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Article

Simulation-Based Optimization: Implications of Complex Adaptive Systems and Deep Uncertainty

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Abstract: Within the modeling and simulation community, simulation-based optimization has often been successfully used to improve productivity and business processes. However, the increased importance of using simulation to better understand complex adaptive systems and address operations research questions characterized by deep uncertainty, such as the need for policy support within socio-technical systems, leads to the necessity to revisit the way simulation can be applied in this new area. Similar observations can be made for complex adaptive systems that constantly change their behavior, which is reflected in a continually changing solution space. Deep uncertainty describes problems with inadequate or incomplete information about the system and the outcomes of interest. Complex adaptive systems under deep uncertainty must integrate the search for robust solutions by conducting exploratory modeling and analysis. This article visits both domains, shows what the new challenges are, and provides a framework to apply methods from operational research and complexity science to address them. With such extensions, simulation-based approaches will be able to support these new areas as well, although optimal solutions may no longer be obtainable. Instead, robust and sufficient solutions will become the objective of optimization processes.

Keywords: optimization; heuristics; uncertainty; complex adaptive systems; deep uncertainty



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1. Introduction

The term optimization is used in a multitude of contributions to the Modeling and Simulation (M&S) Body of Knowledge (BoK), which was recently commissioned by the Society for Modeling and Simulation [1]. To optimize something is generally understood to mean the modification of something until it exists in its most desirable state. In the mathematical world, though, the definition can be more rigorous, as the optimum of a function is definable as the point of the domain where the value in the range is maximized. In engineering disciplines, optimization problems cope with the selection and configuration of the best group of elements regarding a criterion. Typically, a utility function projecting the selected alternative into the range of utility allows the application of mathematical optimization principles.

For a long time, we assumed that the function describing the targeted value of a system would remain constant, or at least that the change would occur in an observable and understandable context. However, with the realization that more and more modern-day challenges are complex and potentially even adaptive, our understanding of optimization has also had to change. We often use computational complex adaptive systems to help us understand the natural systems of interest. There are multitudes of natural complex adaptive systems, such as society [2], the ecosystem and biosphere [3], supply networks [4], human language [5], health care [6], and climate change [7], to name just a few. Using computational representations of such systems to simulate their dynamics is a well-recognized method for developing a better understanding of them. Two of the leading organizations in complexity science, the Santa Fe Institute and the New England Complex Systems Institute, heavily rely on computer simulations for their work.

An additional driver for simulationists to be interested in addressing complexity is the need for more interdisciplinary work to address complex challenges, as is discussed in the report of the National Academy of Sciences [8]. The report notes that four factors are driving this development:

1. The recognition of the inherent complexity of nature and society and the inability of reductionism to cope with these challenges;
2. Exploring problems and questions that are not confined to a single discipline;
3. Growing societal problems that require a broader approach on a shorter time scale; and
4. The emergence of new technologies applicable in more than one discipline.

An example of this is the support given to policymakers when they make decisions. Gilbert et al. state, “Where the costs or risks associated with a policy change are high, and the context is complex, it is not only common sense to use policy modeling to inform decision making, but it would be unethical not to” [9]. Such support requires the simulation of complex socio-technical systems.

A recent literature review on optimization techniques for adaption planning in adaptive systems provides several examples of complex adaptive systems in cyber-physical systems, the internet of things, smart cities, and more. Henrichs et al. [10] describe several methods, but simulation-based optimization of complex adaptive systems is not discussed at any great length. Indeed, while the effectiveness of simulation-based optimization at solving industrial engineering problems is well established [11] and is often supported as a capability by industrial simulation applications, this is not yet the case for complex adaptive problem domains. Although there are promising applications of data assimilation that configure and calibrate the control parameters of a system, some of them even using real-time data to do so, as shown in [12], as well as using stochastic adaptive search methods to address complexity [13], the structure of the simulation remains untouched, as the system is perceived to remain constant.

This article therefore presents insights on optimality in the context of complex adaptive systems under deep uncertainty and derives implications for simulation-based optimization.

2. The Problem Domain: New Insights on Optimality

To understand why revisiting simulation-based optimization is necessary, this section begins by addressing how our understanding of optimal solutions has changed in recent years. This does not imply a new definition of optimality; indeed, the mathematical frame introduced earlier remains valid. However, what the supported decision makers consider to be the “best solution under the given constraints” does change. The most important constraint that changes is the nature of the system for which and in which a decision is made. To demonstrate this need, this section will focus on the insights gleaned from the field of complex adaptive systems and deep uncertainty when addressing systems of interest.

2.1. *Optimal Solutions in Complex Adaptive Systems*

In his introduction to complexity, Page [14] employs a metaphor in which he compares the response surface within a solution space of an optimization problem to landscapes. The task, he asserts, is to find the highest elevation within such landscapes.

The typical undergraduate examples of this are the landscapes of Mount Fuji and Mount Kilimanjaro. These solution spaces have a conical shape with a clear optimum that can be found by “climbing the mountain” using gradient-based algorithms, as described in [15]. Many machine learning algorithms use such approaches [16].

