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Simulation-Based Optimization: A Comprehensive Review of Concept, Method and Its Application

Milad Abolghasemian[1,*], Sedigheh Kaveh[2], Fatemeh Ebrahimzadeh[2]

[1] Department of Industrial Engineering, Ayandegan University, Tonekabon, Iran; abolghasemian@aihe.ac.ir.

[2] Department of Computer Engineering, Ayandegan University, Tonekabon, Iran; s.kaveh@aihe.ac.ir; f.ebrahimzadeh@aihe.ac.ir.

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Abstract

Simulation-Based Optimization (SBO), as a hybrid approach combining simulation modeling and optimization techniques, is a powerful tool for solving complex decision-making problems that cannot, or cannot be reliably, solved by classical methods due to uncertainty, nonlinear and discrete behaviors, high dimensions, and the black-box nature of systems. The combination of simulation's descriptive power and optimization's prescriptive power enables accurate analysis of dynamic, uncertain environments and the identification of optimal or near-optimal decision-making policies. This article provides a comprehensive overview of the fundamental concepts, classification of approaches, and key methods in the field of SBO. In this regard, a variety of optimization methods used alongside simulation—including deterministic and stochastic methods, metaheuristics, machine learning-based approaches, multiobjective frameworks, and constrained optimization techniques—are reviewed. Special attention is paid to derivative-free methods and surrogates, which are common for optimizing expensive, noisy, and non-differentiable models. The role of various simulation approaches, such as discrete-event, continuous-time, agent-based, and Monte Carlo simulations, in shaping the SBO landscape is also discussed. In the applications section, the paper reviews key areas including Supply Chain Management (SCM), healthcare systems, transportation and logistics, energy and environment, and military and defense applications. For each area, it is shown how SBO can improve strategic and operational decision-making under uncertainty, enhance system performance, and increase its resilience. In addition, the significant challenges of SBO, including high computational cost, model uncertainty, data limitations, and high dimensionality, are analyzed. Finally, the article highlights emerging trends, including the integration of machine learning and simulation, the development of digital twins, the use of high-performance computing, and the move towards real-time optimization. Overall, this review aims to provide a comprehensive overview of the theoretical foundations, methodological advances, practical applications, and future research directions in SBO.

Keywords: Simulation, Optimization, Simulation-based optimization.

1 | Introduction

Modern engineering and management systems—from supply chains and transportation networks to healthcare operations and energy systems—are increasingly complex and uncertain. Traditional analytical

Corresponding Author: abolghasemian@aihe.ac.ir

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optimization models often fail to capture the full dynamics of these systems. In contrast, simulation models allow practitioners to replicate real-world variability and system behavior more realistically [1]. The increasing complexity, dynamism, and uncertainty inherent in modern engineering, business, and socio-technical systems have driven a growing reliance on simulation to model real-world operations. Simulation enables analysts to capture stochastic variability, nonlinear relationships, time-dependent interactions, and system behaviors that are often analytically intractable or impossible to express in closed form [2]. While simulation alone provides valuable performance insights, decision makers ultimately require tools that can not only evaluate but also optimize system behavior. This need has led to the emergence and rapid growth of Simulation-Based Optimization (SBO)_a field that integrates computational simulation models with optimization algorithms to guide decision-making in environments where traditional analytical approaches fall short. SBO refers to a family of methods that use simulation models to evaluate potential solutions while optimization algorithms guide the search for the best solution. SBO has become a major research and industrial tool for decision-making under uncertainty [3]. SBO provides a powerful framework for identifying optimal or near-optimal solutions when the objective function is evaluated only through simulation, is noisy, lacks gradient information, or involves complex constraints [4]. SBO encompasses a broad suite of methodologies, ranging from classical derivative-free optimization and stochastic approximation to advanced machine learning and metaheuristic algorithms. These methods can address high-dimensional, multimodal, and non-convex optimization landscapes in which simulation evaluations are computationally expensive and analytically opaque. As a result, SBO has become an indispensable tool across diverse fields, including manufacturing, Supply Chain Management (SCM), healthcare operations, military decision-making, transportation logistics, and energy systems [5].

