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Exploratory modeling for analyzing coupled human-natural systems under uncertainty

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Abstract

Modeling is a crucial approach for understanding the past and exploring the future of coupled human-natural systems. However, uncertainty in various forms challenges inferences from modeling results. Model-based support for decision-making has increasingly adopted an emerging *exploratory* approach. This approach addresses uncertainty explicitly through systematically exploring the implications of modeling assumptions, aiming to enhance the *robustness* of inferences from models. Despite a variety of applications, the extent and the way(s) that exploratory modeling can deal with the challenges that arise from the uncertainty and complexity of decision-making with stakeholders has not yet been systematically framed. We address this gap in two ways. First, we present a taxonomy of the ways that exploratory modeling can be used to inform robust inferences in coupled human-natural systems by mapping the technical capabilities of this approach in relation to the diversity of past applications. This subsequently guides an investigation of the practical benefits and challenges of these capabilities in handling uncertainty and complexity. Second, we discuss different ways for integrating genuine stakeholder engagement into exploratory modeling through transdisciplinary research. Finally we outline some priorities for future expansion of this research area.

Keywords: Decision-making, adaptation, uncertainty, robustness, stakeholder, participatory, sustainability.

1 Introduction

Significant concerns have arisen from impacts of global change on water resources, ecosystems, land use, and food production, worldwide (Eker *et al.*, 2019; Gao & Bryan, 2017; Khazaei *et al.*, 2019; Quinn *et al.*, 2018). Data on the not-yet-experienced states and multi-decadal impacts of global change are limited given the presence of many highly interrelated, complex, variable, and poorly understood human-natural systems and because of the long timescales involved (Funtowicz & Ravetz, 1990; Lamontagne *et al.*, 2019; Oddo *et al.*, 2017; Weaver *et al.*, 2013). Despite the complexity and limited data availability, computer modeling and simulation are widely-used tools to understand environmental and societal risks of global change on human-natural systems (Bilskie *et al.*, 2016; Fischer *et al.*, 2005). For the purpose of this article, we define a *model* as a formal description of human knowledge about the nexus of systems driven by physical, chemical, and biological mechanisms as well as societal, economic, and political forces. A *simulation* means using such a model, running it to inspect how these systems manifest and interact, usually as a function of time. A diverse set of models and model-based inferences is used to underpin decision-making under global change spanning areas such as food and diet (Bijl *et al.*, 2017; Eker *et al.*, 2019; Malek *et al.*, 2020), climate adaptation (JGCRI, 2017; Mayer *et al.*, 2017; Small & Xian, 2018), and land use (Doelman *et al.*, 2018; Gao & Bryan, 2017). Models can play an important role in our understanding of the Earth's climate, water, land dynamics, and energy conditions in the past (e.g., cycles of ice ages over the past two million years) and the ways that this can change in the future (e.g., via global warming). These modeling efforts have underlined the importance of systematically dealing with complexity and uncertainty as defining properties of all human-natural systems (Verburg *et al.*, 2016) and of the policy design process (Mercure *et al.*, 2016). Here we analyze the extent of modeling capabilities, challenges, and opportunities for navigating the complexity and uncertainty that arise in understanding and managing coupled human-natural systems.

The knowledge we put into models is, in most cases (except perhaps *purely* mathematical or logical models), imperfect and uncertain. Uncertainties lurk throughout different facets of modeling and simulation including conceptual framing, boundary conditions, the choice of modeling paradigms, model structures and schematizations, input data, scenario assumptions, and performance metrics, as systematically pointed out by Morgan *et al.* (1990), Walker *et al.* (2003), Lempert *et al.* (2003), McPhail *et al.* (2018), and Khatami *et al.* (2019). Traditionally, a consolidative approach to modeling — as Bankes (1993) stated — incorporates all known facts into a best estimate package which can then be used for predicting system behavior (Lempert & Collins, 2007). Such a consolidative approach frames uncertainty as something that is imaginable. However, future climate and environmental conditions and their societal risks are a not-yet-experienced state of human-natural systems. Therefore, *a priori* calibration of models will not produce reliable long-term forecasts (Weaver *et al.*, 2013). Modeling approaches that rely on things being imaginable — if perhaps improbable and implausible — cannot usually deal with so-called 'Grey Swans' or 'unknown knowns', that is unexpected consequences of that which we already knew (Di Baldassarre *et al.*, 2016). Consolidative approaches also fail when confronted with missing data or inadequate theories (Weaver *et al.*, 2013). Unknown knowns, missing data, and inadequate theories are not amenable to probabilistic characterization and may not even be assigned a likelihood of occurrence (Maier *et al.*, 2016). Their values are either unknowable at present, or no agreement can be reached about their values because of the presence of multiple stakeholders with different, often contrasting views. This range of uncertainties which cannot be meaningfully couched as probabilities, initially discussed in the context of Knightian uncertainty (Knight, 1921), has been recently termed *deep uncertainty* (Lempert *et al.*, 2003) or *severe uncertainty* (Ben-Haim, 2006).

Exploratory modeling is an approach, a philosophy, of modeling which is concerned specifically with dealing with deep uncertainty and complexity (Bankes, 2002b; Lempert *et al.*, 2003). The approach was conceived and pioneered at the RAND Corporation, notably by Hodges (1991), Hodges and Dewar (1992), Bankes (1993), Bankes (2002b), Lempert (2002), Lempert *et* *al.* (2003), and Bankes *et al.* (2013). The central idea of exploratory modeling is to let go of the ideal of a model as a predictive tool which turns best available knowledge into a best estimate, and to abandon the notion of a good model being one that gives an accurate prediction of the most likely development of the system (Kwakkel & Haasnoot, 2019). Rather, a model is seen as a thinking aid where the aim is to capture relevant uncertainties by enumerating a range of possible assumptions and systematically exploring the implications of these assumptions via large numbers of computational experiments.

The core idea of exploratory modeling has been adopted in theory and model development aimed at explaining a potential phenomenon of interest or to test and refine a set of hypotheses and assumptions (de Haan *et al.*, 2016). This corresponds to Bankes (1993) *data-driven* and *model-driven* exploratory modeling. The former aims to reveal regularities, patterns, goodness-of-fit, and structure of a dataset, while the latter asks whether and under what conditions several models of the same phenomenon can produce similar behavior (Auping *et al.*, 2016). Exploratory modeling has been adopted much more widely in model-based decision support for a variety of human-natural systems under deep uncertainty (Helgeson, 2020), for example in water resource management (Gold *et al.*, 2019; Trindade *et al.*, 2017; Trindade *et al.*, 2019) and in supporting climate-related decisions (Isley *et al.*, 2015; Lamontagne *et al.*, 2019; Sriver *et al.*, 2018; Weaver *et al.*, 2013). Exploratory modeling is also a key model-based approach for supporting the design of adaptive policy pathways that aim to combine low-regret, short-term actions with long-term solutions to adapt (if needed) to uncertain future change (Haasnoot *et al.*, 2013; Trindade *et al.*, 2019; Wise *et al.*, 2014). This approach enables the investigation of the efficacy of monitoring systems for adapting to global change (Haasnoot *et al.*, 2018; Raso *et al.*, 2019). These widely-used applications of exploratory modeling are *question-driven* and case-based (Boero & Squazzoni, 2005), designed to illuminate robust policy choices and develop adaptation plans for a specific decision problem.

Several studies have attempted to inform exploratory modeling through detailed classifications of decision support frameworks (Herman *et al.*, 2020; Herman *et al.*, 2015; Kwakkel & Haasnoot, 2019; Moallemi *et al.*, 2020b), scenario approaches (Guivarch *et al.*, 2017; Trutnevyte *et al.*, 2016), robustness metrics (McPhail *et al.*, 2018), and scenario selection (McPhail *et al.*, 2020). However, these have either been sector-specific (e.g., water), method-specific, or focused on a particular topic (e.g., scenarios) rather than discussing the bigger picture and the synthesis of different topics. This has led to a major gap where exploratory modeling, as an emerging field with interlinkages between its different areas, has not yet been systematically framed to guide a broader audience in extending and combining its capabilities in new sectoral domains (e.g., integrated assessment modeling (Obersteiner *et al.*, 2016)). This situation has an analogy with the related area of sensitivity analysis where there are similar concerns around being mostly method- or domain-focused (Saltelli *et al.*, 2019).