The second type introduced by Page is rugged landscapes. The European Alps, the Asian Himalayas, or the American Rocky Mountains are rugged landscapes characterized by many peaks. The highest point in these landscapes is not obvious, and gradient-based algorithms can easily get stuck in a local optimum. Additional heuristics, such as simulated annealing [17] or genetic algorithms [18], increase the probability of finding the highest

peak. Depending on the time available for the search, it is possible not only to find the highest peak but also many additional solutions that are sufficient for practical application.

The third type is “dancing landscapes,” which are landscapes that change over time. Accordingly, peaks keep moving as well, and the highest elevation at one point in time can sink while another point in the landscape can rise. Examples of this are dunes in the Sahara, snow hills during a blizzard, or ocean waves. This metaphor best describes the solution space of a complex adaptive system, as the components that build the system are constantly adapting, learning, and optimizing, resulting in a change of the system. The optimal solution is not fixed but changes with the adaption process in the system. The three landscapes are depicted in Figure 1.



Figure 1. Three Landscape Types as Introduced in Page’s Metaphor.

The main challenge is that any optimal solution in a complex adaptive system may only be temporary. What is the best way to act in one moment can become suboptimal moments later. Instead of looking for the optimal temporal solution, decision makers are increasingly interested in solutions that are applicable even under the change of the system. A stable solution with sufficiently good results is often more desirable than the optimal solution that only provides the best solution under very specific and quickly changing conditions.

2.2. Effects of Deep Uncertainty on Optimal Solutions

Practical applications of simulation optimization [19] focus predominantly on solutions for stable systems. However, some allow their simulated entities to choose different strategies, particularly for supporting business operations [20] or simulation applications in the defense and security domain [21]. They also take advantage of stochastic modeling of simulated process times and outcomes in order to evaluate the likelihood of observed outcomes. This approach enables the handling of stochastic uncertainties.

However, as observed in [22], stochastic uncertainties are a well-understood form of uncertainties, and statistics provide many tools and methods to address them. Multiple additional categories of uncertainty must be addressed when using simulation-based

optimization approaches. The traditional view is that stochastic simulations represent two types of uncertainty, which are aleatoric and epistemic uncertainty [23]. Aleatoric uncertainty represents the fundamental stochastic nature of a system while epistemic uncertainty results from insufficient knowledge. This understanding must be extended for the systems addressed in this article. Uncertainty is not simply the absence of information; it is more likely the result of inadequate information in the form of inaccurate information, unreliable information, or simply ignorance. There are multiple numerical methods to address this problem, as described in [24], but they all assume that some basic knowledge exists, which is increasingly not the case. When we address natural complex adaptive systems as described in the introduction, we often do not know the necessary detail, and sometimes we may not even know what we do not know.

The operations research community refers to this challenge as deep uncertainty. The term and its definition were introduced in a report by Lempert et al. as conditions “where analysts do not know, or the parties to a decision cannot agree on, (1) the appropriate conceptual models that describe the relationships among the key driving forces that will shape the long-term future, (2) the probability distributions used to represent uncertainty about key variables and parameters in the mathematical representations of these conceptual models, and/or (3) how to value the desirability of alternative outcomes” [25], pp. 3–4.

Since this report, deep uncertainty has been identified as a condition observed in many of the application domains of natural complex adaptive systems, e.g., for climate change assessment [26], the transportation system [27], mitigating epidemics [28], climate change [29,30], and more. New approaches are needed to use simulation-based optimization under this condition, as discussed in the next section. Similar to our observations at the end of the last section, decision makers are more and more interested in stable solutions that provide good results for a great variety of possible conditions under deep uncertainty.

3. Implications for Simulation-Based Optimization: Extending the Methods

The traditional way simulation-based optimization is performed to maximize—or minimize—the performance measures is by manipulating the input decision variables under certain constraints. The system of interest, including the constraints, is modeled in a simulation system with input parameters representing the input decision variables and output parameters that enable the calculation of the desired performance measures. Often, control parameters can configure the simulation so that it can be applied to evaluate a variety of constraints. Figure 2 shows the general structure of this method, using input, control, and output parameters.

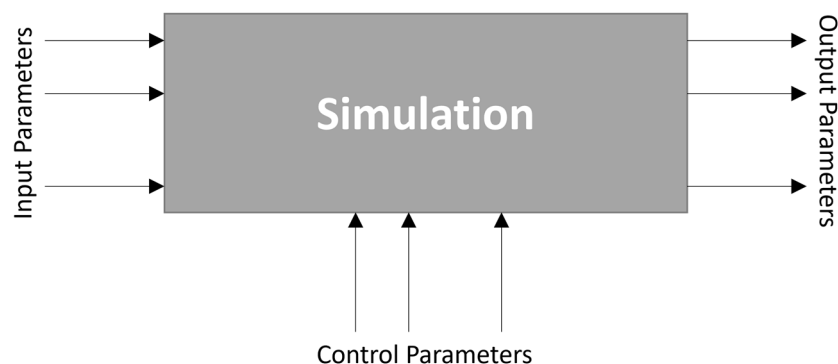


Figure 2. Structure of Simulation-based Optimization.