The increasing availability of high-performance computing, parallel simulation engines, and data-driven modeling techniques has further accelerated the evolution of SBO. Recent advancements—including surrogate-assisted optimization, Bayesian Optimization (BO), reinforcement learning, and digital twins—have expanded the scope, speed, and capability of simulation-driven decision technologies. Despite these advancements, fundamental challenges persist in balancing accuracy and computational cost, handling stochastic noise, scaling to high-dimensional problems, and ensuring convergence guarantees [6]. The roots of SBO trace back to early Monte Carlo experiments in the 1950s and the rise of Discrete-Event Simulation (DES) in the 1960s, when researchers began recognizing simulation's potential not only to evaluate but also to improve system performance. Early stochastic optimization techniques—such as stochastic approximation [7] and finite-difference gradient estimators—laid theoretical foundations for optimizing noisy objective functions. By the 1980s and 1990s, the proliferation of affordable computing power enabled large-scale simulation studies, leading to renewed interest in derivative-free optimization, Design of Experiments (DoE), and metamodel-based approaches. The 2000s witnessed the rise of metaheuristics (Genetic Algorithms (GAs), Particle Swarm Optimization (PSO), Simulated Annealing (SA)), which proved effective for complex black-box problems. More recently, advances in machine learning, BO, surrogate modeling, and reinforcement learning have substantially expanded SBO's capabilities [8]. Today, the field is rapidly evolving alongside technologies such as digital twins, high-performance computing, and data-driven modeling, positioning SBO as a cornerstone methodology for modern decision science [9].

A general SBO problem can be expressed as [2]:

$$
\begin{aligned}
&\min f(x) = E[L(x, \varepsilon)],\\
&\text{s.t.}\\
&g_i(x) \leq 0, \quad j = 1, \dots, m,
\end{aligned}
\tag{1}
$$

where: 1) x represents the decision variables, 2) $L(x, \varepsilon)$ is the simulation response with random input ε, and 3) $f(x)$ is the expected performance measure the decision-maker seeks to minimize or maximize.

Because $f(x)$ is not available in closed form, and simulation outputs may be noisy, discontinuous, or computationally expensive; classical optimization techniques cannot be directly applied. Instead, SBO frameworks rely on iterative search strategies that repeatedly call a simulation model to evaluate candidate solutions. Several real-world challenges illustrate the importance and necessity of SBO [9]:

I. Healthcare operations: hospitals face uncertainty in patient arrivals, treatment times, and resource availability. Simulation helps model patient flow, while optimization identifies staffing levels, triage strategies, and scheduling policies that improve service quality.

II. Supply chain and logistics: multi-echelon supply chains involve stochastic demand, lead times, and transportation delays. SBO enables organizations to determine optimal inventory levels, network configurations, and routing plans that reduce costs and improve resilience.

III. Manufacturing systems: complex production systems require optimizing batch sizes, sequencing rules, and machine configurations. Simulation captures shop-floor variability; optimization recommends decisions that minimize makespan or maximize throughput.

IV. Energy systems: power grids, renewable energy systems, and smart networks exhibit dynamic, uncertain behaviors. SBO provides tools to manage load balancing, storage scheduling, and energy distribution in uncertain environments.

V. Defense and military applications: mission planning, equipment maintenance, and logistics operations benefit significantly from simulation-enhanced optimization, enabling risk-aware decisions in uncertain operational settings.

In each of these examples, the challenge is similar: the underlying system is too complex or stochastic for analytical optimization, but too critical to manage without systematic decision support. Despite its strength, SBO introduces several challenges [10]:

I. Noise and variability: simulation outputs often exhibit stochastic noise, complicating performance estimation and convergence.

II. Computational cost: high-fidelity simulations can require hours per run, motivating the need for surrogate models and efficient search strategies.

III. Nonconvexity and non-differentiability: many real systems yield simulation responses that lack smoothness or structure.

IV. High dimensionality: as the number of decision variables grows, the search space becomes exponentially harder to explore.