Here we formulate a taxonomy of exploratory modeling approaches for decision-making to map emerging technical capabilities in addressing uncertainty and complexity (Section 2). While past studies have discussed specific details of these capabilities, we focus on the combination of these capabilities and how they can be used to deal with the challenges and opportunities that arise in the modeling of coupled human-natural systems. We analyze several recent studies through the lens of this taxonomy to illustrate the diversity of the field (Section 3). We discuss the strengths of the iterative process of exploratory modeling from which researchers can benefit and reflect on some of the known issues and challenges that remain to be addressed

(Section 4). As a direction for future research, we discuss different ways for engaging with stakeholders in exploratory modeling for the co-creation of model inferences as an emerging and popular topic in the literature and a major gap in the literature (Section 5). Our motivation is to encourage and guide researchers and practitioners across disciplines to adopt exploratory modeling beyond the currently established decision-making frameworks and in new applications for sustainability. A simple and widely accessible description of exploratory modeling can pave the way for its further contribution to decision-making under uncertainty in high-impact international science-policy arenas such as the Sustainable Development Goals (UN, 2015), the Intergovernmental Panel on Climate Change (IPCC, 2019), and the Intergovernmental Platform on Biodiversity and Ecosystem Services (IPBES, 2019).

2 A taxonomy of exploratory modeling for decision support

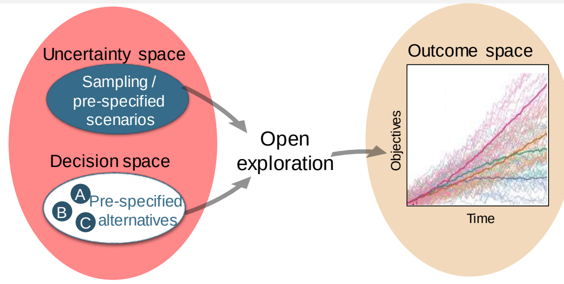
The use of exploratory modeling in supporting decision-making often starts by formulating an initial decision problem that can be revised iteratively throughout the modeling process (Quinn *et al.*, 2017). Typically, the problem formulation involves the specification of scenarios, decision alternatives, robustness metrics, and models (Lempert *et al.*, 2003; Walker, 2000). A scenario, in the context of exploratory modeling, is a fully specified realization of sampled values from the model parameter uncertainty space, representing a future state of the world. An example from climate change scenarios is a multi-dimensional uncertainty space created by the combination of different growth rates for population and the economy and different time series for the price of fossil fuels and renewable energy technology in the future where each point sampled from this space is a single socio-economic scenario (Riahi *et al.*, 2017). A decision alternative is a vector of decision variables/levers in a multi-dimensional decision space that fully specifies all required candidate actions/choices. An example of a lever is a feed-in tariff or renewable energy credit price in the electricity sector, where a vector from a specific value of each lever forms a decision alternative for supporting the renewable energy generation. Models are used to generate computational experiments, analyzing the implications of decision alternatives over the diversity of scenarios in an outcome space. The outcome space contains the (potential) results of the computational experiments (i.e., simulation runs) which could be post-processed using various robustness metrics, indicating how well the system performs under a range of plausible conditions (e.g., absolute performance or regret) (McPhail *et al.*, 2018).

Different exploratory modeling approaches share the core idea of systematically analyzing the implications of decision and uncertainty spaces in the outcome space. However, they can be implemented in different ways through open exploration or directed search. Under uncertainty, there is a large set of possible assumptions from which we need to draw inferences (i.e., decision insights/conclusions that we obtain from results). Open exploration through the *design of experiments* and *stress-testing* is one way of investigating global properties of the assumption set. These approaches involve systematic sampling (e.g., via Latin Hypercube or Monte Carlo Sampling) from the uncertainty/decision space to generate a series of computational experiments with good space filling properties. The experiments are used to run the model and to analyze the model results for policy-relevant inferences. Open exploration generates a broad understanding of the implications and vulnerabilities of alternative assumptions. However, the weakness of open exploration emerges for systems with complex combinations of decisions that require the attainment of high levels of sustained performance often for conflicting objectives. Several studies have shown that in many systems without more formalized directed search, an open exploration is myopic in focusing on a limited set of alternatives and in not capturing key trade-offs (Gold *et al.*, 2019; Zeff *et al.*, 2014). This initially led to early work (Kasprzyk *et al.*, 2009; Reed *et al.*, 2008) on the use of *(many-objective) optimization* algorithms (Halim *et al.*, 2016; Kollat & Reed, 2006; Reed *et al.*, 2013) to search for specific decisions and scenarios which lead to properties of interest in the outcome space. In other words, optimization investigates closely the reasons (assumptions) behind the properties of interest and finds specific inferences. More recent work has shown that including open exploration and deep uncertainties in directed search can yield substantially more robust and effective candidate decisions, which has led to the increasing use of *many-objective robust optimization* (Bartholomew & Kwakkel, 2020; Eker & Kwakkel, 2018; Quinn *et al.*, 2018; Trindade *et al.*, 2019).

Box 1 and Box 2 present the taxonomy of these exploratory modeling approaches, articulating the "what" and "why" of different components of the problem framing and characterizing the *problem type* (i.e., the type of research problem that can be answered), *decision specification* (i.e., how decision alternatives are generated), *uncertainty characterization* (i.e., how scenarios are generated), type of *outcome implication* (i.e., the inferences obtained from the analysis), and an *example* of an application. We also further elaborated three examples from different sectors to show how these approaches lead to different types of robust inferences in Appendix C. While we characterize different exploratory modeling approaches, we avoid rigid divisions (i.e., dichotomy or polychotomy) between them as they can overlap and interact with one another. For example, in Box 1, design of experiments and stress-testing are not mutually exclusive, and they can both use sensitivity analysis. Stress-testing can be implemented using sensitivity analysis to identify those factors that most influence certain properties of interest (Lamontagne *et al.*, 2018). However, stress-testing can be implemented in other ways too, for example using the patient rule-induction method (Guivarch *et al.*, 2016), classification and regression trees (CART) (Lempert *et al.*, 2008), many-objective optimization (Kwakkel, 2019), and logistic regression (Quinn, 2017). Conversely, not all sensitivity analysis processes in exploratory modeling are for the purpose of stress-testing. Sensitivity analysis can also be used in the design of experiments for investigating how variation in model output can be attributed to variations in inputs to identify the most important decision alternatives or scenarios. See Appendix B for a further discussion about sensitivity analysis in relation to exploratory modeling.

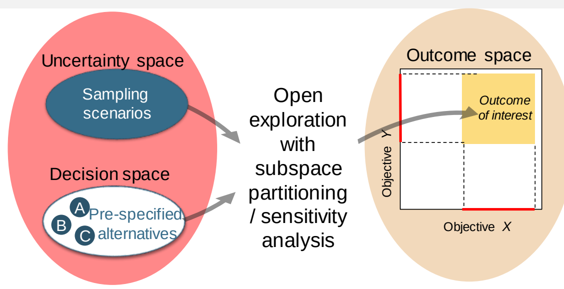
Box 1. **Exploratory modeling approaches**. (a) design of experiments, (b) stress-testing.

a) Design of experiments (i.e., quasi-random sampling)



Problem type: how sensitive is the fulfilment of objectives to alternatives/scenarios?
Decision specification: a set of pre-specified alternatives is selected a priori (by experts or from literature) to be evaluated under many scenarios.
Uncertainty characterization: random values from the uncertainty space are systematically sampled to generate/represent many possible scenarios/states of the world.
Outcome implication: identifying the specific alternatives that can leverage performance the most.
Example: Moallemi and Köhler (2019) used design of experiments and sensitivity analysis to identify the most important household behavioral factors that could promote transitions to sustainable mobility in the UK.

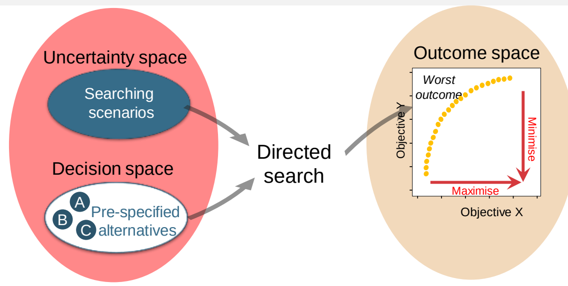
b) Stress-testing (i.e., adaptation tipping points and scenario discovery)



Problem: under what scenarios does a decision alternative fail to achieve objectives (or certain outcomes of interest)?
Decision specification: a set of pre-specified alternatives is selected a priori, but they are refined iteratively for improvement in their robustness to future vulnerabilities.
Uncertainty characterization: random values are systematically sampled from the uncertainty space to generate/represent many possible scenarios. The generated scenarios are then investigated with subspace partitioning (Bryant & Lempert, 2010) or sensitivity analysis (Lamontagne et al., 2018) for stress-testing and scenario discovery.
Outcome implication: specifying scenarios when certain performance thresholds are passed or a specific outcome of interest is observed (e.g., when and how to adapt a decision).
Example: Lamontagne et al. (2018) used statistical scenario discovery to identify global climate change scenario assumptions that are most relevant to the outcomes of interest of high or low mitigation costs.