As Law and McComas [31] discuss, this structure enables the use of solvers to generate input parameter sets that optimize the result measured by the output parameters for a system simulated under the constraints configured by the control parameters. Many professional simulation frameworks are providing this functionality. Carson and Maria [32] provide a taxonomy of simulation optimization methods, shown in Figure 3, and describe

the various methods in detail. Although the taxonomy is neither complete nor exclusive, it provides an overview of a wide range of methods used in practice.

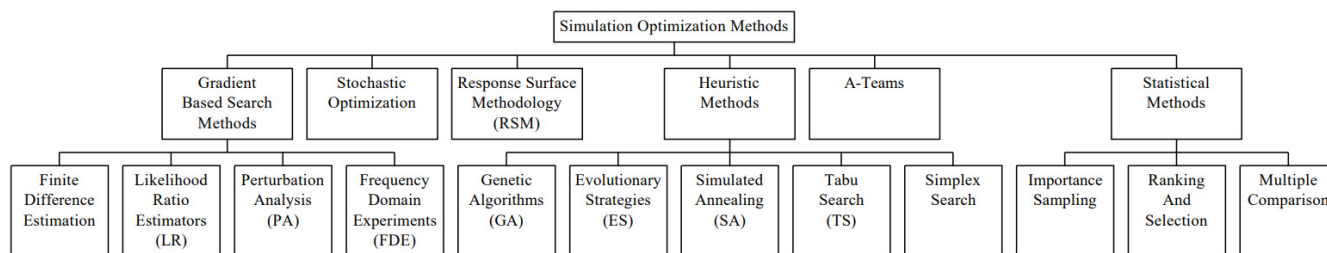


Figure 3. Taxonomy of Simulation Optimization Methods ([32], p. 119).

These traditional approaches, including probabilistic methods as described among others in [33], are applicable to problems with a solution space like Mount Fuji. Many others, meanwhile, apply to the category of rugged landscapes, but they are of limited value in addressing the third category of dancing landscapes.

The methods also assume a clear understanding of the system, so problems with deep uncertainty cannot be successfully addressed. For defense applications, Davis [34] summarized two types of uncertainty: parametric and structural uncertainty. Within the parametric uncertainty category, he captured all the operational challenges that make up the parameters of the otherwise well-known combat challenges. As such, parametric uncertainty can be summarized as having the right model but being uncertain about the input values. Structural uncertainty, though, is worse, as it is based on uncertainty about the phenomenon, meaning that it requires the consideration of possible spaces or even alternative models and conceptualizations.

In summary, deep uncertainty requires a broader evaluation of the solution space using not just a single simulation system addressing the parametric uncertainties but rather multiple simulation systems to address possible situations of interest representing possibilities under structural uncertainties. Each of these simulations represents a complex adaptive challenge. Understanding these assumptions and constraints and how they affect the uncertainties in the solution space is a novel challenge for simulation-based optimization. Instead of providing an optimal point estimate, a clear understanding of the topology of the solution space is needed to identify solutions or strategies that are sufficient under a much wider variety of possibilities derived from the uncertainties.

These kinds of questions require additional methods, as it becomes more important to find solutions that are sufficient while also being stable and robust when the underlying system changes. This observation does not imply that the traditional approaches are no longer necessary or useful. On the contrary, the heuristics and probabilistic methods can be used to gain valuable insight into the solution space and need to remain in the toolbox of the experts conducting the analysis. They do, however, need to be complemented with new approaches, some of which are discussed in the following sections.

3.1. Addressing Optimal Solutions in Complex Adaptive Systems

3.1.1. Applicable Engineering Methods

The complexity primer of the International Council of Systems Engineering (INCOSE) guides systems engineers by “applying key concepts from complex systems science to systems engineering to suggest new methods that can handle complexity rather than assuming it away” [35], p. 1. The focus of the primer is to recommend systems modeling methods to better analyze, diagnose, model, and synthesize under complexity. They follow Shalizi’s [36] recommendation to add new tools that address complexity in addition to the already applied and trusted traditional methods. Table 1 below shows the recommended methods, several of which are simulation methods used to model natural or engineered complex systems.

Table 1. Methods Recommended for Systems Engineering to Deal with Complexity [35], p. 9.