This review synthesizes the foundational theories, methodological developments, application domains, and emerging directions of SBO [11]:

I. Core SBO concepts and categories

II. State-of-the-art optimization techniques suitable for simulation settings

III. Practical applications across industry and research

IV. Performance evaluation strategies

V. Future opportunities driven by machine learning, digital twins, and hybrid modeling

The aim is to provide a cohesive, accessible, and comprehensive reference that supports both academic inquiry and practical implementation. Recognizing these challenges, the field has developed a spectrum of methodologies—from metamodel-based approaches and heuristics to advanced learning-based optimization—to improve convergence efficiency, robustness, and scalability [12]. This paper provides a comprehensive review of SBO, synthesizing methodological foundations, algorithmic developments, classification frameworks, real-world applications, and emerging trends. The objective is to offer researchers, practitioners, and graduate students a cohesive, accessible understanding of the field's current state, potential, and future directions [13]. By integrating perspectives from optimization theory, simulation modeling, artificial intelligence, and applied operations research, this review aims to serve as a foundational reference for both academic study and practical implementation of SBO tools. This review highlights key concepts, methods, and applications of SBO and provides a structured perspective for newcomers and experts in the field [14].

2 | Foundations of Simulation-Based Optimization

2.1 | Simulation Models

Simulation models can be categorized into several fundamental types, each designed to capture specific characteristics of real-world systems. The four most widely used categories in SBO are DES, continuous simulation, Agent-Based Simulation (ABS), and Monte Carlo simulation. Each approach provides unique strengths depending on the nature of the system being studied and the type of uncertainty involved. Simulation models can be classified into [15]:

I. DES: models systems where state changes occur at discrete points in time.

II. Continuous simulation: models based on differential equations.

III. ABS: models autonomous interacting agents.

IV. Monte Carlo simulation: uses repeated sampling to model stochastic systems.

These models can capture nonlinearities, randomness, and high-dimensional dependencies. DES represents systems in which state changes occur only at specific points in time, typically triggered by discrete events. Between these events, the system remains unchanged. DES models are structured around an event calendar that schedules and processes events such as arrivals, service completions, failures, and state transitions. This approach is particularly well-suited for operational systems that involve queues, resource sharing, and workflows [16]. DES is widely applied in manufacturing systems, healthcare operations, call centers, transportation terminals, and supply chain networks. For instance, in a hospital emergency department, patient arrivals, triage decisions, and treatment completions can be represented as discrete events, enabling analysts to evaluate performance metrics such as waiting times, resource utilization, or throughput [17].

Continuous simulation is used to model systems whose states evolve continuously over time, typically described by differential equations. Unlike DES, which captures discrete transitions, continuous simulation models physical, chemical, or biological processes in which changes occur continuously. These models often involve Ordinary Differential Equations (ODEs), differential-algebraic equations, or, in some cases, Stochastic Differential Equations (SDEs) [18]. Continuous simulation is commonly employed in engineering fields such as fluid dynamics, thermal and chemical processes, epidemic modeling, and environmental systems. For example, the spread of a contaminant in a river or the progression of an infectious disease within a population can be modeled using continuous dynamics that track state variables continuously.

ABS models a system as a collection of autonomous, interacting agents, each with its own behaviors, attributes, and decision-making rules [19]. Unlike DES or continuous models, which focus on processes or equations, ABS emphasizes individual-level interactions that collectively generate emergent system-level behaviors. Agents may represent people, vehicles, animals, robots, or any entity capable of making independent decisions [20].

ABS is beneficial for complex adaptive systems where heterogeneity and decentralized interactions are significant factors. Applications include social behavior modeling, financial markets, crowd dynamics, ecological systems, and multi-robot coordination. For example, in epidemiological modeling, each person can be represented as an agent whose health state and movement patterns influence disease transmission dynamics [21].

Monte Carlo simulation is a stochastic modeling technique based on repeated random sampling. Instead of modeling the detailed dynamics of a system, Monte Carlo methods repeatedly generate random inputs to approximate the distribution of uncertain outcomes. With sufficient iterations, this method provides statistically reliable estimates of expected performance, variability, and risk [22].

Monte Carlo simulation is widely used in finance, risk analysis, reliability engineering, environmental modeling, and decision-making under uncertainty. For example, in investment portfolio analysis, random draws of market conditions are simulated to evaluate the distribution of potential returns and risks [23].

2.2 | Optimization Methods

Optimization techniques used in SBO span a broad spectrum—from classical mathematical methods to modern machine learning-driven algorithms. These approaches vary in their assumptions, computational requirements, and suitability for deterministic or stochastic environments. The major categories include deterministic optimization, metaheuristics, machine learning–based optimization, and stochastic optimization [23].