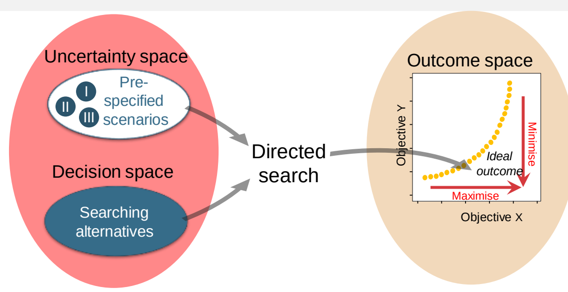
Box 2. Exploratory modeling approaches (cont'd). (c) worst-case scenario discovery, (d) many-objective optimization, and (e) many-objective robust optimization.

c) Worst-case scenario discovery



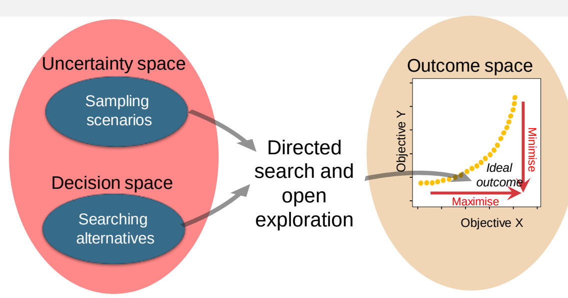
Problem: what are the worst possible outcomes and under which scenarios do they appear?
Decision specification: a set of pre-specified alternatives is selected a priori to be tested under worst-case conditions.
Uncertainty characterization: the uncertainty space is searched for specific scenarios that could lead to the worst outcome.
Outcome implication: identifying a set of small changes that substantially deteriorate the outcome of each candidate alternative.
Example: Halim et al. (2016) assessed the implications of various uncertainties that could substantially affect the competitive position of European ports in the global container transport system.

d) Many-objective optimization



Problem: what are 'good' decisions that can trade-off between a set of conflicting objectives under reference scenarios?
Decision specification: the decision space is searched for specific alternatives that can capture key trade-offs between conflicting objectives.
Uncertainty characterization: a set of pre-specified scenarios can be selected a priori for the evaluation of the decision alternatives.
Outcome implication: identifying decisions which can make good trade-offs between multiple objectives under reference scenarios.
Example: Kasprzyk et al. (2009) analyzed the trade-offs associated with managing the urban water supply risks under growing demand and drought.

e) Many-objective robust optimization



Problem: what decisions can robustly trade-off between a set of conflicting objectives over many scenarios?
Decision specification: the decision space is searched for specific alternatives that can capture key trade-offs between conflicting objectives.
Uncertainty characterization: random values are systematically sampled from the uncertainty space to generate/represent many possible scenarios for testing the robustness of the decision alternatives.
Outcome implication: identifying decisions which can make good trade-offs between multiple objectives over many scenarios in the uncertainty space.
Example: Trindade et al. (2017) used robust optimization for regional water portfolio planning in North Carolina, USA.

How do these different exploratory modeling approaches fit together? There has been a growing interest in combining exploratory modeling approaches to better address complex policy questions. For example, Watson and Kasprzyk (2017) used the strength of scenario discovery in vulnerability assessment to complement the analysis of candidate decisions identified through many-objective optimization. This combination of exploratory modeling approaches has led to new ways to support decision-making, broadly categorized into two (not mutually exclusive) groups (Herman *et al.*, 2020; Kwakkel & Haasnoot, 2019): *robustness frameworks* that often focus on static plans and suggest decisions which work under a range of uncertain futures, and; *adaptation frameworks* that focus on the importance of flexibility in decision-making and suggest adaptive decisions that can respond to emerging challenges and opportunities over time (Figure 1).

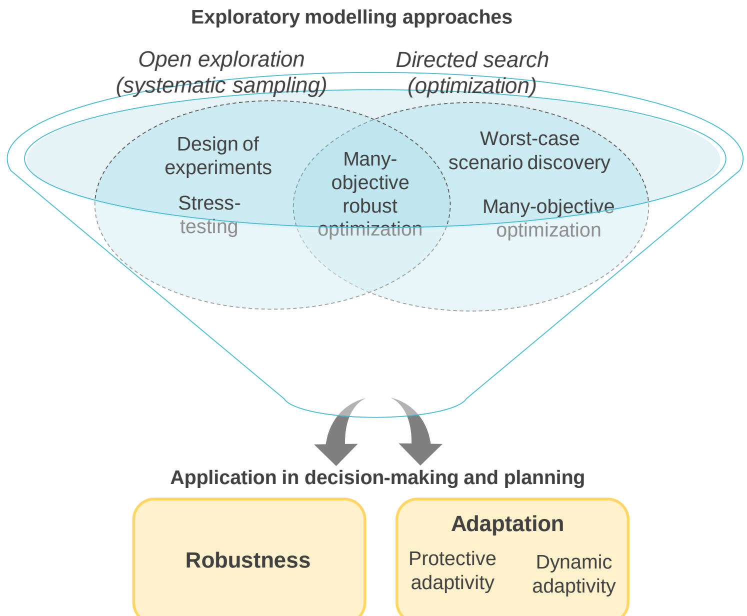


Figure 1. **An overview of potential approaches of exploratory modeling and their applications in decision-making and planning**. Different types of exploratory modeling approaches can be combined with one another in support of robust or adaptive decision-making.

Examples of robustness frameworks include Robust Decision Making (Lempert *et al.*, 2003), Info-Gap (Ben-Haim, 2019) and Decision Scaling (Brown *et al.*, 2012). They often use stress-testing (Lempert *et al.*, 2013) or worst-case scenario discovery (Halim *et al.*, 2016) to identify system vulnerabilities under deep uncertainty and then use the design of experiments (Moallemi *et al.*, 2017) or many-objective (robust) optimization (Trindade *et al.*, 2017) to recommend decisions with robust performance over scenarios. The process of designing a plan with robustness frameworks is often less dependent on uncertainty characterization due to the presence of the uniformly sampled values from the uncertainty space and the assessment of decision alternatives over the ensemble of sampled scenarios. Adaptation frameworks recommend decision alternatives that can be adapted over time in response to a clear signal that they are necessary from new information collected. Some adaptation frameworks propose a basic plan with protective contingency measures to be implemented if needed (protective adaptivity), for example in Assumption-based planning (Dewar *et al.*, 1993) and Dynamic Adaptive Planning (Kwakkel *et al.*, 2010). Others propose a series of decisions with possible transfers between them that should be implemented depending on how the future unfolds (i.e., dynamic adaptivity), for example in Dynamic Adaptive Policy Pathways (Haasnoot *et al.*, 2013). In both cases, stress-testing and worst-case scenario discovery are often used to identify when the contingency measures for a basic plan may be needed or when a decision fails to meet the objectives and a different decision is required. Design of experiments and many objective (robust) optimization can also be used in optimizing the sequence, timing, and threshold values of a variable to adapt a decision through triggering a contingency measure or transferring to a new decision (Fletcher *et al.*, 2019; Kwakkel *et al.*, 2015). The decision-making process in adaptation frameworks is generally more dependent on uncertainty specification as it requires specifying the uncertainty range as well as the sequences of decision alternatives over time (Herman *et al.*, 2020).

3 Applying the taxonomy

In this section we demonstrate the diverse applications of exploratory modeling as a field according to the proposed taxonomy and provide specific examples analyzing coupled human-natural systems under uncertainty using various exploratory modeling approaches. We summarized selected studies that have used exploratory modeling (Table 1), organized under the framing of the taxonomy (Boxes 1 and 2), their context (i.e., water, climate, energy and transport, infrastructure, and land use and food), and type of case study (i.e., illustrative/hypothetical or real-world). The list of selected studies in Table 1 is not meant to be exhaustive nor represent the entire literature on exploratory modeling, but rather illustrates the use of our taxonomy and the diversity of the field across different contexts (see Appendix C for the rationale behind selecting these papers). We refer readers interested in a systematic review to recent reviews on scenario analysis (Guivarch *et al.*, 2017), decision-making/planning (Herman *et al.*, 2020; Kwakkel & Haasnoot, 2019), sensitivity and uncertainty analysis (Maier *et al.*, 2016; Pianosi *et al.*, 2016), and many-objective optimization algorithms (Maier *et al.*, 2019; Reed *et al.*, 2013), where exploratory modeling is used as model-based support. We also provide a detailed description of three exploratory modeling studies (Appendix C) from water, infrastructure, and energy contexts to further familiarize modelers with the implementation process and the type of results and insights obtained.