Analyze	Diagnose	Model	Synthesize
Data Mining	Algorithmic Complexity	Uncertainty Modeling	Design Structure Matrix
Splines	Monte Carlo Methods	Virtual Immersive Modeling	Architectural Frameworks
Fuzzy Logic	Thermodynamic Depth	Functional/Behavioral Models	Simulated Annealing
Neural Networks	Fractal Dimension	Feedback Control Models	Artificial Immune System
Classification and Regression Trees	Information Theory	Dissipative Systems	Particle Swarm Optimization
Kernel Machines	Statistical Complexity	Game Theory	Genetic Algorithms
Nonlinear Time Series Analysis	Graph Theory	Cellular Automata	Multi-Agent Systems
Markov Chains	Functional Information	System Dynamics	Adaptive Networks
Power Law Statistics	Multi-scale Complexity	Dynamical Systems	
Social Network Analysis		Network Models	
		Agent-based Models	
		Multi-Scale Models	

The challenge identified before is the temporal nature of an optimal solution. Depending on the speed of change, traditional solutions can still play an important role. Suppose in the business world that it takes several weeks for a business to identify, analyze, and adapt to a new environment. In such a case, ample time would remain to analyze the currently valid and relatively stable situation as if the system were static. The more agile the system is, and the more rapidly that changes occur, the more important becomes the aspect of temporary optima. What establishes rapid changes depends in this context on the decision’s length and effect time. If the decision cycle is only a few minutes long and creates a single effect, a system that changes every two weeks is de facto stable. However, if, e.g., a new building is constructed, system changes twice a year are considered rapid. As such, the context of the problem becomes tremendously important.

If the system changes rapidly in the context of the optimization question, then understanding the topology of the solution space becomes more important than identifying an optimal solution. Based on methods enumerated in Table 1, the topology captures information about the various points or regions of the solution space regarding three questions:

1. What is the probabilistic distribution within the current point or region?
2. What is the sensitivity, including the probabilistic distribution of the neighbored points and region?
3. How do these characteristics change over time, particularly in regard to the time span in which and for which a decision needs to be made?

If time and computational capabilities allow a complete parameter sweep, sensitivity does not have to be calculated explicitly, as all points of the solution space are calculated. However, heuristics like genetic algorithms must likely be used for larger problems in order to quickly establish an overview of the general structure of the solution space. By doing this, only promising regions are evaluated. However, where such promising regions are located may change over time.

In addition to these challenges of multi-criteria optimization under uncertainty, not every optimization problem has only one performance measure. As a rule, the analyst must optimize multiple objectives, which may be competitive, meaning that trade-offs are necessary. A good overview of multi-objective optimization is captured in [37]. This approach is not a unique characteristic of complex adaptive systems. Decision makers tend to focus on the most urgent problem and thereby ignore the effects a decision has on the additional performance measures. Due to their high degree of non-linearity and interconnectedness, in complex adaptive systems under uncertainty, such behavior may lead rapidly to unintended negative consequences.

3.1.2. Principles of Graphical Representation

Simulation-based optimization in the context of complex adaptive systems has a much more important role in representing and managing the uncertainty underlying a problem than the traditional approaches did. Again, this is not directed at the application

or contribution of these approaches; it is merely to say that they need to be augmented, as using probabilistic methods and sensitivity analyses for optimal solutions is no longer sufficient because the response surface of the performance metrics changes with parameters as well as with structural changes.

Davis [38] describes being forthcoming about assumptions as an ethical imperative when using simulation-based approaches to support analysis for decision makers. However, he also observes that “viewgraphs with long lists of assumptions are not exactly welcomed by busy officials” ([38], p. 5). Instead, he recommends visualizing how results vary under different assumptions, both parametric and structural. He gives an example depicted in Figure 4, originally published in [39]. The figure presents a two-dimensional possibility space that captures two main uncertainties that define the dimension. The response surface of the performance parameter has been mapped to success likely (green area), success possible (yellow area), and failure likely (red area). The figure shows two alternatives for strategy A on the left side and strategy B on the right side. It also references the most likely as the “standard case” with the highest likelihood of being observed, shown on the lower left of each strategy.

