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 1354 EarthsFuture_2022_MSD_Uncertainty](https://github.com/david0811/EarthsFuture_2022_MSD_Uncertainty).

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