Optimization approaches in SBO can be broadly grouped into:

I. Deterministic optimization: gradient-based, convex, or exact methods.

II. Metaheuristics: Evolutionary Algorithms (EAs), PSO, SA.

III. Machine learning-based optimization: surrogate modeling, BO.

IV. Stochastic optimization: Sample Average Approximation (SAA), stochastic gradient methods.

Due to the absence of closed-form objective functions, SBO must rely on simulation outputs for performance evaluation [24].

Deterministic optimization methods assume that the system is fully known, mathematically well-defined, and free from randomness. These models rely on exact functional relationships and typically aim to find a global or local optimum using analytical or numerical tools [25].

Gradient-based methods

Gradient-based optimization methods use first-order (or second-order) derivative information to guide the search direction. Algorithms such as gradient descent, Newton's method, quasi-Newton methods (e.g., BFGS), and interior-point methods iteratively improve the objective by following gradients. These methods are efficient and fast, but they require differentiable objective functions and may become trapped in local optima [26].

Convex optimization

Convex optimization focuses on problems in which the objective function and the feasible region are convex. Such problems guarantee a globally optimal solution, which can be found using efficient algorithms such as the ellipsoid method, subgradient methods, or interior-point methods. Convex optimization is widely used in engineering design, control systems, and large-scale linear or quadratic programming [27].

Exact optimization methods

Exact methods deliver provably optimal solutions. These include branch-and-bound, dynamic programming, cutting plane methods, Mixed-Integer Linear Programming (MILP), and combinatorial optimization techniques. Although exact methods are mathematically rigorous, they often become computationally expensive for large or nonlinear systems [28].

Metaheuristics are high-level, problem-independent search frameworks designed to explore large, complex, and potentially non-convex search spaces. They do not require gradient information, making them suitable for SBO where objective functions are often noisy, black-box, or highly nonlinear [29].

Evolutionary algorithms

EAs mimic the principles of natural evolution, including selection, crossover, and mutation. GAs are the most widely known example. EAs maintain a population of candidate solutions and evolve them over generations. They are robust, easy to implement, and excel in complex search spaces, but can require substantial computational effort [30].

Particle swarm optimization

The collective movement of birds or fish inspires PSO. A population of "particles" moves within the search space, adjusting velocities based on their own experience and the best-known global solution. PSO is simple, computationally efficient, and effective for continuous optimization problems [31].

Simulated annealing

The annealing process inspires SA in metallurgy. It probabilistically accepts worse solutions early in the search to escape local minima, gradually reducing randomness as the temperature parameter decreases. SA is effective for combinatorial optimization and rugged search landscapes [32]. As simulation models become more computationally expensive, machine learning–based optimization methods provide efficient ways to approximate or optimize complex objective functions [33].

Surrogate modeling

Surrogate modeling involves constructing an approximate model of the objective function—called a surrogate or meta-model—to replace expensive simulations. Popular surrogate models include Gaussian processes, radial basis functions, polynomial regression, and neural networks. Optimization is performed on the surrogate model rather than the real simulation, drastically reducing computational costs [34].

Bayesian optimization

BO is a powerful framework for optimizing expensive black-box functions. It models uncertainty using Gaussian processes and selects new evaluation points using an acquisition function that balances exploration and exploitation. BO is widely used for hyperparameter optimization, engineering design, and high-computational-cost simulation [35]. Stochastic optimization deals with problems involving randomness in parameters, models, or objective functions. These methods are essential when uncertainty cannot be eliminated or when the system is inherently probabilistic [36].

Sample average approximation

SAA approximates the expected objective function by averaging over multiple scenarios (samples). As the number of samples increases, the approximation converges to the true expectation. SAA is widely used in risk management, logistics, and stochastic programming, especially when paired with deterministic solvers [37].

Stochastic gradient methods

These methods generalize gradient descent to stochastic environments by using noisy or partial gradient estimates. Prominent examples include Stochastic Gradient Descent (SGD), mini-batch gradient methods, and variance-reduction techniques such as SVRG and ADAM-like adaptive optimizers. Stochastic gradients are efficient in large-scale problems and foundational in machine learning [8].

3 | Categories of Simulation-Based Optimization

3.1 | Black-Box Optimization

In many cases, simulation models provide only output responses without revealing internal mathematical structure. Black-box optimization treats the simulation as an opaque function [2].