Table 1. Examples of recent studies focused on exploratory modeling of different types, contexts, and applications. The examples are selected and categorized in the table based on the authors' knowledge of studies and they do not represent a comprehensive overview of the literature (see Appendix C for the selection process).

Examples	Stress-testing	Design of experiments	Worst-case scenario discovery	Many-objective optimization	Many-objective robust optimization	Water	Climate	Energy & mobility	Infrastructure	Land use (also food)	Illustrative	Case study
Giudici et al. (2020)	●				●			●				●
Lamontagne et al. (2019)	●	●			●		●					●
Hall et al. (2019)	●	●					●		●			●
Gold et al. (2019)	●				●	●			●			●
Moallemi and Köhler (2019)		●						●				●
Groves et al. (2019)	●					●	●					●
Eker et al. (2019)	●	●								●		●
Babovic and Mijic (2019)	●						●		●			●
Sriver et al. (2018)	●	●					●		●			●
Lamontagne et al. (2018)	●	●					●				●	
Eker and Kwakkel (2018)	●				●	●					●	
Marcos-Martinez et al. (2018)		●					●			●		●
Quinn et al. (2018)	●				●	●	●					●
Kwakkel (2017)	●	●	●	●	●	●					●	
Gao and Bryan (2017)		●				●	●	●		●		●
Watson and Kasprzyk (2017)	●				●	●						●
Quinn et al. (2017)			●		●	●	●		●			●
Trindade et al. (2017)	●				●	●	●		●			●
Moallemi et al. (2017)	●	●						●				●
Berntsen and Trutnevyte (2017)	●							●				●
Bryan et al. (2016)		●					●			●		●
Zeff et al. (2016)	●				●	●	●		●			●
Herman et al. (2016)	●				●	●	●		●			●
Gao et al. (2016)		●					●			●		●
Carlsen et al. (2016)	●				●	●	●		●			●
Guivarch et al. (2016)	●						●				●	
Grundy et al. (2016)		●					●			●		●
Eker and van Daalen (2015)	●				●			●				●
Kwakkel et al. (2015)	●				●	●	●		●		●	
Halim et al. (2016)	●		●						●			●
Borgomeo et al. (2014)	●	●				●	●		●			●
Herman et al. (2014)	●				●	●	●		●			●
Zeff et al. (2014)					●	●	●		●			●
Castelletti et al. (2014)					●	●	●		●			●
Zhao et al. (2014)		●					●			●		●
Giuliani et al. (2014)					●	●			●			●
Rozenberg et al. (2014)	●						●				●	
Hamarat et al. (2014)					●			●				●
Whateley et al. (2014)	●					●	●					●
Hamarat et al. (2013)	●				●			●			●	
Kasprzyk et al. (2013)	●				●	●	●		●			●
Song et al. (2013)		●								●		●
Lempert et al. (2013)	●	●					●		●			●
Nazemi et al. (2013)	●	●				●	●					●
Song et al. (2012)		●								●		●
Lempert and Groves (2010)	●	●				●	●		●			●
Bryant and Lempert (2010)	●	●						●			●	
Kasprzyk et al. (2009)				●		●	●		●			●
Kollat and Reed (2006)				●		●					●	

The trend of the selected studies in Table 1 shows that the treatment of uncertainty improved over time by re-appropriating established approaches such as sensitivity analysis and many-objective optimization for exploratory purposes under deep uncertainty, for example, through stress-testing and many-objective robust decision-making (Hall *et al.*, 2019; Lamontagne *et al.*, 2018; Watson & Kasprzyk, 2017). There is also a growing interest in capitalizing on the strengths of one approach to compensate for the limitations of others and the integrated use of different types of exploratory modeling (Moallemi *et al.*, 2018), for example, through combining stress-testing and robust optimization in decision-making frameworks (Eker & Kwakkel, 2018; Gold *et al.*, 2019; Trindade *et al.*, 2017). The abundance of various applications on real-world problems in Table 1 supports the practicality of exploratory modeling approaches and encourages their further use for decision-making across other applications and for new modeling purposes. While the contexts in which exploratory modeling has been applied are diverse, so far not all types of exploratory modeling have been widely used across different sustainability areas. There is, therefore, an opportunity for enhancing modeling under uncertainty in new contexts such as food and land systems, biodiversity, health, and ecology, beyond the standard use of scenario analysis and sensitivity analysis. Eker *et al.* (2019) provides a recent example of an exploratory modeling application in these emerging contexts where they used scenario discovery to identify a set of behavioral factors that can shift the global food system towards a more sustainable diet.

4 Benefits and challenges of exploratory modeling in practice

We investigate the motivations and the potential benefits of using exploratory modeling in support of good modeling practice and robust decision-making. We enumerate the benefits to argue for the further adoption of exploratory modeling addressing sustainability contexts more widely across coupled human-natural systems. We also discuss current limitations and potential challenges that modelers may face in the use of exploratory modeling. Reflection on current issues can highlight the areas for further improvement and direct future research in the field.

We frame the discussion of potential benefits and challenges in the context of the iterative process of model-based decision-making to clarify the impacts (Figure 2). According to Sterman (2000), model-based policy analysis typically starts by *problem articulation* for identifying the decision problem, requirements, and the current situation. It continues by *system conceptualization* for developing a conceptual model that can represent the problem at hand. The conceptual model, supported by data, is used in *model formulation* for setting up a simulation model. The formulated model, after *testing and validation* under uncertainty, works as a simulation engine in exploratory modeling to generate the system response under different assumptions. The validated model is used for the *policy evaluation* of decisions and scenarios to obtain robust inferences.

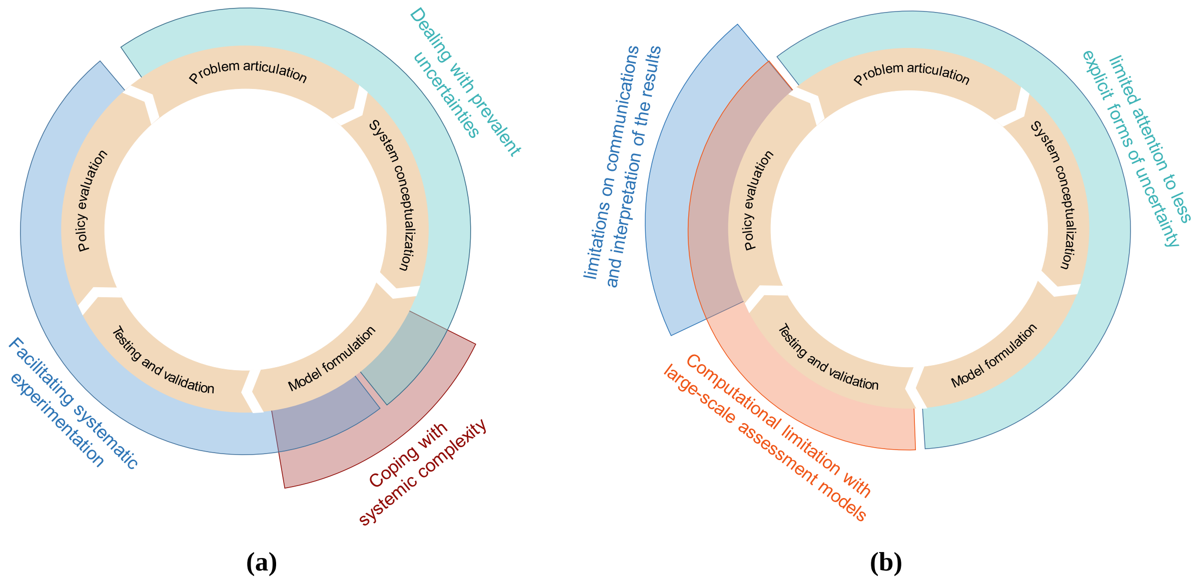


Figure 2. An overview of the benefits and challenges of exploratory modeling. (a) shows benefits and (b) shows challenges. The circular arrows represent the iterative steps in the general modeling process. The rings around the arrows show where potential benefits/challenges overlap with the modeling step(s).

4.1 Handling uncertainty

Coupled human-natural systems work in a context of multiple interacting climatic, technological, socio-economic, and political uncertainties (Quinn, 2017). Exploratory modeling has a major advantage in '*dealing with the prevalent uncertainties'* of these systems, through evaluating models as hypotheses (Khatami *et al.*, 2020) and by a systematic exploration of the diversity of (model and dataset) assumptions with minimum prior judgements about their ranking or probability. This variety of assumptions can be reflected in different parts of the modeling process. Uncertainty can occur in framing a problem (problem articulation) (Quinn *et al.*, 2017), the implications of different datasets and system conceptualizations (in system conceptualization) (de Haan *et al.*, 2016; Moallemi *et al.*, 2017), and in the multiple alternative models of the same problem (in model formulation) (Auping *et al.*, 2016; Pruyt & Kwakkel, 2014).