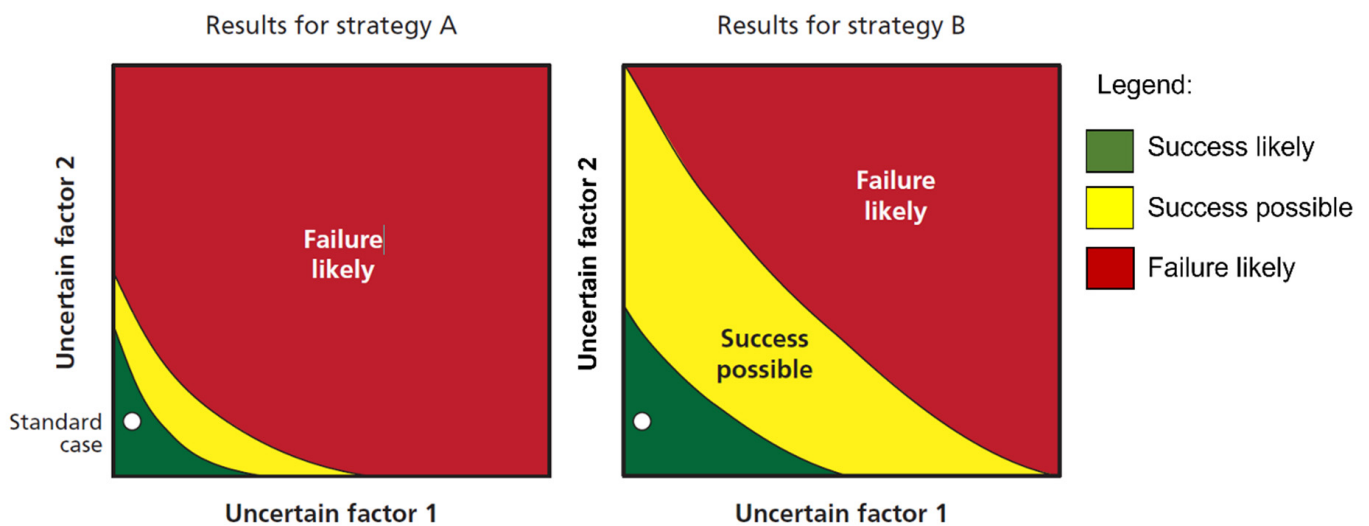


Figure 4. Comparing the Success of Two Strategies across Two Uncertainty Factors ([39], p. x).

If analysts are only looking at the standard case, the two strategies appear to be equally successful, and strategy A may even be preferable as long as we are looking for a point solution. However, as soon as we consider the uncertainty factors, the situation changes. While only a small fraction of the possible solution space results in a likely or possible success when choosing strategy A, strategy B seems more robust and preferable. Suppose more information about the uncertainty factors is available, such as a probability distribution implying that not all parts of the response surface are equally likely. In such a case, this can be visualized as well, e.g., by the height of the surface or the intensity of the colors. Furthermore, it is worth noting that the constraints are most likely affected by the choice of our strategies as well, as the system will adapt and change. When we are looking at tradeoffs between strategies, we cannot keep all other parameters as they are, as the parameters themselves are affected by the decision. The notion of comparing two alternatives with everything else being equal may not be valid under complexity and deep uncertainty.

In their work on decision space visualization (DSV) to support option awareness, Drury et al. [40] emphasize the need to root DSV in the different sets of principles of human–computer interaction (HCI), such as Nielsen’s ten usability heuristics [41], Norman’s fundamental principles [42], and the design strategies of Shneiderman et al. [43]. In their research, based on years of prototyping and experimentation [44], they identify seven principles to guide decision space visualization:

1. Allow users to apply their mental models to their situational observations and provide input parameter values. Do not require users to set input parameter values for information that can be accurately and automatically obtained elsewhere.
2. Let the user apply their real-world knowledge to set weights or values for the scoring function (the criteria for ranking the options).
3. Provide an overview of the several top options and allow users to employ their pattern recognition, judgment, and values to choose the desired option.
 - (a) Do not have the visualization identify a single, firm recommendation to users.
 - (b) Do not provide a particularly wide range of options, especially when many of them are much less desirable and thus unlikely to warrant serious consideration.
4. When constructing DSVs, tradeoff unnecessary fidelity in favor of speed of response. Determine the required fidelity level based on whether DSVs generated from models of a lower fidelity level would lead to the same decision as DSVs constructed from data obtained via a higher-fidelity model.
5. Show the consequences of choosing one option versus another under a variety of possible conditions rather than a single set of “most likely” conditions.
 - (a) Use a frequency-based presentation, not a probability-based presentation.
 - (b) Reveal the shapes of the distribution of outcomes.
6. Provide interactive filtering and sorting for viewing subsets of the data that underlie the decision space.
7. Support comprehension of the factors and relationships mediating the consequences of choosing one option versus another.

As before, it is good practice to follow these principles to gain the group’s full support because the visualization is driven by their needs, options, and metrics. They support the creation of visualizations that capture the effect of uncertainties and drive the options that a decision maker has. As such, they can create a helpful shell around simulation-based optimization applications.

To summarize, the objective of addressing optimal solutions in complex adaptive systems is the decision-centered understanding of the solution space and the uncertainties that drive the change of the response surface to changes in the underlying system. Graphical representations that are meaningful to the decision maker and communicate the effects of uncertainties are pivotal for success.

3.2. Addressing Optimal Solutions under Deep Uncertainty

Optimal solutions under deep uncertainty must address all the aspects described thus far, whilst also applying various methods and techniques to address the structural uncertainties that result from the lack of consensus regarding the structure and conceptual principles describing the system of interest.

Marchau et al. [22] introduce five levels of uncertainty that span the gap between total certainty and total ignorance about a system of interest. Their levels extend the work of Courtney et al. [45], who introduced four levels of uncertainty:

1. A clear enough future allowing for a single forecast;
2. Alternate futures with a few discrete outcomes allowing for traditional decision analysis and game theory;
3. A range of futures with a range of possible outcomes, not connected by common scenarios; and
4. True ambiguity with no basis to forecast the future.