3.2 | Derivative-Free Optimization

In many SBO problems, the objective function is noisy, non-differentiable, discontinuous, or computationally expensive, making traditional gradient-based methods impractical or unusable. Derivative-Free Optimization (DFO) refers to a class of optimization techniques that do not rely on explicit gradient information. Instead, they use direct search strategies, function evaluations, or probabilistic sampling to explore the decision space. DFO methods include pattern search, Nelder–Mead simplex, trust-region methods for black-box functions, response-surface methods, and various stochastic search algorithms. Because they rely solely on input–output evaluations of the simulation model, these methods are particularly suitable for complex systems such as supply chains, manufacturing processes, and engineering design problems where the functional form of the objective is unknown. A key advantage of DFO is its robustness to noise and non-smoothness, which are common characteristics of simulation outputs. However, DFO methods can be computationally intensive, as they may require many simulation replications to achieve reliable results—especially in high-dimensional or highly stochastic environments [14].

3.3 | Multi-Objective Simulation-Based Optimization

Real-world decision-making often involves multiple, conflicting objectives, such as minimizing cost while maximizing service quality or throughput. Multi-Objective Simulation-Based Optimization (MOO-SBO) extends traditional single-objective optimization by evaluating trade-offs between competing goals. Instead of producing a single optimal solution, MOO-SBO aims to approximate the Pareto front, which represents the set of efficient solutions where no objective can be improved without degrading another [38].

Approaches for MOO-SBO include:

I. Pareto-based metaheuristics, such as NSGA-II, SPEA2, and MOO-PSO

II. Scalarization techniques, which convert multiple objectives into a single weighted objective

III. Evolutionary Multi-Objective optimization (EMO), which is well-suited to non-smooth or noisy simulation outputs

IV. Surrogate-assisted MOO, in which surrogate models approximate multiple outputs simultaneously to reduce simulation cost

MOO-SBO is widely used in engineering system design, environmental modeling, healthcare planning, and logistics optimization, where decision-makers must evaluate trade-offs among efficiency, cost, robustness, reliability, and sustainability [1].

3.4 | Constrained Simulation-Based Optimization

In practical applications, optimization problems rarely exist without constraints.

These constraints may be [18]:

I. Explicit mathematical constraints (e.g., linear constraints on resources)

II. Implicit constraints, such as feasibility rules or operating limits embedded in the simulation logic

III. Simulation-based constraints, which require simulation evaluation to determine feasibility (e.g., "the probability that waiting time exceeds 10 minutes must be below 5%")

Constrained SBO incorporates such limitations into the search process. Because constraints may also be stochastic, non-differentiable, or observable only through noisy simulation outputs, specialized methods are required.

Common approaches include [22]:

I. Penalty-function methods, which incorporate constraint violations into the objective function

II. Feasibility restoration approaches, which guide the search toward feasible regions

III. Chance-constrained optimization, where constraints must hold with a specified probability

IV. SAA for estimating constraint probabilities

V. Surrogate-based constraint modeling, where classifiers or regressors approximate feasible and infeasible regions

Constrained SBO is essential in systems such as queuing networks with service-level agreements, manufacturing systems with capacity limits, energy systems with safety thresholds, and transportation models with regulatory constraints [23].

3.5 | Model-Based and Surrogate-Based Optimization

Surrogate modeling approximates simulation outputs using: 1) kriging (Gaussian process regression), 2) radial basis functions, and 3) neural networks. This reduces the number of simulation runs needed. Metamodeling, also known as surrogate or response surface modeling, is a powerful strategy for approximating the relationship between decision variables and performance measures when direct simulation is computationally expensive. Instead of repeatedly running high-fidelity simulations—which may take minutes or hours per replication—meta-models provide a fast-to-evaluate analytical or statistical approximation of the simulation output. In SBO, each evaluation of the objective function can be extremely costly. Metamodeling addresses this challenge by [33]:

I. Reducing computational burden

II. Allowing extensive exploration of the decision space

III. Supporting optimization algorithms that require many function evaluations

IV. Providing analytical insight into system behavior

By replacing the simulation with a mathematical approximation, metamodeling enables efficient optimization even under tight computational budgets. The general process of metamodeling is as follows [38].

I. DoE: select input points (sample designs) at which simulation runs will be performed. Techniques include factorial designs, Latin Hypercube Sampling, and space-filling designs.