Given these uncertainties, an exploratory approach helps modelers to investigate a wide range of assumptions which otherwise might have remained uninvestigated. A key advance of exploratory modeling in decision-making over conventional predict-then-act approaches is in where and how uncertainty is treated. Conventional approaches to decision-making address uncertainty *a priori* when decision-maker preferences and knowledge are elicited and imposed before performing any analysis (Tsoukiàs, 2008). In contrast, the adoption of exploratory modeling is more consistent with *a posteriori* analysis that opens up the space of alternative assumptions that can be made, in pursuit of increasing the robustness of inferences across a large range of possible uncertainties (Dessai & Hulme, 2007; Huskova *et al.*, 2016). In other words, robust inferences are obtained after a thorough exploration and a diverse search over rival framings of a problem, conflicting objectives, and divergent stakeholder preferences (Hadjimichael *et al.*, 2020b; Herman *et al.*, 2015). Shortridge and Zaitchik (2018) and Taner *et al.* (2019) are two recent examples of *a posteriori* analysis of likelihood after stress testing. Conventional approaches also rely on the maximization of expected utility and an optimal performance as the criterion for a 'good' decision against a predicted future with the best-estimate probability distributions (Lempert, 2019). Instead, exploratory modeling uses robustness and flexibility as the mark of quality — that is whether a set of decisions performs well across many possible futures (Herman *et al.*, 2015; Herman *et al.*, 2014; Maier *et al.*, 2016; McPhail *et al.*, 2018), and whether decision performance remains insensitive to (or minimizes regret) and flexible in response to unforeseen futures (Weaver *et al.*, 2013).

Despite the potential to incorporate various forms of uncertainties, previous exploratory modeling studies usually only considered uncertainties in input parameters. This has led to the current gap in the literature, that is a '*limited attention to less explicit forms of uncertainty*', which are often non-parametric. Such uncertainties can be reflected in different ways of valuing outcomes (in problem articulation) (Giuliani & Castelletti, 2016; McPhail *et al.*, 2018), variation in model structural relationships and equations (in model formulation) (Auping *et al.*, 2016; Moallemi *et al.*, 2017; Pruyt & Kwakkel, 2014), and disagreement in theories and conceptual frameworks underpinning the models (in problem articulation and conceptualization) (de Haan *et al.*, 2016; Quinn *et al.*, 2017). The further incorporation of these uncertainties within the computational process of modeling can enable more robust decision-making.

When exploratory modeling is used to investigate a wide range of assumptions through batch simulations, it can result in very large data outputs which need to be analyzed and understood in decision-making. Statistical and data-mining techniques can be used to analyze big data from exploratory modeling. However, current exploratory modeling approaches do not provide much guidance for how their outputs should be interpreted. Here a gap exists between results and decision-making (in policy evaluation), leading to another challenge, that is the '*limitations in communication and interpretation of the results'*. The visualization limitation in the communication of multi-dimensional data and the limited cognitive capacity of humans (i.e., model users and decision-makers) in examining the multiple dimensions of data at once can make the interpretation of the exploratory modeling results even more challenging. Understanding the results often requires techniques for viewing highly multi-dimensional data. The use of advanced visualization techniques (Brodlie *et al.*, 2012; Bryan *et al.*, 2016; Reed & Kollat, 2013; Woodruff *et al.*, 2013), which allow users to explore data graphically in multiple dimensions, can be a way to mitigate this challenge and assist in interpretation. One example is Kasprzyk *et al.* (2013) where they used Interactive Visual Analytics to support collaboration with users and to improve their ability to effectively analyze many decisions generated by an exploratory modeling approach. The use of data-mining methods such as clustering which summarizes multi-dimensional data into distinct groups is also another way to address this challenge (de Haan *et al.*, 2016; Gerst *et al.*, 2013; Guivarch *et al.*, 2016; Rozenberg *et al.*, 2014).

4.2 Managing complexity

Real-world human and natural systems are complex. Complex systems are often characterized as incorporating many parts, comprising causally interrelated elements within multiple social, technical, and economic dimensions (Bunge, 1997). While this holds true to the etymology of the term *complex*, systems and models can exhibit complexity yet look deceptively simple. The logistic map, a fully deterministic, one-variable, discrete, iterated equation, is a classic example. However, for certain values of its only parameter, it exhibits full-blown chaos (Stewart, 1989). In other words, many parts should not be thought of as a necessary condition for complexity. What does seem to be a necessary condition for complexity is non-linearity. It is the non-linearity in the logistic map that is the source of its chaos and if a system of many parts is complex it is due to non-linear interactions, side-effects, and emergent features (Bunge, 2003) amongst those many parts. Given the complexity, these systems are typically hard to predict or explain directly in terms of the behavior of individual elements (de Haan, 2006). A great strength of exploratory modeling is in '*coping with systemic complexity'*. An exploratory approach enhances model formulation by making valid conclusions not necessarily from individually correct models of complex systems, but from an ensemble of different framings of these systems, for example with various interactions between elements and different agent rules. To illustrate, Pruyt and Kwakkel (2014) and Auping *et al.* (2016) have used exploratory modeling for investigating the implications of model (structural) complexity in energy sector and national security contexts, respectively. Real-world systems are also often characterized by a complex combination of decisions that requires a high level of performance for multiple (sometimes conflicting) objectives. Exploratory modeling can enable the investigation the diversity of decision alternatives (instead of a limited set) and capturing key trade-offs (Gold *et al.*, 2019; Mitchell, 2009; Singh *et al.*, 2015; Trindade *et al.*, 2017).

The cognitive complexity of testing various alternative assumptions and observing their consequences in the outcome space manually poses a significant barrier, in addition to the systemic complexity itself. Exploratory modeling can be helpful in dealing with this aspect of complexity in implementation too, by '*facilitating systematic experimentation'*. Exploratory modeling has adopted computational support such as the Python-based Exploratory Modeling Workbench (Kwakkel, 2017) and OpenMORDM (Hadka *et al.*, 2015) amongst other associated libraries (Hadjimichael *et al.*, 2020a; Trindade *et al.*, 2020), for the systematic assessment of assumptions and learning about model behavior in a multi-objective space. Exploratory modeling using these computational supports can enhance analytical capability through managing, tracing, and documenting many quantitative models, large datasets, and conceptual framings. Such computational support can help in quantifying the consequences of many assumptions for outcomes through experimenting in an automated process (Kwakkel, 2017). This can be a helpful feature in model formulation where modelers often experiment with assumptions in an ad hoc manner before they settle on their ultimate set of assumptions that constitute their model. For example, Kwakkel *et al.* (2015) and Fletcher *et al.* (2019) used exploratory modeling (policy search and stochastic dynamic programming) as a computational support to address the combinatorial problem in policy design arising from many ways in which decision alternatives can be sequenced over time and the rules that govern when new decisions are to be triggered in adaptive planning. In this way, exploratory modeling can also help in the uncertainty analysis of model behavior, contributing to the modeling process in policy evaluation.

While exploratory modeling approaches can help in coping with the complexity of systems and experimentation, they can still face some '*computational limitations in working with large-scale assessment models'*. These models often have extensive and complex structures, integrating many interacting components and agents to represent system processes. Examples can be found among established environmental models, such as energy and climate models, commonly used in global or regional integrated assessment (IPCC, 2018; UN, 2019). Complexity may be even greater in agent-based models, which are assumed to have a capacity to model and capture in detail the multiple interactions of human-natural systems (Bankes, 2002a, 2002b; Lempert, 2002). Agent-based models can feature a large number of input parameters for different classes of agents, which can significantly expand the size of the assumption space for a model to search through (Moallemi & Köhler, 2019). Producing even a few scenarios with such models can sometimes take several days. Such a slow simulation process can impose a challenge for some of these large-scale models in adopting exploratory modeling that requires a wide exploration/search over various assumptions. One obvious approach to mitigate this challenge is the use of efficient algorithms, parallel processing, and high-performance computing (Bryan, 2013; Reed *et al.*, 2008; Zhao *et al.*, 2013). Another way is via the use of meta-models for screening and analyzing an ensemble of model behaviors and observing interesting model outcomes (Haasnoot *et al.*, 2014). This can lead to a multi-resolution model of a complex system with a high-level of abstraction which can be used initially to facilitate the exploratory modeling process. The full resolution model can then be used to investigate model behaviors of interest. Adaptive sampling can also be used to search the uncertainty space based on its likelihood of uncertainty estimation and the complexity of the likelihood surface of the uncertainty space; the complexity that results from the interaction of multiple uncertainty dimensions as well as the model structure (Blasone *et al.*, 2008; Islam & Pruyt, 2016; Khu & Werner, 2003).