Table 2 is a slightly modified version of that presented in [22], focusing on the system model and simulation support to address the extended levels of uncertainty. Marchau et al. use an additional level and embed their levels into a broader context. Level 1 borders on total certainty, which implies full information about the system of interest and its context. Level 5 borders on total ignorance, which is even less certain than the unknown future, as, in the unknown future, we at least know that we do not know something now, but we may

expect it to be observed in the future. Total ignorance excludes even knowing what we do not know.

Table 2. Progressive Transition of Levels of Uncertainty and System Implications.

	Level 1	Level 2	Level 3	Level 4	Level 5
Context	A clear enough future (with sensitivity)	Alternate futures (with probabilities)	Alternate futures (with ranking)	A multiplicity of plausible futures (unranked)	Unknown future
System Model	A single system model	A single system model with a probabilistic parametrization	Several system models with different structures with assigned likelihoods	Several system models with different structures	Unknown system model, but we know what we do not know
System Outcomes	Point estimates with sensitivity	Several sets of point estimates with confidence intervals	Several sets of point estimates ranked according to their perceived likelihood	A known range of outcomes	Unknown outcomes, but we know what we do not know
Weights on Outcomes	A single estimate of the weights	Several sets of weights with probabilities assigned	Several sets of weights ranked according to their perceived likelihood	A known range of weights	Unknown weights, but we know what we do not know
Simulation Support	Simulation-based optimization	Probabilistic simulation-based optimization	Simulations for each system model as the basis for probabilistic optimization	Simulations for each system model to generate the range of outcomes and weights	Without a system model, simulation-based optimization is not possible

While rare and extremely rare events can be captured in simulations [46], black swans, as described in [47], are unknown, so they cannot be modeled. This observation is also generally a challenge with simulation-based support under uncertainty: we can only simulate what we can imagine, and we can usually not imagine something we know nothing about. This observation serves as a general epistemological limit on simulations. However, all other types of uncertainty can be captured in a model and can therefore be simulated.

From a practical viewpoint, it is good practice to use the levels of uncertainty to identify the simulation-based optimization support needed to generate the multiple possible outcomes that will shape the decision space. To provide the intended decision support requires an additional step, namely the application of algorithms that make sense of this multitude of data describing many possible futures and—particularly in socio-technical systems—reflect multiple different viewpoints and value systems, resulting in multiple objectives for each possible future scenario. In other words, the process recommended in [25] is still valid, namely iterating through all candidate strategies using the ensemble of plausible scenarios addressing all identified uncertainties. Current computational capabilities support this massive computational effort. The process of identifying the possible alternatives of interest is often addressed as exploratory modeling and analysis [48], the process of designing search or sampling strategies that support valid conclusions or reliable insights needed to address deep uncertainty.

The many objectives robust decision making (MORDM) process was introduced in [49] and provides a reasonable basis to guide analysts through exploratory modeling and analysis. While the original MORDM process started with one scenario of interest and discovered additional possibilities iteratively, alternate future situations already start with multiple possible scenarios. Such observations led to an extension of the MORDM to support better deep uncertainty challenges, as demonstrated in [50]. Figure 5 shows the extended MORDM process.

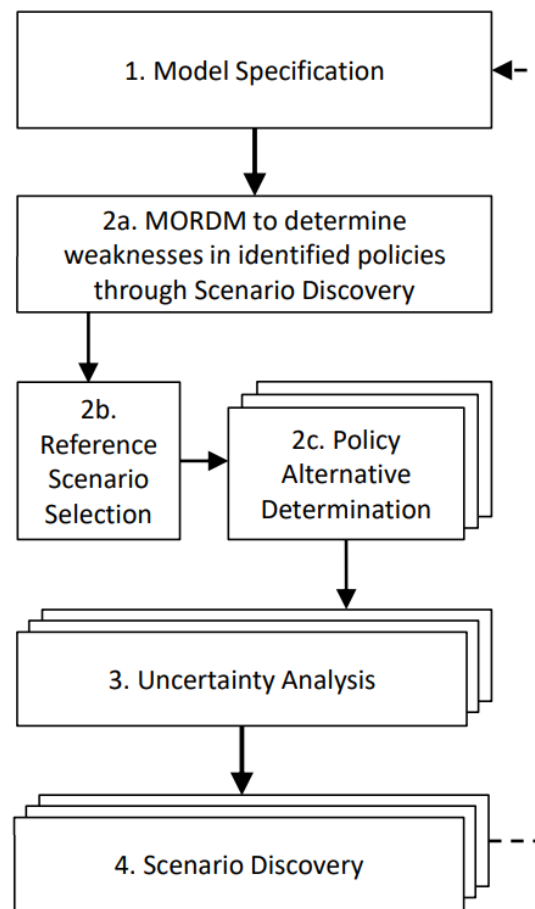


Figure 5. Extended MORDM Process as Introduced in [50].