II. Simulation runs: perform simulation experiments at the selected design points to generate training data.

III. Model construction: fit a meta-model that maps the inputs to outputs based on the simulation results.

IV. Model validation: evaluate accuracy using cross-validation, prediction error metrics, or additional test points.

V. Optimization using the meta-model: use the surrogate in place of the simulation to identify promising regions of the search space, often followed by selective simulation refinement.

4 | Applications of Simulation-Based Optimization

4.1 | Manufacturing Systems

SBO helps improve production scheduling, inventory control, and quality control.

Table 1. Example applications in manufacturing.

Application	Objective	Simulation Type	Optimization Method
Production scheduling	Minimize makespan	DES	GA/PSO
Inventory control	Minimize holding cost	Montecarlo	Bi-objective

4.2 | Supply Chain Management

Simulation plays a critical role in SCM, where systems are highly complex, dynamic, and uncertain. SBO helps decision makers evaluate various policies and structural designs under fluctuating demand, variable lead times, and capacity constraints [3].

I. Demand forecasting: Monte Carlo simulation and stochastic demand models are commonly used to capture seasonal patterns, demand variability, and uncertainty. SBO methods help determine optimal inventory levels, safety stocks, and reorder policies that minimize cost while ensuring service-level performance.

II. Facility location and network design: DES enables evaluation of alternative network configurations, warehouse locations, and distribution strategies. SBO helps planners identify configurations that minimize transportation and facility costs while meeting delivery performance targets.

III. Transportation planning: simulation supports route planning, fleet optimization, and carrier selection under variable travel times, traffic, and fuel costs. Metaheuristic and surrogate-assisted optimization methods are frequently used to evaluate routing policies in large-scale networks.

IV. Warehouse operations: DES is widely used to model picking strategies, material-handling equipment, storage policies, and labor planning. SBO optimizes workforce shifts, layout designs, and automation technologies to increase throughput and reduce congestion.

Overall, SBO helps supply chains become more agile, cost-efficient, and resilient to disruptions.

4.3 | Healthcare Systems

Resource constraints, unpredictable patient arrivals, and strict quality-of-care requirements characterize healthcare systems. Simulation provides a safe and cost-effective environment to test operational improvements without disrupting real operations [8].

I. Capacity planning: DES models support long-term decisions regarding bed capacity, staffing levels, diagnostic equipment, and operating rooms. SBO identifies optimal capacity-expansion strategies or staff-allocation plans under uncertain demand.

II. Patient flow optimization: simulation helps analyze bottlenecks in emergency departments, outpatient clinics, and surgical pathways. Combined SBO techniques optimize triage rules, treatment prioritization, and patient routing schemes to reduce waiting times and improve service quality.

III. Scheduling: surgical scheduling, appointment booking, and nurse rostering are optimized using DES, ABS, and metaheuristics. SBO supports balancing patient satisfaction, resource availability, and operational efficiency.

IV. Resource allocation: in pandemic or disaster scenarios, simulation evaluates allocation of ventilators, hospital beds, vaccines, or medical personnel. Stochastic optimization methods help design policies that remain effective even in the face of uncertain demand surges.

Healthcare SBO ultimately improves patient outcomes, operational resiliency, and system-wide efficiency.

4.4 | Transportation and Logistics

Transportation and logistics systems involve complex interactions between vehicles, infrastructure, and human operators. Simulation helps model real-world variability such as traffic congestion, weather effects, and system disruptions [9].

I. Fleet management: simulation models evaluate vehicle allocation, maintenance policies, and dispatching strategies. SBO is used to minimize operating costs, energy consumption, and turnaround times.

II. Route optimization: traffic-aware routing, last-mile delivery optimization, and multimodal transport planning often involve massive search spaces. Simulation-based metaheuristics (e.g., GAs, PSO) produce near-optimal routing decisions under uncertainty.

III. Traffic flow modeling: microscopic and macroscopic traffic simulations analyze congestion dynamics, signal timing, lane usage, and infrastructure planning. SBO assists in optimizing traffic control strategies and reducing travel delays.

IV. Airport operations: DES is used for runway scheduling, gate assignment, baggage handling, and passenger movement. SBO ensures efficient coordination among airlines, airport authorities, and ground operations to improve reliability and safety.

Simulation enables transportation systems to adapt to increasing demand, technological evolution, and environmental constraints [28].