5 Exploratory modeling with stakeholders

Policy agencies and science funding organizations increasingly require scientists and stakeholders (e.g., practitioners, policy/decision-makers, civil society, interest groups) to *co-create* the knowledge for dealing with the complex challenges of coupled human-natural systems (Game *et al.*, 2018; Mauser *et al.*, 2013; Moallemi *et al.*, 2020a; Moser, 2016; Norström *et al.*, 2020). Co-creation of knowledge has been discussed in the context of participatory modeling and decision-making (Halbe *et al.*, 2020; Halbe *et al.*, 2018; Jordan *et al.*, 2018; Voinov *et al.*, 2018). Within the context of exploratory modeling, several previous studies have discussed co-creation, implicitly or explicitly, through embedding stakeholder input into the iterative process of modeling and combining computational and human capabilities interactively (Eker *et al.*, 2017; Kasprzyk *et al.*, 2013; Lempert *et al.*, 2003; Moallemi & Malekpour, 2018; van Bruggen *et al.*, 2019). In the context of decision-making, they urged deliberation with analysis where model users can interact with the computational process, observe counterintuitive results based on a shared vision of the problem, and inform the improvement of results (National Research Council, 2009). Some recent studies also further investigated nuances of modeling social/psychological dimensions, discussing human factors (such as biases and hidden preferences) that shape decision-making (Moallemi *et al.*, 2020b; Zare *et al.*, 2020). Despite this growing interest, deliberation with analysis in exploratory modeling remains a black box and the co-creation of knowledge with stakeholder participation in the robust decision context remains a topic of lively debate (Alrøe & Noe, 2016; Döll & Romero-Lankao, 2017; Glynn *et al.*, 2017, 2018; Walker *et al.*, 2018). Learning from previous work (Landström *et al.*, 2011; Lane *et al.*, 2011) and building on the Mauser *et al.* (2013) framework for knowledge co-creation, we discuss some of the ways for stakeholder participation in exploratory modeling, aiming to contribute to better approaches for *socially* robust inference.

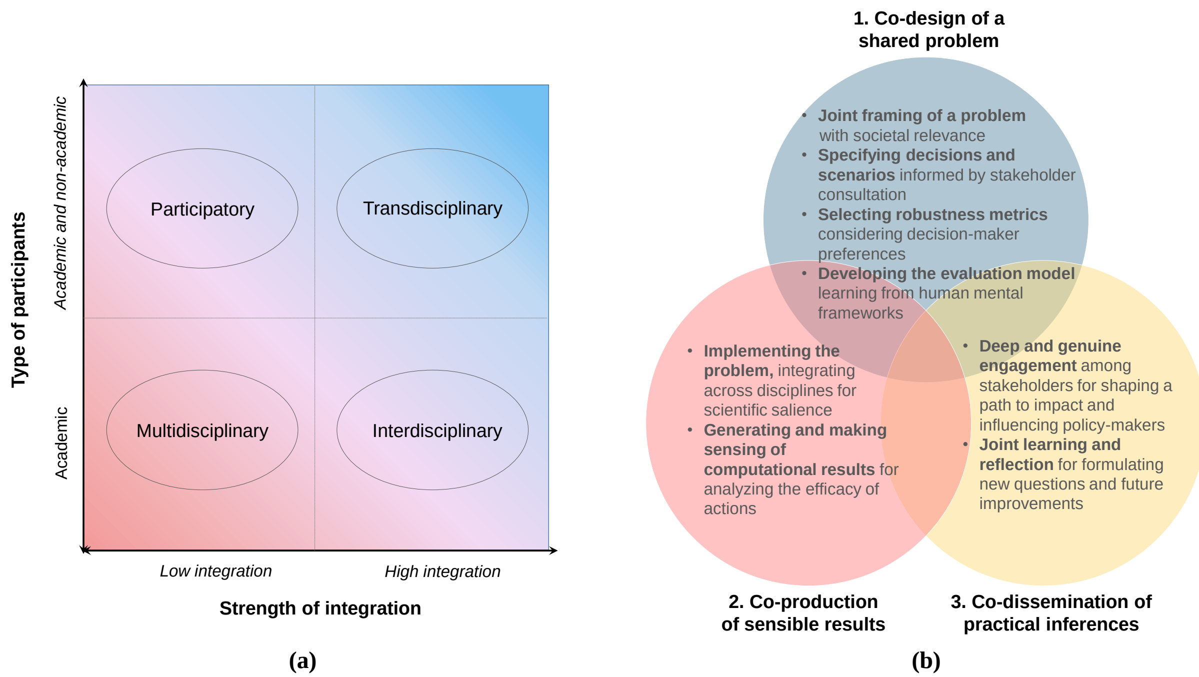


Figure 3. The co-creation of knowledge with stakeholders. (a) shows different forms of stakeholder participation, based on Tress *et al.* (2005). The color hue shows participation with diverse participant groups and a high integration of knowledge forms from various sources (blue) versus participation with narrow participant groups and a low integration (red); (b) shows the three ways for the co-creation of knowledge in exploratory modeling, with their varying forms of stakeholder participation.

Tress *et al.* (2005) argued that different forms of stakeholder participation can be imagined (see Figure 3a), varying based on the type of participants (who is involved?) and the strength of integration across research concepts (what is the diversity of incorporated language and forms of knowledge?). From these different forms, interdisciplinary and transdisciplinary research often involves a stronger integration compared to multidisciplinary and participatory approaches. There is also a wider and more inclusive incorporation of academics and non-academics (e.g., civil society, policy-makers, practitioners) in participatory and transdisciplinary research for enhancing legitimacy and accountability among stakeholders. Conversely, multidisciplinary and interdisciplinary aim to improve the consistency and salience of the research across scientific disciplines, and therefore often focus more on engagement with different academic communities (Mauser *et al.*, 2013; Tress *et al.*, 2005). We argue that exploratory modeling can learn from these approaches for the co-creation of knowledge to *co-design* a shared problem, *co-produce* sensible results for the problem, and *co-disseminate* robust sensible inferences (Figure 3b).

The co-design of a shared decision problem involves the joint framing of a pressing sustainability challenge from relevant societal sectors through *participatory* processes (e.g., workshops, brainstorming). Co-design also involves the translation of the real-world sustainability challenge into an abstract problem that can be analyzed with models. The required knowledge for the specification of problem components (i.e., decisions, scenarios, robustness metrics, models) can be obtained through the interaction of scientific methods with social contexts (Lempert *et al.*, 2003). For example, scientists and stakeholders can together identify a range of feasible candidate decisions (e.g., through SWOT analysis and multi-criteria decision analysis) and influential but uncertain factors in future scenarios (e.g., participatory scenario development and scenario discovery). Depending on the confidence of stakeholder knowledge and agreement among different views, the decision and scenarios can be specified by human judgement *a priori* to analysis (de Neufville *et al.*, 2019) or in an iterative process where the initial list of pre-specified decisions are refined based on the feedback from the analytical results (Kasprzyk *et al.*, 2013). The selection of appropriate robustness metrics and models is also sensitive to stakeholder participation. There are different elicitation tools (Morris *et al.*, 2014; Reichert *et al.*, 2013) that can help in defining appropriate robustness metrics by obtaining knowledge of context (e.g., about the relevancy of absolute performance or regret measures) and decision-maker preferences (e.g., about preferred risk aversion level) (McPhail *et al.*, 2018). Eliciting mental models and assumptions of various academic and non-academic participants about underlying causal interactions of the problem can also help to delineate meaningful boundaries and develop relevant evaluation models in decision-making (Mayer *et al.*, 2017). Here the modeling literature has several examples of model development with stakeholders through conceptual and cognitive mapping (Gray *et al.*, 2012), system dynamics modeling (Zare *et al.*, 2019), and other participatory modeling approaches (Basco-Carrera *et al.*, 2017; Voinov, 2017).

The co-production of exploratory modeling results is about the generation of sensible and credible outcomes from the quantification of the costs and benefits, not necessarily in monetary terms, of various decisions under future scenarios. Co-production involves the interaction of *interdisciplinary* teams to integrate different methods in a way that best serves the problem at hand. The integration in exploratory modeling can be as simple as the independent applications of two methods and frameworks on the same problem and the comparative analysis of the results (Halim *et al.*, 2016). It can also be more sophisticated in design, from a sequential integration where the output from one is used as input to another (Glasgow *et al.*, 2018), to a full integration where new frameworks emerge from two-way interactions between multiple methods and frameworks (Watson & Kasprzyk, 2017). Co-production also involves the generation of computational experiments and making sense of the results of the experiments for analyzing the efficacy of various decisions and making trade-offs between multiple objectives. Collaborations among various scientific expertise can broaden perspectives and expand choices of suitable analytical (e.g., sampling and optimization) algorithms (Maier *et al.*, 2019; Reed *et al.*, 2013) and toolboxes for their implementation (Hadka *et al.*, 2015; Kwakkel, 2017).