The model specification phase defines the research question. It identifies the problems, possible strategies, and scenarios to evaluate them in a multi-objective context. This approach includes identifying the level of uncertainty. Each model results in a simulation for which the uncertain parameters can now be specified to the degree the team is aware of them: parameters are estimated, probability functions are identified, and missing concepts and attributes are inserted. The second phase has been improved by allowing multiple alternative determinations, resulting from the iterative process supported by simulation-based optimization of the strategy/scenario combinations. While phase one defines the models, phase two focuses on the strategies and how well they perform under the constraints of these models. The following uncertainty analysis for each alternative discovers new scenarios, i.e., additional models, strategies, or both, resulting in additional iterative loops. The integration of the decision maker into this loop is pivotal, as the understand the problem domain and can avoid possible, but not always meaningful combinations. As a result, the MORDM helps us to discover the strengths and weaknesses of the alternative strategies in alternate futures. Figure 6 illustrates how this process has been applied to show the likelihood of success for three different strategies under various scenarios. As the reader is already familiar with it, we use the same visualization as that used in the examples provided in [39].

When comparing the three strategies, it quickly becomes apparent that strategy C is a bad choice under all conditions. Strategies A and B, meanwhile, both have their advantages and disadvantages, although A seems to be more robust and is superior to strategy B except in the scenario shown in the top of the stack. It is this kind of insight that the simulation-based optimization must provide for complex adaptive systems under deep uncertainty.

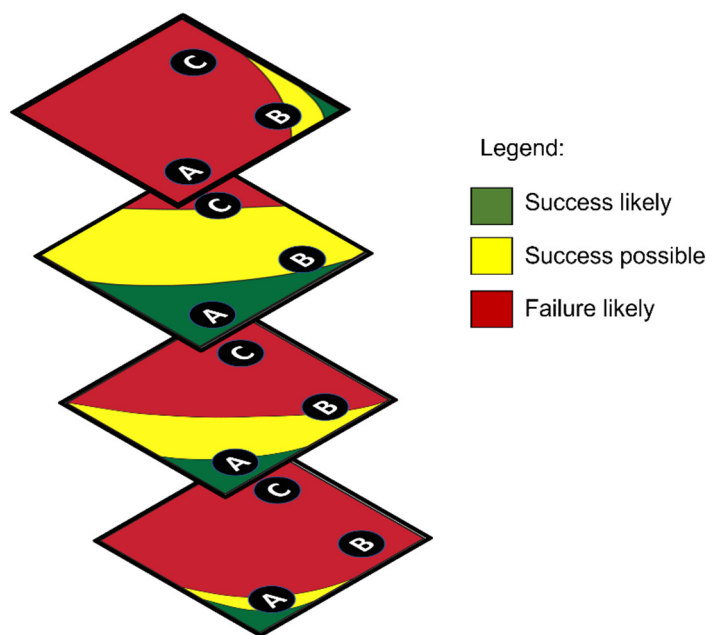


Figure 6. Likelihood of the Success of Three Alternative Strategies under Four Scenarios.

Another question that is worth exploring is which uncertainties matter for the decision to be supported? Simulation can provide answers by conducting parameter sweeps to gain insights into how sensitive the model is to uncertainty in parameters. Using models with different structures also enables the analyst to address epistemic as well as aleatoric uncertainty. The main insight here is that we should attempt to develop a better understanding of which parameters really matter in regard to the objectives, and as a corollary, does it matter if a great deal of effort is put into reducing uncertainty regarding these parameters? In the context of decision making, we must answer the following question: Although we may not know something, would it matter if we did? Additionally, if it matters, is it worth allocating resources in attempt to reduce that uncertainty? Option awareness [44] emphasizes the role of humans in this process, as humans are aware of the context of the decision, which is not necessarily the case for simulations rooted in simplifications and abstractions.

To further support the need to create better awareness, it may be possible to adapt business visualization strategies, as they are already used to support decision making under complexity and uncertainty, such as Wardley maps [51]. Examples of state-of-the-art visualization methods for multi-dimensional uncertainty have been compiled in [52,53]. Some additional promising research results on decision space visualization and extended use of simulation have been published in [54]. Furthermore, there are open-source workbench solutions that support these processes [55]. Augmenting these processes and workbench solutions through simulation solutions in order to enable even better simulation-based optimization support under deep uncertainty is an ongoing research topic.

4. Conclusions and Discussion

Being faced with complexity is not a new problem. However, until recently, the dimensions in which we dealt with our challenges were limited enough to allow the use of methods that do not have to consider complexity and adaption. We also knew enough about our systems to avoid deep uncertainty concerns. However, with the increasing capabilities and the new structures created by interconnected systems, we can no longer ignore complex adaptive challenges. Furthermore, supporting decision makers often requires dealing with socio-technical systems that exhibit complex and adaptive characteristics. Simulation-based optimization must play a part in addressing this issue by incorporating methods from complexity science and exploratory modeling and analysis applications.