4.5 | Energy and Environmental Systems

Energy and environmental sectors face challenges such as increasing renewable energy penetration, climate variability, and regulatory constraints. SBO supports both strategic and operational decisions [36].

I. Renewable energy integration: simulation evaluates wind, solar, and hybrid renewable systems under stochastic weather patterns. SBO optimizes storage sizing, grid reliability, and power dispatch strategies.

II. Carbon reduction and emissions planning: scenario-based simulation supports policy evaluation, carbon trading mechanisms, and decarbonization pathways. Optimization identifies the least-cost strategies for meeting emissions targets while maintaining system reliability.

III. Energy system resilience: simulation assesses the system's vulnerability to extreme weather, equipment failures, and cyber threats. SBO helps design resilient infrastructure, backup generation, and adaptive load management strategies.

IV. Environmental impact modeling: agent-based and continuous simulation models represent ecological systems, pollution dispersion, and environmental remediation. Optimization helps balance economic and environmental objectives in sustainable development projects.

Energy and environmental SBOs are essential for managing the transition toward low-carbon, reliable, and sustainable energy systems.

4.6 | Defense and Military Applications

Defense and military systems are inherently uncertain, high-risk, and mission-critical. Simulation provides a safe environment to evaluate strategies, technologies, and operational plans before execution [11].

I. Mission planning: ABS models adversary behavior, terrain conditions, and operational risks. SBO supports selecting mission routes, resource utilization plans, and tactical decisions.

II. Military logistics: simulation models supply chain operations, maintenance policies, fuel consumption, and equipment deployment. SBO optimizes logistics networks to ensure rapid and reliable support for military operations.

III. Resource allocation: personnel deployment, equipment scheduling, and emergency response planning are optimized using DES and stochastic optimization techniques.

IV. System reliability and performance: simulation assesses weapon system reliability, repair policies, and lifecycle performance. SBO identifies optimal maintenance strategies, redundancy levels, and upgrade schedules.

Military organizations use simulation to reduce operational risk, improve decision-making, and evaluate new technologies without exposing personnel or assets to danger.

5 | Conclusion

SBO has emerged as a powerful paradigm for analyzing, designing, and improving complex systems that exhibit uncertainty, nonlinearity, and dynamic interactions. This review has provided a comprehensive examination of the conceptual foundations, methodological developments, and diverse applications of SBO across multiple domains. By integrating simulation models with optimization techniques, SBO enables decision makers to evaluate alternative strategies in environments where analytic methods are insufficient or infeasible. From the methodological perspective, the field encompasses a broad spectrum of approaches—ranging from deterministic and stochastic optimization to metaheuristics, machine learning–based methods, multi-objective frameworks, and constrained optimization techniques. Derivative-free and surrogate-based methods have proven particularly valuable for computationally intensive simulations or non-differentiable objective functions. Moreover, advances in multi-objective and constrained SBO provide practical tools for addressing real-world trade-offs and operational limitations. The continued integration of machine learning, Bayesian modeling, and high-performance computing is further expanding the scope and efficiency of SBO methodologies. The application review demonstrates that SBO plays a critical role in sectors such as SCM, healthcare operations, transportation and logistics, energy and environmental systems, and defense. In each domain, SBO supports data-driven decision-making by capturing system complexity, evaluating uncertainty, and optimizing performance metrics such as cost, quality, resilience, safety, and sustainability. As global systems become more interconnected and subject to rapid technological and environmental changes, the importance of SBO is expected to grow. Looking ahead, several opportunities exist for advancing the field. These include developing more scalable surrogate models for high-dimensional problems. These hybrid optimization frameworks combine mathematical rigor with learning-based exploration, and real-time SBO enabled by digital twins and advanced computing architectures. Furthermore, research efforts are needed to improve the interpretability, robustness, and generalizability of SBO models in practice. Finally, SBO provides a rigorous and flexible foundation for solving complex decision problems in uncertain and dynamic environments. By bridging simulation and optimization, it offers a transformative toolkit for both researchers and practitioners, enabling deeper insight and more effective strategies across a broad range of industries and scientific disciplines. As systems become increasingly complex, the role of SBO in decision-making is likely to expand even further.

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Data Availability

The data supporting the findings of this study are available from the corresponding author upon reasonable request.

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