The co-dissemination of exploratory modeling results aims to enhance the ownership and accountability of outcomes and helps to influence policymakers' decisions via deep and genuine engagement with stakeholders. This can be achieved through a *transdisciplinary* approach that brings scientific and stakeholder groups together for shaping a path to impact on the ground. Collaborative efforts between academics and non-academics can help in translating the abstract results into practical inferences, with an accessible and comprehensive language for different audiences. Interaction with these stakeholder groups, for example via role-playing games (d'Aquino & Bah, 2013), visual analytics (Reed & Kollat, 2013), and web applications (Nativi *et al.*, 2013), can enable joint learning and ongoing reflection of the results. This can also help to create new research questions and improve problem framings for the future, contributing to the iterative cycle of human deliberation with model-based analysis.

Future studies can further advance this discussion by translating it in the context of different decision-making frameworks and by implementing it in applications. Collaborating with stakeholders with different characteristics, such as willingness to participate, strategic thinking maturity, and divergence of values, can pose practical limitations on knowledge co-creation that need to be addressed within the case studies (Hurlbert & Gupta, 2015; Jordan *et al.*, 2018; Smajgl & Ward, 2015).

6 Conclusions

There is inherent complexity in the interactions and processes in the sustainability of coupled human-natural systems, such as climate, land-use, energy, and water (Howells *et al.*, 2013). These systems are also surrounded by uncertainties arising from the multiple factors including long time-scales, spatial heterogeneity, environmental change versus natural variability, alternative theories and models of human-nature interactions, contextual contingencies, and contested views of stakeholders. The presence of complexity and deep uncertainty has challenged the relevance of conventional modeling approaches (which use prior information) for understanding the behavior of these systems and for informing decisions towards sustainability. Conventional approaches can prematurely close down the assumption space in the pursuit of a best-estimate scenario. Through this pre-mature closure, the modeler may also forego the ability to even assess how good the best-estimate scenario is and how robust inferences are. Exploratory modeling can address the challenges posed by complexity and deep uncertainty by modeling coupled human-natural systems under uncertainty and informing decision-making for sustainability by generating robust inferences. While exploratory modeling can face challenges in practice, such as computational limitations with large-scale assessment models and limitations on communications and interpretation of the results, it still offers great benefits to modeling and model-based decision-making. There is substantial potential for the further use of this approach by researchers and practitioners in new applications spanning multiple sustainability contexts. Our taxonomy can guide this wider adoption by illustrating the ways in which exploratory modeling can be used across different areas. We hope that the proposed taxonomy can be used as a benchmark framework for enhancing robust inferences about the impacts of global change on sustainability priorities through recognizing and implementing rival ways of modeling under uncertainty.

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Appendix A

A note on terminology: The literature uses various—sometimes inconsistent—terms to refer to exploratory modeling practices. The terminology we adopt in this article uses the terms: *approach* for referring to a philosophical position to modeling providing context and logics (e.g., consolidative modeling vs. exploratory modeling approaches in Bankes (1993)); *method/technique/algorithm* for a structured set of processes that can be used for a particular purpose in exploratory modeling (e.g., PRIM or CART in scenario discovery (Lempert *et al.*, 2008)); *framework* for a mix of methods that interact to support decision-making (e.g., Robust Decision Making (Lempert, 2019)); *toolkit (tool)* for well-defined and documented resources (e.g., programming libraries) that are external to users and can support the exploratory modeling process (e.g., the Exploratory Modeling Workbench (Kwakkel, 2017) and Rhodium (Hadka *et al.*, 2015)).

What we are discussing in this article as optimization is the *simulation-based* optimization (Amaran *et al.*, 2016) which is connected to Monte Carlo simulation, reliability engineering, and evolutionary optimization (Beyer & Sendhoff, 2007; Maier *et al.*, 2014; Nicklow *et al.*, 2010; Reed *et al.*, 2013). This class of optimization has been used widely in the deep uncertainty literature for policy search (Gold *et al.*, 2019; Herman *et al.*, 2015; Quinn *et al.*, 2017; Trindade *et al.*, 2017). Here we do not discuss stochastic dynamic programming that has been used for policy design through optimizing the sequence and timing of decision variables to trigger adaptation (Fletcher *et al.*, 2019). We also do not discuss earlier works that go back to robust linear programming of the 1980s in operations research (Ben-Tal & Nemirovski, 1998; Ben-Tal & Nemirovski, 1999).

Appendix B

Exploratory modeling can overlap with other areas that also use model-based experimentation to analyze the implications of conflicting objectives and alternative assumptions, such as multi-objective optimization (Reed *et al.*, 2013), design of experiments (Montgomery, 2017), and sensitivity analysis (Borgonovo & Plischke, 2016; Saltelli *et al.*, 2008; Saltelli *et al.*, 2000). Therefore, a range of existing methods from other areas can be re-appropriated to support exploratory modeling for new exploratory purposes.

As an example, exploratory modeling overlaps with, and can use methods from, sensitivity analysis (Giuliani *et al.*, 2014; Kasprzyk *et al.*, 2013; Lamontagne *et al.*, 2018; Moallemi *et al.*, 2018c; Reed & Kollat, 2013; Singh *et al.*, 2015). Sensitivity analysis, in general, can be performed in four settings (Jaxa-Rozen & Kwakkel, 2018; Saltelli *et al.*, 2008):

- *Factor prioritization* to specify important model inputs contributing to output uncertainties (Loucks *et al.*, 2005);
- *Factor fixing* to determine the model inputs with the least influence on output uncertainties (Saltelli *et al.*, 2008);
- *Variance cutting* to search for input values under which output uncertainty remain below a threshold (Saltelli & Tarantola, 2002); and
- *Factor mapping* to identify areas of input uncertainty responsible for a given output (also related to scenario discovery) (Guivarch *et al.*, 2016; Lamontagne *et al.*, 2018).

The sensitivity analysis literature often uses methods in these four settings for different purposes: to enhance model structure (Iman *et al.*, 2005) in a *consolidative* paradigm by discarding non-influential inputs (Felli & Hazen, 2004); to inform model calibration and further data collection (Saltelli *et al.*, 2000); and to identify the direction of change in the behavior of model outputs (Anderson *et al.*, 2014). In contrast, exploratory modeling adopts sensitivity analysis for different purposes. For example, it uses similar methods (e.g., factor mapping) for identifying scenario assumptions that can lead to policy relevant outcomes of interest (Lamontagne *et al.*, 2018). Exploratory modeling also uses sensitivity analysis methods for *stress-testing* to identify unexpected model behavior in outcome space (e.g., adaptation tipping points) and generating a hypothesis about it (Hall *et al.*, 2019). Sensitivity analysis methods can be also used in an exploratory setting for scenario decomposition to generate a small number of scenarios as model response to extreme variations of inputs (e.g., worst-case, best-case scenario discovery) (Tietje, 2005). While the difference between exploratory modeling and other areas is sometimes just one of disciplinary terminology or purpose, there are also more fundamental differences related to the treatment of uncertainty. For example, standard uncertainty analysis tends to rely on well-characterized uncertainties where the joint or marginal probability distribution of input parameters is known, for example estimated by statistical techniques (e.g., histograms) or expert judgement (Loucks *et al.*, 2005). In contrast, exploratory modeling uses probability distributions *a posteriori* to summarize and describe experiments generated based on quasi-random samples from the assumption space.

Appendix C

C.1 Selecting papers for representing the taxonomy

Exploratory modeling has been used in a variety of methodological (improvement) work with illustrative case applications (Kwakkel & Cunningham, 2016; Kwakkel & Jaxa-Rozen, 2016; Rozenberg *et al.*, 2014) as well as in real-world case studies for informing planning and decision-making (Kwakkel, 2010; Lempert *et al.*, 2013; Lempert *et al.*, 2016). The (illustrative and real-world) case applications have been across different sectoral domains, including energy (Auping *et al.*, 2016; Eker & van Daalen, 2015; Moallemi *et al.*, 2017a), climate change mitigation (Enserink *et al.*, 2013; Greeven *et al.*, 2016; Guivarch *et al.*, 2016; Lempert *et al.*, 1996; Rozenberg *et al.*, 2014), transportation planning (Halim *et al.*, 2016; Kwakkel *et al.*, 2010), flood risk management (Kwakkel *et al.*, 2016; Lempert *et al.*, 2013), water resource management (de Haan *et al.*, 2016; Huskova *et al.*, 2016; Matrosov *et al.*, 2013), defense planning (Brooks *et al.*, 1999; Lempert *et al.*, 2016; Moallemi *et al.*, 2018a; Moallemi *et al.*, 2018b; Niese & Singer, 2014), and health management and disease prevention (Auping *et al.*, 2017; Manheim *et al.*, 2016). From these many previous studies, in Section 3 of the manuscript, we only used some to demonstrate our proposed taxonomy in practice and to represent the diversity of the field across different types of exploratory modeling (but not covering all previous work as we were not undertaking a review). For example, there are many studies that use exploratory modeling for stress-testing, some of which cited in Table 1. We tried to cover examples of stress-testing across different sectoral domain (e.g., water and energy) and with different methodological innovations (e.g., stress-testing with sensitivity analysis versus stress-testing with many-objective optimization). In selecting the articles, we focused on diversity rather than coverage as we aimed to inform modelers about a variety of the ways that exploratory modeling has been used in the past and can be also used in the future.