Thus, this article enumerates some methods that can potentially contribute to new solutions. While many of the methods are already known, their combined use to allow for simulation-based optimization of complex adaptive systems under deep uncertainty is a new notion that must be put to the test in future research. As exemplified in *Nature* magazine [56], blindly applying statistical cookbook solutions without understanding the application domain or the validity contexts of the methods can lead to insufficient or incorrect interpretations. This challenge is exaggerated for decisions in complex adaptive systems under deep uncertainty. For every solution generated to address an aspect of deep uncertainty, the result still exposes many additional parametric uncertainties that change over time due to the adaptive nature of the decision environment.

Representing these multidimensional uncertainties that influence the effects of a decision over time to decision makers is the subject of ongoing research. Instead of presenting one optimal point solution and conducting single-objective optimization, the objective must be to find robust solutions that work effectively for many constellations or that eliminate bad solutions that do not work under any or only a few unlikely constraints. As summarized in recent recommendations for policy decision making in complex systems, the “recommendation is those policy analysts . . . should prioritize serious uncertainty analysis, to include addressing uncertainty and disagreement about conceptual models that underlie the analysis. This observation means analysis to find strategies that are flexible, adaptive, and robust . . . , i.e., strategies that are expected to do well across the range of assumptions about inputs, how the world works, and how alternative policies would affect outcomes over time” [57], pp. 194–195. Following this advice is also good practice for simulation-based optimization.

One aspect that is important for the application of simulation for optimization that was not addressed explicitly in this paper is the aspect of trust. Decision makers must trust the simulation to trust the resulting data and recommendations. Harper et al. [58] only recently compiled a review of applicable methods. However, trust does not imply that the computational teammate is always superior and should always be followed. Instead, it implies that the recommendations are well founded on trusted algorithms and reliable data but that human intuition cannot be replaced by computational rigor. Furthermore, for socio-technical systems, the question of how to validate them, particularly under deep uncertainty, is an ongoing research topic. As discussed in [59], our view on validation may have to be revisited.

Finally, simulation-based optimization, as described here, provides a multitude of data under uncertainty. These data need to be presented to the decision maker in an understandable and actionable form. To make the simulation insights applicable to decision makers, they must clearly understand policy levers representing various policies and alternatives. Rouse [60] proposes making the system immersive and interactive so that it becomes the “flight simulator for decision makers.” Haberlin and Page [61] describe large-scale, highly configurable visualization facilities. Placing the decision maker into such an interactive and immersive display results in a better understanding of the solution space and even provides experience of the possible side effects of policies. As decision makers use dashboards to visualize real-world data for understanding the current situation better, sometimes augmented by methods used in their profession to investigate available decision options and their consequences, familiar dashboards should be part of these presentations. However, dashboards and other traditional methods often fall short of visualizing uncertainties. These uncertainties are a vital part of the insights that can be provided using simulation-based optimization, requiring the augmentation of the dashboards accordingly. Visual representation of uncertainties is a topic of ongoing research that requires us to follow developments for the best support of communicating uncertainties and related risks to the decision maker.

Using a simulation-based approach to support making decisions under deep uncertainty is not the only aspect. As already mentioned before, integrating the decision maker more into the decision process and get their inputs early has been recognized as good prac-

tice. Dynamic adaptive planning [62] and dynamic adaptive policy pathways [63] provide a new approach for decision making under uncertainty of interest to the simulation-based optimization community, as they describe a new paradigm to follow.

All these proposed methods and tools are complementary methods to the established simulation-based optimization approaches, as captured by Fu in [64] and by Nelson and Pei in [65]. These traditional methods, which are also addressed in the BoK [1], remain essential to solving optimization challenges using simulation. What needs to be changed, then, is our view of systems as stable constructs. Instead of highly optimized point solutions, understanding how the topology and response surface may change to support stable and good solutions that take multiple objectives and uncertainties into account is needed. With socio-technical and complex adaptive systems serving as the systems of interest, and in the presence of deep uncertainty, the era of point solutions based on single models must come to an end. Even terms like “prediction” and “optimal” should be avoided, as they suggest a certainty of the recommended solutions we no longer can provide. We need to clearly communicate that we mean improvement towards something better when we use the term optimization in the context of complex adaptive systems under deep uncertainty.

The implications are not limited to the discipline of M&S but are also of interest to the many disciplines that are using M&S to support them [66]. Of particular interest is the discipline of systems engineering, as new paradigms like system-of-systems [67] and the Internet-of-Things (IoT) [68] are placing systems increasingly into complex, adaptive, and deeply uncertain environments. Although systems engineering is increasingly starting to address such new challenges, as among others described in [69], the need for better support is recognized. Particularly the challenge of emergence gains increasingly publicity, in theoretical [70] as well as practical domains [71]. Emergence—understood as a behavior exposed by the system but not by any of its components—adds a new dimension to unpredictability that needs to be considered by decision makers, and as Darley defines in [72], “a true emergent phenomenon is one for which the optimal means of prediction is simulation,” so simulation-based optimization will have its role addressing these challenges as well.

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