The way we selected the articles was guided by the authors' informed judgement from the recent literature in the three following steps:

1. We firstly solicited an initial list of representative articles that could exemplify different types of exploratory modeling in our taxonomy. We identified this initial list by looking at the modeling papers in the Decision-Making Under Deep Uncertainty (DMDU) literature (Marchau *et al.*, 2019), as it was the main and closest research community to exploratory modeling in decision support.

2. We discuss the initial list within the author team to add new papers to the list based on the less represented areas of the literature. In improving the initial list, we decided to include the studies where original data and new decision insights are created (rather than conceptual discussion), the focus is on a method improvement and/or a new application (rather than a review), and the context of the study is human and natural systems. Given these selection criteria, we did not to include the original introductory studies that discussed the foundations and concepts (Bankes, 2002a, 2002b; Bankes *et al.*, 2001; Brown *et al.*, 2012). We did not include the review studies as their primary aim was to provide an overarching overview of the field rather than generating decision insights for a specific application (Giuliani & Castelletti, 2016; Guivarch *et al.*, 2017; Herman *et al.*, 2020; Herman *et al.*, 2015; Kwakkel & Haasnoot, 2019; Reed *et al.*, 2013; Trutnevyte *et al.*, 2016). We excluded examples from other areas rather than human-natural systems (e.g., engineering systems and defense planning) as they were not aligned with the

article's aim and the journal's scope. We also did not consider articles from the broader areas of sensitivity analysis and optimization (Bryan & Crossman, 2013; Jaxa-Rozen & Kwakkel, 2018; Pianosi *et al.*, 2016; Pye *et al.*, 2015) as they were of the secondary importance for the specific purpose of the current article.

3. We reviewed each paper in the list to specify its position in Table 1 with respect to type of exploratory modeling, context, and application. We cross-checked the results within the author team to make sure about the correct understanding of the position of the papers in the table. We also acknowledged that the position of the selected studies in the table is based on the authors' judgement and according to the proposed taxonomy.

C.2 Examples from exploratory modeling applications

This rest of this appendix briefly summarizes three examples from the variety of exploratory modeling applications: long-term policy analysis of energy systems, future adaptive planning for flood risk management, and theory testing of water systems management from a historic perspective. We choose these three examples as they represent some of the diversity of exploratory modeling applications discussed in Section 3.

Example I – Policy analysis in energy transitions modeling

The first example combines a methodological work with a real-world case application in energy sector and is from Moallemi *et al.* (2017a). The study is about how qualitative narratives of sustainability transitions can support the computational process of exploratory modeling in long-term policy analysis. The study also analyses future transition pathways towards renewable electricity in India for meeting 100 GW solar electricity and 60 GW wind electricity in a period from 1990 to 2030. This transition unfolds in a context where multiple techno-economic uncertainties (e.g., fuel prices) and socio-political uncertainties (such as electricity demand) challenge a robust understanding of possible future pathways. Therefore, it is important to understand how future transition pathways pan out (i.e. whether the renewable targets will be met or not) and what conditions can redirect this transition towards the targets.

The study initially develops qualitative narratives, developed based on the interpretation of raw data from available documents through the lens of sustainability transitions theories (Moallemi *et al.*, 2017b). These narratives differentiate among different structure of the electricity sector (whether it would be dominated by market or government control) and the priorities for the electricity sector (e.g., energy equity, energy security, and sustainability) and use them to guide the development of some deliberate assumption spaces of future in which transition could unfold. Computational experiments are performed within each deliberate assumption space—each experiment corresponds to a single transition pathway. Many transition pathways are analyzed across assumption spaces to assess the fulfilment of wind and solar targets across different pathways.

The analysis of experiments using scenario discovery (Bryant & Lempert, 2010) and multi-dimensional clustering (Gerst *et al.*, 2013) shows that the realization of the 100 GW solar electricity by 2022 is unlikely while it is most likely around 2028. However, meeting the 60 GW target for wind electricity by 2022 is closer to reality as the most-likely time for the fulfilment of this target is around 2024. The analysis also shows that a transition pathway towards a renewable—mainly solar—electricity is more likely under conditions when the structure for the electricity sector is government controlled through systemic coordination of renewable initiatives and when energy security and sustainability are dual priorities.

Example II – Adaptive planning in flood risk management

The second example combines methodological work with an illustrative application in flood risk management and is from Kwakkel *et al.* (2015). The study is about how many-objective robust optimization can computationally support the design of adaptive plans within the Dynamic Adaptive Policy Pathways framework (Haasnoot *et al.*, 2013). There are two challenges with the original design of this framework: how to choose a sequence of actions—known as pathways which remain valid under transient scenarios? and how to cope with the combinatorial problem which arises from the multiplicity of ways which actions can be concatenated? This computational support is intended to help in identifying the most promising pathways with respect to multiple objectives using many-objective optimization and assessing the robustness of pathways over many scenarios by sampling over uncertainty space. The study uses a hypothetical case in Rhine Delta in the Netherlands over the next 100 years. The flood risk management in this case is surrounded by uncertain factors, such as socio-economic development factors (e.g., population and economic growth), global climate change (e.g., droughts and increase in temperature), and land use (e.g., de-urbanization or fast urbanization).

The design of adaptive plan starts initially by identifying policy actions, such as flood prevention measures, heightening the dikes, and strengthening the dikes, for meeting objectives regarding costs, causalities, and damages. Many adaptation pathways can be constructed based on different concatenation of these policy actions and by considering possible various transfers between actions at actions' sell-by dates. The study formulates a many-objective optimization problem and uses optimization (metaheuristic) evolutionary algorithms to enumerate different concatenation of these policy actions—in the form of policy pathways—which minimize the costs, causalities, and damages under two constraints of limiting maximum damages and maximum causalities. The study generates transient scenarios by sampling from uncertainty space and then runs computational experiments to test the robustness of enumerated pathways over generated scenarios. The final result is an adaptation map representing different sequences of actions (pathways) with their respective sell-by dates leading to specific futures. Decision makers could decide which sequence of actions to choose based on their preference or a cost-benefit analysis.

Example III – Theory testing in urban water management

The third example combines methodological innovation with a real-world case application and is from de Haan *et al.* (2016). The study is an application of exploratory modeling to theory testing (non-decision support) on a historical case, which is a less investigated use of exploratory modeling in the literature. The exploratory model—called STM (Societal Transitions Module)—generates scenarios of transition pathways, more precisely put: the uptake and phasing out of servicing solutions (types of technology) in urban water systems. STM implements a theory of change known as the Multi-Pattern Approach by de Haan and Rotmans (2011) and, perhaps atypically, the model exploits the acknowledged uncertainties in this theory, rather than in estimated parameter values. The theory states that, given certain conditions, at any point in time, one of *several* patterns of change may follow—the theory is agnostic as to which pattern is more likely.

Exploratory modeling for STM amounts to producing a portfolio of scenarios starting from one initial condition. For example, 50 time steps with six patterns possible at each time step would yield about 6^{50} scenarios. This produces two problems: (1) this is computationally infeasible, and (2) what should be the interpretation of such a multitude of possibilities? Can these scenarios give any meaningful information about pathways at all? The former issue is easily solved by sampling the solution space, limiting the runs to, e.g., 2000-5000 scenarios. The latter issue is addressed by performing a cluster analysis on the produced scenarios. It turns out that although each scenario is different, many are very much alike and the thousands of possible outcomes can be grouped into a handful of clusters. This is the idea behind the title of this study 'Many Roads to Rome', there are many scenarios that, though different in detail, lead to qualitatively similar outcomes.

The STM is set up to re-produce a known historical trajectory of green infrastructure uptake in Melbourne's urban water management system from 1960-2010. Though STM produces several clusters of pathways, one matches the historical data well. The other clusters can be interpreted as alternative histories, developments that could have been.

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